Waves 2022

The 15th International Conference on Mathematical and Numerical Aspects of Wave Propagation

July 24-29, 2022

Book of Abstracts
Version: July 17th
The 15th International Conference on Mathematical and Numerical Aspects of Wave Propagation

Local Organizing Committee

Eliane Bécache  Marc Bonnet  Anne-Sophie Bonnet-Ben Dhia
Stéphanie Chaillat  Corinne Chen  Patrick Ciarlet
Marie Enée  Luiz Faria  Sonia Fliss (co-chair)
Laure Giovangigli  Christophe Hazard (co-chair)  Patrick Joly
Maryna Kachanovska  Nicolas Kielbasiewicz  Eric Lunéville
Pierre Marchand  Axel Modave  Julienne Moukalou
Magalie Quet  Hélène Tranchant

Scientific Committee

Daniel Apello  Adrianna Gillman  Wangtao Lu
Tilo Arens  Dan Givoli  Ya Yan Lu
Lehel Banjai  Marcus Grote  Bruno Lombard
Alex Barnett  Bojan Guzina  Paul Martin
Timo Betcke  Houssem Haddar  Andrea Moiola
Liliana Borcea  Thomas Hagstrom  Peter Monk
Oscar Bruno  David Hewett  Lothar Nannen
Fioralba Cakoni  Ralf Hiptmair  Vincent Pagneux
Maxence Cassier  Marlis Hochbruck  Konstantin Pankrashkin
Simon Chandler-Wilde  Thorsten Hohage  Ilaria Perugia
Lucas Chesnel  Lise-Marie Imbert-Gérard  Karim Ramdani
Bérengère Delourme  Sébastien Impériale  Jerónimo Rodríguez García
Bruno Després  Steven Johnson  Claire Scheid
Julien Diaz  Manfred Kaltenbacher  Euan Spence
Martin Gander  Andreas Kirsch  Chrysoula Tsogka
Christophe Geuzaine  Olivier Lafitte  Michael Weinstein

Conference Homepage

http://www.waves2022.fr/

Credits for the Book of Abstracts

\LaTeX{} editor: Nicolas Kielbasiewicz
Preface

The biannual WAVES conference series is a major venue for disseminating the latest advances in theoretical and computational modeling of wave phenomena, catering to the emerging problems in science and technology.

The themes of the conference, which may concern any kind of waves (acoustic, electromagnetic, elastic, etc.), include, but are not limited to, the following:

- photonics and optics,
- flow-acoustic interaction,
- water waves and coastal modeling,
- medical and seismic imaging,
- non-destructive testing,
- waveguides,
- nonlinear wave phenomena,
- imaging and inverse problems,
- scattering problems,
- periodic and random media,
- asymptotic models and homogenization,
- high-frequency approximations,
- integral equations,
- absorbing boundary conditions,
- domain decomposition methods,
- boundary element methods,
- discontinuous discretization methods,
- fast computational techniques.

**WAVES 2022 : A scientific and human meeting to celebrate a double anniversary**

The 2022 edition of the WAVES series is organized at ENSTA Paris in Palaiseau (about 20kms in the south of Paris) by the POEMS team (acronym for “Propagation des Ondes: Étude Mathématique et Simulation” *), a research team associated with CNRS, INRIA and ENSTA Paris. The very first conference, held in 1991 in Strasbourg (France), was initiated by members of POEMS. The current team is glad to host this particular edition, which will be an opportunity to celebrate a double anniversary: the 15th occurrence of the conference, which coincides with its 30+1 years birthday!

Palaiseau, July 2022

*The WAVES 2022 Organizing Team*
## Contents

### Plenary lectures

Runborg Olof - *Solving Helmholtz Equation Using the Temporal Wave Equation* ................. 17  
Nigam Nilima, Wakeling James - *Elasticity, skeletal muscle, and waves?* ......................... 22  
Krejcirik David - *The virial theorem and the method of multipliers in spectral theory* .......... 26  
Biondi Biondo - *Robust seismic imaging by full-waveform inversion with model time extension: time-domain and frequency-domain formulations* ........................................ 32  
Darbas Marion - *Fast solvers for time-harmonic high-frequency elastic wave propagation problems* ................................................................. 38  
Melenk Markus - *Wavenumber-explicit hp-FEM for Helmholtz problems in piecewise smooth media* .......................................................... 44  
Claeys Xavier - *Generalized optimized Schwarz methods in arbitrary non-overlapping subdomain partitions* ......................................................... 56

### Minisymposia

#### New trends in nonlinear acoustics and related phenomena ........................................... 63  
Rozanova-Pierrat Anna, Hinz Michael, Dekkers Adrien, Teplyaev Alexander - *Well-posedness and shape optimization for the Westervelt Robin boundary problem on domains with non-Lipschitz boundaries* ..................................... 64  
Garcke Harald, Mitra Sourav, Nikolić Vanja - *A phase-field approach to shape and topology optimization of nonlinear acoustic waves* ........................................ 66  
Meliani Mostafa, Nikolić Vanja - *Analysis of shape optimization problems for the Kuznetsov equation* ........................................................ 68  
Bongarti Marcelo, Lasiecka Irena - *Boundary stabilization of critical nonlinear JMGT equation with undissipated Neumann boundary* ............................................. 70  
Racke Reinhard, Hu Yuxi, Wang Na - *Formation of singularities for relaxed compressible Navier-Stokes equations* ................................................. 72  
Scholle Markus, Gaskell Philip, Ismail-Sutton Sara - *Obtaining nonlinear acoustic models from non-conventional variational principles in fluid mechanics* .......... 74  
Baker Katherine, Banaji Lehel, Ptashnyk Mariya - *A fast time-stepping method for the Westervelt equation with time-fractional damping* ......................... 76  
Rauscher Teresa - *Modeling and simulation of nonlinear wave propagation in ultrasound imaging* ................................................................. 78

**Wave propagation in ab initio molecular simulation** ...................................................... 81  
Dupuy Mi-Song, Levitt Antoine - *Finite-size effects in response functions of molecular systems* ................................................................. 82  
Joubert-Doriot Loïc - *Quantum dynamics beyond the Born-Oppenheimer approximation in molecular systems* ..................................................... 84  
Colbrook Matthew, Horning Andrew, Thicke Kyle, Watson Alex - *Computing Spectral Properties of Topological Insulators with Disorder* ......................... 86
Letournel Eloïse, Levitt Antoine, Genovese Luigi, Duchemin Ivan, Ruget Simon - Computation of resonances in locally perturbed periodic quantum systems .... 88

Contributed talks

Monday, July 25, Morning Session .......................................................... 93

Letournel Eloïse, Levitt Antoine, Genovese Luigi, Duchemin Ivan, Ruget Simon - Computation of resonances in locally perturbed periodic quantum systems .... 88

Imbert-Gérard Lise-Marie, Sylvand Guillaume - Three types of quasi-Trefftz functions for the 3D convected Helmholtz equation: construction and theoretical approximation properties ................................................ 94

Sirdey Margot, Tordeux Sébastien, Pernet Sébastien - Iterative Trefftz Method For Three-dimensional Electromagnetic Waves Simulation ............................. 96

Parolin Emile, Huybrechs Daan, Moiola Andrea - Stable approximation of Helmholtz solutions with evanescent plane waves ........................................ 98

Chandler-Wilde Simon, Caetano Antonio, Gibbs Andrew, Hewett David, Moiola Andrea - A Hausdorff-measure boundary element method for scattering by fractal screens I: Numerical Analysis .......................................................... 100

Gibbs Andrew, Moiola Andrea, Hewett David - A Hausdorff-Measure Boundary Element Method for Scattering by Fractal Screens II: Numerical Quadrature .......... 102

Florian Francesc, Hiptmair Ralf, Sauter Stefan - A new theory for acoustic transmission problems with variable coefficients modeled as stable integral equations .... 104

Villalobos Guíllen Cristóbal, Baratchart Laurent, Haddar Houssem - Inverse problem for the Helmholtz equation and singular sources in the divergence form 106

Gerber-Roth Anthony, Munnier Alexandre, Ramdani Karim - A reconstruction method for the inverse gravimetric problem .............................................. 108

Nemaire Masimba, Asensio Paul, Badier Jean-Michel, Leblond Juliette, Marmorat Jean Paul - A layer potential approach to functional and clinical brain imaging ... 110

Després Bruno, Nicolopoulous Anouk, Thierry Bertrand - On corner matrices for high order DDMs ................................................................. 112

Lucero Lorca Jose Pablo, Gillman Adrianna - A comparison between Hierarchical Poincaré-Steklov approaches for the 3D Helmholtz equation with variable coefficients116

Erath Christoph, Mascotto Lorenzo, Melenk Markus, Perugia Ilaria, Rieder Alexander - dGFEM-BEM mortar coupling for the Helmholtz problem in three dimensions . 118

Bonizzoni Francesca, Pradovera Davide, Ruggeri Michele - Rational-based MOR methods for Helmholtz frequency response problems with adaptive nite element snapshots 120

Sauter Stefan, Bernkopf Maximilian, Torres Céline, Veit Alexander - Solvability of Discrete Helmholtz Equations .................................................. 122

Monday, July 25, First Afternoon Session .................................................. 125

Anderson Thomas G., Bruno Oscar P. - Decay Theory and Numerical Analysis for Hybrid Frequency/Time Methods in Long-Time Transient Wave Scattering .... 126

Rosas Alejandro, Joly Patrick, Cassier Maxence - Long time behaviour for electromagnetic waves in dissipative Lorentz media ................................. 128

Jerez-Hanckes Carlos, Escapil-Inchauspé Paul - Bi-Parametric Operator Preconditioning and Applications .......................................................... 130

Fierro-Piccardo Ignacia, Betcke Timo - An OSRC Preconditioner for the EFIE .... 132

Baek Youngsoo, Aquino Wilkins, Mukherjee Sayan - Probabilistic Wave Inversion Using Gibbs Posterior: Application in Ultrasound Vibrometry ......... 134

Bellam Muralidhar Nanda Kishore, Rauter Natalie, Mikhailenko Andrei, Lammering Rolf, Lorenz Dirk A. - Damage Identification in Fiber Metal Laminates with Guided Ultrasonic Wave using Bayesian Inference and Model Order Reduction. 136

Millien Pierre, Baldassari Lorenzo, Vanel Alice - Modal approximation for plasmonic resonators in the time domain ........................................ 138
Kachanovska Maryna - Asymptotic models for time-domain scattering by small particles ........................................ 140
Kirsch Andreas, Hu Guanghui - Radiation Conditions for Periodic Waveguides .................................................. 142
Schweizer Ben - Energy method approach to existence results for the Helmholtz equation
in periodic waveguides ........................................................................................................................................ 144

**Monday, July 25, Second Afternoon Session**

Appelö Daniel, Peng Zhichao - EM-WaveHoltz: A time-domain frequency-domain solver
for Maxwell’s equations ........................................................................................................................................ 148
Chaumont-Frelet Théophile, Grote Marcus J., Tang Jit H., Lanteri Stéphane - A
controllability method for Maxwell’s equations ................................................................................................. 150
Stolk Chris - A time-domain preconditioner for the Helmholtz equation: Analysis and
performance on GPUs ........................................................................................................................................ 152
Bagur Laura, Chaillat Stéphanie, Semblat Jean-François, Stefanou Ioannis - Fast boundary
element method for fault mechanics and earthquake control .............................................................................. 154
Carvalho Camille, Kim Arnold, Moitier Zoïs - Quadrature by Parity Asymptotic exPan-
sions (QPAX) for light scattering by high aspect ratio plasmonic particle .................................................... 156
Arrieta Rodrigo, Faria Luiz, Perez Arancibia Carlos, Turc Catalin - A High-order Density-
Interpolation-Based Nyström Method for Three-Dimensional Electromagnetic Boundary Integral Equations
.............................................................................................................................................................................. 158
Demaldent Edouard, Bonnet Marc - Eddy-current asymptotics of the Maxwell PMCHWT
formulation: the multi-body case .......................................................................................................................... 160
Knöller Marvin - Maximizing the electromagnetic chirality for metallic nanowires in the
visible spectrum ...................................................................................................................................................... 162
Gaucher Samuel, Guiffaut Christophe, Reineix Alain, Cessenat Olivier - Angle-dependent
SIBC model of metamaterial in FDTD method .................................................................................................. 164
Stellin Filippo, Filoche Marcel, Dias Frederic - Localization landscape for interacting
Bose gases in one-dimensional speckle potentials ............................................................................................... 166
Karnezis Aristeidis, Gower Artur L. - Complex Effective Wavenumbers of Isotropic
Particulate Materials .......................................................................................................................................... 168
Goepfert Quentin, Garnier Josselin, Giovangiğli Laure, Millien Pierre - Speckle statistics
in stochastic homogenization regime .................................................................................................................. 170
Gomez Sergio, Moiola Andrea - A space–time Trefftz discontinuous Galerkin method for
the linear Schrödinger equation .......................................................................................................................... 172
Lee Spencer, Appelö Daniel - Implicit Filon Methods for Highly Oscillating Problems
and Controlled Qubits ...................................................................................................................................... 174
Eriksson Gustav, Werpers Jonatan, Niemelä David, Wik Niklas, Zethrin Valter, Mattsson
Ken - Stable finite differences for the piecewise homogeneous dynamic beam equation ............................... 176

**Tuesday, July 26, Morning Session**

White Tom, Assier Raphael, Parnell William - Sound Propagation in Slowly-Varying
Lined Ducts ............................................................................................................................................................. 179
Bourgeois Laurent, Fliss Sonia, Fritsch Jean-François, Hazard Christophe, Recoquillay
Arnaud - Scattering in a partially open waveguide: the forward problem .................................................... 182
Fritsch Jean-François, Bourgeois Laurent, Recoquillay Arnaud - Scattering in a partially
open waveguide: the inverse problem .................................................................................................................. 184
Niclas Angèle, Bonnetier Éric, Seppacher Laurent, Vial Grégory - High sensitivity imaging
defects in elastic waveguides using near resonance frequencies ..................................................................... 186
Barucq Hélène, Calandra Henri, Diaz Julien, Vasanthan Vinduja - On the construction
of Shape Functions for Spacetime Trefftz-DG Formulations of Wave Problems
with Perfectly Matched Layers .......................................................................................................................... 188
Li Jichun - Analysis and FDTD simulation of a perfectly matched layer for the Drude
metamaterial ......................................................................................................................................................... 190
Bécache Eliane, Kachanovska Maryna, Wess Markus - Stability and convergence of
time-domain perfectly matched layers in dispersive waveguides .................................................................... 192
Cousin Theau, Gout Christian, Tomnoir Antoine, Fauchard Cyrille - Perfectly Matched Layers for second order Maxwell’s equations in time domain 194
Hochbruck Marlis, Köhler Jonas, Kumbhar Pratik - Locally Implicit Preconditioning for Maxwell equations on a locally refined spatial grid 196
Beni Hamad Akram, Imperiale Sébastien, Joly Patrick - Efficient numerical method for time domain electromagnetic wave propagation in thin co-axial cables 198
Law Yann-Meing, Appelö Daniel - The Hermite-Taylor Correction Function Method for Maxwell’s Equations 200
Moiola Andrea, Imbert-Gérard Lise-Marie, Stocker Paul - A space-time quasi-Trefftz DG method for the wave equation with smooth coefficients 202

Tuesday, July 26, First Afternoon Session 205
Halla Martin, Lehrenfeld Christoph, Stocker Paul - Numerical treatment of the vectorial equations of stellar oscillations 206
Latham Benjamin, Kim Arnold, Carvalho Camille - Capturing plasmonic behaviors in light scattering by spheres using finite element methods and asymptotic quadrature 208
Arnold Anton, Geevers Sjoerd, Perugia Ilaria, Ponomarev Dmitry - Revisiting the limiting amplitude principle for the wave equation with variable coefficients 210
Burkhard Sélima, Dörich Benjamin, Hochbruck Marlis - Gaussian wave packets for the magnetic Schrödinger equation 212
Aimi Alessandra, Desiderio Luca, Di Credico Giulia, Guardasoni Chiara - Recent Advances in Elastodynamics by Time-Domain Energetic Boundary Element Method 214
Haider Anita, Schanz Martin - Experiences with the 3D-ACA in a CQM based Time Domain Boundary Element Method 216
Quaine Kieran, Gimperlein Heiko - Enriched Space-Time Finite Element Methods for the Wave Equation 218
Bignardi Paolo, Moiola Andrea - A space-time continuous and coercive variational formulation for the wave equation 220

Tuesday, July 26, Second Afternoon Session 223
Phillips Oliver, Langdon Stephen, Chandler-Wilde Simon - An iterative hybrid numerical-asymptotic boundary element method for high-frequency scattering by multiple screens 224
Bonnet-Ben Dhia Anne-Sophie, Allouko Amond, Baronian Vahan, Fliss Sonia - A high-frequency approach for the acceleration of the Half-Space Matching method 226
Hewett David, Smynshyaev Valery - The inflection point problem - from modal to scattering behaviour 228
Naqvi Shiza, Ayton Lorna - Homogenisation of perforated plates 230
Cornaggia Rémi, Lombard Bruno - Homogenization for transient waves in 1D periodic media: dispersion, interfaces and point sources 232
Rotem Amit, Appelö Daniel, Runborg Olof - The WaveHoltz Heterogeneous Multiscale Method for the Helmholtz Equation 234
Le Louër Frédérique, Ivanyshyn Yaman Olha - Modeling and analysis of an inverse boundary value problem in a two dimensional viscoelastic medium 236
Arens Tilo, Hagemann Felix, Hettlich Frank - Domain Derivatives in Electromagnetism and Optimal Design of Chiral Objects 238
Asensio Paul, Baratchart Laurent, Leblond Juliette, Olivi Martine, Seyfert Fabien - Surface identification through back-scattering of an electromagnetic planar wave, by rational approximation 240
Dubois Juliette, Imperiale Sébastien, Sainte-Marie Jacques - Propagation of acoustic and gravity waves in the ocean: a new derivation for a general model 242
Boyaval Sébastien - Symmetric-hyperbolic conservation laws modelling viscoelastic flows 244
Moufid Ilyes, Matignon Denis, Roncen Rémi, Piot Estelle - Stability analysis of the JCAPL equivalent fluid model equations for porous media 246
Wednesday, July 27, Morning Session

Martin Paul, Skvortsov Alex - Scattering by a Body in a Pipe

Berggren Martin, Mousavi Abbas, Wadbro Eddie - Waveguide acoustic black holes: non-helpful and helpful damping mechanisms

Thibault Alexis, Chabassier Juliette, Boutin Henri, Hélie Thomas - Thermoviscous acoustic propagation in thin rough tubes

Moufid Ilyes, Matignon Denis, Roncen Rémi, Piot Estelle - Multipole-model approximation of the equivalent fluid model equations for porous media in the time domain

Bruno Oscar P. - Efficient numerical solvers for frequency- and time-domain electromagnetic simulation, optimization and design

Cortes Elsle, Carvalho Camille, Tsogka Chrysoula - Boundary Integral Equation Methods for Optical Cloaking Models

Labarca Ignacio, Hiptmair Ralf - Coupled Single-Trace Formulations with Volume Integral Operators for Acoustic Transmission Problems

Bannister Joshua, Gibbs Andrew, Hewett David - Volume integral equations on fractal domains and the Koch snowlake transmission problem

Giovangigli Laure, Fliss Sonia, Boucart Amandine - Homogenization of a thin layer of randomly distributed nano-particles: effective model and error estimates

Rohan Eduard, Lukeš Vladimir - Modelling acoustic metasurfaces using homogenization of fluid-structure interaction on strongly heterogeneous perforated plates in thin layers

Bellis Cédric, Lombard Bruno, Touboul Marie, Assier Raphael - Effective dynamics for low-amplitude transient elastic waves in a 1D periodic array of non-linear interfaces

Touboul Marie, Assier Raphael, Lombard Bruno, Bellis Cédric, Cotterill Philip, Nigro David, Parnell William - High-frequency homogenisation in periodic media with imperfect interfaces and elastodynamic co-dipole metaclusters

Chesnel Lucas, Heleine Jérémy, Nazarov Sergei A. - Design of a mode converter using thin resonant ligaments

Ruiz Matias, Bonnet-Ben Dhia Anne-Sophie, Hazard Christophe - Spectral analysis of generalized normal modes

Briet Philippe - Sheared nanoribbons

Naderi Kiyan, Pankrashkin Konstantin - A trace theorem on an infinite p-adic tree

Ritzenthaler Valentin, Cantin Pierre, Ferrière Xavier, Pernet Sébastien, Guillaume Puigt - Spectral Difference method on Structured-Grids for Maxwell’s Equations in Time Domain

Delaunay Tiphaine, Imperiale Sébastien, Moireau Philippe - Stabilization of the high-order discretized wave equation for data assimilation problems

Fraschini Sara, Moiola Andrea, Sangalli Giancarlo - Stability of space–time isogeometric methods for wave propagation problems

Weber Ivy, Kreiss Gunilla - A comparison of Hermite and Lagrange finite element methods for the wave equation

Thursday, July 28, Morning Session

Amenoagbadji Pierre, Fliss Sonia, Joly Patrick - Wave propagation in unbounded quasiperiodic media, Part 1: the absorbing case

Joly Patrick, Fliss Sonia, Amenoagbadji Pierre - Wave propagation in unbounded quasiperiodic media, Part 2: the non-absorbing case

Guzina Bojan B., Oudghiri-Idrissi Othman, Meng Shixu - Asymptotic analysis of Berry phase governed by the scalar wave equation

Shafieeabaneh Nasim, Zhang Ruming - Numerical solution for non-periodic scattering problem in the 3D periodic structure
<table>
<thead>
<tr>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>A data compact representation for frequency dependent BEM matrices</td>
<td>300</td>
</tr>
<tr>
<td>Numerical Modelisation of Interaction between Plasma Thruster Plume</td>
<td>302</td>
</tr>
<tr>
<td>and Antennas on Small Satellites</td>
<td></td>
</tr>
<tr>
<td>A FFT-based Kernel-independent Directional Fast Multipole Library for</td>
<td>304</td>
</tr>
<tr>
<td>Arbitrary Particle Distributions at All Frequency Regimes</td>
<td></td>
</tr>
<tr>
<td>Massively Parallelized Interpolated Factored Green Function Method</td>
<td>306</td>
</tr>
<tr>
<td>Adaptive Spectral Decomposition for Time-Dependent Inverse Problems</td>
<td>308</td>
</tr>
<tr>
<td>Solving inverse source wave problem: from observability to observer</td>
<td>312</td>
</tr>
<tr>
<td>design</td>
<td></td>
</tr>
<tr>
<td>Iterative helioseismic holography-Inversions for solar differential</td>
<td>314</td>
</tr>
<tr>
<td>rotation</td>
<td></td>
</tr>
<tr>
<td>Solution of a non-linear eigenvalue problem for Photonic Crystal</td>
<td>316</td>
</tr>
<tr>
<td>Fiber applications</td>
<td></td>
</tr>
<tr>
<td>Modal computation for open waveguides</td>
<td>318</td>
</tr>
<tr>
<td>Computing eigenvalues of the Laplacian on rough domains</td>
<td>320</td>
</tr>
<tr>
<td>Maximum norm error bounds for the full discretization of non-autonomous wave equations</td>
<td>324</td>
</tr>
<tr>
<td>Order-preserving non-conforming grid interfaces for boundary-optimized summation-by-parts operators</td>
<td>326</td>
</tr>
<tr>
<td>Linearly implicit energy consistent time discretisation for nonlinear wave equations</td>
<td>328</td>
</tr>
<tr>
<td>Non-conforming and moving grids for the simulation of waves in viscous fluids</td>
<td>330</td>
</tr>
<tr>
<td>Computing eigenvalues of the Laplacian on rough domains</td>
<td></td>
</tr>
<tr>
<td>Maximum norm error bounds for the full discretization of non-autonomous wave equations</td>
<td></td>
</tr>
<tr>
<td>Order-preserving non-conforming grid interfaces for boundary-optimized summation-by-parts operators</td>
<td></td>
</tr>
<tr>
<td>Linearly implicit energy consistent time discretisation for nonlinear wave equations</td>
<td></td>
</tr>
<tr>
<td>Non-conforming and moving grids for the simulation of waves in viscous fluids</td>
<td></td>
</tr>
<tr>
<td>Thursday, July 28, First Afternoon Session</td>
<td>333</td>
</tr>
<tr>
<td>Efficient Iterative High Order Numerical Method for Multiple Scattering</td>
<td>334</td>
</tr>
<tr>
<td>Asymptotic analysis for sound-hard acoustic scattering by two closely-situated spheres</td>
<td>336</td>
</tr>
<tr>
<td>Analysis and Approximation of Electromagnetic Surface Waves in Nonlinear Dispersive Media</td>
<td>338</td>
</tr>
<tr>
<td>Wave power farm made of many rigid floating structures in Boussinesq regime</td>
<td>340</td>
</tr>
<tr>
<td>Log-stability results for inverse coefficients problem associated with time harmonic magnetic Schrödinger operator</td>
<td>342</td>
</tr>
<tr>
<td>Numerical methods for a Schrodinger equation inverse eigenvalue problem</td>
<td>344</td>
</tr>
<tr>
<td>Acoustic passive cloaking using thin resonant ligaments</td>
<td>346</td>
</tr>
</tbody>
</table>
Fornerod Jean, Nguyen Hoai-Minh - The Weyl Law of transmission eigenvalues and the completeness of the generalized transmission eigenfunctions without the complementing conditions .......................................................... 348
Rouxelin Nathan, Barucq Hélène, Tordeux Sébastien - Low-order Absorbing Boundary Conditions in HDG discretization of the convected Helmholtz equation .......................................................... 350
Faria Luiz, Anne Alexis, Bonnet-Ben Dhia Anne-Sophie - Solving the water-waves problem with Laplace’s free-space Green’s function .......................................................... 352

Thursday, July 28, Second Afternoon Session .................................................................. 355
Mandel Rainer, Moitier Zoïs, Verfürth Barbara - Nonlinear Helmholtz equations with sign-changing diffusion coefficient .......................................................... 356
Bonnet-Ben Dhia Anne-Sophie, Chesnel Lucas, Rihani Mahran - 3D scalar transmission problem in presence of a conical tip of negative material .......................................................... 358
Bonnet-Ben Dhia Anne-Sophie, Chesnel Lucas, Rihani Mahran - Maxwell’s equations in presence of a tip of material with negative permittivity .......................................................... 360
Jerez-Hanckes Carlos, Pinto Jose, Yin Tao - Exponentially Convergent Spectral Galerkin BEM for Elastic Wave Scattering of Cracks .......................................................... 362
Montanelli Hadrien, Haddar Houssem, Aussal Matthieu - Computing singular and near-singular integrals in high-order boundary elements .......................................................... 364
Turc Catalin - Robust boundary integral equations of Helmholtz decomposition formulations of elastic scattering problems .......................................................... 366
Recoquillay Arnaud - On the use of phased array data for the Linear Sampling Method in an elastic waveguide .......................................................... 368
Boukari Yosra, Haddar Houssem, Jenhani Nouha - Identification of a local perturbation in unknown periodic layers .......................................................... 370
Monk Peter, Lähivaara Timo, Selgas Virginia - The Time Domain Linear Sampling Method for Maxwell’s equations .......................................................... 372
Banon Jean-Philippe, Pelletier Pierre, Weisbuch Claude, Mayboroda Svitlana, Filoche Marcel - Wigner-Weyl description of radiative processes in correlated disordered semiconductor alloys .......................................................... 374
Gower Artur L., Kristensson Gerhard, Hawkins Stuart C. - Modelling and validating average waves in random particulate materials .......................................................... 376
Boucart Amandine, Fliss Sonia, Giovangigli Laure, Stupfel Bruno - Modeling scattering from a random thin coating: asymptotic model and numerical simulations .......................................................... 378
Tamber Jagdeep, Matt Tranter - Scattering of an Ostrovsky Wave Packet in a Delaminated Waveguide .......................................................... 382
Margenberg Nils, Kärtner Franz, Bause Markus - Higher Order Variational Time Discretizations for Nonlinear Dispersive Wave Equations .......................................................... 384

Friday, July 29, Morning Session ......................................................................................... 387
Lafitte Olivier - High frequency analysis of the Dirichlet to Neumann operator for the Helmholtz equation on a coated cylinder or elliptic cylinder .......................................................... 388
Londoño Mauricio, Rodriguez-Cortés Francisco - Oscillatory RBF for Helmholtz problems with large wavenumber .......................................................... 390
Galkowski Jeffrey, Marchand Pierre, Spence Euan - High-frequency estimates and error bounds on the h-BEM for the Helmholtz exterior Neumann problem .......................................................... 392
Oudghiri-Idrissi Othman, Guzina Bojan B. - Effective Wave Motion in Periodic Origami Structures .......................................................... 394
Cassier Maxence, Weinstein Michael I. - TE band structure for honeycomb media in a high contrast regime .......................................................... 396
Delourme Bérangère, Fliss Sonia - Dislocation model for hexagonal periodic graphs perturbed along the Zig Zag direction .......................................................... 398
Benjamin Harold, De Pascalis Riccardo - Acoustoelasticity of soft viscoelastic solids and phononic crystals ................................................................. 400
Bécache Eliane, Bonnet-Ben Dhia Anne-Sophie, Fliss Sonia, Tonnoir Antoine - The Half-space Matching method and the Perfectly Matched Layers for scattering problem in anisotropic elastic media ........................................... 402
Halla Martin - Radial complex scaling/PML for anisotropic scalar resonance problems 404
Bériot Hadrien, Modave Axel - A PML implementation for convex domains of general shape in time-harmonic acoustics .................................................. 406
Hohage Thorsten, Preuß Janosch, Lehrenfeld Christoph - Learned Infinite Elements .... 408
Nassor Alice, Bonnet Marc, Chaillat Stéphanie - Transient, global-in-time, convergent iterative coupling of acoustic BEM and elastic FEM .......................... 410
Givoli Dan, Rabinovich Daniel - Dirichlet-to-Neumann Coupling for 2D-1D Time-Dependent Wave Problems ................................................................. 412
Desiderio Luca, Falletta Silvia, Ferrari Matteo, Scuderi Letizia - One-equation coupling of Curvilinear Virtual Element and Boundary Element methods for the wave equation in unbounded domains .................................................. 414
Labat Justine, Pujols Agnès, Collino Francis - Discontinuous Galerkin-based domain decomposition method for boundary integral equations in electromagnetism . . 416
Hales Alistair, Ayton Lorna - Reduction of Leading-Edge Noise by Tailored Turbulence Anisotropy ................................................................. 418
Ruello Maëlys, Rudel Clément, Pernet Sébastien, Brazier Jean-Philippe - One-Way methods for wave propagation in complex flows ........................................ 420
Putz Felician, Zhang Yi, Oberlack Martin - Instability and over-reflection of acoustic waves in compressible boundary layer flows ........................................ 422
Hägg Linus, Berggren Martin - Accounting for viscothermal boundary losses in time-domain acoustics ................................................................. 424
Plenary lectures
Solving Helmholtz Equation Using the Temporal Wave Equation

Olof Runborg

1Department of Mathematics, KTH, Stockholm, Sweden

Abstract

We consider iterative methods for the Helmholtz equation that are based on the related time domain wave equation. In each iteration, the solution to the wave equation with a time-periodic forcing is computed and filtered in time. For Dirichlet and Neumann problems the iteration corresponds to a linear and coercive operator which, after discretization, is recast as a positive definite linear system of equations that can be solved with the conjugate gradient method.

Keywords: Helmholtz, Wave Equation.

1 Introduction

Designing efficient iterative solvers for the Helmholtz equation is a challenging problem, in particular when the frequency is high. The main difficulties stem from the resolution requirements and the highly indefinite character of the discretized problem. For detailed reviews see the articles by Ernst, Gander, Zhang and Erlangga [6,7,9].

Computational costs and memory requirements increase rapidly with the frequency $\omega$. To maintain a fixed accuracy with a $p$-th order method at frequency $\omega$ the number of grid points per wavelength must scale as $\omega^{1/p}$ due to the pollution errors. The total number of degrees of freedom is then proportional to $\omega^{d(1+1/p)}$ in $d$ dimensions. At high frequencies this leads to large scale problems that require parallel high-performance computers. It is thus important that solver implementations work well on such platforms. Moreover, solvers should be based on high order accurate methods, or the extra penalty $\omega^{d/p}$ due to pollution errors can become prohibitive, in particular in 3D.

As discretizations of Helmholtz give rise to indefinite linear systems, the conjugate gradient (CG) method cannot be used and the method of necessity becomes the generalized minimal residual method (GMRES). Without preconditioning, the convergence is, however, very slow and the iteration typically stagnates. Efficient preconditioners tailored to the Helmholtz equation must be used to accelerate the convergence. Many such preconditioners have been developed in the past two decades, for instance the analytic incomplete LU [8], shifted laplacian [5], and sweeping [4] preconditioners, to mention a few. Specialized, and efficient, preconditioners give faster convergence, but they can be harder to reconcile with the need for high order implementations that can use high performance computers to good advantage.

2 Time-domain methods

In this talk I will discuss time-domain methods, which is a less explored type of iterative method for the Helmholtz equation that exploits its connection to the time-dependent wave equation. Specifically, I will consider the WaveHoltz method that was developed in [2].

There are many advantages to solving the time dependent wave equation rather than the Helmholtz equation. Algorithms for solving the wave equation are memory lean. They are easy to parallelize and scale well. There are also many provably stable and high order accurate methods available. Compared to discretizations of Helmholtz, time domain methods can therefore more easily deal with large scale high-frequency problems.

In the simplest time-domain method one runs the wave equation for a long time to get a Helmholtz solution. The theoretical underpinning of this approach is the limiting amplitude principle [12] which says that every solution to the wave equation with an oscillatory forcing, in the exterior of a domain with reflecting boundary conditions tends to the Helmholtz solution. However, this method generally does not work for interior problems and becomes very slow for problems with trapping waves.

The Controllability Method (CM) is an alternative approach. It was originally proposed by Bristeau et al. [3] and was further developed by Heikkola et al. [11] as well as Grote and Tang [10]. In CM the solution to the Helmholtz equation is found by solving a convex constrained least-squares minimization problem where the
deviation from time-periodicity is minimized in
the classic wave equation energy. The basic it-
eration step in CM includes the solution of a
forward and a backward wave equation over one
time-period. In some versions one must also
solve a symmetric coercive elliptic (and wave
number independent) problem.

3 The WaveHoltz method

The WaveHoltz method is inspired by CM. It
only requires a single forward wave equation solve
per iteration, and no elliptic solves. For Dirich-
let and Neumann problems it leads to a positive
definite linear system that can be solved with
CG or other Krylov methods. Below we de-
scribe the simplest version of the method for the
Helmholtz equation. It can also be generalized
to other frequency domain wave equations, such
as the elastic wave equation and the Maxwell
equations [1,13].

Consider the Helmholtz equation in a bounded
open smooth domain \( \Omega \),

\[
\nabla \cdot (c^2 \nabla u) + \omega^2 u = f, \quad \text{in } \Omega, \quad (1)
\]

with either Dirichlet or Neumann boundary con-
ditions,

\[
u = 0 \quad \text{or} \quad \vec{n} \cdot \nabla u = 0, \quad \text{on } \partial \Omega.
\]

In this formulation no energy leaves the domain
and for (1) to be well-posed, \( \omega \) must not be a res-
onant frequency, i.e. \( \omega \) cannot be an eigenvalue
of the operator \(-\nabla \cdot (c(x)^2 \nabla)\). We assume non-
resonance, \( f \in L^2(\Omega) \) and \( c \in L^\infty(\Omega) \) bounded
away from zero, which ensures that there is a
unique weak solution \( u \in H^1(\Omega) \) to (1).

This energy conserving case is typically the
most difficult one for iterative Helmholtz solvers.
Moreover, the limiting amplitude principle does
not hold, and one can thus not obtain the Helm-
holtz solution by solving the wave equation over
a long time interval.

To motivate the methods, we first note that
if \( u \) solves (1) then the function

\[
w(t, x) := u(x) \cos(\omega t),
\]

is a \( T = 2\pi/\omega \)-periodic (in time) solution to the
forced scalar wave equation

\[
\begin{align*}
w_{tt} &= \nabla \cdot (c^2(x) \nabla w) - f(x) \cos(\omega t), \\
w(0, x) &= v_0(x), \quad w_t(0, x) = 0,
\end{align*}
\]

where \( v_0 = u \). The domain and boundary con-
ditions are the same as in (1). Based on this
observation, our approach is to find \( w \) instead
of \( u \). We could thus look for initial data \( v_0 \) such
that \( w \) is a \( T \)-periodic solution to (2). However,
there may be several such \( w \), see [10], and we
therefore impose the alternative constraint that
a certain time-average of \( w \) should equal the ini-
tial data. More precisely, we introduce the op-
erator \( \Pi \) acting on the initial data \( v_0 \in H^1(\Omega) \)
as

\[
\Pi v_0 = \frac{2}{T} \int_0^T \left( \cos(\omega t) - \frac{1}{4} \right) w(t, \cdot) dt, \quad (3)
\]

where \( w \) satisfies the wave equation (2) with ini-
tial data \( w = v_0 \) and \( w_t = 0 \). The result of
\( \Pi v_0 \) can thus be seen as a filtering in time of \( w \)
around the \( \omega \)-frequency. By construction, the
solution \( u \) of Helmholtz is a fixed point of \( \Pi \),

\[
u = \Pi u,
\]

and the basic method amounts to solving this
equation with the fixed point iteration

\[
v^{n+1} = \Pi v^n, \quad v^0 \equiv 0 \quad (4)
\]

Provided this iteration converges and the fixed
point is unique we obtain the Helmholtz solution
as \( u = \lim_{n \to \infty} v^n \).

Remark 1 Note that each iteration is inexpen-
sive and that \( T \) is reduced by the reciprocal of
\( \omega \) as \( \omega \) grows. If we assume that the number of
degrees of freedom in each dimension scales with
\( \omega \) and that we evolve the wave equation with an
explicit method this means that the number of
timesteps per iteration is independent of \( \omega \). Also
note that the iteration is trivial to implement (in
parallel or serial) if there is already a time do-
main wave equation solver in place. The integral
in the filtering (3) is carried out independently
for each degree of freedom and simply amounts
to adding up a weighted sum (e.g. a trapezoidal
sum) of the solution one timestep at a time. Fi-
nally, note that the time-domain iteration allows
all the advanced techniques that have been de-
veloped for wave equations (e.g. local timestep-
ning, non-conforming discontinuous Galerkin fi-
nite elements h- and p-adaptivity etc.) to be
transferred to the Helmholtz equation and other
time harmonic problems.
4 Analysis

We will now make a simple analysis of the iteration (4). Consider the Helmholtz solution \( u \) and the wave equation solution \( w \) with initial data \( w = v, u_t = 0 \) and forcing \( f \). Let \( \phi_j \) and \( \lambda_j^2 \) be the eigenfunctions and corresponding eigenvalues of \(-\nabla(c^2(x)\nabla)\). We can then expand the functions

\[
u(x) = \sum_{j=0}^{\infty} \hat{u}_j \phi_j(x), \quad v(x) = \sum_{j=0}^{\infty} \hat{v}_j \phi_j(x),
\]

\[
w(t, x) = \sum_{j=0}^{\infty} \hat{w}_j(t) \phi_j(x), \quad f(x) = \sum_{j=0}^{\infty} \hat{f}_j \phi_j(x).
\]

The modes of the wave equation solution \( w \) can be written explicitly as functions of time,

\[
\hat{w}_j(t) = (\hat{v}_j - \hat{u}_j) \cos(\lambda_j t) + \hat{u}_j \cos(\omega t),
\]

and the filtering step (3) gives

\[
\Pi v = \sum_{j=0}^{\infty} \tilde{v}_j \phi_j(x), \quad \tilde{v}_j = \beta(\lambda_j)(\hat{v}_j - \hat{u}_j) + \hat{u}_j,
\]

where

\[
\beta(\lambda) := 2 \int_0^T (\cos(\omega t) - \frac{1}{4}) \cos(\lambda t) dt.
\]

(Note that \( \beta(\omega) = 1 \).) Upon defining the linear operator \( S \) by

\[
S \sum_{j=0}^{\infty} \hat{u}_j \phi_j(x) := \sum_{j=0}^{\infty} \beta(\lambda_j) \tilde{u}_j \phi_j(x),
\]

we can then write the iteration as

\[
v^{n+1} = \Pi v^n = S(v^n - u) + u. \tag{5}
\]

The operator \( S \) is self-adjoint and has the same eigenfunctions \( \phi_j(x) \) as \(-\nabla \cdot (c^2(x)\nabla)\) but with the (real) eigenvalues \( \beta(\lambda_j) \). The convergence properties of the iteration depend on these eigenvalues and it is therefore of interest to study the range of the filter transfer function \( \beta \). Figure 1 shows a plot of \( \beta \) which indicates that the eigenvalues of \( S \) are inside the unit interval, with a few of them being close to 1 (when \( \lambda_j \approx \omega \)), and most of them being close to zero (when \( \lambda_j \gg \omega \)). In fact, one can show that \( \beta(\lambda) \in [-0.5, 1] \) and

\[
\beta(\omega + \varepsilon \omega) \approx 1 - c\varepsilon^2, \quad |\varepsilon| \ll 1. \tag{6}
\]

We can now derive a convergence result. We quantify the non-resonance condition by letting

\[
\delta = \inf_{j} \frac{|\lambda_j - \omega|}{\omega} > 0,
\]

be the relative size of the smallest gap between \( \lambda_j \) and the Helmholtz frequency. Then we introduce

\[
\rho = \max_{j} |\beta(\lambda_j)| = \beta(\omega \pm \delta \omega) \approx 1 - c\delta^2,
\]

where the last step follows from (6), assuming \( \delta \ll 1 \). We can rearrange (5) and obtain

\[
v^{n+1} - u = S(v^n - u).
\]

Then,

\[
||v^{n+1} - u||_{L^2(\Omega)}^2 = \sum_{j=0}^{\infty} \beta(\lambda_j)^2 (\tilde{v}_j^n - \hat{u}_j)^2
\]

\[
\leq \rho^2 \sum_{j=0}^{\infty} (\tilde{v}_j^n - \hat{u}_j)^2
\]

\[
= \rho^2 ||v^n - u||_{L^2(\Omega)}^2,
\]

which shows that \( v^n \) converges to \( u \) in \( L^2 \) with rate \( \rho = 1 - O(\delta^2) \). Thus, not surprisingly, the smallest gap, \( \delta \), determines the convergence factor. It is straightforward to also get convergence in \( H^1 \). In the end we obtain the following theorem, [2].

**Theorem 2** The iteration (4) converges in \( H^1(\Omega) \) for the Dirichlet and Neumann problems away from resonances to a unique fixed point which is the solution of the Helmholtz equation (1). The convergence rate is \( 1 - O(\delta^2) \).
The iteration operator is an affine operator of the form
\[ \Pi v = Sv + b, \quad b = u - Su. \]
Setting \( A = I - S \) we can reformulate the fixed point problem \( v = \Pi v \) as a linear equation
\[ Av = b. \tag{7} \]
Further analysis of \( S \) shows that it is a bounded, linear, self-adjoint, compact operator from \( H^1(\Omega) \) to \( H^1(\Omega) \), whose eigenvalues lie in the interval \([-0.5, \rho]\). Therefore, \( A \) is a bounded, linear, self-adjoint operator from \( H^1(\Omega) \) to \( H^1(\Omega) \), which is positive and coercive, with eigenvalues in the interval \((1 -\rho, 3/2]\). Its condition number is of size \( O(1/(1 - \rho)) = O(1/\delta^2) \).

**Krylov acceleration.** We note that \( b = \Pi 0 \) in (7) and can therefore easily be pre-computed. Furthermore, we can then evaluate the action of \( A \) as
\[ A v = v - \Pi v + b. \]
Thus, we can simply carry out the evaluation of \( Av \) by evolving the wave equation for one period in time with \( v \) as the initial data and then subtract the filtered solution from the sum of the initial data and the right hand side \( b \). This makes it possible to replace the simple fixed point iteration (4) with accelerated Krylov methods. Since \( A \) is positive and self-adjoint one can use the conjugate gradient (CG) method.

Although the formulation (7) is mathematically equivalent to the original Helmholtz equation (1) for the interior Dirichlet and Neumann problems away from resonances, there are two striking differences:

- The linear equation (7) is positive definite, not indefinite.
- Since \( S \) is compact, the condition number of \( A \) after discretization is essentially independent of the grid size \( \Delta x \). This means that, similar to many boundary integral methods, the number of iterations needed for convergence is also virtually independent of \( \Delta x \).

For CG the number of iterations needed to obtain a fixed accuracy scales as the square root of the condition number of \( A \), i.e. as \( 1/\delta \). To further understand how \( \delta \) may depend on the frequency \( \omega \), consider the asymptotic distribution of large eigenvalues. By the work of Weyl we know that the eigenvalues of elliptic operators grow asymptotically as \( \lambda_j \sim j^{1/d} \) in \( d \) dimensions. For large \( j \) the eigenvalues thus become more dense in dimensions \( j \geq 2 \). The average relative gap \( \delta \) when \( \omega \approx \lambda_j \) can be estimated as
\[ \delta \approx \frac{\lambda_{j+1} - \lambda_j}{\omega} \sim \omega^{-d}. \]
Thus, for high frequencies, one expects the number of iterations with an (unconditioned) CG method to grow as \( O(\omega^d) \). However, in numerical experiments we observe slightly better complexity.

**Remark 3** The iteration count above is for the interior energy conserving case, which is ill-posed for resonant \( \omega \). Moreover, when \( d \geq 2 \) the problem will be closer and closer to resonance as \( \omega \) grows. To have a physically relevant model at high frequencies some damping may be required, for instance by adding a term \( \iota \omega \eta u \) to (1). In this case, we observe that the number of iterations for the corresponding WaveHoltz method grows as just \( O(\omega) \) in all dimensions.

**Impedance case.** For open, non energy conserving problems, the Dirichlet or Neumann boundary conditions, are replaced by the impedance condition
\[ i\omega u + \vec{n} \cdot \nabla u = 0, \quad \text{on } \partial \Omega. \]
This is a common situation in practical applications. In this case the boundary conditions in the wave equation (2) should be
\[ w_1 + \vec{n} \cdot \nabla w = 0, \quad \text{on } \partial \Omega. \]
Moreover, also the initial data for the time-derivative \( u_t(0, x) = v_1(x) \) must be included in the iteration:
\[ \begin{bmatrix} v_0 \\ v_1 \end{bmatrix}^{(n+1)} = \Pi \begin{bmatrix} v_0 \\ v_1 \end{bmatrix}^{(n)}, \quad \begin{bmatrix} v_0 \\ v_1 \end{bmatrix}^{(0)} = 0, \]
where \( v_t^{n+1} \) is the time-filter of \( w_t \) (3) in the same way as \( v_0^{n+1} \) is the time-filter of \( w \) in (3). The resulting operator \( A \) is no longer self-adjoint, and GMRES must be used instead of CG to solve (7). For these open problems we observe convergence but do not yet have a complete theory.
explaining it. Since the operator in the wave equation in this case does not have a point spectrum, nor an eigen basis, the simple analysis used above fails. However, numerical experiments show that the number of iterations for fixed accuracy generally grows as $O(\omega)$ independent of $\Delta x$ and dimension $d$.

We note finally that the convergence rates reported above are all for the unconditioned case. As for frequency domain methods, preconditioners could potentially improve these rates significantly.

References


Elasticity, skeletal muscle, and waves?

Nilima Nigam$^{1,*}$, James Wakeling$^{1,2}$

$^1$Department of Mathematics, Simon Fraser University, Burnaby, Burnaby, Canada
$^2$Department of Biomedical Physiology and Kinesiology, Simon Fraser University, Burnaby, Canada

$^*$Email: nigam@math.sfu.ca

Abstract

In this talk, we survey recent work on the modeling, simulation and validation of a fully 3-D continuum elasticity approach for skeletal muscle dynamics. Skeletal muscle is modelled as a fibre-reinforced hyperelastic material, with other connective tissues such as aponeurosis and tendon being similarly described. These fibres are capable of nonlinear activation. After discretization (semi-implicit in time, FE in space), the model is validated against physiological data, and then used to understand the impact of muscle architecture, mass and tissue properties on questions of physiological interest.

Keywords: Nonlinear elasticity, skeletal muscle mechanics, three-field formulation.

1 Background

Skeletal muscles exhibit fascinating structural and mechanical properties. Skeletal muscle is composed of cells collectively referred to as fibers, which themselves contain contractile proteins arranged longitudinally into sarcomeres (Fig.1). These latter respond to signals from the nervous system, and contract; this leads to a strong mechanical anisotropy in the system. Muscles react to mechanical forces - they contain connective tissue and fluid, and are linked via tendons to the skeletal system - but they also are capable of activation via stimulation (and hence, contraction) of the sarcomeres. The restorative along-fibre force depend on departures from a characteristic length of the sarcomeres; diseases such as cerebral palsy cause this characteristic length to change, thereby impacting muscle force.

Prior to the landmark paper by A.V. Hill [1], it was believed a stimulated muscle was like an elongated spring that has the capacity to contract and do work. However, this failed to explain an important distinction between ‘usual’ elastic materials and skeletal muscle: the force exerted by a pure elastic body depends on its strain; however, in muscle fibres, force is additively dependent on the velocity of contraction. Hill’s paper showed that even for isometric (fixed length) contractions, muscles fibres are capable of shortening. Hill suggested that skeletal muscles have two distinct kinds of elastic components in series with each other: a contractile component that shortens when stimulated and a nonlinear elastic component which lengthens under tension. The resulting 1-D mathematical model (see Fig.2) proposed by him was both simple and remarkable in its predictive capabilities. Since then, experimentalists have gained much insight into mammalian skeletal muscle especially at small scales such as those of sarcomeres, single fibres and small muscles. Experimental data on muscle contraction is typically determined assuming the muscle is fully active, changes length at constant velocity, and considers forces and length changes in only the longitudinal direction. This information, incorporated into refinements of Hill’s model, has lead to important advances in biomechanics.

In Hill’s 3-element model Fig 2, a muscle fibre of total length $L$ is described as $L = L_{PE} = L_{SE} + L_{CE}$, where $L_{PE}$, $L_{CE}$ and $L_{CE}$ are the lengths of the passive, contractile and series elements. The force in the contractile element depends on both the stretch $\lambda$ and the time rate
Figure 2: Hill’s 3-element model: PE denotes the passive element, CE is the (nonlinear) contractile element, SE encapsulates the elastic properties of the fibre.

of stretch $\lambda$:

$$F_{CE}(L_{CE}, v) = F_{\text{max}} \left[ a(t) \hat{F}_v(\lambda) \hat{F}_a(\lambda) \right] + F_{\text{passive}} \hat{F}_p(\lambda).$$

The springs themselves are assumed massless, and to move in 1 direction.

Skeletal muscles consist of many fibres, arranged in a striated manner (in contrast to cardiac muscle). We know surprisingly little about large muscles contract, particularly when they are not fully active or contract with varying velocities. We also do not know, in detail, what the effects of changing shape, muscle density or material properties (fat infiltration, stiffening due to neuromuscular diseases) have on muscle force output. Understanding how the contractile elements interact with the tissue properties of the whole muscle, how deformations may arise in all three dimensions during contraction, and how transverse compression/shape changes affect force output are questions which cannot be answered by 1-D models. For example, experimental evidence suggests that the Hill-type approximation yields poor force predictions for larger muscles, [11]. Additionally, it has been experimentally observed that elastic waves may propagate through the muscle; this is not possible to explain the single-fibre model of muscle.

Some of the pioneering works on a fully 3-D model of muscle include [4,6,7], who considered a 3-D constitutive model for incompressible biological soft tissues within an isometric setting, and FEM implementations. In this talk, we’ll first present a brief review of the existing work on 3-D modelling of skeletal muscle mechanics. We’ll describe our model, and some of the experimental data used to fit parameters. The discretization of the highly nonlinear system is via a semi-discretization in time, and a finite element discretization in space.

2 Mathematical model

We focus on length scales larger than those of individual fibres, which allows us to capture the role of structure and tissue properties on large muscle mechanics. Muscle is represented as a fiber-reinforced hyperelastic material, where the fibre properties are governed by the myofilament contractile forces described Hill-type models, and the composite properties are represented a Neo-Hookean 'base material' encapsulating properties of muscle tissue across several scales, including intracellular stiffness and extracellular material. This muscle is encased, as needed, by connective tissues (tendon/aponeurosis) modelled as Yeoh-type materials.

Our work builds on that of [6,7]. We work with a three-field variational formulation pioneered in [2,3] (see also [5]). The implementation is within the deal.ii finite element library, and is based on the excellent tutorial on finite deformations in an isotropic Neo-Hookean material, [8].

We first discuss quasi-static deformations, consistent with an isometric system in which neither muscle mass nor velocity is involved. We use a mixed Jacobian formulation ([2,3]) to solve for the unknown displacement $u$, the pressure $p$, and a dilation $D$ in the current configuration $\Omega$, with $\Pi := (u, p, D) \in (H^1(\Omega))^3 \times L^2(\Omega) \times L^2(\Omega)$. We seek the state $\Pi$ which is a stationary point of a potential (as in [8]).

The constitutive relations for hyperelastic materials are given, as is standard, in terms of the Helmholtz free energy density $W(B)$, which depends on the left Cauchy-Green tensor $B$. We can split the energy density into a volumetric and isochoric part; the latter is then split into the along-fibre and base material contributions

$$W(B) = W_{\text{vol}}(J) + W_{\text{iso}}(B) = W_{\text{vol}}(J) + W_{\text{fibre}} + W_{\text{base}}.$$ 

See, for instance, [6,12]. The precise dependance
of $W$ on different invariants of $B$ are obtained via fitting to experimental data; details can be found in [9, 10, 12, 14, 15]. As an instance: in order to obtain the energy $W_{fibre}$ (which is consistent with the original Hill-type model), we consider single-fibre data. In the laboratory setting, what is measured is the dependance of along-fibre stress with isochoric stretch $\lambda_{iso}$. So, we must first fit the stress to the data (Fig 3 [11]; we’d then use the relation

$$\lambda_{iso} \frac{\partial W_{fibre}(\lambda_{iso})}{\partial \lambda_{iso}} = \sigma_{fibre}(\lambda)$$

to obtain $W_{fibre}$. A similar procedure is carried out for the other components of the model. In some, the experimental data is directly in terms of the strain energy; in others (as for the fibre), it is not.

The Euler-Lagrange equations for stationarity of the potential for the isometric setting can then be written as

$$-\text{div}(\sigma(\mathbf{u})) = \mathbf{b} \quad \text{(static equilibrium)} \tag{1}$$

$$D = \text{det}(J + \nabla \mathbf{u}) =: J(\mathbf{u}) \quad \text{(dilation)} \tag{2}$$

$$p = \frac{\delta(W_{\text{vol}}(D))}{\delta D} \quad \text{(pressure response)} \tag{3}$$

We prescribe either zero traction boundary conditions on the faces, or Dirichlet conditions (depending on the experiment). We also allow for the combination of distinct tissues - muscles, aponeurosis and tendon - for which the constitutive laws have to be obtained.

As in [8], we use a total Lagrangian formulation. The Euler-Lagrange equations leads to a (nonlinear) weak formulation. We use a finite element approach, combined with a Newton-Raphson strategy to solve the nonlinear system; the system is implemented within the deal.II library.

In case of a fully dynamic system, inertial effects due to mass become important. In addition, the along-fibre contributions to the stress are given by a (nonlinear) relationship involving both the stretch and the stretch rate; this is due to Hill’s model. For this reason, we must directly work with the dynamic system with the additional unknown velocity $\mathbf{v}$.

$$\frac{\partial}{\partial t} (\rho \mathbf{v}) = -\text{div}(\rho \mathbf{v} \otimes \mathbf{v}) + \text{div}(\sigma(\mathbf{u})) + \mathbf{b},$$

$$D = J(\mathbf{u}),$$

$$p = \frac{\delta(W_{\text{vol}})}{\delta D}.$$  

Once again, zero traction and (possible inhomogenous) Dirichlet conditions are allowed. We use a semi-implicit discretization in time, and a $Q1 \times P0 \times P0$ discretization in space.

### 3 Results

Our mathematical models, and associated finite element implementations, allow for an exploration of a range of questions in physiology. A first and important question to address is: in pennate muscles (those in which the line-of-action of a load is not long the direction of fibres), does the curvature of fibres change? This has been observed in MRI studies, and cannot be readily explained by 1-D Hill-type models.

As a next investigation, we examine the mechanical energy within a muscle. During muscle contraction, chemical energy is converted to mechanical energy, which in turn is distributed and stored in the tissue as the muscle deforms or is used to perform external work. We showed how energy is distributed through contracting muscle during fixed-end contractions; subsequently, we study the distribution of tissue energy when mass effects are taken into account. Some of these results will be described in the talk, and also form the basis of validation of our model, [12, 14, 15].

As a final demonstration, we will describe recent work on cerebral palsy. In this condition, there are changes to the size, shape and stiffness of the tissues; additionally, the length of the sacromeres changes (resulting in changes to the curves in Fig. 2). MRI data is used to
generate hexahedral meshes, and we are able to assess the impact of these changes to the mechanical work done by muscles. [16].

References


The virial theorem and the method of multipliers in spectral theory

David Krejčiřík\textsuperscript{1,*}

\textsuperscript{1}Department of Mathematics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Trojanova 13, 12000 Prague 2, Czech Republic

*Email: david.krejcirik@fjfi.cvut.cz

Abstract

We provide a link between the virial theorem in quantum mechanics and the method of multipliers in theory of partial differential equations. After giving a physical insight into the techniques, we show how to use them to deduce the absence of eigenvalues and other spectral properties for electromagnetic Schrödinger operators. We focus on our recent developments in non-self-adjoint settings, namely on Schrödinger operators with matrix-valued potentials, relativistic operators of Pauli and Dirac types, and complex Robin boundary conditions.

Keywords: virial theorem, method of multipliers, absence of eigenvalues, uniform resolvent estimates, electromagnetic Schrödinger and Dirac operators, non-self-adjoint perturbations, Robin boundary conditions

1 Quantum-mechanical background

In quantum mechanics, physical states and observables are represented by vectors and self-adjoint operators in a Hilbert space \( \mathcal{H} \), respectively. The expectation value of an observable \( A \) to be in a state \( \Psi \) is given by the inner product \( \langle A \rangle := (\Psi, A\Psi) \) and the outcomes of measuring are the spectrum of \( A \). The most prominent observable is the Hamiltonian \( H \) representing the total energy of the system. It determines the evolution of states in time \( t \) through the Schrödinger equation

\[
\frac{d\Psi}{dt} = H\Psi. \tag{1}
\]

The eigenvalues \( \lambda \) of \( H \) are energies of the system for which (1) admits stationary solutions of the type \( e^{-i\lambda t}\psi \), where \( \psi \) is an eigenvector of \( H \) corresponding to \( \lambda \); it is customarily called a bound state (or trapped mode). The exclusion of eigenvalues constitutes a first step in justifying transport for a quantum system.

2 The virial theorem

How to achieve the absence of eigenvalues of a given operator \( H \)? A powerful tool is represented by an abstract version of the virial theorem (see [10, Sec. 13 & Notes] for a historical background). Let us present a formal statement first.

Let \( T \) be another self-adjoint operator in \( \mathcal{H} \). Assume that the commutator of \( T \) with \( H \) is positive in a sense. For instance, in a very restrictive sense, that there exists a positive number \( a \) such that (we do not care about operator domains for a moment)

\[
i[H,T] \geq a I \tag{2}
\]

in the sense of quadratic forms in \( \mathcal{H} \).

Now, let \( \lambda \) be an eigenvalue of \( H \) corresponding to an eigenvector \( \psi \), normalised to 1 in \( \mathcal{H} \). That is, the stationary Schrödinger equation

\[
H\psi = \lambda\psi \tag{3}
\]

holds. Then we get a contradiction

\[
a \leq \langle \psi, i[H,T]\psi \rangle = \langle H\psi, T\psi \rangle - i\langle T\psi, H\psi \rangle = i\langle \lambda\psi, T\psi \rangle - i\langle T\psi, \lambda\psi \rangle = 0, \tag{4}
\]

where the first and last equalities employ the self-adjointness of \( H \) and \( T \). Note that our convention is that the inner product \( (\cdot, \cdot) \) of \( \mathcal{H} \) is linear in the second component.

Hence, the positivity of the commutator prevents the existence of eigenvalues. This is the formal statement of the virial theorem. Schematically:

existence of eigenvalues \( (2) \implies \sigma_p(H) = \emptyset \),

where \( \sigma_p(H) \) denotes the point spectrum of \( H \), i.e. the set of eigenvalues.
3 The method of multipliers

The virial theorem is closely related with the method of multipliers, usually attributed to the original development of Morawetz [9].

Take an inner product of both sides of (3) with the vector \( \phi := iT \psi \) (this is the multiplier of the method) and take twice the real part of the obtained identity:

\[
(\psi, [H, T] \psi) = (iT \psi, H \psi) + (H \psi, iT \psi)
\]

\[
= 2\Re(\phi, H \psi)
\]

\[
\pm \lambda 2\Re(\phi, \psi)
\]

\[
= \lambda \left[ (iT \psi, \psi) + (\psi, iT \psi) \right]
\]

\[
= 0
\]

(here the arrow points to the initial identity, the other equalities are manipulations). In this way we have arrived at the same identity as in (4) and the same contradiction under the positivity hypothesis (2).

4 An evolution interpretation

Why the positivity of the commutator is related to the (total) absence of eigenvalues? How to choose the auxiliary (so-called conjugate) operator \( T \)? It is useful to get a physical insight first.

Differentiating the expectation value of \( T \) with respect to time \( t \) and using (1), we (formally) get

\[
\frac{d}{dt} \langle T \rangle = \left( \frac{d}{dt}, T \Psi \right) + \langle T, \frac{d}{dt} \Psi \rangle
\]

\[
= \left( -iH \Psi, T \Psi \right) + \left( \Psi, (T - iH) \Psi \right)
\]

\[
= i \langle \Psi, HT \Psi \rangle - i \langle \Psi, T H \Psi \rangle
\]

\[
= \langle \Psi, i[H, T] \Psi \rangle
\]

\[
= \langle i[H, T] \rangle.
\]

(5)

Hence the evolution of the expectation value of \( T \) is given by the expectation value of the commutator with \( H \) multiplied by \( i \) (without this multiplication, the commutator \([H, T]\) is actually skew-adjoint).

It follows from (5) and (2) that the differential inequality

\[
\frac{d}{dt} \langle T \rangle > a
\]

holds (assuming the normalisation \( \| \Psi \| = 1 \)), which in turn implies

\[
\langle T \rangle(t) > \langle T \rangle(0) + at
\]

for all times \( t \geq 0 \). Consequently,

\[
\lim_{t \to +\infty} \langle T \rangle(t) = +\infty.
\]

In summary, the positivity of the commutator (2) implies that the expectation value of \( T \) diverges.

5 The free Hamiltonian

To answer the pertinent questions at the beginning of Section 4, let us focus on the Hamiltonian of a free (i.e. no forces) non-relativistic (i.e. no spin) particle. It is customarily represented by the operator

\[
H_0 := -\Delta \quad \text{in} \quad L^2(\mathbb{R}^d),
\]

which is self-adjoint provided its domain is chosen to be the Sobolev space \( W^{2,2}(\mathbb{R}^d) \). Note that \( H_0 = P_0^2 := P_0 \cdot P_0 \), where the dot denotes the scalar product in \( \mathbb{R}^d \) and \( P_0 := -i \nabla \), with domain being the Sobolev space \( W^{1,2}(\mathbb{R}^d) \), represents the momentum of the particle. In this representation, the position of the particle is represented by the maximal operator of multiplication \( X \) by the space variable \( x \), i.e.

\[
X \psi(x) = x \psi(x).
\]

Now, let \( T_0 \) be the quantum counterpart of the radial momentum of the particle:

\[
T_0 := \frac{X \cdot P_0 + P_0 \cdot X}{2} = -i x \cdot \nabla - \frac{d}{2}.
\]

(8)

Note that we had to take a symmetrised version of the classical radial momentum \( X \cdot P_0 \) (in order to make \( T_0 \) self-adjoint, at least formally), since the observables \( X \) and \( P_0 \) do not commute in quantum mechanics. Then (6) can be interpreted in physical terms as that the particle escapes to infinity of \( \mathbb{R}^d \) for large times (for the radial derivative diverges). That is, the particle is not bound, it propagates. More specifically, the stationary solutions of the Schrödinger equation (1), corresponding to initial data being eigenfunctions, do not exist.

It remains to analyse the validity of (2) for the free Hamiltonian (7) and the radial momentum (8). It is easily verified that (still formally)

\[
i[H_0, T_0] = 2H_0.
\]

Here the right-hand side is non-negative because, by an integration by parts,

\[
(\phi, H_0 \phi) = (\phi, -\Delta \phi) = \| \nabla \phi \|^2 \geq 0
\]

(9)
for every $\phi \in W^{2,2}(\mathbb{R}^d)$. However, it is not positive in the strict sense (2) for $\sigma(H_0) = [0, \infty)$. Nonetheless, a contradiction in the spirit of (4) is still in order:

$$2 \|\nabla \psi\|^2 = (\psi, 2H_0\psi) \geq (\psi, i[H_0, T_0]\psi) = 0,$$

whenever $\psi$ is an eigenfunction of $H_0$. Indeed, from this identity we deduce that $\psi$ is constant, which is not possible for a non-trivial function in $L^2(\mathbb{R}^d)$.

In summary, commutators arise in evolution processes in quantum mechanics and the natural choice for the conjugate operator for the free Hamiltonian $H_0$ is given by the radial momentum (8).

6 Dispersion

There is yet another support for the choice (8), at least if we deal with the Laplacian and its perturbations. In fact, the conjugate operator $T_0$ by itself arises as a commutator with the Laplacian:

$$T_0 = i \left[ H_0, \frac{X^2}{4} \right].$$

Consequently,

$$\frac{d^2}{dt^2} \left\langle \frac{X^2}{4} \right\rangle = \frac{d}{dt} \langle T_0 \rangle = \langle i[H_0, T_0] \rangle,$$

so the positivity of the commutator $i[H_0, T_0]$ actually shows that the expectation value of the square of the magnitude of the position is a convex function in time: there is a dispersion.

7 Rigorous implementation

There are certainly a number of formal manipulations in the arguments given above. Let us now show how to justify them for the free Hamiltonian. The eigenvalue equation (3) for the free Hamiltonian precisely means that there exists a non-trivial function $\psi \in W^{2,2}(\mathbb{R}^d)$ such that

$$(\nabla \phi, \nabla \psi) = \lambda(\phi, \psi).$$

for any choice $\phi \in W^{1,2}(\mathbb{R}^d)$. This is just a weak formulation of the Helmholtz equation in $\mathbb{R}^d$.

First of all, notice that we may restrict to $\lambda \geq 0$ due to the self-adjointness of $H_0$ and (9).

In other words, the existence of non-real and negative eigenvalues is easily disproved.

Following the arguments given above, our aim is to choose $iT_0\psi$ for the test function (the multiplier) $\phi$, where the conjugate operator $T_0$ is given by (8). However, it is not clear that $\psi$ belongs to the domain of $T_0$ (the domain of $T_0$ has not been even discussed) and, even if so, that $\phi \in W^{1,2}(\mathbb{R}^d)$. Indeed, the problem is the unbounded position operator $x$ in the definition of $T_0$.

To proceed rigorously, we therefore choose the regularised multiplier

$$\phi := x \cdot \nabla(\xi_\nu \psi) + \frac{d}{2} \psi,$$

where $\xi_\nu$ is the cut-off function satisfying, for every $n \in \mathbb{N}^*$, $\xi_\nu(x) := \xi(x/n)$, where $\xi \in C_0^\infty(\mathbb{R}^d)$ is such that $0 \leq \xi \leq 1$, $\xi(x) = 1$ for every $|x| \leq 1$ and $\xi(x) = 0$ for every $|x| \geq 2$. Then $\phi \in W^{1,2}(\mathbb{R}^d)$ because $\psi \in W^{2,2}(\mathbb{R}^d)$ and the multiplication by $x$ is bounded on the support of $\psi_n$. Then we get the ultimate identity $\|\nabla \psi\| = 0$ of (10) after taking the limit $n \to \infty$.

The specialty of the free Hamiltonian $H_0$ is that the elliptic regularity implies that the eigenfunction $\psi$ belongs to $W^{2,2}(\mathbb{R}^d)$. Without this extra result (which will be particularly the case when we deal with electromagnetic perturbations below), we only have $\psi \in W^{1,2}(\mathbb{R}^d)$. Then an extra regularisation of the multiplier $iT_0\psi$ consists in replacing the gradient in (12) by difference quotients, as originally proposed in our work [5]. Altogether, proceeding rigorously with the regularised multiplier and taking the limits in the right order is rather painful. This is probably the reason why necessary regularisation schemes are usually omitted in the literature, except for the recent work [5].

8 Electromagnetic perturbations

Of course, the absence of eigenvalues of the free Hamiltonian $H_0$ can be proved more straightforwardly by using the Fourier transform. However, the advantage of the present method based on the virial theorem is that it is much more robust. In particular, the same conjugate operator $T_0$ applies to electric perturbations of $H_0$ and its magnetic version enables one to deal with magnetic perturbations of $H_0$, too.

Given a scalar function (electric potential) $V : \mathbb{R}^d \to \mathbb{R}$ and a vector-valued function (mag-
electric potential) $A: \mathbb{R}^d \to \mathbb{R}^d$, consider the electromagnetic Hamiltonian
$$H_{A,V} := (-i\nabla - A)^2 + V.$$ Under the minimal hypotheses $V \in L^1_{\text{loc}}(\mathbb{R}^d)$ and $A \in L^2_{\text{loc}}(\mathbb{R}^d)$ together with a relative smallness of the negative part of $V$ with respect to the magnetic Laplacian $-\Delta_A := (-i\nabla - A)^2$, the operator $H_{A,V}$ is customarily realised as a self-adjoint operator in $L^2(\mathbb{R}^d)$ with the form domain of $H_{A,V}$ being the magnetic Sobolev space $W^{1,2}_{A,V}(\mathbb{R}^d) := \{\psi \in L^2(\mathbb{R}^d) : \nabla_A \psi \in L^2(\mathbb{R}^d)\}$, where $\nabla_A := \nabla - iA$ is the magnetic gradient. Of course, $H_{0,0} = H_0$ is the free Hamiltonian.

**Electric perturbations**

In the magnetic-free case, one has
$$i[H_{0,V}, T_0] = 2H_0 - x \cdot \nabla V,$$
so the virial identity reads
$$2 \|\nabla \psi\|^2 - \int_{\mathbb{R}^d} x \cdot \nabla V \, |\psi|^2 = 0 \quad (13)$$
whenever $\psi$ is an eigenfunction of $H_{0,V}$.

Clearly, the pointwise repulsivity condition
$$x \cdot \nabla V \leq 0$$
implies a contradiction, therefore the absence of eigenvalues of $H_{0,V}$. Less restrictively, it is enough to assume the smallness of the positive part $(x \cdot \nabla V)_+$ in the following integral sense: There exists a positive number $a < 2$ such that
$$\int_{\mathbb{R}^d} (x \cdot \nabla V)_+ |\psi|^2 \leq a \int_{\mathbb{R}^d} |\nabla \psi|^2 \quad (14)$$
holds for every $\psi \in W^{1,2}(\mathbb{R}^d)$. Our regularisation scheme described in Section 7 requires the extra regularity condition
$$V \in W^{1,p}_{\text{loc}}(\mathbb{R}^d), \quad (15)$$
where $p = 1$ if $d = 1$, $p > 1$ if $d = 2$ and $p = d/2$ if $d \geq 3$.

The repulsivity condition (14) can be replaced by the following smallness condition, in which case (15) is not needed: There exists a positive number $a < 2/(d+2)$ such that
$$\int_{\mathbb{R}^d} |V| |\psi|^2 \leq a \int_{\mathbb{R}^d} |\nabla \psi|^2; \quad \int_{\mathbb{R}^d} |x|^2 |V|^2 |\psi|^2 \leq a^2 \int_{\mathbb{R}^d} |\nabla \psi|^2, \quad (16)$$
hold for every $\psi \in W^{1,2}(\mathbb{R}^d)$. Indeed, it is enough to integrate by parts in the second term on the left-hand side of (13) and use the Schwarz inequality.

Let us summarise the obtained results into the following theorem.

**Theorem 1** Assume (14) with $a < 2$ or (16) with $a < 2/(d+2)$. In the former case assume in addition (15). Then $\sigma_p(H_{0,V}) = \emptyset$.

This theorem is a very special case of a series of recent results obtained in [6, Thm. 3] and [4, Thm. 3.4]. However, a first rigorous proof of (13) (under alternative regularity hypotheses about $V$) goes back to Weidmann [11].

**Magnetic perturbations**

When there is a magnetic field, the conjugate operator (8) should be replaced by its magnetic version
$$T_A := \frac{X \cdot P_A + P_A \cdot X}{2} = -i x \cdot \nabla_A - i \frac{d}{2},$$
where $P_A := -i\nabla_A$ is the magnetic momentum. For simplicity, let us consider purely magnetic perturbations of the free Hamiltonian. Then
$$i[H_{A,0}, T_A] = 2H_{A,0} + (x \cdot B) \cdot P_A + P_A \cdot (x \cdot B),$$
where $B := \nabla A - \nabla A^T$ is the magnetic tensor. Consequently, the virial identity reads
$$2 \|\nabla_A \psi\|^2 + 23 \int_{\mathbb{R}^d} (x \cdot B) \cdot \psi \nabla A \psi = 0$$
whenever $\psi$ is an eigenfunction of $H_{A,0}$.

Using the Schwarz inequality, we get a contradiction, and therefore the absence of eigenvalues of $H_{A,0}$, provided that the following smallness condition holds: There exists a positive number $a < 1$ such that
$$\int_{\mathbb{R}^d} |x|^2 |B|^2 |\psi|^2 \leq a^2 \int_{\mathbb{R}^d} |\nabla_A \psi|^2 \quad (17)$$
holds for every $\psi \in W^{1,2}_{A}(\mathbb{R}^d)$. Our regularisation scheme described in Section 7 requires the extra regularity condition
$$A \in W^{1,2p}_{\text{loc}}(\mathbb{R}^d), \quad (18)$$
where $p$ is as below (15).

We have therefore established the following theorem.
Theorem 2 Assume (17) with $a < 1$ and (18). Then $\sigma_p(H_{A,0}) = \emptyset$.

It is important that the fundamental hypothesis (17) is gauge invariant (i.e. it does not depend on the choice of $A$ for a given magnetic field $B$).

Theorem 2 is a very special case of a series of recent results obtained in [6, Thm. 3] and [4, Thm. 3.4]. The sufficient conditions which guarantee the absence of eigenvalues of $H_{A,V}$ follow from a full electromagnetic virial identity there.

Low versus high dimensions

It is interesting that spectral conclusions can be obtained on the basis of functional inequalities of the type (14), (16) and (17). Because of the criticality of the Laplacian in dimensions $d = 1, 2$, the conditions (16) cannot be satisfied for a non-trivial $V$ in these low dimensions. On the other hand, explicit sufficient conditions to verify the functional inequalities in high dimensions $d \geq 3$ follow by the Hardy inequality. What is more, hypothesis (17) (and other sufficient conditions stated in terms of the magnetic Laplacian $\nabla_A$) is non-void even in dimension $d = 2$ due to the existence of magnetic Hardy inequalities [3].

9 Non-self-adjoint perturbations

There are recent motivations to consider complex electromagnetic fields, including quantum mechanics [8]. It is clear already from the manipulations in (4) that the idea based on the virial theorem becomes useless in this case. On the other hand, the method of multipliers turns out to be more flexible.

Let us demonstrate it on the eigenvalue problem for the magnetic-free Hamiltonian

$$H_{0,V} \psi = \lambda \psi,$$ (19)

where both the potential $V$ and the eigenvalue $\lambda$ are allowed to be complex now. We set $\lambda_1 := \Re \lambda$ and $\lambda_2 := \Im \lambda$, and analogously for $V$. For simplicity, let us assume the following subordination condition: There exists a positive number $b < 1$ such that

$$\int_{\mathbb{R}^d} (|\partial V| + |3V|) |\psi|^2 \leq b \int_{\mathbb{R}^d} |\nabla \psi|^2$$ (20)

holds for every $\psi \in W^{1,2}(\mathbb{R}^d)$. Then the numerical range of $H_{0,V}$ is contained in the cone $|\lambda_2| \leq \lambda_1$, so it enough to explore the presence of eigenvalues there.

As in Section 3 (and disregarding the necessary regularisation procedures), take an inner product of both sides of (19) with the function $i T_0 \psi$, where $T_0$ is given by (8), and take twice the real part of the obtained identity. This leads to the identity

$$2 \|\nabla \psi\|^2 - \int_{\mathbb{R}^d} x \cdot \nabla V_1 |\psi|^2 - 2 \Im \int_{\mathbb{R}^d} V_2 x \cdot \psi - \nabla \psi = 0,$$ (25)

which is a non-self-adjoint counterpart of (13).

The idea of [1] is to compensate the appearance of the imaginary part of the inner product on the second line of (21) with no obvious sign by further identities obtained by using different multipliers. First, taking an inner product of both sides of (19) with the function $\psi$ and taking the real part of the obtained identity, we get

$$\|\nabla \psi\|^2 + \int_{\mathbb{R}^d} V_1 |\psi|^2 = \lambda_1 \|\psi\|^2.$$ (22)

Second, taking an inner product of both sides of (19) with the function $x|\psi$ and taking the real and imaginary part of the obtained identity, we respectively get

$$\int_{\mathbb{R}^d} |x| |\nabla \psi|^2 - \frac{d - 1}{2} \int_{\mathbb{R}^d} |\psi|^2 + \int_{\mathbb{R}^d} |x| V_1 |\psi|^2 = \lambda_1 \int_{\mathbb{R}^d} |x| |\psi|^2.$$ (23)

and

$$\Im \int_{\mathbb{R}^d} \frac{x}{|x|} \cdot \overline{\psi} \nabla \psi + \int_{\mathbb{R}^d} |x| V_2 |\psi|^2 = \lambda_2 \int_{\mathbb{R}^d} |x| |\psi|^2.$$ (24)

By taking the clever sum

$$(21) - (22) + \frac{|\lambda_2|}{\sqrt{\lambda_1}} (23) - 2 \sqrt{\lambda_1} \text{sgn}(\lambda_2) (24),$$

we arrive at the ultimate identity

$$\|\nabla \psi^-\|^2 + \frac{|\lambda_2|}{\sqrt{\lambda_1}} \int_{\mathbb{R}^d} |x| \left( |\nabla \psi^-|^2 - \frac{d - 1}{2} \frac{|\psi|^2}{|x|^2} \right) - \int_{\mathbb{R}^d} \frac{x}{|x|} \cdot \nabla(|x| V_1) |\psi|^2 + \frac{|\lambda_2|}{\sqrt{\lambda_1}} \int_{\mathbb{R}^d} |x| V_1 |\psi|^2$$

$$- 2 \Im \int_{\mathbb{R}^d} V_2 x \cdot \psi \nabla \psi^- = 0,$$ (25)
where
\[ \psi^-(x) := e^{-i\sqrt{\lambda_1} \text{sgn}(\lambda_2)|x|} \psi(x). \]

Various sufficient conditions for the absence of eigenvalues of \( H_{0,V} \) can be derived from (25). This has been done in a series of recent papers [4, 6, 7], including the magnetic field and obtaining uniform resolvent estimates.

For instance, let \( d \geq 3 \), so that the second term on the first line of (25) is non-negative by a weighted Hardy inequality, and assume that the potential \( V \) is purely imaginary. Then \( H_{0,V} \) has no eigenvalues in the cone \( |\lambda_2| \leq \lambda_1 \) provided that there exists a positive number \( a < 1/2 \) such that
\[ \int_{\mathbb{R}^d} |x|^2 |\nabla V|^2 |\psi|^2 \leq a^2 \int_{\mathbb{R}^d} |\nabla \psi|^2 \] (26)
holds for every \( \psi \in W^{1,2}(\mathbb{R}^d) \).

**Theorem 3** Let \( d \geq 3 \) and \( \Re V = 0 \). Assume conditions (26) with \( a < 1/2 \) and (20) with \( b < 1 \). Then \( \sigma_p(H_{0,V}) = \emptyset \).

10 Relativistic operators

The approach described in the preceding section can be adapted to electromagnetic Schrödinger operators with matrix-valued potentials. This has been done in [4], where we also applied the results to establish the absence of eigenvalues of Pauli and Dirac operators.

11 Boundary perturbations

The flexibility of the method of multipliers, particularly due to the developments described in Section 9, enables one to consider elliptic operators constrained to subdomains of the Euclidean space. In [5], we developed the method to study spectral properties of the Laplacian in the half-space \( \mathbb{R}^{d-1} \times (0, \infty) \), subject to Robin boundary conditions
\[ -\frac{\partial \psi}{\partial x_d} + \alpha \psi = 0, \]
where \( \alpha : \mathbb{R}^{d-1} \times \{0\} \to \mathbb{C} \) plays the role of a strongly localised potential. For instance, there are no eigenvalues provided that \( \alpha \) is repulsive in the sense that
\[ \alpha \geq 0 \quad \text{and} \quad x \cdot \nabla \alpha \leq 0. \]

Moreover, we derive uniform resolvent estimates.

The half-space can be regarded as a degenerate situation of conical domains intensively studied in recent years. In this respect, let us particularly mention the proof of the absence of eigenvalues of the Laplacian in non-convex conical sectors, subject to no specific boundary conditions [2]. On the other hand, it is easy to construct square-integrable solutions to the eigenvalue problem in a half-space.

**References**


Robust seismic imaging by full-waveform inversion with model time extension: time-domain and frequency-domain formulations

Biondo Biondi1,∗, Guillaume Barnier,1, Rustam Akmadhev1, Robert G. Clapp1, Ettore Biondi1,2

1Geophysics Department, Stanford University, Stanford, USA
2Seismological Laboratory, Caltech, Pasadena, USA
∗Email: biondo@stanford.edu

Abstract

Seismic full waveform inversion is formulated as non-convex optimization problem that converges to useful solutions only when the starting velocity is close to the true velocity and/or the data contain unrealistic low frequencies. A time-extension of the velocity model leads to waveform inversion algorithms that are more robust than the conventional full waveform inversion algorithms. Waveform inversion with time extension can be formulated in either the time domain or the temporal-frequency domain. The time-domain algorithm has been successfully tested with several datasets. A simple numerical example illustrates the characteristics of the proposed method and provides intuition on the convergence properties of the long wavelengths of the velocity model.

Keywords: seismic, waveform inversion, non-convex optimization

1 Introduction

Since its introduction in the early 80s [12, 20] full waveform inversion (FWI) has been appealing for the simplicity of its formulation. FWI is defined as the search of the velocity model that minimizes the differences between the data recorded in the field and data modeled by using a waveform modeling operator. FWI practical applications have been hampered by three main challenges: 1) computational cost, 2) data quality (e.g. poor spatial sampling), and 3) unreliable convergence to a useful model when the starting model is inaccurate and the data do not contain unrealistic low frequencies. Modern computational and data-acquisition technology have mostly solved the first two of these challenges. Progress in ray-based velocity estimation methods and progress in low-frequency and long-offsets data acquisition have reduced the practical impact of the third and enabled the successful application of FWI to many datasets.

However, there are many datasets acquired over complex geology that still defy modern FWI algorithms because of lack of convergence.

Several examples of algorithmic solutions of the convergence problem have been proposed; for some useful algorithmic solutions see [4, 9, 14, 21]. This paper presents two methods, which are closely related to each other, to overcome the convergence challenges of conventional FWI by using the concept of velocity-model extension. The idea of using velocity-model extensions to estimate the long wavelengths of the velocity model is rooted in the concept of prestack images. The goal of conventional velocity estimation is to focus prestack images obtained by seismic migration [6]. In a waveform inversion framework, prestack images are estimates of the short-wavelength component of an extended velocity model. Adding to the data-fitting goal of FWI the additional goal of focusing prestack images leads to waveform inversion methods that can robustly update the long wavelength of the velocity model [5, 15–18].

Symes [19] generalized the velocity-model extension idea beyond extended images to a velocity space-extension that includes all scales of the model. Biondi and Almomin [7] showed that extending the model in time yields a practical algorithm for robustly estimating all the wavelengths in the model. However, their optimization algorithm requires the tuning of several hyperparameters. Barnier et al. [6] introduced a more robust and general algorithm based on variable projection [11] that can be applied to both space and time extension of the model.

In this paper we focus on the time extension of the model and present two waveform-inversion methods. The first one is based on the time-domain solution of the acoustic wave equation and the second one on the temporal-frequency domain solution. The time-domain method is the time-extension instance of the
more general FWI with model extension (FWIME) method presented in [1–3].

2 Full waveform inversion with time extension (FWITE)

Conventional full-waveform inversion (FWI) is performed by solving the following optimization problem

\[
\min_{s^2} J (s^2),
\]

where:

\[
J (s^2) = \frac{1}{2} \| \mathcal{L} (s^2, f) - d \|_2^2,
\]

and \( s^2 \) is a vector of gridded slowness-squared values. \( \mathcal{L} \) is a wave-equation operator whose solutions are nonlinear with respect to slowness perturbations but linear with respect to the source function, \( f \), which is function of time, \( t \). The data vector \( d \) is a subset of the pressure-field vector \( p \) that is defined on the same spatial grid as \( s \) and on a discretized time. The data are extracted from the pressure field at the receivers’ locations through a linear sampling operator \( K \); such as \( d = Kp \).

For the sake of simplicity, we assume that \( \mathcal{L} \) is the acoustic and isotropic wave-equation operator. A generalization of the concepts presented in this paper to problems that require more complex wave-equation operators such as elastic and/or anisotropic is possible in principle, although it is not straightforward.

To define full waveform inversion with time extension (FWITE) we introduce a new "extended-model" wave operator \( \tilde{\mathcal{L}} \) defined by the extended acoustic wave equation:

\[
\nabla^2 p (t, x) - \tilde{s}^2 (t, x) \frac{\partial^2}{\partial t^2} p (t, x) = f (t).
\]

In equation 2 the symbol \( \ast \cdot \) signifies convolution in time between the pressure field and the time-extended slowness-squared model, \( \tilde{s}^2 \). When \( \tilde{s} \) is different from zero only at \( \tau = 0 \) equation 2 reduces to the conventional wave equation that describes the physical phenomenon of wave propagation in an acoustic medium.

We define FWITE as the minimization of the following objective function,

\[
\tilde{J} (\tilde{s}^2) = \frac{1}{2} \| \tilde{\mathcal{L}} (\tilde{s}^2) - d_\omega \|_2^2 + \epsilon \| \tau \tilde{s}^2 \|_2^2.
\]

We introduce the second term in 3 to constrain the solution to be "physical"; that is, to satisfy the conventional wave-equation without extension, and \( \epsilon \) is a trade-off parameter between the two terms in the objective function.

The formulation of FWITE as the minimization of the objective function 3 presents several theoretical and practical problems. The most fundamental challenge concerns the stability of the solution of the extended-model wave equation in 2. In the next section we present practical solution of these challenges based on a first-order Born linearization of 2 that leads to a robust, though computationally expensive, variable-projection inversion algorithm.

**Frequency-domain time extension**

To avoid the hurdles of the time-domain formulation of FWITE and to reduce the computational cost of the method, we are developing a frequency-domain based on the one-way approximation of the Helmholtz equation. Claerbout [10] introduced one-way wave propagation in the early 1970s. Since then, the seismic exploration community has developed many efficient numerical schemes for one-way wave propagation in the frequency domain. The use of the one-way wave equation for waveform inversion is more recent [4]. We believe that our frequency-domain method could be generalized to solutions of the full Helmholtz equation, which is more accurate, but also substantially more expensive to solve, in particular in three dimensions.

FWITE can be defined in the temporal frequency, \( \omega \), domain by extending a complex valued \( \tilde{s}^2 \) along \( \omega \). In that case the convolution in equation 2 becomes a simple multiplication and the weight by \( \tau \) in the second term of the objective function 3 becomes a derivative with respect to frequency.

FWITE in the frequency domain minimizes the following objective function,

\[
\tilde{J} (\tilde{s}^2) = \frac{1}{2} \| \tilde{\mathcal{L}}_\omega (\tilde{s}^2) - d_\omega \|_2^2 + \epsilon \| i \omega \tilde{s}^2 \|_2^2,
\]

where \( \tilde{\mathcal{L}}_\omega \) is a frequency-domain wave operator based on the one-way wave equation and \( d_\omega \) is the recorded data in the frequency domain. The stability of the one-way modeling operator can be ensured by imposing the constraint \( \Re (\tilde{s}^2) \leq 0 \).
3 FWITE algorithms

In this section we discuss two different optimization algorithms for solving the time-domain and the temporal-frequency domain formulations of FWITE.

Variable-projection optimization for time-domain FWITE

As mentioned in the previous section, an important challenge of minimizing the objective function 3 is computing numerical solutions to equation 2. Because of the large dimension of the computational grid needed in reflection seismology, practical algorithms for solving the wave equation in time domain are based on explicit finite differences; implicit finite-differences algorithms are too computationally intensive in 3D for being practical. Explicit finite-differences solutions of equation 2 would be unstable.

The solution to this problem is to approximate the wave operator \( \hat{L} \) with its first-order Born linearization, \( \hat{L} \), around a background physical (i.e. not extended) slowness model \( s_b^2 \); that is, using the following approximation

\[
\hat{L} \left( s_b^2 + \Delta s^2 \right) \approx L \left( s_b^2 \right) + \hat{L} \left( s_b^2 \right) \Delta s^2.
\]  

The objective function 3 then becomes

\[
\tilde{J}_t \left( s_b^2, \Delta s^2 \right) = \frac{1}{2} \left\| L \left( s_b^2 \right) + \hat{L} \left( s_b^2 \right) \Delta s^2 - d \right\|_2^2 + \epsilon \left\| \left( (\tau^*) + \alpha \right) \Delta s^2 \right\|_2^2.
\]  

This new objective function is then minimized by applying a variable projection scheme [11]. Notice the addition of the small positive scalar \( \alpha \) in the objective function 6. It ensures that the Hessian of the variable projection step is a positive-definite matrix.

At each iteration of the optimization, we first fix \( s_b^2 \) and iteratively solve the quadratic problem in \( \Delta s^2 \) by applying a conjugate gradient method to estimate an optimal \( \Delta s^2 \). A conjugate-gradient solution requires applications of \( \hat{L} \) and of its adjoint \( L^T \) to vectors in the slowness space and data space, respectively. These matrix-vector products are computed using algorithms based on adjoint-state methods that are similar to the ones used for conventional FWI. Given the solution \( \Delta s_b^2 \) of the variable-projection step, we then perform a single step of L-BFGS to update the background model \( s_b^2 \).

We stop the iterative process when the differences between the data modeled using the new background model and the recorded data are sufficiently small.

The analysis of the structure of the gradient for the outer iterations illuminates the nature of the FWITE process and provides intuition on the way that the methods overcome the convergence challenges of conventional FWI [1–3]. The gradient is the sum of two different components and can be written as:

\[
\nabla \tilde{J}_t = (T^* + L^*) \left( L \left( s_b^2 \right) + \hat{L} \left( s_b^2 \right) \Delta s^2 - d \right),
\]  

where \( L^* \) is the adjoint of the first-order Born linearization of \( L \), and \( T^* \) is the adjoint of a data-domain tomographic operator that connects the long-wavelength of the slowness model to data perturbations [7]. When \( s_b^2 \) is far from the “true” model and \( \Delta s_b^2 \) is far from being focused around \( \tau = 0 \), the first term drives the long-wavelengths of the model towards the correct solution. In contrast, when \( s_b^2 \) is close to the “true” model and \( \Delta s_b^2 \) is well focused around \( \tau = 0 \), the contributions of the tomographic term to the gradient are small, and the iterations approximate standard FWI iterations.

Constrained optimization for frequency domain FWITE

The frequency-domain objective function 4 can be directly minimized using a gradient-based optimization scheme for complex variables, such as an L-BFGS optimization scheme. To avoid instability in the computation of the forward operator \( \hat{L}_\omega \), we ensure that the condition \( \Im \left( s_b \right) \leq 0 \) is always fulfilled by projecting the gradients onto the feasible subspace.

4 Numerical example

The time-domain algorithm outlined in the previous section has successfully been tested on several challenging synthetic examples as well as on a 3D field dataset [3]. In this section we show one of the examples from Barnier [3] that is an archetypal example in reflection seismology [13]. It has the advantage of simplicity and thus it lends itself to illustrating some of the salient characteristic of the method.

Figure 1 shows the 2D velocity model assumed for numerical modeling a reflection dataset solving a constant-density acoustic wave equation. The velocity in the circle in the middle is substantially lower (2,25 km/s) than the back-
ground velocity (2.7 km/s). The source had the unrealistic frequency range between 20 and 50 Hz to ensure that conventional multi-scale FWI [9] fails to retrieve the true model. Indeed, when the starting model is homogeneous and set to the background velocity of 2.7 km/s, conventional FWI employing the well-known frequency bootstrapping procedure that starts with the low frequency to improve convergence [9], produces the model shown in Figure 2. In contrast, a multi-scale FWITE algorithm [2] yields the accurate model shown in Figure 3, after two scale refining steps. The graphs shown in Figures 4 and 5 compare the result of FWI (magenta lines) and FWITE (blue lines) at the constant fixed horizontal location of 2 km and at the fixed depth of 0.6 km, respectively. The FWITE result is close to the true model (black lines) notwithstanding the starting model was far from accurate and the missing low frequencies in the data.

Examining the tomographic component of the first outer-loop iteration gradient (equation 7) provides some intuition on the reason why FWITE converges to an excellent model even when the starting model is grossly inaccurate and the data miss the low frequencies. Figure 6 shows the tomographic component (first term in equation 7) of the search direction (opposite sign of the gradient). The tomographic component is already moving the long-wavelengths of the model in the right direction of decreasing the velocity in the low-velocity anomaly in the middle. The gradient tomographic component does not cycle skip as it would the conventional FWI gradient because the data residuals that are back-projected by equation 7 have been corrected by the addition of the term $\tilde{L}\Delta s^2_o$.

The nature of the long-wavelength contribution of the tomographic component is further illustrated by the complex modulus of the Fourier transform of the search direction shown in Figure 7. Comparing this wavenumber-domain spectrum with the similar spectrum of the difference between true and starting models shown in Figure 8, we can see how the tomographic component starts to fill in the low wavenumbers, in particular around the horizontal direction, of the velocity anomaly missing from the starting model. These results are consistent with the generalization of the classical wavenumber-domain analysis of first-order scattering [22] by Biondi et al. [8] and summarized by the diagram shown in Figure 9. The area shaded in orange in the Figure corresponds to the model wavenumber components that are illuminated by second order scattering when the data are recorded with source and receivers located at the surface.

5 Conclusions

Full waveform inversion with model time extension can be a powerful algorithmic solution to the convergence problems of conventional full waveform inversion. The time-domain version of the method is solved with a variable projection algorithm after a modification of the objective function based on a Born linearization of the modeling operator with respect to the extended model. The frequency-domain formulation holds the promise of enabling a direct solution of the optimization problem formulated with non-linear extended modeling operator.

6 Acknowledgements

We would like to thank the Stanford Exploration Project affiliate companies for financial support and the Stanford Center for Computational Earth and Environmental Sciences (CEES) for providing computational resources.

References


Figure 1: Velocity model assumed to compute synthetic seismograms for test dataset.

Figure 2: Velocity model produced by conventional FWI employing a frequency bootstrap algorithm to improve convergence [9].


Figure 3: Velocity model produced by the time-domain FWITE algorithm presented in this paper.

Figure 4: Vertical slice taken at the lateral location of 2 km through the initial model (red), FWI model (magenta), FWITE model (blue), and true model (black).

Figure 5: Horizontal slice taken at depth of 0.6 km through the initial model (red), FWI model (magenta), FWITE model (blue), and true model (black).

Figure 6: Tomographic component of the first search direction of the FWITE optimization process.

Figure 7: Complex modulus of the Fourier transform of the search direction shown in Figure 6.

Figure 8: Complex modulus of the Fourier transform of the difference between the true and the starting models.

Figure 9: Diagram showing the areas (orange) in the wavenumber plane that are illuminated by second order scattering (tomographic operator) when the data are recorded with source and receivers located at the surface.
Fast solvers for time-harmonic high-frequency elastic wave propagation problems

Marion Darbas

LAGA UMR CNRS 7539, Sorbonne Paris Nord University, France

*Email: darbas@math.univ-paris13.fr

Abstract

This talk provides an overview of several results dedicated to the development of fast solvers for elastic wave propagation problems using the integral equation method. They are issued from different collaborations (cited hereafter) over the past few years.

Keywords: boundary integral methods, analytical preconditioners, domain decomposition, scattering problems, transmission problems.

1 Introduction

The accurate numerical modeling of highly oscillatory elastic wave problems is a very challenging task due to the variety of possible applications (for example medical diagnosis, seismic imaging or non-destructive testing).

To solve elastodynamic scattering problems in unbounded domains, a possibility is to use the method of boundary integral equations. The main advantage is to reformulate the exterior boundary value problem as an integral equation on the boundary of the scatterer. Thus, the dimensionality of the problem is reduced by one. Still, the method has its drawbacks. The discretization matrix of a boundary integral operator is dense. Furthermore, in order to capture the oscillatory phenomenon, one has to fix typically about ten discretization points per wavelength per dimension. The solution of these large and fully-populated complex linear systems is handled by iterative solvers, namely GMRES. The motivating question is: how to get a fast convergence of GMRES independently of the frequency, the characteristics of the medium and the discretization parameters?

The talk focuses first on the numerical resolution of scattering problems by an impenetrable object. Analytical preconditioning techniques are addressed. The second part is dedicated to an ongoing work on multitrace boundary integral formulations for transmission problems.

2 The Navier exterior problem and standard boundary integral equations

Let us consider the time-harmonic scattering problem of an incident elastic wave \( u^{inc} \) by an impenetrable body \( \Omega^+ \) in \( \mathbb{R}^d \), \( d = 2, 3 \), with a closed boundary \( \Gamma := \partial \Omega^+ \) of class \( C^2 \) at least. Let \( \Omega^- \) denote the exterior domain \( \mathbb{R}^d \setminus \overline{\Omega}^+ \) and \( n \) the outer unit normal vector to the boundary \( \Gamma \). The elastic medium is assumed to be isotropic and homogeneous. It is characterized by three positive constants: the Lamé parameters \( \mu \) and \( \lambda \), and the density \( \rho \). We are interested in finding the scattered field \( u \) solution to the exterior Navier problem [8]

\[
\begin{align*}
\Delta^* u + \rho \omega^2 u &= 0, &\text{in } \Omega^+, \\
\mathbf{u} &= -u^{inc} &\text{on } \Gamma, \\
\lim_{r \to \infty} r \left( \frac{\partial u_p}{\partial r} - i \kappa_p u_p \right) &= 0, & r = |x|, \\
\lim_{r \to \infty} r \left( \frac{\partial u_s}{\partial r} - i \kappa_s u_s \right) &= 0, & r = |x|,
\end{align*}
\]

with \( \Delta^* u := \mu \Delta u + (\lambda + \mu) \nabla \cdot \mathbf{u} \) and \( \omega > 0 \) the angular frequency. The displacement field \( \mathbf{u} \) is decomposed into a longitudinal field \( \mathbf{u}_p \) with vanishing curl and a transverse divergence-free field \( \mathbf{u}_s \), both solutions to the Helmholtz equation with respective wavenumbers \( \kappa_p^2 = \rho \omega^2 (\lambda + 2\mu)^{-1} \) and \( \kappa_s^2 = \rho \omega^2 \mu^{-1} \). The Neumann trace, defined by \( t_{\Gamma} := T \mathbf{u} \), is given by the traction operator

\[
T = 2\mu \frac{\partial}{\partial n} + \lambda \mathbf{n} \cdot \nabla + \mu \mathbf{n} \times \text{curl}
\]

and we set \( t_{\Gamma}^{inc} = T u^{inc} \). For existence and uniqueness results, we refer to Kupradze [8].

The first main difficulty arising in the numerical solution to the exterior boundary value problem (1) is related to the unbounded computational domain \( \Omega^+ \). Integral equation methods are one of the possible tools to overcome this issue. For a solution \( \mathbf{u} \) of the Navier equation in \( \Omega^+ \), that satisfies the Kupradze boundary conditions, one can derive the Somigliana integral representation formula:

\[
\mathbf{u}(x) = D \mathbf{u}_{\Gamma}(x) - S t_{\Gamma}(x), \quad x \in \Omega^+. \tag{2}
\]
The single- and double-layer potential operators are defined respectively by
\[
S\phi = \int_{\Gamma} \Phi(x, y)\varphi(y) ds(y),
\]
\[
D\psi = \int_{\Gamma} [T_y\Phi(x, y)]^T \psi(y) ds(y),
\]
where \(\Phi\) is the fundamental solution of the Navier equation and \(T_y = T(n(y), \partial_y)\) and \(T_y\Phi(x, y)\) is the tensor obtained by applying the traction operator \(T_y\) to each column of \(\Phi(x, y)\). The Cauchy data \((u_{\text{inc}}, t_{\text{inc}})\) become the new unknowns of the problem. The displacement field \(u\) on \(\Omega^+\) is uniquely determined from the knowledge of these two surface fields. Given vector densities \(\varphi\) and \(\psi\), the boundary integral operators \(S, D, D'\) and \(N\) are defined, for \(x \in \Gamma\), by
\[
S\varphi(x) = \int_{\Gamma} \Phi(x, y)\varphi(y) ds(y),
\]
\[
D\psi(x) = \int_{\Gamma} [T_y\Phi(x, y)]^T \psi(y) ds(y),
\]
\[
D'\varphi(x) = \int_{\Gamma} T_x\Phi(x, y)\varphi(y) ds(y),
\]
\[
N\psi(x) = \int_{\Gamma} T_x\{[T_y\Phi(x, y)]^T \psi(y)\} ds(y).
\]
By applying the exterior Dirichlet and Neumann traces to \(S\) and \(D\), we have
\[
(S\varphi)|_\Gamma = S\varphi, \quad (TS\varphi)|_\Gamma = \left( -\frac{1}{2} + D' \right)\varphi,
\]
\[
(D\psi)|_\Gamma = \left( \frac{1}{2} + D \right)\psi, \quad (TD\psi)|_\Gamma = N\psi,
\]
where \(I\) is the identity operator.

3 Analytical preconditioners and regularized CFIE for scattering problems

This section presents results [2–5] obtained in collaboration with Stéphane Chaillat (POEMS laboratory, CNRS-INRIA-ENSTA) and Frédérique Le Louër (LMAC, Sorbonne Universités, Université de technologie de Compiègne). We propose well-conditioned boundary integral equations for the resolution of (1). We focus on Combined Field Integral Equations (cal-led CFIE). The standard CFIE consists in finding \(\psi := - (t_{\text{inc}} + t_{\text{inc}})|_{\Gamma} \in H^{-1/2}(\Gamma)\) solution to
\[
\left( \frac{1}{2} + D' + i\eta S \right)\psi = - (t_{\text{inc}} + i\eta u_{\text{inc}})|_{\Gamma}, \quad \text{on } \Gamma.
\]
CFIE is well-posed for any frequency and any non-zero real parameter \(\eta\). However, the condition number of the CFIE operator depends on the frequency \(\omega\). Hence the iterative resolution of the corresponding linear system, after a discretization by means of Boundary Element Methods (BEM), is slow at high frequencies.

We regularize it through analytic preconditioning. More precisely, the principle of the approach is the following. Let us describe the main steps in the case of a Dirichlet boundary condition \(u = -u_{\text{inc}}\) on \(\Gamma\). Consider the exterior Dirichlet-to-Neumann (DtN) map
\[
\Lambda_{\text{ex}} : u_{\text{inc}}^+ \in H^{1/2}(\Gamma) \mapsto t_{\text{inc}} := \Lambda_{\text{ex}}^{-1} u_{\text{inc}}^+ \in H^{-1/2}(\Gamma).
\]
By taking the Dirichlet trace on \(\Gamma\) of the integral representation (2) of the scattered field, we obtain
\[
u_{\text{inc}}(x) = \left( \frac{1}{2} + D - S\Lambda_{\text{ex}} \right) u_{\text{inc}}^+(x), \quad x \in \Gamma,
\]
and we deduce
\[
\frac{1}{2} + D' - \Lambda_{\text{ex}}' S = I, \quad \text{on } \Gamma.
\]
Assume that \(\omega\) is not an eigenfrequency of the Navier equation in \(\Omega^-\) with either the Dirichlet or the Neumann homogeneous boundary condition, the adjoint DtN map is expressed in terms of boundary integral operators on \(\Gamma\) by
\[
\Lambda_{\text{ex}}' = - \left( \frac{1}{2} I - D' \right)^{-1} S^{-1} \left( \frac{1}{2} I + D' \right)^{-1} N,
\]
and, in view of (5), provides a natural and efficient analytical preconditioner for the CFIE operator. However, it is expensive to consider the exact operator (6) for a numerical purpose. Instead, an approximation \(\Lambda'\) of \(\Lambda_{\text{ex}}'\), given in terms of surface differential operators, is introduced to construct a preconditioned CFIE: find the trace of total field \(\varphi := -(t_{\text{inc}} + t_{\text{inc}})|_{\Gamma}\) solution to
\[
\left( \frac{1}{2} + D' - \Lambda' S \right)\varphi = - (t_{\text{inc}} + \Lambda' u_{\text{inc}})|_{\Gamma}, \quad \text{on } \Gamma.
\]
elasticity has to be overcome. The double-layer boundary integral operator $D$ and its adjoint $D'$ are not compact even for sufficiently smooth boundaries. We propose to work in a modified potential theory which consists in replacing the traction operator $T$ with $T - \alpha \mathcal{M}$ where $\alpha$ is a real-valued constant and

$$
\mathcal{M} = \frac{\partial}{\partial n} - n \text{div} + n \times \text{curl}
$$

is the tangential Günter derivative. The double-layer boundary integral operator becomes: for $x \in \Omega$

$$
D_\alpha \varphi(x) = \int_{\Gamma} [(T_y - \alpha \mathcal{M}) \Phi(x, y)]^T \varphi(y) ds(y).
$$

It can be proved that $D'_\alpha$ is compact for the choice $\alpha = \tilde{\alpha} = (2\mu^2)/(\lambda + 3\mu)$ [6]. With this good property in hand, an approximate adjoint DtN map is given by

$$
\Lambda' = \left( \frac{1}{2} + P_0(D'_\alpha) \right)^{-1} P_1(N_\alpha) + \tilde{\alpha} \mathcal{M}
$$

(8)

where the operators $P_0(D'_\alpha)$ and $P_1(N_\alpha)$ are respectively the principal parts of the boundary integral operators $D'_\alpha$ and $N_\alpha$ (hypersingular operator in the modified potential theory). They are expressed in terms of surface differential operators, square-root operators and their inverse. As illustration, the first term of $R_0(D'_\alpha)$ is given by [5]

$$
I_1 = \frac{i}{2} \left( n(\Delta_I + \kappa^2_I) \right)^{-\frac{1}{2}} \text{div}_I I_1
$$

$$
- \nabla_I (\Delta_I + \kappa^2_I)^{-\frac{1}{2}} n \cdot I_n
$$

where $I_n = n \otimes n$ and $I_1 = I - I_n$.

Using (8), we construct three preconditioned CFIEs:

- the **Low-Order preconditioned CFIE** (LO P-CFIE) with $\Lambda' = i((\lambda + 2\mu)\kappa s I_n + \mu s I_k)$ where $I_n = n \otimes n$ and $I_k = I - I_n$.

- the **High-Order preconditioned CFIE with one term** (HO(1) P-CFIE) with

$$
\Lambda' = 2P_1(N_\alpha) + \tilde{\alpha} \mathcal{M}.
$$

The contribution of $P_0(D'_\alpha)$ is omitted.

- the **High-Order preconditioned CFIE with two terms** (HO(2) P-CFIE) with the complete approximation (8).

We combine such analytic preconditioners with a Fast Multipole-BEM solver to solve 3D exterior scattering problems for different geometries and incident fields. The mechanical parameters are defined such that the wavenumbers satisfy $\kappa_s = 1.5\kappa_p$ (i.e. $\mu = 1, \mu = 1$ and $\lambda = 0.1$). The density of points per S-wavelength $\lambda_s = 2\pi/\kappa_s$ is fixed to about $n\lambda_s = 10$. First, we consider the diffraction of incident plane waves by a unit sphere. A spectral decomposition, in terms of the vector spherical harmonics, of the elementary integral operators can be obtained.

We compare in Figure 1 the distribution of the eigenvalues of the standard CFIE ($\eta = 1$) and the P-CFIEs for $\kappa_s = 16\pi$. The three preconditioners are performant. The best spectral configuration is offered by considering the approximation (8) of the adjoint DtN map. We observe an excellent eigenvalue clustering around the point $(1, 0)$ for any mode (propagating, grazing and evanescent) whereas a penalizing cluster of small eigenvalues close to zero for the standard CFIE is seen.

![Figure 1: Unit sphere. Distribution of the eigenvalues of the standard and different P-CFIEs.](image-url)
of iterations without any preconditioner drastically increases with the frequency. The three P-CFIEs are very efficient as expected after the spectral observations.

<table>
<thead>
<tr>
<th>ω</th>
<th>#iter</th>
<th>#iter</th>
<th>#iter</th>
<th>#iter</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>14</td>
<td>10</td>
<td>9</td>
<td>9 (13)</td>
</tr>
<tr>
<td>5</td>
<td>40</td>
<td>12</td>
<td>10</td>
<td>9 (13)</td>
</tr>
<tr>
<td>11</td>
<td>120</td>
<td>13</td>
<td>10</td>
<td>9 (12)</td>
</tr>
<tr>
<td>16</td>
<td>&gt;500</td>
<td>49</td>
<td>19</td>
<td>11 (13)</td>
</tr>
</tbody>
</table>

Table 1: Diffraction of P-waves by a cube. Number of GMRES iterations for a fixed density of 10 points per wavelength.

This preconditioning method has been successfully applied for a Neumann boundary condition too. 2D numerical results attest that the dependence on the frequency after preconditioning is reduced (see Table 2).

<table>
<thead>
<tr>
<th>ω</th>
<th>#iter CFIE</th>
<th>#iter LO</th>
<th>#iter HO(1)</th>
<th>#iter HO(2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2π</td>
<td>57</td>
<td>19</td>
<td>11</td>
<td>10(25)</td>
</tr>
<tr>
<td>4π</td>
<td>103</td>
<td>25</td>
<td>15</td>
<td>11(35)</td>
</tr>
<tr>
<td>6π</td>
<td>134</td>
<td>30</td>
<td>21</td>
<td>13(42)</td>
</tr>
<tr>
<td>8π</td>
<td>177</td>
<td>36</td>
<td>28</td>
<td>15(52)</td>
</tr>
<tr>
<td>16π</td>
<td>287</td>
<td>55</td>
<td>19</td>
<td>11(80)</td>
</tr>
</tbody>
</table>

Table 2: Unit square. Diffraction of incident P-waves. Number of GMRES iterations for a fixed density of points $n_{A_0} = 20$.

Remark: The approximate DtN maps (8) play also a concluding role in domain decomposition methods [9]. This is a joint work with Christophe Geuzaine (UCL, Liège) and Vanessa Mattesi (UCL, Liège).

4 Multitrace boundary integral formulations for transmission problems

This section is devoted to an on-going joint work with Stéphanie Chaillat. The aim is to construct local multiple trace boundary integral formulations for transmission problems. Such formalism has been proved to be powerful in acoustics (e.g. [7]). It relies on local traces on subdomains and weak enforcement of transmission conditions. The unknowns are the interior and exterior Cauchy data. We are interested in studying the scattering of time-harmonic elastic plane waves by a bounded penetrable object $Ω (d = 2, 3)$. It is composed of $p$ non-overlapping subdomains denoted by $Ω_i, i = 1, \ldots, p$, each with its own material properties. We denote by $Ω_0$ the associated unbounded exterior domain of propagation, an homogeneous and isotropic elastic medium. The resulting elastic field (namely the total field in $Ω$ and the scattered field in $Ω_0$) is solution to a multiple transmission problem: seek $u$ solution to

\[
\begin{cases}
\Delta_s u + \rho \omega^2 u = 0 \text{ in } Ω_i \cup Ω_f^c,
+ \text{inhomogeneous transmission conditions on } \Gamma = \partial Ω,
+ \text{homogeneous transmission conditions on all interfaces } Ω_i \cap Ω_j,
+ \text{radiation conditions for } |x| \to +\infty.
\end{cases}
\]

We define a main ingredient for writing multitrace boundary integral formulations: the Calderón projectors. To this end, consider a single domain $Ω_i$. We seek $u \in H^1_{loc}(Ω_i \cup Ω_f)$ such that

\[
\begin{cases}
\Delta_s u + \rho \omega^2 u = 0 \text{ in } Ω_i \cup Ω_f^c,
+ \text{radiation conditions at infinity.}
\end{cases}
\]

The solution $u$ is expressed by: for $x \in \mathbb{R}^d \setminus \partial Ω_i$

\[
u(x) = D^i([γ_D u]|_{∂Ω_i}) - S^i([γ_N u]|_{∂Ω_i}), \quad (9)
\]

where $S^i$ and $D^i$ are the single- and double-layer potential operators respectively (see (3)) and the trace jump operator across the boundary $∂Ω_i$ are given on $∂Ω_i$ by

\[
[γ u]|_{∂Ω_i} := \begin{bmatrix}
[γ_D u]|_{∂Ω_i}
[γ_N u]|_{∂Ω_i}
\end{bmatrix} = \begin{bmatrix}
γ_D^c u - γ_D^i u
γ_N^c u - γ_N^i u
\end{bmatrix}
\]

with $γ_D^i, N$ the Dirichlet and Neumann traces on $∂Ω_i$ taken from within $Ω_i$, and $γ_D^c, N$ traces taken from the complementary domain $Ω_f^c$. When taking the interior traces of the integral representation (9), we get the following relations

\[
\begin{align*}
γ_D^i u &= \left(\frac{1}{2}I - D_i\right)γ_D^i u + S_N^i u
γ_N^i u &= N_N^i γ_D^i u + \left(\frac{1}{2}I + D_i\right)γ_N^i u
\end{align*}
\]

involving the four elementary boundary integral operators (4). They read on $∂Ω_i [1]

\[
\begin{bmatrix}
γ_D^i u \\
γ_N^i u
\end{bmatrix} = C_i \begin{bmatrix}
γ_D^i u \\
γ_N^i u
\end{bmatrix} = \frac{1}{2}I + A_i \begin{bmatrix}
γ_D^i u \\
γ_N^i u
\end{bmatrix}
\]

(10)
where the multitrace matrix $A_i$ of operators is defined by
\[
A_i = \begin{pmatrix} -D_i & S_i & N_i & \ldots \end{pmatrix} : V_i \rightarrow V_i.
\]
with $V_i := H^2(\partial \Omega_i) \times H^{-\frac{\pi}{2}}(\partial \Omega_i)$. The relation (10), called Calderón identity, gives a characterization of the Dirichlet and Neumann traces, for weak solutions of the Navier equation.

Let us now explain how to use Calderón identity for writing a local Multiple Trace Formula (MTF) in the case of an homogeneous scatterer ($p = 1$). Consider a bounded domain $\Omega$ and the associated exterior propagation domain $\Omega_0 = \mathbb{R}^d \setminus \overline{\Omega}$ with interface $\Gamma = \Gamma_0 = \partial \Omega$. The two media are characterized by different material properties $(\rho_0, \lambda_0, \mu_0) \neq (\rho_1, \lambda_1, \mu_1)$ and wavenumbers $(k_{p,0}, k_{s,0}) \neq (k_{p,1}, k_{s,1})$. We want to solve the Navier transmission problem: given a field $f = (f_D, f_N) \in V := H^2(\Gamma) \times H^{-\frac{\pi}{2}}(\Gamma)$, seek $u \in H_{loc}(\Omega_0 \cup \Omega_1)$ such that
\[
\begin{align*}
\Delta u + \rho_0 \omega^2 u &= 0, \quad \text{in } \Omega_0, \\
\Delta u + \rho_1 \omega^2 u &= 0, \quad \text{in } \Omega_1, \\
[\gamma u]_\Gamma &= f, \quad \text{on } \Gamma,
\end{align*}
\]
(11)
The transmission conditions $[\gamma u]_\Gamma = f$ across the interface $\Gamma$ read
\[
[\gamma u]_\Gamma = \left( [\gamma D u]_\Gamma, [\gamma N u]_\Gamma \right) = \left( \gamma_D^0 u - \gamma_D^1 u, -\gamma_N^0 u - \gamma_N^1 u \right) = (f_D, f_N).
\]
We define an endomorphism on the product space $V$:
\[
X := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}: V \rightarrow V.
\]
Consequently, the transmission conditions can be expressed as
\[
\begin{pmatrix} \gamma_D^0 u \\ \gamma_N^0 u \end{pmatrix} = X \begin{pmatrix} \gamma_D^1 u \\ \gamma_N^1 u \end{pmatrix} + X \begin{pmatrix} f_D \\ f_N \end{pmatrix} \text{ on } \Gamma
\]
or
\[
X \begin{pmatrix} \gamma_D^0 u \\ \gamma_N^0 u \end{pmatrix} = \begin{pmatrix} \gamma_D^1 u \\ \gamma_N^1 u \end{pmatrix} + \begin{pmatrix} f_D \\ f_N \end{pmatrix} \text{ on } \Gamma.
\]
On the other hand, using local Calderón projectors (10), it holds
\[
\frac{1}{2} \begin{pmatrix} \gamma_D^0 u \\ \gamma_N^0 u \end{pmatrix} = A_i \begin{pmatrix} \gamma_D^1 u \\ \gamma_N^1 u \end{pmatrix}, \quad i = 0, 1.
\]
Thus, we get on the transmission boundary $\Gamma$
\[
2A_0 \begin{pmatrix} \gamma_D^0 u \\ \gamma_N^0 u \end{pmatrix} - X \begin{pmatrix} \gamma_D^1 u \\ \gamma_N^1 u \end{pmatrix} = X \begin{pmatrix} f_D \\ f_N \end{pmatrix}
\]
and
\[
-X \begin{pmatrix} \gamma_D^0 u \\ \gamma_N^0 u \end{pmatrix} + 2A_1 \begin{pmatrix} \gamma_D^1 u \\ \gamma_N^1 u \end{pmatrix} = - \begin{pmatrix} f_D \\ f_N \end{pmatrix}.
\]
Set $X_i := \begin{pmatrix} \gamma_D^0 u \\ \gamma_N^0 u \end{pmatrix}, \quad i = 0, 1$ and $V := V \times V$. Finally, the Navier transmission problem (11) becomes in variational form: seek $\lambda = (\lambda_0, \lambda_1) \in V$ such that, $\forall \varphi \in V$,
\[
m(\lambda, \varphi) := \langle M \lambda, \varphi \rangle_X = \left\langle \frac{1}{2} \begin{pmatrix} Xf \\ -f \end{pmatrix}, \varphi \right\rangle_X,
\]
where
\[
M := \begin{pmatrix} A_0 & -\frac{1}{2}X \\ -\frac{1}{2}X & A_1 \end{pmatrix} : V \rightarrow V
\]
and $\langle \cdot, \cdot \rangle_X$ the duality product of $V$ with itself. The following theorem holds
\[\textbf{Theorem 1} \quad \text{For all } f \in V, \text{ there exists a unique solution } \lambda \in V \text{ such that } \langle M \lambda, \varphi \rangle_X = \left\langle \frac{1}{2} \begin{pmatrix} Xf \\ -f \end{pmatrix}, \varphi \right\rangle_X, \quad \forall \varphi \in V.\]

The proof of the uniqueness is based on extension using single and double-layer potentials inside $\Omega_0$ and $\Omega_1$ and the uniqueness of the Navier radiating solution. Furthermore, a coercitivity property for the matrix operator $A_i$ is required [1]. Then, the existence is obtained by the Fredholm alternative.

We present first preliminary 2D numerical results. We consider incident plane P-waves. The interior domain $\Omega$ is the unit disk. The physical parameters are $\rho_1 = \mu_0 = 1$, $\lambda_1 = \lambda_0 = 2$ and $\rho_0 = 0.5$. We report in Tables 3 and 4 the number of GMRES iterations with respect to the frequency $\omega$ for two different material contrasts. As expected, the convergence depends on a frequency increase and on the constraint between the two media. Preconditioning is required. In Figure 2, real part of the first and second components of the field are presented taking $\omega = 2\pi$ and $\rho_1 = 10$.

Local MTF have been obtained for composite scatterers ($p > 1$) too. As for $p = 1$, the diagonal of operator matrix $M$ is composed of block
boundary integral operators associated with each subdomain. The problem is decoupled. This is a very interesting feature of the local MTF in view of a preconditioning. This work is underway.

5 References

References


wavenumber-explicit \( hp \)-FEM for Helmholtz problems in piecewise smooth media

Maximilian Bernkopf\(^6\), Théophile Chaumont-Frelet\(^2\), Jens Markus Melenk\(^1\)*

\(^1\) TU Wien, Wien Austria
\(^2\) INRIA

*Email: melenk@tuwien.ac.at

Abstract

We analyze the \( hp \)-FEM applied to Helmholtz problems with piecewise analytic coefficients and a variety of boundary conditions. We show that quasi-optimality is reached under the following conditions on the mesh size \( h \) and the approximation order \( p \): a) \( kh/p \) is sufficiently small and b) \( p \gtrsim \log k \).

Keywords: Helmholtz equation, heterogeneous media, high frequency problems

1 Introduction

Time-harmonic wave propagation problems play an important role in a wide range of physical and industrial applications. A prominent example is the Helmholtz equation, which arises, e.g., in acoustics. The heterogeneous Helmholtz equation

\[
-\nabla \cdot (A(x)\nabla u) + k^2 n^2(x) u = f
\]

with coefficients \( A, n \) describes time-harmonic acoustic waves in inhomogeneous media comprising materials with different acoustic properties (e.g., density, speed of sound). An important parameter in this model is the wavenumber \( k > 0 \), which is proportional to the underlying frequency.

A key issue with numerical methods for such equations are dispersion errors, which manifest themselves in the fact that, as the wavenumber \( k \) increases, the discrepancy between the error of the numerical method and the best approximation widens. In particular for homogeneous media, i.e., the Helmholtz equation with constant coefficients, this “pollution effect”, [12], has been analyzed on translation invariant meshes, [1] and on unstructured meshes [18,19] where it has been shown that high order Galerkin methods are better suited to deal with dispersion errors than low-order methods. In fact, while fixed order methods cannot be “pollution-free”, [2], the \( hp \)-version of the Galerkin method (\( hp \)-FEM) achieves quasi-optimality if the following scale-resolution condition

\[
\frac{kh}{p} \leq c_1 \quad \text{and} \quad p \geq c_2 \log k \quad (2)
\]

holds, [10,18,19]. Here, \( c_2 > 0 \) is an arbitrary constant and \( c_1 \) is required to be sufficiently small. In the present work we extend this result to the case of piecewise analytic coefficients \( A, n \). For globally smooth coefficients \( A, n \), such a result has recently been shown in [11,14,15] using different techniques based on semiclassical analysis.

The insight underlying [18,19] and its generalization here to the heterogeneous Helmholtz equation is a splitting of solutions of Helmholtz problems into a part with finite regularity and good \( k \)-dependence and an analytic part with explicit control in terms of \( k \) ("regularity by decomposition"). This idea has been successfully applied in a variety of related contexts such as problems with corner singularities [5,10], discontinuous Galerkin [17], continuous interior penalty [9,24], FEM-BEM coupling, [21], and multiscale [6] methods. The technique of regularity by decomposition proves useful also in the context of a posteriori error estimation [4,8] and in other wave propagation problems [7,16,20].

2 Main result

2.1 Problem formulation and notation

We consider a bounded Lipschitz domain \( \Omega \subset \mathbb{R}^d, d \in \{2,3\} \). We assume \( \Gamma := \partial \Omega \) is analytic. We assume that \( \Omega \) is partitioned into a set \( \mathcal{P} \) of non-overlapping Lipschitz subdomains such that \( \bigcup_{P \in \mathcal{P}} P = \Omega \). We introduce the internal interface \( \Gamma_{\text{interf}} := \bigcup_{P \in \mathcal{P}} \partial P \setminus \Gamma \) and require the pieces \( \partial P, P \in \mathcal{P}, \) to be analytic. We say that a function \( G \) is piecewise analytic if, for some \( C_G, \gamma_G > 0 \) and all \( P \in \mathcal{P} \)

\[
\|D^\beta \! G\|_{L^\infty(P)} \leq C_G \gamma_G |\beta|! \quad \forall \beta \in \mathbb{N}_0^d.
\]

For \( T \subset \mathbb{R}^d \) we introduce the \( k \)-dependent analyticity class \( \mathfrak{A}(C, \gamma, T) \) consists of functions \( G \)
with \( \|D^\beta G\|_{L^2(T)} \leq C_\gamma |\beta| \max\{||\beta|,k|\beta| |\beta| \) \( \forall \beta \in \mathbb{N}_0^d \). We write \( u \in A(C,\gamma,P) \) to indicate that the function \( u \) defined on \( \Omega \) satisfies \( u \in A(C,\gamma,P) \) for all \( P \in \mathcal{P} \). We consider

\[
- \nabla \cdot (A(x)\nabla u) - k^2 n^2 u = f \quad \text{on} \quad \Omega, \tag{3}
\]

\[
\partial_{n_A} u - ik u = g \quad \text{on} \quad \Gamma, \tag{4}
\]

where \( A \in L^\infty(\Omega,\text{GL}(\mathbb{C}^{d\times d})) \) satisfies for some \( c_{\min} > 0 \)

\[
\inf_{\xi \in \Omega} \text{Re} \xi^H A(x)\xi \geq c_{\min} |\xi|^2 \quad \forall \xi \in \mathbb{C}^d
\]

and both \( A, n \) are piecewise analytic. With the outer normal vector \( n \) on \( \Gamma \) we denote by \( \partial_{n_A} u := n^T A(x) \nabla u \) the co-normal derivative. Our analysis is carried out in the norm

\[
\|v\|_{L^2(\Omega)}^2 := \|\nabla u\|_{L^2(\Omega)}^2 + k^2 \|u\|_{L^2(\Omega)}^2.
\]

We will require the following

**Assumption 1 (polynomial well-posedness)**

There are \( \theta \geq 0 \) and \( C > 0 \) such that for \( k \geq 1 \), (3), (4) has a unique solution \( u \in H^1(\Omega) \) with

\[
\|u\|_{1,k} \leq C k^\theta \left( \|f\|_{L^2(\Omega)} + k^{1/2} \|g\|_{L^2(\Gamma)} \right).
\]

**2.2 Quasi-optimality of hp-FEM**

We consider meshes \( T_h \) that satisfy the assumptions spelled out explicitly in [18, Sec. 5]. Essentially, these meshes are such that with the reference simplex \( K \) the element maps \( F_K : \bar{K} \to K \in T \) can be factored \( F_K = R_K \circ A_K \) for some affine maps \( A_K \) with \( \|A_K\|_h \sim h \) and \( \|A_K^{-1}\| \sim h^{-1} \) and analytic maps \( R_K \) whose analyticity properties can be controlled uniformly in \( K \) and \( h \). Additionally, we require the mesh to conform with the partition \( \mathcal{P} \), i.e., for each \( K \in T \) there is \( P \in \mathcal{P} \) such that \( K \subset P \).

With the space \( P_p \) of polynomials of degree \( p \), we introduce the approximation space \( V_N := S^{p^1}(T) := \{v \in H^1(\Omega) \mid v|_K \circ F_K \in P_p \ \forall P \in \mathcal{P}\} \). The \( hp \)-FEM approximation to the solution of (3) (4) is: Find \( u_N \in S^{p^1}(T_h) \) such that

\[
b(u_N,v) = \ell (v) \quad \forall v \in S^{p^1}(T_h), \tag{5}
\]

\[
b(u_N,v) := \int_\Omega A(x) \nabla u_N \cdot \nabla v - k^2 n^2(x) u_N v + ik \int_\Gamma u_N v, \]

\[
\ell (v) := \int_\Omega f v + \int_\Gamma g v.
\]

**Theorem 2 ( [3])** Let \( u \) denote the solution of (3), (4) and \( u_N \) the Galerkin approximation from (5). Under the assumptions above, given \( c_2 > 0 \) there are \( C, c_1 > 0 \) independent of \( k, h, p \) such that under the scale resolution assumption

\[
\frac{kh}{p} \leq c_1 \quad \text{and} \quad p \geq c_2 \log k \tag{6}
\]

there holds the quasi-optimality

\[
\|u - u_N\|_{1,k} \leq C \inf_{v \in S^{p^1}(T_h)} \|u - v\|_{1,k}.
\]

As the sesquilinear form \( b \) satisfies a Gårding inequality, the proof of this theorem relies on a duality argument (“Schatz argument”) as worked out in [18, 19]. Specifically, one introduces the dual solution operator \( f \mapsto S^*(f) \) by

\[
b(v,S^*(f)) = (v,f)_{L^2(\Omega)} \quad \forall v \in H^1(\Omega)
\]

and the adjoint approximation property

\[
\eta := \sup_{f \in L^2} \inf_{v \in S^{p^1}(T_h)} \|S^*(f) - v\|_{1,k} \|f\|_{L^2(\Omega)}.
\]

Then, one estimates for the Galerkin error \( e_N := u - u_N \) using Galerkin orthogonality

\[
\|e_N\|_{L^2}^2 = |b(e_N,S^*(e_N))| = \inf_{v \in V_N} |b(e_N,S^*(e_N) - v_N)| \lesssim \|e_N\|_{1,k} \|e_N\|_{L^2},
\]

which leads to \( \|e_N\|_{L^2} \lesssim \eta \|e_N\|_{1,k} \). Hence,

\[
\|e_N\|_{1,k}^2 \lesssim \inf_{v \in V_N} |b(u_N,v)| + k^2 \|e_N\|_{L^2}^2 \lesssim \inf_{v \in V_N} |b(u - v, e_N)| + (k\eta \|e_N\|_{1,k})^2 \lesssim \inf_{v \in V_N} \|u - v\|_{1,k} \|e_N\|_{1,k} + (k\eta \|e_N\|_{1,k})^2.
\]

We conclude Thm. 2 if \( k\eta \) is sufficiently small.

This argument reduces the proof of the quasi-optimality result to the analysis of \( \eta \). In turn, the best approximation problem in the definition of \( \eta \) requires the understanding of the regularity properties of the solution \( S^*(f) \) of the adjoint problem. This adjoint problem is again a Helmholtz problem with the same structure as (3), (4). The following Theorem 3 shows that \( S^*(f) \) can be written as \( S^*(f) = u_{H^2} + u_3 \) with \( \|u_{H^2}\|_{H^2(\Omega;\Gamma_{inter}))} \lesssim \|f\|_{L^2} \) and \( u_3 \in A(C\|f\|_{L^2}k^p,\gamma, P) \). Control of \( \eta \) is achieved by approximating \( u_{H^2} \) and \( u_3 \) from \( S^{p^1}(T_h) \).
2.3 Regularity by decomposition

Underlying the proof of Theorem 2 is the following decomposition result:

**Theorem 3 ([3])** Under the above assumptions, for every \((f, g) \in L^2(\Omega) \times H^{1/2}(\Gamma)\) the solution \(u\) of (3), (4) can be written as \(u = u_{H^2} + u_\infty\) with

\[
\|u_{H^2}\|_{H^2(\Omega \setminus \Gamma_{\text{interf}})} \leq C \left( \|f\|_{L^2(\Omega)} + \|g\|_{H^{1/2}(\Gamma)} \right),
\]

\(u_\infty \in \mathcal{A}(C \|f\|_{L^2} + \|g\|_{H^{1/2}}, \gamma, \mathcal{P})\)

for some \(C, \gamma > 0\) independent of \(k\).

2.4 Ingredients of the proof of Thm. 3

The proof of Thm. 3 relies on an auxiliary problem: Let \(w = S^+(f, g)\) be the solution of

\[
-\nabla \cdot (A(x) \nabla w) + k^2 w = f \quad \text{on} \ \Omega, \\
\partial_{n,h} w = g \quad \text{on} \ \Gamma.
\]

By Lax-Milgram the operator \(S^+\) is well-defined, and \(S^+(f, g)\) is piecewise \(H^2\) with

\[
\|S^+(f, g)\|_{H^2(\Omega \setminus \Gamma_{\text{interf}})} \lesssim \|f\|_{L^2} + \|g\|_{H^{1/2}}
\]

with implied constant independent of \(k\). A second ingredient of the proof of Thm. 3 are filter operators:

**Lemma 4 ([3])** For each \(\eta > 1\) there operators \(H_\eta : L^2(\Omega) \to L^2(\Omega)\) and \(H_\eta^\Gamma : L^2(\Gamma) \to L^2(\Gamma)\) such that for \(\varepsilon \in [0, 1/2)\) and \(0 \leq \varepsilon' \leq \varepsilon\) and \(L_\eta := 1 - H_\eta\) and \(L_\eta^\Gamma := 1 - H_\eta^\Gamma\).

1. \(\|H_\eta\|_{L^{-1}(\Omega)} \leq C_\varepsilon(\eta k)^{\varepsilon} \|f\|_{L^2(\Omega)}\).
2. \(\|H_\eta^\Gamma f\|_{L^2(\gamma)} \leq C \xi(\eta k)^{\varepsilon} \|f\|_{H^1(\Gamma)}\).
3. \(L_\eta f \in \mathcal{A}(C \|f\|_{L^2(\Omega)}, \eta, \Omega)\).
4. \(L_\eta^\Gamma f\) is the restriction to \(\Gamma\) of a function \(F \in \mathcal{A}(C \|f\|_{H^{1/2}(\Gamma)}, \gamma, T)\) for some tubular neighborhood \(T\) of \(\Gamma\).

To prove Thm. 3 one introduces the solution operator \(S^-\) by denoting \(S^- (f, g)\) the solution of (3), (4) with data \(f, g\). Then, one writes

\[
u = S^+(H_\eta f, H_\eta^\Gamma g) + S^- (L_\eta f, L_\eta^\Gamma g) + \varepsilon.
\]

By (9), one has

\[
\|u_{H^2,0}\|_{H^2(\Omega \setminus \Gamma_{\text{interf}})} \lesssim \|H_\eta f\|_{L^2} + \|H_\eta^\Gamma g\|_{H^{1/2}} \lesssim \|f\|_{L^2} + \|g\|_{H^{1/2}}
\]

with implied constants independent of \(k, \eta\). By the piecewise analyticity of the data \(A, n, \mathcal{P}\) and the analyticity of \(\Gamma_{\text{interf}}, \Gamma\), the function \(u_{H^2,0}\) is piecewise analytic, and [3] asserts

\[
u_{H^2,0} \in \mathcal{A}(CK^\Theta (\|f\|_{L^2} + \|g\|_{H^{1/2}}), \gamma, \mathcal{P})
\]

for some \(K > 0\) independent of \(k\). Finally, the remainder \(\varepsilon\) satisfies

\[-\nabla \cdot (A(x) \nabla \varepsilon) - k^2 n^2 \varepsilon = 2k^2 u_{H^2,0} =: f_1 \quad \text{on} \ \Omega,
\]

\[
\partial_{n,h} \varepsilon - ik \varepsilon = ik u_{H^2,0} =: g_1 \quad \text{on} \ \Gamma.
\]

Lax-Milgram and the properties of the operators \(H_\eta, H_\eta^\Gamma\) then allow one to show with \(\varepsilon = 1/4\)

\[
\|f_1\|_{L^2} + \|g_1\|_{H^{1/2}} \leq C \eta^{-\gamma} [\|f\|_{L^2} + \|g\|_{H^{1/2}}]
\]

with a \(C > 0\) independent of \(\eta\). We may thus select \(\eta > 1\) such that \(C \eta^{-\gamma} \leq 1/2 < 1\). In conclusion, we have shown with this choice of \(\eta\)

\[
S^- (f, g) = u_{H^2,0} + u_\infty + S^-(f_1, g_1)
\]

with \(\|f_1\|_{L^2} + \|g_1\|_{H^{1/2}} \leq 1/2 \|f\|_{L^2} + \|g\|_{H^{1/2}}\).

The decomposition can be repeated for \(S^- (f_1, g_1)\), and a geometric series argument then concludes the proof.

2.5 Extensions of Thm. 3

The proof of Thm. 3 relies on a few principles that open the door to more general settings. Consider, for some boundary operator \(T_k\) the problem

\[
L_k^- u := -\nabla \cdot (A(x) \nabla u) - k^2 n^2 u = f \quad \text{on} \ \Omega, \\
\partial_{n,h} u - T_k^- u = g \quad \text{on} \ \Gamma.
\]

For its analysis, introduce the auxiliary problem

\[
L_k^+ u := -\nabla \cdot (A(x) \nabla u) + k^2 u = f \quad \text{on} \ \Omega, \\
\partial_{n,h} u - T_k^+ u = -g \quad \text{on} \ \Gamma
\]

for some boundary operator \(T_k^+\). One can generalize the procedure of Section 2.4 to this setting, if the following requirements are satisfied:

1. \(L_k^-\) and \(L_k^+\) have the same principal part (which they do);
2. \(T_k^- - T_k^+\) is an operator of order zero of the form \(T_k^- - T_k^+ = kB + a\), where the zero-th order operator \(B\) is controlled uniformly in \(k\) and \(a\) maps into a class of analytic functions in the sense that \(aa\) is the restriction to \(\Gamma\) of a function \(A \in \mathcal{A}(CK^\Theta \|u\|_{L^2(\Gamma)}, \gamma, \mathcal{P})\) for some tubular neighborhood \(T\) of \(\Gamma\) and some \(\beta\).
3. the solution operator \( S^+ \) for the auxiliary problem admits the shift theorem (9) uniformly in \( k \);

4. the solution \( S^- (f,g) \) is in an analyticity class \( \mathfrak{A}(Ck^d, \gamma, P) \) for some \( \beta \in \mathbb{R} \) if \( f \in \mathfrak{A}(C_1, \gamma, P) \) and \( g \) is the restriction to \( \Gamma \) of a function \( G \in \mathfrak{A}(C_\gamma, \gamma_0, T) \) for some tubular neighborhood \( T \) of \( \Gamma \).

**Example 5 (exact b.c. for \( d = 3 \))** Let \( \text{DtN}_k \) be the exterior Dirichlet-to-Neumann operator given by \( \text{DtN}_k : g \mapsto \partial_n v \), where \( v \) solves the homogeneous Helmholtz equation with Sommerfeld radiation condition:

\[
-\Delta v - k^2 v = 0 \quad \text{in } \mathbb{R}^d \setminus \overline{T}, \quad v|_\Gamma = g, \\
\partial_n v - ikv = o(|x|^{-1}) \quad \text{for } |x| \to \infty.
\]

Select \( T_k^+ \) := \( \text{DtN}_k \). The corresponding operator \( T_k^+ \) is then taken as the Dirichlet-to-Neumann operator \( \text{DtN}_0 \) for \( k = 0 \), where the radiation condition required in the definition of \( \text{DtN}_0 \) is such that \( v = O(1/|x|) \). A decomposition result similar to Thm. 3 is then asserted in [3].

**Example 6 (2\textsuperscript{nd} order ABC)** A possible choice for \( T_k^+ \) is \( T_k^+ u = \alpha \Delta u - \beta u \) with \( \Delta u \) being the Laplace-Beltrami operator on \( \Gamma \) and \( \alpha, \beta \in \mathbb{C} \) parameters with \( \text{Re } \alpha \sim 1/k \), \( \text{Re } \beta = O(k^{-2}) \). One may choose \( T_k^+ \) as the leading order term of \( T_k^- \), i.e., \( T_k^- u = \alpha \Delta u \). A decomposition result similar to Thm. 3 can be achieved, [3]. The analysis is performed in the norm \( \| v \|_{1,k,1} := \| v \|_{1,k} + k^{-1/2} \| v \|_{H^2(\Gamma)} \).

### 3.2 Scale resolution condition

We consider for the unit ball \( \Omega = B_1(0) \) for \( d \in \{1,2\} \) the problem

\[
-\Delta u - k^2 (2 - x^2) u = f \quad \text{in } \Omega, \\
\partial_n u - iku = g \quad \text{on } \Gamma
\]

with prescribed solution \( u(x) = \sin(kx) \) for \( d = 1 \) and \( u(x,y) = \sin(k(x+y)) \) for \( d = 2 \). For \( k_0 = 2 \) for \( d = 1 \) and \( k_0 = 2.1 \) for \( d = 2 \), select for each polynomial degree \( p \geq 2 \) the wavenumber \( k = k_0^p \) and the quasi-uniform mesh size \( h \) such that a prescribed number of degrees of freedom per wavelength \( N_\lambda \) is achieved. Fig. 2 presents the ratio of the Galerkin error and the best approximation error for different values of \( N_\lambda \sim 1/c_1 \) and indicates the necessity to require \( c_1 \) to be sufficiently small.

### References


[2] I. Babuška and S. Sauter. Is the pollution effect of the FEM avoidable for the
Figure 1: $h$-FEM for $p = 1, 2, 3, 4$ for heterogeneous Helmholtz equation with 2$^{nd}$ order ABCs


Abstract

High intensity (focused) ultrasound HIFU is used in numerous medical and industrial applications ranging from lithotripsy and thermotherapy via ultrasound cleaning and welding to sonochemistry. We will highlight some mathematical and computational aspects related to the relevant nonlinear acoustic phenomena, namely

- modeling of high intensity ultrasound phenomena as second and higher order wave equations
- some parameter asymptotics
- absorbing boundary conditions for the treatment of open domain problems
- optimal shape design
- imaging with nonlinear waves

The contents is based on joint work with Vanja Nikolić, Gunther Peichl, William Rundell, Igor Shevchenko, and Mechthild Thalhammer.

Keywords: nonlinear acoustics, singular limits, absorbing boundary conditions, shape optimization, nonlinearity parameter imaging.

1 Models of nonlinear acoustics

Our work on partial differential equations (PDEs) modeling nonlinear acoustic wave propagation is motivated by numerous applications of high intensity focused ultrasound ranging from lithotripsy and thermotherapy via welding and sonochemistry to ultrasound cleaning.

The following brief derivation of the fundamental acoustic equations closely follows the review [14]. More details can be found, e.g., in [9, 10].

The main physical quantities involved in the description of sound propagation are

- the acoustic particle velocity \( \vec{v} \);
- the acoustic pressure \( p \);
- the mass density \( \rho \);

that can be decomposed into their constant mean and a fluctuating part

\[ \vec{v} = \vec{v}_0 + \vec{v}_\sim, \quad p = p_0 + p_\sim, \quad \rho = \rho_0 + \rho_\sim, \]

where \( \vec{v}_0 = 0 \) in the absence of a flow.

These quantities are interrelated to each other by the following physical balance and material laws:

- the Navier Stokes equation (balance of momentum) which under the assumption \( \nabla \times \vec{v} = 0 \) reads

\[ \rho \left( \vec{v}_t + \nabla |\vec{v}|^2 \right) + \nabla p = \left( \frac{4\mu V}{3} + \zeta V \right) \Delta \vec{v}, \tag{1} \]

where \( \zeta V \) is the bulk viscosity and \( \mu V \) the shear viscosity;

- the equation of continuity (balance of mass)

\[ \nabla \cdot (\rho \vec{v}) = -\rho_t; \tag{2} \]

- the equation of state relating the acoustic pressure and density fluctuations \( p_\sim \) and \( \rho_\sim \):

\[ \rho_\sim = \frac{p_\sim}{c^2} = \frac{1}{\rho_0 c^2} \frac{B}{2A} \rho_\sim^2 - \frac{\kappa}{\rho_0 c^2} \left( \frac{1}{c_p^2} - \frac{1}{c_V^2} \right) p_\sim t, \tag{3} \]

where \( B/A \) is the parameter of nonlinearity, \( \kappa \) the adiabatic exponent, and \( c_p, c_V \) the specific heat capacitance at constant pressure and constant volume, respectively.

Analogously to the derivation of the linear wave equation from the linearized versions of these equations, we proceed by subtracting the divergence of (1) from the time derivative of (2) to eliminate the linear velocity term, and inserting the state equation to eliminate the mass density. In the resulting second order in time PDE, we may neglect higher order terms, according to a certain hierarchy, which in nonlinear acoustics is known as Blackstock’s scheme [2, 27] and distinguishes between the following categories:
• **First order.** These are linear with respect to the fluctuating quantities and are not related to any dissipative effect;

• **Second order.** Terms of this order are obtained as the union of quadratic and dissipative linear terms (that is, those terms that contain the viscosities as pre-factors);

• **Higher order.** All remaining terms.

Blackstock’s scheme therefore prescribes that one should retain only first and second order terms. Additionally, a result called the substitution corollary allows us to replace any quantity in a second- or higher order term by its first order approximation.

This yields Kuznetsov’s equation [25, 26]

\[ p_{tt} - c^2 \Delta p_{\sim} - b \Delta p_{\sim t} = \left( \frac{1}{\rho_0 c^2} \frac{B}{2A} \|^2 \right)_{tt} \]  (4)

where \( b \) is the diffusivity of sound, \( b = \frac{1}{\rho_0} \left( \frac{4\nu c^2}{3} + \zeta_v + \frac{\beta_s}{\rho_0 c^2} \right) \) and we have related the velocity to the pressure via the linearization of (1),

\[ \rho_0 \hat{v}_t = -\nabla p_{\sim} , \]  (5)

which together with the substitution corollary allowed us to replace \( c^2 \nabla \cdot \Delta \vec{v} = \nabla \cdot \vec{v}_{tt} = -\frac{1}{\rho_0} \Delta p_{\sim t} \); moreover, again using the substitution corollary we set \( \rho_0 \| \vec{v} \|^2 = \rho_0 \| \vec{v} \|^2_{tt}\).

If we ignore local nonlinear effects modeled by the quadratic velocity term, thus approximating \( \rho_0 \| \vec{v} \|^2_{tt} \approx \frac{1}{\rho_0 c^2} p_{tt}^\sim \), we arrive at the Westervelt equation

\[ p_{tt} - c^2 \Delta p_{\sim} - b \Delta p_{\sim t} = \frac{\beta_a}{\rho_0 c^2} \frac{p_{tt}^2}{p_{tt}^\sim} \]  (6)

with \( \beta_a = 1 + B/(2A) \), cf., [33]. Under the already made assumption \( \nabla \times \vec{v} = 0 \) on a simply connected domain there exists an acoustic velocity potential \( \psi \) with \( \vec{v} = -\nabla \psi \), whose constant part by (5) can be chosen such that

\[ \rho_0 \psi_t = p . \]  (7)

Hence both equations (4) and (6) can as well be written in terms of the acoustic velocity potential

\[ \psi_{tt} - c^2 \Delta \psi_{t} - b \Delta \psi_t = \frac{1}{c^2} \left( \beta_a (\psi_t)^2 + s_{WK} \left\{ c^2 \| \nabla \psi \|^2 - (\psi_t)^2 \right\} \right)_{tt} \]  (8)

with \( s_{WK} = 0 \) for (6) and \( s_{WK} = 1 \) for (4).

Further simplifications of the model lead to the Khokhlov-Zabolotskaya-Kuznetsov (KZK) equation [35]

\[ 2c p_{\sim t} - c^2 \Delta_{yz} p_{\sim} - \frac{b}{c^2} p_{\sim tt} = -\frac{\beta_a}{\rho_0 c^2} p_{tt}^2 \]  (9)

(with the coordinate system possibly rotated so that \( x \) is the direction of sound propagation and \( \Delta_{yz} \) the Laplace operator with respect to the coordinates orthogonal to the propagation direction) and the well-known Burgers’ equation in one space dimension, [5].

On the other hand, taking into account interdependence of further quantities such as entropy, heat flux and temperature, we arrive at higher order models of nonlinear acoustics, such as the Blackstock-Crighton equation [2, 4, 9]

\[ (\partial_t - a\Delta) \left( \psi_{tt} - c^2 \Delta \psi - b \Delta \psi_t \right) - r \Delta \psi_t = - \left( \frac{B}{2Ac^2} (\psi_t^2 + |\nabla \psi|^2) \right)_t \]  (10)

where \( a = \frac{\nu}{\rho c^2} \) is the thermal conductivity or the Jordan-Moore-Gibson-Thompson equation JMGT [8, 12, 13, 31]

\[ \tau \psi_{tt} + \psi_{tt} - c^2 \Delta \psi - b \Delta \psi_t = - \left( \frac{B}{2Ac^2} (\psi_t^2 + |\nabla \psi|^2) \right)_t \]  (11)

where \( \tau \) is the relaxation time, that allows to counteract the infinite speed of propagation paradoxon arising in (4) and (6). Also replacement of the strong damping term \( b \Delta \psi_t \) by fractional order derivatives leads to refinements of the model, such as, e.g., the fractional JMGT equation

\[ \tau^\alpha D_t^{2+\alpha} \psi + \psi_{tt} - c^2 \Delta \psi - (\delta + \tau^\alpha c^2) D_t^{\alpha} \psi \]

\[ = \left( \frac{B}{2Ac^2} (\psi_t^2 + |\nabla \psi|^2) \right)_t \]  (12)

or Kuznetsov’s equation with Caputo-Wismer Kelvin damping

\[ \psi_{tt} - c^2 \Delta \psi - \delta \Delta D_t^\alpha \psi \]

\[ = \left( \frac{B}{2Ac^2} (\psi_t^2 + |\nabla \psi|^2) \right)_t \]

taking into account power law frequency dependence of the attenuation.

Challenges in the analysis of these models arise from the fact that they exhibit potential
degeneracy or equivalently nonlinear state dependence of the wave speed. Let us illustrate this by means of the Westervelt equation (with $u$ denoting the pressure)

$$u_{tt} - c^2 \Delta u - b \Delta u_t = -\frac{k}{2} (u^2)_t = -ku_{tt} - k(u_t)^2$$

that is,

$$(1 + ku)u_{tt} - c^2 \Delta u - b \Delta u_t = -k(u_t)^2$$

This reveals the fact that degeneracy occurs for $u \leq -\frac{1}{k}$ and similar considerations hold for the other equations mentioned above (Kuznetsov, JMGT, Blackstock-Crighton). The equation above also illustrates state dependence of the effective wave speed, since we can rewrite it as

$$u_{tt} - c^2 \Delta u - \tilde{b}(u) \Delta u_t = f(u)$$

with $\tilde{c}(u) = \frac{\epsilon}{\sqrt{1 + ku}}$, $\tilde{b}(u) = \frac{k}{1 + ku}$, $f(u) = \frac{k(u_t)^2}{1 + ku}$ as long as $1 + ku > 0$ – otherwise the model loses its validity.

2 Singular limits

We are interested in the question whether some of the above models can be recovered as limits of others as certain parameters tend to zero. Examples of such singular limits are vanishing thermal conductivity $a \searrow 0$ in the Blackstock-Crighton equation (10) or vanishing relaxation time $\tau \searrow 0$ in the JMGT equation (11). In both cases the formal limit is obviously Kuznetsov’s equation (4). Mathematically, this leads to the question in which function spaces the limits of $\psi^\alpha$ and $\psi^\tau$ exist and at which rate convergence occurs. Interestingly, but also intuitively, this requires a compatibility condition on the initial data in case of (10), while this is not needed for (11), where the highest order time derivative term vanishes as in the limiting case, which is not the case for (10). Further examples are the limit as $\alpha \searrow 1$ in (12) with limit equation (11), where the leading derivative order in the PDE changes with $\alpha$; the limit as $\delta \searrow 0$ in (6) or (4), which leads to a change of the qualitative behaviour from global in time well-posedness to potential blow up in finite time.

Details on this can be found, e.g., in [3, 15–19, 24]

3 Absorbing boundary conditions

Whenever a physical acoustic domain is truncated for computational purposes, appropriate boundary conditions have to be imposed in order to avoid spurious reflections at the artificial boundary, see, e.g., Fig. 1 for a typical computational setup in the simulation of ultrasound waves focused by an array of piezoelectric transducers. The vast majority of approaches for this purpose fall under one of the two categories of perfectly matched layers PML or absorbing boundary conditions ABC. We here focus on the latter paradigm. The derivation of ABCs is based on (formal) pseudodifferential calculus to approximately factorize the wave differential operator, which for this purpose has to be linearized for any of the above models. In case of the Westervelt equation in two space dimensions, this leads to the following zero and first order conditions

$$
\begin{align*}
    u_n &= -\frac{1}{\pi} \sqrt{1 + ku} u_t \\
    u_{n tt} &= -\frac{1}{\pi} \sqrt{1 + ku} u_{ttt} + \frac{1}{\pi} \sqrt{1 + ku} u_{t \theta t} \\
    &+ \frac{k}{x \sqrt{1 + ku}} (u_t - \frac{1}{\pi} \sqrt{1 + ku} u_n) u_{tt} \\
    &- \frac{k}{x \sqrt{1 + ku}} \left( \left( \frac{1}{\pi} \sqrt{1 + ku} u_n \right) u_{t \theta} \right)
\end{align*}
$$

on $\partial \Omega$, where $n$ is the normal and $\theta$ the tangential direction. An analysis of the damping properties of the resulting boundary conditions can be carried out by means of energy estimates. Details and computational results can be found in [23, 30].

4 Optimization problems related to ultrasound focusing

The task of focusing the nonlinearly propagating waves in HIFU leads to PDE constrained optimization problems. As an example, consider

![Figure 1: Computational setup with absorbing boundary $\Gamma_A$](image-url)
shape optimization of an acoustic lens, see Fig. 2. Taking into account acoustic-acoustic coupling between lens and fluid domain, as well as power law damping $D(\nabla u_t) = b(1 + \delta |\nabla u_t|^{\alpha-1})\nabla u_t$, this leads to the problem

$$\min_{\Omega \in \mathcal{O}_{\text{ad}}} \int_0^T \int_{\Omega} (u - u_d)^2 \, dx \, ds$$

subject to

$$\begin{aligned}
&\begin{cases}
\frac{1+\kappa_0}{\lambda} u_{tt} - \text{div}(\frac{1}{\rho} \nabla u) - \text{div}(D(\nabla u_t)) = -\frac{k}{2}(u_t)^2 & \text{in } \Omega_+ \cup \Omega_- \\
[[u]] = 0 & \text{on } \Gamma = \partial \Omega_+ \\
\left[\left[\frac{1}{\rho} \frac{\partial u}{\partial n_+} + D(\nabla u_t) \cdot n_+\right]\right] = 0 & \text{on } \Gamma = \partial \Omega_+ \\
u = 0 & \text{on } \partial \Omega \\
(u, u_t)|_{t=0} = (u_0, u_1)
\end{cases}
\end{aligned}$$

where $[\cdot]$ denotes the jump over the interface, $\mathcal{O}_{\text{ad}}$ is a set of admissible domains and the coefficients $\lambda, \rho, b, k$ take different values in the two subdomains, that is, $\lambda = \begin{cases} \lambda_+ & \text{in } \Omega_+ \\ \lambda_- & \text{in } \Omega_- \end{cases}$.

Using the method of mappings, one can define domain deformations that allow to compute a shape derivative in (a) strong and (b) weak form, respectively; that is, as a functional (a) concentrated on the interface $\Gamma$, or (b) distributed over the domain $\Omega$. Based on this, gradient descent methods for computing improved shapes can be derived. For details we point to [20, 28].

5 Imaging with nonlinear ultrasound waves

We finally dwell on recent work on nonlinearity parameter imaging [1, 6, 7, 11, 29, 32, 36, 37], which leads to the inverse problem of identifying the space-dependent coefficient $k(x)$ in Westervelt equation

$$\begin{aligned}
(u + k(x)u^2)_{tt} - c_0^2 \Delta u - \delta \Delta D_p^a u &= r \\
&\quad \text{in } \Omega \times (0, T) \\
&\quad u = 0 \text{ on } \partial \Omega \times (0, T), \\
&\quad u(0) = 0, \quad u_t(0) = 0 \quad \text{in } \Omega
\end{aligned}$$

(with excitation $r$) from boundary observations

$$g = u \quad \text{on } \Sigma \times (0, T),$$

where $\Sigma \subset \Omega$ represents the receiving transducer array. Challenges in this problem result from the fact that the model equation is nonlinear, with the nonlinearity occurring in the highest order term. The unknown coefficient $k(x)$ actually appears in this nonlinear term. Moreover, $k(x)$ is spatially varying whereas the data $g(t)$ is in the “orthogonal” time direction. This is well known to lead to severe ill-conditioning of the inverse problem. In [21, 22], we carry out investigations on the degree of this ill-posedness as well as its dependence on the fractional order $\alpha \in [0, 1]$ of attenuation. Moreover, a uniqueness result for the linearized problem (see also [34]) as well as some preliminary reconstruction results based on Newton’s method are provided.

References


[23] Barbara Kaltenbacher and Igor Shevchenko. Well-posedness of the Westervelt equation with higher order


Generalized Optimized Schwarz Methods in arbitrary non-overlapping subdomain partitions

Xavier Claeys\textsuperscript{1,}\textsuperscript{*}, Emile Parolin\textsuperscript{2}, Francis Collino

\textsuperscript{1}Sorbonne Université, Université Paris-Diderot SPC, CNRS, Inria, Laboratoire Jacques-Louis Lions, équipe Alpèce
\textsuperscript{2}Dipartimento di Matematica, Università degli Studi di Pavia, Italia

*Email: xavier.claeys@sorbonne-universite.fr

Abstract

Optimized Schwarz Methods (OSM) stand among the most popular substructuring domain decomposition strategies for the simulation of wave propagation in harmonic regime. Considering arbitrary non-overlapping subdomain partitions with such methods, the presence of so-called cross points, where three or more subdomains could be adjacent, have raised serious practical and theoretical issues.

We will describe a novel approach to OSM that provides a systematic and robust treatment of cross points as well as a complete analytical framework. A salient new feature is the use of a non-local exchange operator to enforce transmission conditions and maintain subdomain coupling. The associated theory covers several pre-existing variants of OSM, including Després’ original algorithm, and yields new convergence bounds.

Keywords: domain decomposition, substructuring, Optimized Schwarz, cross points

1 Optimized Schwarz Method

When considering a wave propagation problem
\begin{equation}
\Delta u + \omega^2 u = -f \text{ in } \Omega \subset \mathbb{R}^d \text{ with } \partial_\Omega u = 0 \text{ on } \partial \Omega,
\end{equation}
substructuring strategies start from a partition \( \Omega = \bigcup_{j=1}^J \Omega_j \) into non-overlapping subdomains \((\Omega_j \cap \Omega_k = 0 \text{ for } j \neq k)\) to derive a collection of local subproblems, for \( j = 1 \ldots J \),
\begin{equation}
\Delta u + \omega^2 u = -f \text{ in } \Omega_j, \\
\partial_\Omega u = 0 \text{ on } \partial \Omega_j \cap \partial \Omega
\end{equation}
supplemented with transmission conditions through interfaces: denoting \( \Gamma_j := \partial \Omega_j \) and \( n_j \) the normal to \( \Gamma_j \) pointing outside \( \Omega_j \), for all \( j, k \) with \( j \neq k \) we impose
\begin{equation}
\partial_{n_j} u|_{\Gamma_j} = -\partial_{n_k} u|_{\Gamma_k} \\
u|_{\Gamma_j} = u|_{\Gamma_k} \text{ on } \Gamma_j \cap \Gamma_k
\end{equation}
The main idea of the Optimized Schwarz Method
\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{Figure1.png}
\caption{A subdomain partition with cross-points as considered in this work}
\end{figure}
as la Després \cite{12} is to reformulate (1)-(2) in terms of tuples of ingoing/outgoing Robin traces
\begin{equation}
p_{\pm} = (\pm \partial_{n_j} u|_{\Gamma_j} + i \omega u|_{\Gamma_j})_{j=1\ldots J}.
\end{equation}
As regards local wave equations, this is achieved by means of scattering maps \( S_j \) defined by their action on solutions to the homogeneous wave equation
\begin{equation}
S_j(-\partial_{n_j} \psi|_{\Gamma_j} + i \omega \psi|_{\Gamma_j}) := \partial_{n_j} \psi|_{\Gamma_j} + i \omega \psi|_{\Gamma_j} \\
\forall \psi \text{ satisfying: } \Delta \psi + \omega^2 \psi = 0 \text{ in } \Omega_j, \\
\partial_{n_j} \psi = 0 \text{ in } \partial \Omega_j \cap \partial \Omega
\end{equation}
Grouping local scattering maps in a block-diagonal matrix, (1) can be expressed in condensed vector form (with appropriate source term \( \text{rhs} \))
\begin{equation}
p_+ = S(p_-) + \text{rhs},
\end{equation}
with \( S := \text{diag}(S_1, \ldots, S_J) \).

By a simple linear combination involving the impedance coefficient \( i \omega \), the transmission conditions (2) can also be re-arranged in terms of Robin traces
\begin{equation}
-\partial_{n_j} u|_{\Gamma_j} + i \omega u|_{\Gamma_j} \\
= \partial_{n_k} u|_{\Gamma_k} + i \omega u|_{\Gamma_k} \text{ on } \Gamma_j \cap \Gamma_k.
\end{equation}
for all $j, k = 1 \ldots J, j \neq k$ and, again, (5) can be written in vector form as
\begin{equation}
    p_- = \Pi_{\text{loc}}(p_+)
\end{equation}
where the so-called local exchange operator $\Pi_{\text{loc}}$ simply consists in swapping traces, on each interface, from one side to the other. The wave propagation problem is then reformulated by combining (4) and (6)
\begin{equation}
    (\text{Id} - S_{\Pi_{\text{loc}}})p_+ = \mathbf{r}_{\Pi_{\text{loc}}}
\end{equation}
This equation, posed skeleton of the subdomain partition, is the standard form of OSM and Desp"es’ algorithm consists in applying a linear solver to it.

2 Choice of the impedance operator

As a key feature, the skeleton formulation (7) enjoys a positivity property. When considering $L^2$-based scalar product for the traces (3), both $S$ and $\Pi_{\text{loc}}$ are contractive, so that the operator in (7) takes the form "Id + contraction", and
\begin{equation}
    \Re \{ (\text{Id} - S_{\Pi_{\text{loc}}})p, p \}_{L^2(\Gamma)} \geq 0
\end{equation}
This property can be exploited to prove convergence of linear solvers. However, in practice, the convergence can be poor because of a lack of coercivity.

This situation is improved by considering variants of (7) stemming from a different choice of Robin traces
\begin{equation}
    p_{\pm} = (\pm \partial_n u |_{\Gamma_j} + i T_j(u |_{\Gamma_j}))_{j=1 \ldots J}
\end{equation}
with $S_j$’s modified accordingly. The impedance coefficients $T_j$ can be chosen as scalar multiplicative factors, or more generally as (potentially non-local) operators.

The impedance operators $T_j$ appear as parameters of the method that can be tuned so as to improve the convergence of linear solvers, and many contributions of the literature have investigated the best possible choices of $T_j$’s in this respect [1, 10, 17]. State of the art in this direction points towards a choice of $T_j$’s as approximations of exterior Dirichlet-to-Neumann maps based on Padé expansions.

For non-scalar operator valued impedances, a generic convergence theory was proposed in [6, 10, 11] for impedances $T_j$ whose real part is positive definite on $H^{3/2}(\Gamma_j)$. However this theory could not cover the presence of cross points in the subdomain partition, see fig.2.

3 The cross point issue

In both the analysis and the actual implementation of OSM algorithms, cross points (fig.2) have long remained a persistent issue that can spoil convergence [15]. While these points are isolated in 2D, they form a wire-basket network of curves in 3D.

As regards continuous analysis, this issue stems from the local exchange operator $\Pi_{\text{loc}}$ losing its contractivity property in the trace spaces $H^{3/2}(\Gamma_j)$ naturally arising with operator valued impedances [10].

Concerning algorithmic treatments that should be adopted at cross points - at least when degrees of freedom are located there - although recent contributions have proposed effective procedures [13, 14, 18-20], these are restricted to either checkerboard partitions or 2D geometries.

Such difficulties in dealing with cross points are problematic because virtually any subdomain partition of practical relevance involves such feature and the geometry of the (wire basket of) cross points can be very complicated.

4 New form of transmission conditions

In this talk, based on [3, 4, 7, 9], we shall describe a novel approach to OSM that can cope with general non-overlapping subdomain partitions with guaranteed convergence, no matter the presence of cross points. This approach resorts on several new ideas.

The first ingredient is a new manner to impose transmission conditions. While all pre-existing
contributions on OSM imposed transmission conditions by means of the local exchange operator \( \Pi_{\text{loc}} \) like in (5)-(6), we formulate these conditions as

\[
p_+ = \Pi(p_+) \quad \text{where} \\
p_\pm = (\pm \partial_n u |_{\Gamma_j} + iT_j(u|_{\Gamma_j}))_{j=1,...,J} \tag{10}
\]

with an exchange operator \( \Pi \) that does not necessarily reduce to swapping unknowns from each side of each interface:

\[ \Pi \neq \Pi_{\text{loc}} \quad \text{a priori.} \]

The construction of \( \Pi \) depends on the choice of the impedance operators \( T_j \)'s and follows the principles of the Multi-Trace Formalism (MTF) previously developed [5, 8] to deal with boundary integral formulations in multi-domain geometries with possible presence of cross points.

A new variant of OSM then stems from (10) and leads to a skeleton formulation completely analogous to (7)

\[
(\text{Id} - \Pi)p_+ = \text{rhs}. \tag{11}
\]

In fact, if there is no cross point and if impedance operators \( T_j \)'s coincide through each interface, then \( \Pi = \Pi_{\text{loc}} \) and (11) reduces to (7).

In general, the operator \( \Pi \) is non-local, and may be defined implicitly through the solution to a symmetric positive definite system which makes effective numerical solution to (11) more involved.

5 New convergence bounds

Another novelty of our approach concerns the convergence analysis of OSM. Building on [10] combined with our treatment of cross-points, a new idea here is to conduct the analysis in terms of the norms induced by the impedance operators \( T_j \), assuming that \( p_j, q_j \mapsto (T_j^{-1}(p_j), T_j^{-1}(q_j)) ) \) are scalar products on \( H^{-1/2}(\Gamma_j) \), and considering

\[
\|p\|_{T^{-1}} := \langle T_j^{-1}(p_j), T_j^{-1}(q_j) \rangle \tag{12}
\]

on tuples of Neumann traces \( p = (p_1, \ldots, p_J) \). In this norm, contractivity properties of scattering and exchange operators are restored

\[
\|\Pi(p)\|_{T^{-1}} = \|p\|_{T^{-1}}, \\
\|S(p)\|_{T^{-1}} \leq \|p\|_{T^{-1}}.
\]

The analysis can be conducted both at the continuous and the discrete level. In the discrete case, if the impedances \( T_j \) are scalar products, the skeleton formulation is proved to be systematically coercive \((\alpha > 0)\) for the corresponding norm

\[ \Re\{\langle p, (\text{Id} - \Pi) p \rangle \}_{T^{-1}} \geq \alpha \|p\|_{T^{-1}}^2. \]

We shall discuss in detail this coercivity estimate. It leads directly to convergence bounds for classical linear solvers applied to (11), and it suggests certain choices of impedance operators which are confirmed by numerical results.

References


Minisymposia
New trends in nonlinear acoustics and related phenomena
Well-posedness and shape optimization for the Westervelt Robin boundary problem on domains with non-Lipschitz boundaries

Anna Rozanova-Pierrat\textsuperscript{1,4}, Adrien Dekkers\textsuperscript{1,1}, Michael Hin\textsuperscript{2,2}, Alexander Teplyaev\textsuperscript{3,3}

\textsuperscript{1}MICS, Department of Mathematics, CentraleSupélec, University Paris-Saclay, Gif-sur-Yvette, France
\textsuperscript{2}Department of Mathematics, Bielefeld University, Bielefeld, Germany
\textsuperscript{3}Department of Mathematics, University of Connecticut, Storrs, USA

\textsuperscript{4}Email: anna.rozanova-pierrat@centralesupelec.fr

Abstract

We obtain the global on-time well-posedness of the Robin type boundary valued problem for the Westervelt equation on a bounded domain with a non-Lipschitz boundary. The obtained weak solutions are considered in the domain of Laplacian and thus are more regular than $H^1$. The irregularity of the boundary does not allow the usual $H^2$-regularity. We consider the shape optimization problem for this ultrasound wave propagation model to minimize the system’s total acoustic energy by the shape of the boundary for fixed source and initial data. For the Robin boundary, modeling the reflection, we prove the existence of an optimal shape realizing the infimum of the acoustic energy in a class of Lipschitz boundaries. Using its relaxation on the regular class of domains, we prove the existence of an optimal shape realizing the minimum. Keywords: Westervelt equation; Robin boundary condition; fractals; shape optimization; Mosco convergence

1 Westervelt model and assumptions

Westervelt equation [14] is one of the models of non-linear acoustics describing the ultrasound propagation. We study it in a bounded domain $\Omega \subset \mathbb{R}^n$, $n = 2, 3$ with Robin-type boundary conditions:

\[
\begin{aligned}
\begin{cases}
\frac{\partial^2}{\partial t^2} u - c^2 \Delta u - \nu \Delta \partial_t u = \alpha u \partial_t^2 u + \alpha (\partial_t u)^2 + f, \\
\frac{\partial}{\partial n} u + a(x)u = 0 \quad \text{on} \quad \partial \Omega \times [0,T], \\
u(0) = u_0, \quad u_t(0) = u_1 \quad \text{in} \quad \Omega.
\end{cases}
\end{aligned}
\]

(1)

Here the coefficients $c, \nu, \alpha$ are positive constants (corresponding respectively to the sound speed in the air, the viscosity, and non-linear effects coefficient), and the reflection coefficient $a(x) > 0$ is a continuous in $\overline{\Omega}$ function. We don’t suppose any particular regularity on $\Omega$ and its boundary. Precisely, we assume that $\Omega$ is a Sobolev extension domain and its boundary $\partial \Omega$ is the support of a positive Borel measure $\mu$, supposed $d$-upper regular with a real $d \in [n-1, n)$. It means that there exists a constant $c_d > 0$ such that

\[
\mu(B_r(x)) \leq c_d r^d, \quad x \in \partial \Omega, \quad 0 < r \leq 1,
\]

where $B_r(x)$ is the Euclidian ball centered in $x$ of radius $r$.

This condition allows to have boundaries with the Hausdorff dimension $\text{dim}_{H} \partial \Omega \geq d$, i.e. $d$-sets, fractals, multi-fractals, regular boundaries. The Sobolev extension property does not allow the boundary to have infinitely small collapsing parts, as fractal trees do.

2 Weak well-posedness

In the regular case of $C^2$-boundary, there are different well-posedness results [8, 9, 12]. Here, in the absence of the usual $H^2(\Omega)$-regularity for the elliptic problems, we propose an alternative way to solve it following [1, 3, 4], using the domain of Laplacian. One way of the proof is based on a variant of a fixed point theorem [13], once we have the well-posedness of the linear problem by the Galerkin method. Another way is to use the Mosco convergence of the variational formulations on the regular domains to an irregular one to obtain the existence of a weak solution. To prove the unicity, it is sufficient to apply an $L^2$-stability estimate (see (8) from [2, Theorem 1.1]). The main difficulty is the absence of a part of the Dirichlet boundary, ensuring the Poincaré inequality and uniform, on boundary geometry, control estimates of the solution. Thanks to its generalization [6], we handle this problem.

3 Shape optimization: existence

The interest in modeling ultrasound propagation comes from ultrasound imaging (HIFU), lithotripsy, or thermotherapy. Recently [10] in the lithotripsy framework was considered a shape
optimization problem for the Westervelt equation considering the shape derivative on a regular boundary. The existence of such optimal shape was open, and we solved it. We define the admissible class of shapes in which we are searching for the minimum of our energy functional presenting an equivalent $H^1$-norm. This problem as in [10] can also be viewed in the sense of minimization of the difference between the solution $u$ and the reference state $g$ by $H^1([0, T] \times \Omega)$ norm since $w = u - g$ is a solution of the Westervelt equation with just a different source term and the homogeneous initial data. We follow [5, 7, 11] to prove the existence of an optimal shape realizing the infimum of the acoustic energy in a class of Lipschitz boundaries and the minimum on a compact class of uniform domains.

References


A phase-field approach to shape and topology optimization of nonlinear acoustic waves

Harald Garcke1, Sourav Mitra2, Vanja Nikolić3,*
1Faculty of Mathematics, University of Regensburg, Germany
2Institute of Mathematics, University of Würzburg, Germany
3Department of Mathematics, Radboud University, The Netherlands
*Email: vanja.nikolic@ru.nl

Abstract
We investigate the problem of finding the optimal shape and topology of a system of acoustic lenses in a dissipative medium, where the sound propagation is governed by a general semilinear strongly damped wave equation. We introduce a phase-field formulation of this problem through diuse interfaces between the lenses and the surrounding fluid. The resulting formulation is shown to be well-posed and we rigorously derive first-order optimality conditions for this problem. Additionally, we establish a relation between the diuse interface problem and a perimeter-regularized sharp interface shape optimization problem via the Γ-limit of the reduced objective. The talk is based on [1].

Keywords: shape and topology optimization, nonlinear acoustics, phase-field methods, optimality conditions, Γ-convergence

1 Introduction
We consider an acoustic lens system in a thermostatic fluid. A number of acoustic lenses \(\Omega_{1}, \ldots, \Omega_{n}\) of the same material are immersed in an acoustic fluid \(\Omega_f\), \(n \in \mathbb{N}\); see Figure 1. The material parameters corresponding to the lens are given by \((c_i, b_i, k_i)\) and to the fluid by \((\varepsilon_f, b_f, k_f)\). Here \(c_i > 0\) is the speed of sound, \(b_i > 0\) the sound diffusivity, and \(k_i \in \mathbb{R}\) is the nonlinearity coefficient, where \(i \in \{1, f\}\).

The goal is to determine the number and shape of acoustic lenses so that we reach the desired pressure distribution \(u_{t}\) in \(L^2(0, T; L^2(\Omega))\) in some region of interest \(D \subset \Omega\), where \(\Omega \subset \mathbb{R}^d\), \(d \in \{2, 3\}\), is a hold-all domain, assumed to be Lipschitz regular. Let \(T > 0\) denote the final time of propagation. Assuming that we have a high-intensity or high-frequency sound source, the propagation of sound waves is nonlinear. We can obtain the pressure field \(u\) by solving

\[\alpha(x, t)u_{tt} - \text{div}(c^2\nabla u) - \text{div}(b\nabla u_t) = f(u_t)\]

on \(\Omega \times (0, T)\), with the right-hand side nonlinearity given by \(f(u_t) = 2ku_t^2\). The medium parameters are piecewise constant functions, defined as

\[
\begin{align*}
    c &= \alpha x_1 + c_f(1 - \alpha x_1), \\
    b &= b_f(1 - \alpha x_1), \\
    k &= k_f(1 - \alpha x_1),
\end{align*}
\]

with \(\Omega_l = \bigcup_{j=1}^{n} \Omega_{l,j}\). We assume that the coefficient \(\alpha\) does not degenerate, that is, we assume that there exist \(\underline{\alpha}, \overline{\alpha} > 0\), such that

\[
\underline{\alpha} \leq \alpha(x, t) \leq \overline{\alpha} \quad \text{a.e. in } \Omega \times (0, T).\quad (2)
\]

Equation (1) can be seen as a semi-linearization of the Westervelt equation obtained by freezing the term \(\alpha(u) = 1 - 2ku\). The sound waves are excited via boundary in form of Neumann boundary conditions

\[
c^2 \frac{\partial u}{\partial n} + b \frac{\partial u}{\partial n} = g \quad \text{on} \quad \Gamma = \partial \Omega,\quad (3)
\]

where \(n\) denotes the unit outward normal to \(\Gamma\) and the problem is additionally supplemented with initial conditions.

2 A phase-field approach
We next introduce a continuous material representation between lenses and fluid by employing diuse interfaces \(\xi_i\), \(i \in \{1, n\}\), with thickness proportional to \(\varepsilon > 0\). We define a partition

\[\Omega = \Omega_f \cup \xi \cup \Omega_l\]

of \(\Omega\), where \(\xi = \bigcup_{i=1}^{n} \xi_i\) and then also introduce a phase-field function \(\varphi\) such that

\[
\begin{align*}
    \varphi(x) &= 1 \quad \text{for} \quad x \in \Omega_f, \\
    0 \leq \varphi(x) &\leq 1 \quad \text{for} \quad x \in \xi, \\
    \varphi(x) &= 0 \quad \text{for} \quad x \in \Omega_l.
\end{align*}
\]

(4)
see Figure 1. In the phase-field setting, the fluid region Ωf and the lens region Ωl are hence separated by a diffuse interface. On the diffuse interface, the material properties are interpolated with respect to the phase-field function as follows:
\[
c^2 = c_f^2 + \varphi(x)(c_l^2 - c_f^2), \\
b = b_f + \varphi(x)(b_l - b_f), \\
k = k_l + \varphi(x)(k_f - k_l),
\]
where we assume \( c_l < c_f, b_l < b_f, \) and \( k_l < k_f. \)

![Figure 1: The acoustic lens system with a phase-field interface.](image)

To formulate the problem, we employ a tracking-type objective and use a perimeter penalization to overcome ill-posedness of the sharp interface problem. We approximate it in the diffuse interface setting by a multiple of the Ginzburg-Landau energy \( E_\varepsilon \):

\[
E_\varepsilon(\varphi) = \begin{cases} 
\frac{\varepsilon}{2} |\nabla \varphi|^2 + \frac{1}{\varepsilon} \Psi(\varphi)dx, & \text{if } \varphi \in H^1(\Omega), \\
+\infty, & \text{otherwise.}
\end{cases}
\]

Here \( \Psi \) is a double obstacle potential given by

\[
\Psi(\varphi) = \begin{cases} 
\Psi_0(\varphi) & \text{if } 0 \leq \varphi \leq 1, \\
+\infty, & \text{otherwise,}
\end{cases}
\]

with

\[
\Psi_0(\varphi) = \frac{1}{2} \varphi(1 - \varphi).
\]

The shape optimization problem then has the following phase-field formulation:

\[
\min_{(u,\varphi)} J^\varepsilon(u, \varphi) = \frac{1}{2} \int_0^T \int_D (u - u_0)^2 \, dx \, ds + \gamma E_\varepsilon(\varphi),
\]

where \( \gamma > 0 \) is a weighting parameter, with \( \varphi \in \Phi_{\text{ad}} = \{ \varphi \in H^1(\Omega) \cap L^\infty(\Omega) : 0 \leq \varphi \leq 1 \, \text{a.e.} \}, \)

\( u \in U = \{ u \in L^\infty(0,T;H^1(\Omega)) : u_t \in L^\infty(0,T;H^1(\Omega)) \}, \)

such that

\[
\begin{align*}
\alpha u_{tt} - \text{div}(c^2(\varphi)\nabla u) - \text{div}(b(\varphi)\nabla u_t) &= 2k(\varphi)u_t^2, \\
c^2(\varphi) \frac{\partial u}{\partial n} + b(\varphi) \frac{\partial u_t}{\partial n} &= g \text{ on } \Gamma, \\
(u,u_t)|_{t=0} &= (0,0),
\end{align*}
\]

is satisfied (in a weak sense) and the medium parameters satisfy (5).

The function \( \varphi \in \Phi_{\text{ad}} \) is thus the design variable with \( \{ x \in \Omega : \varphi(x) = 1 \} \) modeling the fluid region and \( \{ x \in \Omega : \varphi(x) = 0 \} \) the lenses.

For the well-posedness of the state problem and the corresponding adjoint problem as well the proof of the existence of a minimizer, we refer to [1].

**Theorem 1 (Optimality system)** Let \( \varphi \in \Phi_{\text{ad}} \) be the minimizer of the optimal control problem (2)--(6) and \( u \) and \( p \) the associated state and adjoint variables, respectively. Then the functions \( (u,\varphi,p) \in U \times \Phi_{\text{ad}} \times H^1(0,T;H^1(\Omega)) \) satisfy the following optimality system in the weak sense: the state problem (6), the adjoint problem

\[
\begin{align*}
\alpha p_{tt} - \text{div}(c^2(\varphi)\nabla p) + \text{div}(b(\varphi)\nabla u_t) &= -4k(\varphi)u_t + 2(\alpha + 2k(\varphi)u_t)u_t \\
\quad + (u - u_t)\chi_D &\text{ in } \Omega \times (0,T), \\
c^2(\varphi) \frac{\partial p}{\partial n} - b(\varphi) \frac{\partial u_t}{\partial n} &= 0 \text{ on } \Gamma, \\
(p,u_t)|_{t=T} &= (0,0),
\end{align*}
\]

and the gradient inequality

\[
\gamma \varepsilon \int_\Omega \nabla \varphi \cdot \nabla (\tilde{\varphi}_- - \varphi) \, dx + \frac{\gamma}{\varepsilon} \int_\Omega \Psi'(\varphi) (\tilde{\varphi}_- - \varphi) \, dx
\]

\[
- \int_0^T \int_\Omega (2c(\varphi)c'(\varphi)(\tilde{\varphi}_- - \varphi)\nabla u(t) + b'(\varphi)(\tilde{\varphi}_- - \varphi)\nabla u_t(t)) \cdot \nabla p \, dx \, ds
\]

\[
+ \int_0^T \int_\Omega 2k'(\varphi)(\tilde{\varphi}_- - \varphi)u_t^2(t) \, p \, dx \, ds 
\geq 0, \quad \forall \tilde{\varphi} \in \Phi_{\text{ad}}.
\]

**Theorem 2** Under the assumptions of the well-posedness of state and adjoint problems, the reduced cost functionals \( \{ j_\varepsilon \}_{\varepsilon > 0} \), where \( j_\varepsilon = j_\varepsilon(\varphi) \), \( \Gamma \)-converge in \( L^1(\Omega) \) to \( j_0 \) as \( \varepsilon \to 0 \).

**References**

Analysis of shape optimization problems for the Kuznetsov equation

Mostafa Meliani1,∗, Vanja Nikolić1

1Department of Mathematics, Radboud University, Nijmegen
∗Email: m.meliani@math.ru.nl

Abstract
In various biomedical applications, precise focusing of nonlinear ultrasonic waves is crucial for efficiency and safety of procedures. This work analyzes a class of shape optimization problems constrained by general quasi-linear acoustic wave equations that arise in high-intensity focused ultrasound (HIFU) applications and extends on the work of [3] on the Westervelt pressure equation. Within our theoretical framework, the Westervelt and Kuznetsovequations of nonlinear acoustics in potential form are obtained as particular cases. To prove the existence of the Eulerian shape derivative, we study the local well-posedness and regularity of the forward problem, uniformly with respect to shape variations. Additionally, we prove Hölder-continuity of the acoustic potential with respect to domain deformations in order to rigorously compute the shape derivative within the variational framework of [1] for different cost-functionals of practical interest. The talk will be based on [2].

Keywords: nonlinear acoustics, shape optimization, Kuznetsov’s equation, energy method, HIFU.

1 Introduction
High-Intensity Focused Ultrasound (HIFU) is emerging as one of the most promising non-invasive tools in treatments of various solid cancers. However, its wide-scale use hinges on the ability to guarantee the desired sound behavior in the focal region. Since these ultrasonic waves are commonly excited by one or several piezoelectric transducers arranged on a spherical surface, changes in their shape directly affect the propagation and focusing of sound waves and give rise to practically relevant optimization problems.

Motivated by this, in the present work we conduct the analysis of a class of shape optimization problems subject to a quasilinear wave model with general quadratic nonlinearities:

\[
(1 - 2k\ddot{\psi})\dddot{\psi} - c^2 \Delta \dot{\psi} - b\Delta \psi - 2\sigma \nabla \psi \cdot \nabla \psi = 0,
\]

(1)

Figure 1: The optimization setup, where \( D = D_S \times (t_0, t_1) \)
on smooth spatial domains, assuming nonhomogeneous Neumann boundary excitation.

Besides, we not only treat the classical \( L^2(L^2)\)-tracking problem on \( D = D_S \times (t_0, t_1) \), where the acoustic velocity potential \( \psi \) should match a desired output \( \psi_D \) on a given spatial focal region \( D_S \) within a certain time interval \( (t_0, t_1) \), i.e.,

\[
J(\psi, \Omega) = \frac{1}{2} \int_0^T \int_\Omega (\psi - \psi_D)^2 \chi_{D_S} \, dx \, ds,
\]

we also consider in this work an \( L^2 \)-matching objective at final time:

\[
J_T(\psi, \Omega) = \frac{1}{2} \int_\Omega (\psi(T) - \psi_D)^2 \chi_{D_S} \, dx.
\]

Additionally, we study an \( L^2(L^2)\)-tracking functional on \( \dot{\psi} \), corresponding (up to a multiplicative constant) to tracking the sound pressure:

\[
J_p(\psi, \Omega) = \frac{1}{2} \int_0^T \int_\Omega (\psi - f_D)^2 \chi_D \, dx \, ds;
\]

see Figure 2 for an illustration of the optimization setup.

2 Well-posedness results
We study, under the hypothesis of small initial and boundary data, the well-posedness of the nonlinear Kuznetsov equation (1) coupled with inhomogeneous Neumann boundary excitation

\[
\frac{\partial \psi}{\partial n} = g,
\]
and initial data
\[ \psi(0) = \psi_0 \in H^3(\Omega), \quad \dot{\psi}(0) = \psi_1 \in H^2(\Omega). \]
g is taken in \( H^2(H^{-1/2}(\partial \Omega)) \cap H^1(H^{1/2}(\partial \Omega)) \) such that \( \dot{g} \in L^\infty(H^{1/2}(\partial \Omega)) \), and \( \Omega \) is a \( C^{2,1} \)-regular domain.

Moreover, we study the well-posedness of the general adjoint problem
\[
\begin{aligned}
\frac{\partial}{\partial t} \left( (1 - 2k\dot{\psi})\dot{\rho} \right) - c^2 \Delta \rho + b\Delta \dot{\rho} \\
- 2\sigma \nabla \cdot (\rho \nabla \psi) &= f \\
\end{aligned}
\]
\[ (2) \]
\[ c^2 \frac{\partial \rho}{\partial n} - b \frac{\partial \dot{\rho}}{\partial n} + 2\sigma g \dot{\rho} = 0 \]
\[ p(T) = p_0, \quad \dot{p}(T) = p_1, \]
which covers the different studied cost functionals for specific choices of \( f, p_0, \) and \( p_1 \); see [2] for details. We then establish sufficient conditions on \( f, p_0, \) and \( p_1 \) for which the adjoint problem is well posed and the shape derivative (given hereafter) is well defined.

3 Shape deformation and sensitivity

To describe shape variations and thus be able to express the shape derivative we use a vector field
\[ h \in \mathcal{D} = \left\{ h \in C^{2,1}(\overline{U}, \mathbb{R}^d) \mid h|_{\partial U} = 0 \right\}, \]
to perturb the identity [4].

![Figure 2: Perturbing the identity](image)

Adopting the variational framework developed in [3], we rely on the Hölder continuity of the potential with respect to domain perturbations. We furthermore show that the Kuznetsov equation is uniformly well posed with regard to small enough shape variations.

Under the assumptions of this and previous sections, we then derive shape derivatives of the form required by the Delfour–Hadamard–Zolésio structure theorem.

**Theorem 1** The shape derivatives for cost functionals \( J, J_p, \) and \( J_F \) exist in the direction of any \( h \in \mathcal{D} \) and are given by
\[
dJ(\Omega)h = \int_0^T \int_{\partial \Omega} \left( \frac{\partial}{\partial n} \left( (c^2 g + b\dot{g})p \right) + (c^2 g + b\dot{g})pk \right) (h \cdot n) d\gamma ds \\
- \int_0^T \int_{\partial \Omega} \left( (1 - 2k\dot{\psi})\dot{\rho} + c^2 \nabla p \cdot \nabla \psi \right. \\
\left. + b\nabla p \cdot \nabla \psi - 2\sigma p \nabla \psi \cdot \nabla \psi \right) (h \cdot n) d\gamma ds, \]
where \( \kappa \) stands for the mean curvature of \( \partial \Omega \) and \( p \) depends on the choice of the cost-functional via (2).

4 Conclusions

In this work, we have analyzed shape optimization problems governed by general wave equations that model nonlinear ultrasound propagation and, as such, arise in HIFU applications. In particular, we have established sufficient conditions for the well-posedness and regularity of the underlying wave models with nonhomogeneous Neumann boundary conditions, uniformly with respect to shape deformations, as well as the Hölder continuity of the solutions. Furthermore, we have studied the corresponding adjoint problems and rigorously computed shape derivatives for several objectives of practical interest.

Future work will be concerned, among others, with the numerical analysis and simulation of the Kuznetsov equation and of the optimization problems presented in this work.

**References**


Boundary stabilization of critical nonlinear JMGT equation with undissipated Neumann boundary

Marcelo Bongarti$^{1,*,}$, Irena Lasiecka$^2$

$^1$Weierstrass Institute for Applied Analysis and Stochastics, Berlin, Germany
$^2$Department of Mathematical Sciences, University of Memphis, Memphis, USA

*Email: bongarti@wias-berlin.de $^1$ & lasiecka@memphis.edu$^2$

Abstract
Boundary feedback stabilization Jordan–Moore–Gibson–Thompson (JMGT) equation in the nonlinear and critical case is considered. The boundary feedback is supported only on a portion of the boundary, while its remaining is left free (available to control actions) and fail to satisfy Lopatinski condition (unlike Dirichlet boundary conditions) making the analysis of uniform stabilization from the boundary to become very subtle and to require careful geometric considerations.

Keywords: boundary feedback stabilization, nonlinear acoustics, JMGT–equation

1 Introduction
The JMGT equation is a third–order (in time) semilinear PDE, a established model for nonlinear acoustics (NLA) which has been recently widely studied [1, 2, 3, 4, 5, 6, 9]. Here, critical refers to the usual case where media–damping effects are non–existent or difficult to measure.

Let $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$) be a bounded domain with smooth boundary $\Gamma := \partial \Omega$ and consider the semilinear JMGT–equation

$$\tau u_{ttt} + \left( (2 \cdot \kappa_{\kappa}) u_{ttt} \right) - c^2 \Delta u - (\delta + \tau c^2) \Delta u_t = 2ku_t^2,$$

where $c, \delta, k > 0$ are constants representing the speed and diffusivity of sound and a nonlinearity parameter, respectively, while the function $\alpha : \Omega \to \mathbb{R}^+$ accounts for natural friction. The parameter $\tau > 0$ accounts for thermal time relaxation.

For the analysis of long–time dynamics the function

$$\gamma : \Omega \to \mathbb{R}, \quad \gamma(x) \equiv \alpha(x) - \frac{\tau c^2}{b}$$

plays a central role. In fact, for zero Neumann or Dirichlet data, if $\gamma(x) \equiv \gamma_0 > 0$ a.e. in $\Omega$ both linear ($k = 0$) and nonlinear dynamics are uniform exponentially stable [8]. If $\gamma < 0$, chaotic solutions might appear [7] and if $\gamma \equiv 0$ then the energy is conserved. What mechanisms could ensure stability when $\gamma(x) \equiv 0$ (critical).

In this work we study the stabilizability property of the following boundary conditions

$$\lambda_\partial u + \kappa_0(x)u = 0 \text{ on } \Sigma_0$$

$$\partial_\nu u + \kappa_1(x)u_t = 0 \text{ on } \Sigma_1$$

with $\Gamma_0, \Gamma_1 \subset \Gamma$ relatively open, $\Gamma_0 \neq \emptyset, \Gamma_0 \cap \Gamma_1 = \emptyset, \lambda > 0, \kappa_0 \in L^\infty(\Gamma_0)$ and $\kappa_1 \in L^\infty(\Gamma_1), \kappa_1(x) \geq \kappa_1 > 0, \kappa_0 > 0$ a.e.

2 Functional Analytic Setting
We consider the system comprised of (1), boundary conditions (3) and initial conditions

$$u(0, \cdot) = u_0, u_t(0, \cdot) = u_1, u_{tt}(0, \cdot) = u_2$$

with regularity to be specified in what follows.

Let $A$ be extension (by duality) of the negative Laplacian with domain

$$\mathcal{D}(A) = \{ \xi \in H^2(\Omega) ; \partial_\nu \xi|_{\Gamma_1} = 0, [\partial_\nu \xi + \kappa_0 \xi|_{\Gamma_0}] = 0 \}$$

and let phase space $\mathcal{H}$ given by

$$\mathcal{H} := \mathcal{D}(A^{1/2}) \times \mathcal{D}(A^{1/2}) \times L^2(\Omega)$$

with

$$||u||^2_{\mathcal{H}(A^{1/2})} := ||\nabla u||^2 + \int_{\Gamma_0} \kappa_0 |u_t|^2 d\Gamma_0 \sim ||u||^2_{H^1(\Omega)}$$

The $u$–problem ($k = 1/2$) can be written as

$$\tau u_{ttt} + \alpha u_{tt} + c^2 Au$$

$$+ bAu_t + c^2 AN(k_1, N^* Au_t)$$

$$+ bAN(k_1, N^* Au_t) = u_t^2 + u_{tt}$$

which we transform into the first order Cauchy–problem

$$\begin{cases}
\Phi_t = A\Phi + \mathcal{F}(\Phi) \\
\Phi(0) = \Phi_0 = (u_0, u_1, u_2)^T
\end{cases}$$

in the variable $\Phi = (u, u_t, u_{tt})^T$ with $\mathcal{F}(\Phi)^T \equiv (0, 0, \tau^{-1}(u_t^2 + u_{tt}))$ and $A$ with action (on $\xi = (\xi_1, \xi_2, \xi_3)^T$) and domain respectively

$$A\xi := \frac{c^2}{\tau} AN(k_1, N^* A) \xi_2 - \frac{b}{\tau} \xi_1$$

$$- \frac{b}{\tau} AN(k_1, N^* A) \xi_3 - \frac{\alpha}{\tau} \xi_1$$

$$- \frac{b}{\tau} AN(k_1, N^* A) \xi_3 - \frac{\alpha}{\tau} \xi_1$$
\[ \left\{ \xi \in [H^2(\Omega)]^2 \times H^1(\Omega); \right. \\
D(\mathcal{A}) = \left\{ \partial_\nu \xi_1 + \kappa_0 \xi_1 \right\}_{\Gamma_0} = \left\{ \partial_\nu \xi_2 + \kappa_0 \xi_2 \right\}_{\Gamma_0} = 0 \] (10)
\[ \left\{ \partial_\nu \xi_1 + \kappa_1 \xi_2 \right\}_{\Gamma_1} = \left\{ \partial_\nu \xi_2 + \kappa_1 \xi_1 \right\}_{\Gamma_1} = 0 \}

In order to treat the nonlinear problem we consider a second phase space and its norm
\[ \mathcal{H}_1 = \left\{ \xi \in H; \Delta \xi \in L^2(\Omega); |\lambda \partial_\nu \xi_1 + \kappa_0 \xi_1 |_{\Gamma_0} = 0; \right. \\
\left. \left[ \partial_\nu \xi_1 + \kappa_1 \xi_2 \right]_{\Gamma_1} = 0 \right\} \] (11)
\[ \| \xi \|_{\mathcal{H}_1} = \| \xi \|_H + \| \Delta \xi \|_2 + \| \partial_\nu \xi_1 \|_{H^{1/2}(\Gamma)} \]

3 Main Results

Assumption 1 The boundary \( \Gamma_0 \) is star–shaped and convex. In addition, there exists a convex level set function which defines \( \Gamma_0 \). See [3, 10].

Theorem 1 (Two level uniform stability) Let Assumption 1 be in force and \( \gamma(x) \geq 0 \). Then the operator \( \mathcal{A} \) generates uniformly exponentially stable semigroups on both \( \mathbb{H} \) and \( \mathcal{H}_1 \).

Given \( T > 0 \), we say that \( \Phi(t) \) is a mild solution for the system (1), (3) and (4) provided \( \Phi \in C([0,T], \mathbb{H}_1) \) and \( \Phi \) is given by the variation of parameter (VopP) formula corresponding to the solution of (8) with underlying semigroup being the one generated by \( \mathcal{A} \) in \( \mathcal{H}_1 \).

Define \( \mathbb{H}_\rho := \left\{ \Phi \in \mathcal{H}_1; \| \Phi \|_\mathcal{H} < \rho \right\} \) (\( \rho > 0 \)).

Theorem 2 (Global Solutions) Let Assumption 1 be in force. Then, there exists \( \rho > 0 \) sufficiently small (depending on the parameters in the equation) such that, given any \( \Phi_0 \in \mathbb{H}_\rho \) the VopP formula defines a continuous \( \mathcal{H}_1 \)-valued mild solution for the system (1), (3) and (4). Moreover, for such \( \rho > 0 \), there exists \( R = R(\| \Phi_0 \|_{\mathcal{H}_1}) \) such that all trajectories starting in \( B_{\mathbb{H}}(0,R) \) remain in \( B_{\mathbb{H}}(0,R_1) \) for all \( t \geq 0 \) and \( R_1 \) such that \( R_1 > R \).

Theorem 3 (Nonlinear Uniform Stability) Let Assumption 1 be in force and assume \( \gamma \in L^\infty(\Omega) \) and \( \gamma(x) \geq 0 \). Then, there exists \( \rho > 0 \) sufficiently small and \( M(\rho), \omega > 0 \) such that if \( \Phi_0 \in \mathbb{H}_\rho \) then
\[ \| \Phi(t) \|_{\mathcal{H}_1} \leq M(\rho)e^{-\omega t}\| \Phi_0 \|_{\mathcal{H}_1}, \quad t \geq 0 \] (12)
where \( \Phi \) is the mild solution given by Theorem 2.

References


Formation of singularities for relaxed compressible Navier-Stokes equations

Yuxi Hu\(^1\), Reinhard Racke\(^2\), Na Wang\(^3\)

\(^1\)Department of Mathematics, China University of Mining and Technology, Beijing, P.R. China
\(^2\)Department of Mathematics and Statistics, University of Konstanz, Konstanz, Germany
\(^3\)School of App. Sci., Beijing Information Science and Technology University, Beijing, P.R. China

Abstract

We investigate the formation of singularities in one-dimensional hyperbolic compressible Navier-Stokes equations, a model proposing a relaxation leading to a hyperbolization through a nonlinear Cattaneo law for heat conduction as well as through the constitutive Maxwell type relations for the stress tensor. We show that there are in general no global smooth solutions for the studied system with some large initial data.

This appears as a remarkable contrast to the situation without relaxation, i.e. for the classical compressible Navier-Stokes equations, where global large solutions exist. It also contrasts the fact that for the linearized system associated to the classical resp. relaxed compressible Navier-Stokes equations, the qualitative behavior is exactly the same: exponential stability in bounded domains and polynomial decay without loss of regularity for the Cauchy problem.

Keywords: singularities; compressible Navier-Stokes equations; large data

1 Nonlinear blow-up

We consider the system of one-dimensional non-isentropic compressible Navier-Stokes equations,

\[
\begin{cases}
\rho_t + (p\rho) u_x = 0, \\
p u_t + p u u_x + p_x = S_x, \\
p e_t + p u u_x + p u_x + q_x = S u_x,
\end{cases}
\]

where \(\rho, u, e, p, S, q\) denote the fluid density, velocity, specific internal energy per unit mass, pressure, stress tensor, heat flux, respectively. Instead of using the classical relations

\[q = -\kappa \theta_x, \quad S = \mu u_x,\]

we shall consider the relaxed versions in form of the (nonlinear) Cattaneo law of heat conduction

\[\tau_1(q_t + u \cdot q_x) + q + \kappa \theta_x = 0,\]

and the Maxwell type constitutive relations for the stress tensor

\[\tau_2(S_t + u \cdot S_x) + S = \mu u_x.\]

The internal energy \(e\) and the pressure \(p\) satisfy

\[
e = C_e \theta + \frac{\tau_1}{\kappa \theta} \rho^2 + \frac{\tau_2}{\mu} S^2, \quad (4)
\]

\[
p = R \rho \theta - \frac{\tau_1}{2 \kappa} \rho^2 - \frac{\tau_2}{2 \mu} S^2. \quad (5)
\]

We study the Cauchy problem for the functions \((\rho, u, \theta, S, q) : \mathbb{R} \times [0, +\infty) \to \mathbb{R}_+ \times \mathbb{R} \times \mathbb{R}_+ \times \mathbb{R} \times \mathbb{R}\) with initial condition

\[
(\rho(x, 0), u(x, 0), \theta(x, 0), S(x, 0), q(x, 0)) = (\rho_0, u_0, \theta_0, S_0, q_0).
\]

Let

\[
F(t) := \int_{\mathbb{R}} x \rho(x, t) u(x, t) dx,
\]

\[
G(t) := \int_{\mathbb{R}} (E(x, t) - \bar{E}) dx,
\]

where

\[E(x, t) := \rho(e + \frac{1}{2} u^2)\]

is the total energy and

\[\bar{E} := \rho(\bar{e} + \frac{1}{2} \bar{u}^2) = C_v.\]

Theorem 1 We assume that the data

\[(\rho_0 - 1, u_0, \theta_0 - 1, q_0, S_0)\]

are compactly supported in \((-M, M)\), and that

\[G(0) > 0.\]

Then, there exists \(u_0\) satisfying

\[
F(0) > \max \left\{ \frac{32 \sigma \max_{\rho_0}}{3 - \gamma}, \frac{4 \sqrt{\max_{\rho_0}}}{\sqrt{3 - \gamma}} \right\} M^2,
\]

\[1 < \gamma := 1 + \frac{R}{C_v} < 3\]

such that the length \(T_0\) of the maximal interval of existence of a smooth solution \((\rho, u, \theta, q, S)\) of (1)-(6) is finite, provided the compact support of the initial data is sufficiently large.
The method we use to prove the blow-up result is mainly motivated by work of Sideris where he showed that any $C^1$ solutions of compressible Euler equations must blow up in finite time. Using the finite propagation speed property allows us to define some averaged quantities and finally show a blow-up of solutions in finite time by establishing a Riccati-type inequality.

2 Linear stability

The linearized system associated to (1)-(3) has the form

\[
\begin{aligned}
\rho_t + u_x &= 0, \\
u_t - S_x + R\theta_x + R\rho_x &= 0, \\
C_s\theta_t + Ru_x + q_x &= 0, \\
\tau_1 q_t + q + \kappa \theta_x &= 0, \\
\tau_2 S_t + S - \mu u_x &= 0.
\end{aligned}
\] (9)

**Case 1: Bounded domain, $x \in (0,1)$**

Here we consider the boundary conditions

\[
u(t,0) = u(t,1) = 0, \quad q(t,0) = q(t,1) = 0.
\] (12)

Without loss of generality, we assume

\[
\int_0^1 \rho_0(x)dx = \int_0^1 \theta_0(x)dx = 0.
\] (13)

Defining

\[
E_1(t) := \int_0^1 \left( \frac{R}{2} \theta^2 + \frac{1}{2} \rho^2 + \frac{C_s}{2} \theta^2 + \frac{\tau_1}{2k} q^2 + \frac{\tau_2}{2\mu} S^2 \right) dx \equiv E_1(t; \rho, \ldots, S),
\]

\[
E_2(t) := E_1(t; \rho_1, \ldots, S_t)
\]

and

\[
E(t) := E_1(t) + E_2(t)
\]

to have the exponential stability:

**Theorem 2** There are constants $C$ and $C_1$ such that for all $t \geq 0$ we have

\[
E(t) \leq CE(0)e^{-\alpha t}.
\]

The proof is obtained by a standard multiplier method. For $\tau = 0$ we have

\[
u_t - R_1u_x = 0,
\]

and in bounded domains: exponential stability, for the Cauchy problem: no loss of regularity. For $\tau > 0$ we have

\[
\tau u_{ttt} + u_t - R_1u_{xx} - (\tau R_1 + \mu)u_{txx} = 0
\]

(Jordan-Moore-Gibson-Thompson type), again: exponential stability in bounded domains and no loss of regularity for the Cauchy problem.

**Theorem 3** There are positive constants $C$ and $C_1$ such that

\[
|\hat{V}(t, \xi)|^2 \leq Ce^{-C_1|\xi|^2} |\hat{V}(0, \xi)|^2,
\] (14)

for $(t, \xi) \in \mathbb{R}^+ \times \mathbb{R}$, where $h(\tau) := \frac{\tau^2}{1+\tau^2}$.

The proof is based on work of Kawashima for symmetric-hyperbolic systems. As a consequence, we obtain the decay rates of solutions to the Cauchy problem.

**Theorem 4** Let $l \geq 0$, and $0 \leq k \leq l$ be integers, and let $p \in [1,2]$. Assume that $V(0) \in H^l(\mathbb{R}) \cap L^p(\mathbb{R})$. Then we have

\[
\|\partial_t^l V(t)\|^2 \leq C \left\{ e^{-C_1t} \|\partial_t^l V(0)\|^2 + (1 + t)^{-2(l+1-k)} \|\partial_t^k V(0)\|_L^2 \right\},
\] (15)

where $\lambda = \frac{1}{2l} - \frac{1}{2}$ and $C_1$ is the same constant as in Theorem 3.

We remark that the isentropic case was discussed by Hu and Wang before,

\[
\begin{aligned}
\rho_t + (\rho u)x &= 0, \\
\rho u_t + \rho uu_x + p_x &= S_x, \\
\tau S_t + S &= \mu u_x.
\end{aligned}
\] (16)

$\tau = 0$: global large solutions exist, $\tau > 0$: blow-up for large data, but again: similarity of the linearized systems,

\[
\begin{aligned}
\rho_t + u_x &= 0, \\
u_t + R_1u_x - S_x &= 0, \\
\tau S_t + S - \mu u_x &= 0.
\end{aligned}
\] (17)

For $\tau = 0$ we have

\[
u_t - R_1u_{xx} - \mu u_{txx} = 0,
\]

and in bounded domains: exponential stability, for the Cauchy problem: no loss of regularity. For $\tau > 0$ we have

\[
\tau u_{ttt} + u_t - R_1u_{xx} - (\tau R_1 + \mu)u_{txx} = 0
\]

(Jordan-Moore-Gibson-Thompson type), again: exponential stability in bounded domains and no loss of regularity for the Cauchy problem.

**References**

Obtaining nonlinear acoustic models from non-conventional variational principles in fluid mechanics

Markus Scholle\textsuperscript{1,*}, Philip H. Gaskell\textsuperscript{2}, Sara Ismail-Sutton\textsuperscript{2}

\textsuperscript{1}Heilbronn University, Institute for Flow in Additively Manufactured Porous Media, D-74081 Heilbronn, Germany.

\textsuperscript{2}Department of Engineering, Durham University, Durham, DH1 3LE, UK.

\textsuperscript{*}Email: markus.scholle@hs-heilbronn.de

Abstract

Starting from various variational formulations of compressible viscous flows, linear and weakly nonlinear equations of acoustic wave propagation are derived and analysed in terms of additional terms compared to the classical wave equations. On the one hand, the focus is on extensions of the classical theory in the direction of viscous flows beyond the local thermodynamic disequilibrium and on small scales up to the limits of the continuum hypothesis; on the other hand, relativistic flows are considered which appear on very large scales. For the latter, the modelling of viscosity in accordance with the causality principle is still a subject of current debates, so that the analysis of acoustic wave propagation can make a valuable contribution to this issue. Keywords: Variational calculus, discontinuous Lagrangian, non-equilibrium Thermodynamics, weakly nonlinear wave equation, causality

1 Variational principles for fluid flow

The formulation of physical theories with variational principles enables a deeper understanding of the physical system in many respects. It can equally serve as a basis for the development of efficient solution methods. Two different approaches for fluid flow are considered below.

1.1 Clebsch potential approach

For compressible viscous flow without thermal conductivity, \cite{1} proposed the Lagrangian:

\begin{equation}
\ell = - \varrho \left[ D_t \Phi + \alpha D_t \beta + \frac{1}{\omega_0} \left( \chi D_t \chi - \frac{\bar{u}^2}{2} \right) + e \right] + \frac{1}{2\omega_0} \ln \sqrt{\frac{\chi}{D \cdot R}},
\end{equation}

where \( e = e(\varrho, s) \) is the specific inner energy of the fluid depending on the mass density \( \varrho \) and \( s = c_\varrho \ln (\chi / c_\varrho T_0) \) the specific entropy, given in terms of the complex thermal excitation \( \chi \) \cite{2}, with temperature \( T_0 \), mass density \( \varrho_0 \) and specific heat \( c_\varrho \) as reference quantities. \( \bar{u} \) denotes the velocity field, \( D_t = \partial / \partial t + \bar{u} \cdot \nabla \) the material time derivative, and \( D \cdot R \) the contraction of the shear rate tensor \( D \) with the friction tensor \( R \), taking viscosity into account.

Two Striking features are the discontinuity due to the logarithmic term, \( \ln \sqrt{\chi / \chi} \), and the additional parameter \( \omega_0 \), both being related to phenomena away from thermodynamic equilibrium and beyond the continuum hypothesis, in particular Brownian molecular motion. In this context, \( 2\pi / \omega_0 \) can be interpreted as a thermodynamic relaxation time. The occurrence of the Clebsch variables \( \Phi, \alpha \) and \( \beta \) as fundamental fields is due to the required Galilei invariance of the Lagrangian \cite{1}.

1.2 Tensor potential approach

If one demands Lorentz invariance in place of Galilei invariance, the following proposal for a Lagrangian, motivated by analogy to Maxwell’s theory, turns out to be suitable \cite{3}:

\begin{equation}
\ell = \left[ (nmc^2 + ne + p) u^\alpha u^\beta + R^\alpha \beta \right] \tilde{a}_{\alpha \beta} - n u^\alpha \partial_\alpha \chi \\
+ \frac{1}{2} \partial^\mu u^\alpha \partial_\mu \tilde{a}_{\alpha \beta} - \partial_\alpha \tilde{a}^{\alpha \beta} \partial^\mu \tilde{a}_{\mu \beta} - \frac{1}{3} \partial_\alpha \tilde{a}^{\alpha \beta} \partial_\beta \Phi \\
- \left[ nmc^2 + ne - 3p + R^\alpha_\alpha \right] \frac{\Phi}{6} + \frac{\partial^\mu \Phi \partial_\mu \Phi}{12},
\end{equation}

with \( n \) the particle density, \( s \) the specific entropy, \( u^\alpha \) the 4-velocity, \( \chi \) a Lagrange multiplier, \( \Phi \) a scalar potential and \( \tilde{a}_{\alpha \beta} \) a traceless symmetric tensor potential. Again \( e = e(\varrho, s) \) is the specific internal energy, \( p = n^2 \partial e / \partial n \) the pressure and \( R^\alpha_\beta \) the friction tensor taking viscosity and heat conduction into account. Both \( e \) and \( R^\alpha_\beta \) depend on the constitutive relationships chosen to underpin the fluid model. Einstein’s summation convention is used consecutively.
2 Derivation of weakly nonlinear acoustic models

Starting from a theory of fluid flow, weakly nonlinear acoustic models are obtained following a set procedure. Usually the first step is the computation of the respective Euler-Lagrange equations from the given Lagrangian, followed by manipulations leading to the equations of motion. The next steps refer to the case of classical flows considered in Sec. 1.1, but can also be applied to the relativistic case shown in Sec. 1.2 after necessary adaptations. As state equation for the pressure is assumed:

$$\frac{\partial p}{\partial \theta} = a_0^2 \left[ 1 + \frac{B}{A} \frac{\varrho - \varrho_0}{\varrho_0} \right], \quad (3)$$

with small-signal sound speed $a_0$ and the non-linearity parameter $B/A$ of the respective fluid. Furthermore, sound waves are regarded as irrotational, $\nabla \times \vec{u} = 0$, implying:

$$\vec{u} = \nabla \Phi. \quad (4)$$

On introducing the condensation $\varepsilon := \ln (\varrho/\varrho_0)$ with equilibrium mass density $\varrho_0$, Taylor expansion w.r.t. $\varepsilon$ and $\Phi$ up to terms of quadratic order while considering friction terms only in linear order, the set of equations can be reduced to one equation only for the potential [4]:

$$a_0^2 \left\{ -\frac{1}{a_0^2} \frac{\partial^2}{\partial \theta^2} + \nabla^2 \right\} \Phi = \frac{\partial}{\partial t} \left[ (\nabla \Phi)^2 + \frac{B}{2Aa_0^2} (\partial_t \Phi)^2 - \bar{\nu} \left\{ 1 + \frac{\pi}{2a_0^2} \right\} \nabla^2 \Phi \right], \quad (5)$$

with $\bar{\nu}$ the diffusivity of sound over mass density. Eq. (5) is a generalisation of Kuznetsov’s equation with an additional term due to thermodynamic non-equilibrium, the effect of which becomes visible in the dispersion relation [4]:

$$k = \frac{\omega}{a_0} \sqrt{\frac{1 + \frac{i \omega}{a_0^2} \left( 1 - \frac{\pi^2 a_0^2}{2a_0^2} \right)}{1 + \left( \frac{\omega}{a_0^2} \right)^2 \left( 1 - \frac{\pi^2 a_0^2}{2a_0^2} \right)}}, \quad (6)$$

resulting from the respective linearised equation. According to Fig. 1, the attenuation coefficient $\Im k(\omega)$ is smaller compared to the classical one.

3 Conclusions and perspectives

Deriving equations for acoustic wave propagation from unconventional fluid flow theories provides an excellent test scenario of such theories:

while in case of the Lagrangian (1) thermodynamic non-equilibrium effects are identified as deviations from the classical theory, an analogue treatment of the relativistic Lagrangian (2) may help to test different constitutive models for the friction tensor $R^{\alpha\beta}$ in terms of causality. Also the role of potentials, for example the tensor potential $a^{\alpha\beta}$, and additional degrees of freedom such as the phase of the complex field $\chi$, could be better understood via such models.

Another promising path could be the direct application of the procedure depicted in Sec. 2 to the Lagrangian density in order to formulate acoustic models by variational principles.

References


A fast time-stepping method for the Westervelt equation with time-fractional damping

Katherine Baker 1, Lehel Banjai 1,*, Mariya Ptashnyk 1
1Maxwell Institute for Mathematical Sciences, Department of Mathematics, Heriot-Watt University, Edinburgh, UK, EH14 4AS
*Email: l.banjai@hw.ac.uk

Abstract
We consider the attenuated Westervelt equation, with the attenuation governed by a non-local in time operator. The non-locality is described by a time convolution with a singular kernel, the simplest case being that of the Riemann-Liouville fractional integral. We describe a time-stepping method and how a recently developed fast and memory efficient method for fractional derivatives can be applied to lessen the impact the non-locality has on the computational costs. Numerical results complete the work.

Keywords: Westervelt, damped wave equation, time-fractional derivative

1 Damped nonlinear wave equation
In this work we consider the damped Westervelt equation on a smooth domain \( \Omega \subset \mathbb{R}^d \), \( d = 2, 3 \),
\[
\partial_t^2 u - \Delta u - a \beta \ast \Delta \partial_t u = k \partial_t^2(u^2),
\]
where
\[
f \ast g(t) = \int_0^t f(t - \tau)g(\tau)d\tau
\]
denotes the one sided convolution, \( a > 0, k > 0 \) constants and \( \beta : \mathbb{R}_+ \to \mathbb{R}_+ \). Westervelt equation is a fundamental model in nonlinear acoustics with, e.g., the above damped equation capable of modelling of ultrasound in lossy media such as human tissue.

We assume that the kernel \( \beta \) satisfies
\[
\beta \in \mathcal{L}^1_{\text{loc}}(0, \infty), \quad \beta \geq 0, \quad \beta' \leq 0
\]
and that its Laplace transform \( \hat{\beta} \) satisfies
\[
\Re \frac{1}{\beta(z)} \geq C_{\beta}(\sigma) > 0 \quad \text{for} \quad \Re z \geq \sigma > 0.
\]
Typical example of \( \beta \) we have in mind is
\[
\beta(t) = \frac{1}{\Gamma(\mu)} t^{\mu-1} e^{-rt},
\]
for constants \( r \geq 0 \) and \( \mu \in (0, 1) \). If \( r = 0 \), then
\[
\beta \ast f = \mathcal{I}^\mu f \quad \text{and} \quad \beta \ast \partial_t f = \partial_t^{\alpha-\mu} f,
\]
where \( \mathcal{I}^\mu \) denotes the Riemann-Liouville fractional integral of order \( \mu \in (0, 1) \) and \( \partial_t^{\alpha-\mu} \) the Caputo derivative of order \( 1 - \mu \in (0, 1) \). The Laplace transform of \( \beta \) in this case is
\[
\hat{\beta}(z) = (z + r)^{-\mu}.
\]
Thus (3) is also satisfied as
\[
\Re \frac{1}{\beta(z)} \geq (\sigma + r)^{\mu} \quad \text{for} \quad \Re z \geq \sigma > 0.
\]
A number of other non-local damping operators can be found in literature. These include combinations of fractional time-derivatives and fractional space derivatives. For a list and existence and uniqueness of solutions to resulting equations, see the recent [5].

We rewrite equation (1) as
\[
(1 - 2ku)\partial_t^2 u - \Delta u - a \beta \ast \partial_t \Delta u(t)ds = 2k(\partial_t u)^2
\]
\[
\text{with} \quad u(0) = u_0, \quad \partial_t u(0) = u_1,
\]
where homogeneous Dirichlet condition is taken for simplicity. Next, we present a time-discretisation of the equations in this form.

2 Time-discretization
Let \( \Delta t > 0 \) be the uniform time-step and \( t_n = n\Delta t \) the discrete times at which \( u_n \) denotes the approximation of \( u(t_n) \). We introduce some notation to more easily present the discretisation:
\[
D u_n = \frac{1}{\Delta t} (u_{n+1} - u_{n-1}),
\]
\[
D^2 u_n = \frac{1}{\Delta t^2} (u_{n+1} - 2u_n + u_{n-1}),
\]
\[
\{u\}_n = \frac{1}{4} (u_{n+1} + 2u_n + u_{n-1}).
\]
We now discretize the equation using the trapezoidal rule (a second-order, A-stable Newmark scheme). The time-discrete system then reads:
\[
(1 - 2k\{u\}_n)D^2u_n - \Delta\{u\}_n - a\beta \ast_{\Delta t} D\Delta u_n = 2k(Du_n)^2,
\]
where \(\beta \ast_{\Delta t} g_n\) denotes a convolution quadrature \([6]\) approximation of \(\int_0^n \beta(t_n - \tau)g(\tau)d\tau\). Similar time-discretization but with explicit time-stepping was analyzed in \([1]\) for the linear case \(k = 0\).

Under the assumptions on \(\beta\), convolution quadrature conserves a certain positivity property of the convolution, namely
\[
\sum_{j=0}^{\infty} \sigma^j \langle v_j, \beta \ast_{\Delta t} v_j \rangle \geq C_{\beta}(\sigma) \sum_{j=0}^{\infty} \sigma^j \|\beta \ast_{\Delta t} v_j\|_2^2,
\]
for any \(\sigma \in (0, 1)\); see \([4]\). If \(\lim_{\sigma \to 0^+} C_{\beta}(\sigma) > 0\), the scaling parameter \(\sigma\) can be set to 1, which simplifies the technicalities involved in analysing the stability and convergence of the above semi-discrete system; see \([2]\). The latter is the case for \(\beta\) as in \((4)\) with \(r > 0\).

3 Oblivious computation of the memory
Convolution quadrature of the time-discretization has the form
\[
\beta \ast_{\Delta t} v_n = \sum_{j=0}^{n} \omega_{n-j} v_j,
\]
where \(\omega_j\) are convolution weights, which in general decay only slowly as \(j \to \infty\). Thus, the numerical scheme needs to keep \(O(N)\) solution vectors \(u_j\) in memory where \(N\) is the number of time-steps and has computational time increasing quadratically with \(N\). This makes realistic computation difficult or impossible. Recent fast and oblivious algorithm for convolution quadrature of fractional integrals presented in \([3]\) is directly applicable in the case \((4)\) with \(r = 0\) and can reduce the memory requirements to \(O(\log N)\) and computational cost to \(O(N \log N)\). The case of \(r > 0\) in \((4)\) can also be dealt with the same algorithm with some small changes.

4 Numerical results
Numerical analysis of the time-discrete system is given in \([2]\) including a number of numerical evidence supporting the analysis. Here we present some basic computational results in 1D. The parameters in \((1)\) are set to \(k = 0.09\), \(a = 0.1\), and \(\mu = 0.5\) and \(r = 0\) in \((4)\). The initial data is a Gaussian
\[
u_0(x) = e^{-40x^2} \quad v_0(0) = 0.
\]

The spatial discretisation is performed by the piecewise linear Galerkin finite element method. The solution is plotted in Figure 1 at various times.

References
\begin{thebibliography}{9}
\bibitem{1} K. Baker and L. Banjai, Numerical analysis of a wave equation for lossy media obeying a frequency power law, in \textit{IMA J. Numer. Anal.}, (2021), online.
\end{thebibliography}
Modeling and simulation of nonlinear wave propagation in ultrasound imaging

Teresa Rauscher

1Department of Mathematics, Universität Klagenfurt, Klagenfurt, Austria

*Email: teresa.rauscher@aau.at

Abstract

Nonlinear ultrasound imaging has become increasingly important in medical but also industrial areas, as it makes the ultrasound beam analysis more accurate and enhances the quality of images. We develop a three dimensional model for nonlinear ultrasound imaging and a numerical algorithm to simulate pressure waveforms based on the KZK-equation. In our case we model the propagation of three dimensional sound beams in water for a rectangular source. With an eigensystem approach for the Laplacian operator on a rectangular domain and an operator splitting method the effects of nonlinearity and diffraction can efficiently be taken into account. To demonstrate the accuracy of the developed model it has been implemented in MATLAB and simulated results are compared to acoustic output measurements performed by a hydrophone.

Keywords: nonlinear wave propagation, ultrasound imaging, KZK-equation

1 Introduction

The pressure waves of ultrasound beams have strong nonlinearities at higher intensities. Figure 1 shows a beam sent out by a linear probe, the intensity of the pressure and the corresponding pressure waveforms at different depths.

Figure 1: Acoustic measurement: overview

The wave steepens, the amplitude of the compressional peak gets higher, whereas the rarefactive peak gets shallower. The waveform distorts because of increasing energy in higher harmonic frequencies. To model this behavior, we consider the KZK-equation as it accounts for diffraction, nonlinearity and absorption and uses a paraxial approach which is especially suitable for directive sound beams [2]. We investigate the wave propagation in water, so attenuation can be neglected and the KZK-equation in integrated form in terms of the pressure \( p \) reduces to

\[
\partial_\tau p = \frac{c_0}{2} \int_{-\infty}^{\infty} \Delta_\perp p \, d\tau + \frac{\beta}{2\rho_0 c_0^2} \partial_\tau p^2,
\]

where \( \tau \) is the retarded time, \( c_0 \) the speed of sound, \( \rho_0 \) the density and \( \beta \) the nonlinearity parameter. The direction of propagation is \( z \), so \( x, y \) are orthogonal coordinates and \( \Delta_\perp = \partial_x^2 + \partial_y^2 \). An efficient numerical method to solve this equation is an operator splitting approach [5], where each physical effect, i.e.

\[
\partial_\tau p = \frac{c_0}{2} \int_{-\infty}^{\infty} \Delta_\perp p \, d\tau,
\]

\[
\partial_\tau p = \frac{\beta}{2\rho_0 c_0^2} \partial_\tau p^2,
\]

is assumed to operate independently of the other over sufficiently small propagation distances.

2 Model equation

The shape of the beam strongly depends on the geometry of the probe [4] which we assume to be rectangular. Since it is symmetrical around its central axis we only consider the first quadrant. Looking at the classical eigenvalue problem for the Laplace operator with Neumann boundary conditions [1] on \( \Omega = [0, a] \times [0, b] \), the eigenvalues and eigenvectors are explicitly given by

\[
\lambda^{jk} = \frac{\pi^2 j^2}{a^2} + \frac{\pi^2 k^2}{b^2},
\]

\[
\phi^{jk}(x, y) = \frac{2}{\sqrt{ab}} \cos \left(j \pi \frac{x}{a}\right) \cos \left(k \pi \frac{y}{b}\right).
\]

The overall pressure at any time \( \tau \) and position \( x, y, z \) is given by

\[
p(x, y, z, \tau) = \sum_j \sum_k \rho^{jk}(z, \tau) \phi^{jk}(x, y).
\]

With these relations solving (2) is equivalently to solve for all \( m, n \) the ODE

\[
p^{mn}(z, \tau) = -\frac{2}{c_0\lambda^{mn}} P^{mn}(z, \tau).
\]

From (4) one can also derive an expression for the source condition.
3 Numerical results

We start our algorithm by applying a discrete cosine transform to the initial data, compare (4). Then we perform the diffraction step over a sufficiently small distance of propagation $\Delta z$, where (5) has been discretized with an implicit finite difference scheme. Next, we change back into time domain by applying the inverse cosine transform. Then we take the effect of nonlinearity with a discretized version of (3) over $\Delta z$ into account and one step is completed. Now, this algorithm has to be carried out until the final plane at depth $z_{\text{out}}$ is reached.

The following simulations were performed with MATLAB based on the proposed algorithm where the initial data was calculated by FIELD II [3]. Figure 2 shows numerical simulations of pressure waveforms on the central axis with the corresponding frequency spectra at various distances based on the proposed numerical algorithm.

Finally, in the following figures we compare on-axis pressure waveforms from acoustic measurements (blue) and simulations (orange) at different depths.

![Figure 2: On-axis pressure waveforms with corresponding frequency spectra at different depths](image)

![Figure 3: waveform at $z=1.5\text{mm}$, $z=16.5\text{mm}$](image)

![Figure 4: waveform at $z=26.5\text{mm}$, $z=39.5\text{mm}$](image)

4 Outlook

Future work is the derivation of a paraxial model based on the KZK-equation for vibro-acoustic imaging, do simulations and to put it into the mathematical framework of inverse problems (more precisely, coefficient identification in PDEs) and regularization.

References


The proof of this theorem is based on a second order linearization of the DtN map and high-frequency isonating profiles in the form of Gaussian beams. Consider \( f = \epsilon_1 f_1 + \epsilon_2 f_2 \) and denote \( U = \partial_t u + \partial_x u \) at \( \epsilon_1 = \epsilon_2 = 0 \). Then \( U \) solves
\[
c^{-2} \partial_t^2 U - \Delta U = \beta \partial_t^2 (u_1 u_2) \quad \text{in} \ (0, T) \times \Omega \quad (5)
\]
where \( u_1 \) and \( u_2 \) solve (1)-(3) with \( \beta = 0 \), and \( f_1 \) and \( f_2 \) replacing \( f \), resp. As a consequence \( \partial_t \partial_x \Lambda_\beta = \partial_t U \). Integration by parts yields,
\[
\int_0^T \int_{\partial \Omega} \partial_t U f_0 = 2 \int_{\Omega} \beta \int_0^T \partial_t (u_1 u_2) \partial_t u_0 \quad (8)
\]
where \( u_0 \) solves the linear wave equation with vanishing Dirichlet boundary condition and vanishing Cauchy data at \( t = T \). The proof of Theorem 1 hinges on the ability to construct special solutions \( u_j, j = 0, 1, 2 \) to make the time-integrals of functions \( \partial_t (u_1 u_2) \partial_t u_0 \) a dense set. Gaussian beams are such functions because they concentrate (at large frequencies) along geodesics of the manifold \((\Omega, g)\). The right-hand side of (8) converges to the line integral
\[
\int_{t_-}^{t_+} \beta (\gamma(t)) e^{3/2 (\gamma(t))} (\det Y(t))^{-1/2} dt \quad (9)
\]
along a geodesic \( \gamma \), and \( Y \) is a known tensor dependent on the metric \( g \). The family of integrals (9) is known as the Jacobi weighted ray transform of \( \beta e^{3/2} \) which is known to be invertible [2].

4 Inversion Algorithm

In the ultrasound transmission setting, the domain \( \Omega \) is isonated on one side and the transmitted wave generated by the nonlinearity is measured on the opposite side. We propose an algorithm to reconstruct \( \beta \) based on the behavior of the wave field at large but finite frequencies.

Take \( u_1 = u_2 = e^{ikx} e^{-i\omega t} \) representing waves propagating in the \( k \)-direction, with wave number \( k \), wave speed \( c \), and angular frequency \( \omega = c|k| \). The transmitted field \( U \) satisfies
\[
\partial_x U - 2ikU + \frac{1}{4nk} \partial^4_x U = \beta e^{2ikx} + O (\omega^{-2}) \quad (10)
\]
which follows the paraxial or one-way wave approximation for waves with a preferred direction of propagation [3].

Our algorithm is analogue to the filtered back-projection to invert the Radon transform,
\[
\beta \approx W^* [h * W[\beta]] \quad (11)
\]
where \( h \) is a suitable filter, \( W \) maps \( \beta \) to \( \partial_t U \), and \( W^* \) is the adjoint of \( W \). Figure 1 shows results of a numerical implementation of the reconstruction algorithm and its ability to back-propagate the wave field, taking into account its spreading to form sharp reconstructed images even at relatively low frequencies. As the frequency increases, the formulation converges to the inversion of the Radon transform.

![Figure 1: Synthetic data using the forward model (10) at angular resolution of 5° and reconstructed profiles using the inversion algorithm (11) for \( L/\lambda = 10 \) (top row) and \( L/\lambda = 100 \) (bottom row) where \( L \) is the size of the image and \( \lambda \) is the wavelength.](image)

References


Wave propagation in ab initio molecular simulation
Finite-size effects in response functions of molecular systems

Mi-Song Dupuy1,∗, Antoine Levitt2
1LJLL, Sorbonne Université, Paris, France.
2Inria Paris, CERMICS (ENPC), Champs sur Marne, France.
∗Email: mi-song.dupuy@sorbonne-universite.fr

Abstract

We consider an electron in a localized potential submitted to a weak external, time-dependent field. In the linear response regime, the response function can be computed using Kubo’s formula. In this paper, we consider the numerical approximation of the response function by means of a truncation to a finite space domain. This is necessarily a singular approximation because of the discreteness of the spectrum of the truncated Hamiltonian, and in practice a suitable regularization has to be used. Our results provide error estimates for the response function past the ionization threshold with respect to both the smoothing parameter and the size of the computational domain.

Keywords: linear response, limiting absorption principle, finite-size effects.

1 Setting and assumptions

The dynamics of $N$ electrons in a molecule, formally modeled by the many-body Schrödinger equation, can be approximated by time-dependent density functional theory, which results in a coupled set of 3-dimensional nonlinear partial differential equations for a set of $L^2$-orthogonal functions $(\psi_1, \ldots, \psi_N)$. In the regime of weak external fields, a linear response approximation yields response functions that describe the reaction of the electrons to an applied field at a particular frequency $\omega$.

In this study, we simplify the problem by considering a single electron. The evolution of $\psi \in L^\infty(\mathbb{R}, L^2(\mathbb{R}^d))$ ($d = 1, 2, 3$) is then given by the time-dependent Schrödinger equation

$$
\begin{cases}
    i\partial_t \psi = (-\Delta + V) \psi + \varepsilon f(t) V p \psi, \\
    \psi(0) = \psi_0.
\end{cases}
$$

(1)

$\psi_0$ is the ground-state of $H = -\Delta + V$ where $V$ is a multiplicative potential.

$V p$ is a perturbation potential, typically an electric field in a direction $e \in \mathbb{R}^d$, $V p(x) = x \cdot e$. The function $f \in L^\infty(\mathbb{R})$ is bounded. All the results in this work are established under the following assumptions

1. the ground-state $\psi_0$ is nondegenerate;
2. $V$ is smooth and bounded;
3. $V$ decays as $1/|x|^{2+\varepsilon}$, $\varepsilon > 0$;
4. the observable $V_0$ and the perturbation $V p$ are smooth and their derivatives are bounded.

2 Linear response theory

Consider $V_0$ a potential representing an observable, to first order in $\varepsilon$, we have for all $t \in \mathbb{R}$ the first order expansion

$$
\langle \psi(t), V_0 \psi(t) \rangle = \langle \psi_0, V_0 \psi_0 \rangle + \varepsilon \langle K \ast f \rangle(t) + O(\varepsilon^2).
$$

(2)

Under the above assumptions, the response function $K$ is defined by the Kubo formula

$$
K(\tau) = -i\theta(\tau) \langle V_0 \psi_0, e^{-i(H-E_0)\tau} V p \psi_0 \rangle + c.c.,
$$

(3)

where $z + c.c.$ is a notation for $z + \overline{z}$, and $\theta$ is the Heaviside function. It is continuous, of at most polynomial growth, and causal. The response function has a Fourier transform at least defined in distribution

$$
\hat{K}(\omega) = \lim_{\eta \to 0^+} \langle V_0 \psi_0, (\omega + i\eta - (H-E_0))^{-1} V p \psi_0 \rangle - \langle V p \psi_0, (\omega + i\eta + (H-E_0))^{-1} V_0 \psi_0 \rangle.
$$

(4)

When $|\omega| \notin \sigma(H-E_0)$, $\hat{K}$ defines an analytic function in a neighborhood of $\omega$. When $|\omega| = E_n - E_0$ for $E_n$ an eigenvalue of $H$, $\lim_{\eta \to 0^+} \hat{K}(\omega + i\eta)$ diverges, and the distribution $\hat{K}$ is singular at $\omega$. When $|\omega| > -E_0$, i.e. above the ionization threshold, we can study the boundary value of the resolvent $(z-H)^{-1}$ as the divergence merely indicates a loss of locality of the associated Green’s function. This is known
as a limiting absorption principle [1] which has a long history in mathematical physics.

Under our assumptions, it is standard to show that $\hat{K}$ is a continuously differentiable function for $|\omega| > -E_0$:

$$|\hat{K}(\omega + i\eta) - \hat{K}(\omega)| \leq C\eta. \quad (5)$$

3 Space truncation and main result

We now truncate our problem (4) by diagonalizing the operator $-\Delta + V$ on a domain $[-L, L]^d$ with Dirichlet boundary conditions. The corresponding approximations $H_L, \psi_{0,L}$ and $E_{0,L}$ give rise to an approximate response function $K_L$ which is a singular approximation of $K$ as the spectrum of the operator $H_L$ is only discrete.

**Theorem 1** (\[2\]) $K_L$ converges towards $K$ in the sense of tempered distributions. Furthermore, for all $\omega \in \mathbb{R}$ there is $\alpha > 0$ such that for all $0 < \eta < 1, L > 0$,

$$|\hat{K}_L(\omega + i\eta) - \hat{K}(\omega)| \lesssim e^{-\alpha\eta L} \eta^2 + \eta. \quad (6)$$

There is a balance of error to set between the size of the domain $L$ and the regularization $\eta$ as can be seen in Figure 1 and Figure 2.

4 Conclusion and perspectives

In this work, we have established the convergence rate of the truncated linear response function $\hat{K}_L$ and the exact one. The homogeneous Dirichlet boundary condition is a simple but crude approximation which can be improved by imposing frequency dependent boundary conditions (absorbing boundary conditions, perfectly matching layers) that better reproduce the continuous spectrum. Another limitation of our work is the linearity of the model that does not reflect what is used in practice. We would need to prove a limiting absorption principle in that case.

References


Quantum dynamics beyond the Born-Oppenheimer approximation in molecular systems

Loïc Joubert-Doriol

1Univ Gustave Eiffel, Univ Paris Est Creteil, CNRS, UMR 8208, MSME, F-77454 Marne-la-Vallée, France
*Email: loic.joubert-doriol@univ-eiffel.fr

Abstract

Representing the wavefunction of quantum systems scales exponentially with the number of particles, which makes quantum simulations of molecules intractable. The Born-Oppenheimer approximation utilizes the difference in timescales’ dynamics of electrons and nuclei to split the problem into two simpler problems associated with each type of particle by using the Born-Oppenheimer representation. While this approximation is a cornerstone of quantum chemistry, it neglects important effects when a molecule undergoes an ultrafast process where both electrons and nuclei evolve on a similar timescale. In this case, one must go beyond this approximation. Unfortunately, the Born-Oppenheimer representation exhibits two major drawbacks that make exact simulations impossible: i) a geometric phase in the electronic wavefunctions, and ii) a non-integrable term in the Hamiltonian. After exposing these problems, I will present an alternative employing time-dependent electronic wavefunctions: the moving crude adiabatic states.

Keywords: Quantum molecular dynamics, Moving Crude Adiabatic

Introduction

Simulation of matter at the molecular scale requires applying quantum mechanical concepts to describe electrons and nuclei. Quantum mechanics describes matter as a wavefunction, which can be understood as a superposition of a large number of possible configurations that span a Hilbert space. Numerical approaches to simulating quantum systems scale exponentially with the number of particles, which makes the simulations intractable. The time evolution of the system is described by the Schrödinger equation

$$\frac{\partial \Psi}{\partial t(t)} = -i\hat{H}\Psi(t)$$,

(1)

where $t$ is the time parameter, $|\Psi(t)\rangle$ is the molecular wavefunction, and $\hat{H}$ is the molecular Hamiltonian where the potential energy is given by the Coulomb interactions between the particles.

Thanks to the mass ratio of the electrons and nuclei, the electronic timescale is much shorter than the nuclear timescale. Then, electrons instantaneously adapt to the motion of the nuclei, while the nuclei experience the average field of the electrons. This separation is achieved by: i) splitting the Hamiltonian into nuclear kinetic energy and the electronic Hamiltonian, $\hat{H}_e(R)$, which contains the remaining terms and depends on the nuclear positions $R$, and ii) imposing that electrons are represented by stationary states, also named adiabatic states, of $\hat{H}_e$ and associated with the electronic eigenenergies $\varepsilon_n(R)$:

$$\hat{H}_e(R)|\varphi_n(R)\rangle = \varepsilon_n(R)|\varphi_n(R)\rangle.$$  \hspace{1cm} (2)

These electronic states form a basis on which one can expand the molecular wavefunction

$$|\Psi(R,t)\rangle = \sum_{n=1}^{\infty} |\varphi_n(R)\rangle \chi_n(R, t).$$ \hspace{1cm} (3)

The Born-Oppenheimer approximation imposes that the electronic part of the total wavefunction is confined in a given electronic state and the total wavefunction reads $|\Psi(R,t)\rangle \approx |\varphi_n(R)\rangle |\chi_n(R, t)\rangle$. This approximation is a cornerstone of chemistry and is often valid for molecular systems close to equilibrium at ambient temperature, where only the ground electronic state is populated. However, this approximation can fail dramatically when the system is excited to a higher electronic state, and strong couplings allow for transitions between electronic states such that more terms in Eq. 3 are required. An interesting case occurs in the presence of geometries named conical intersections, where the electronic states energies are degenerate $\varepsilon_n = \varepsilon_{n+1}$ and the interstate coupling becomes infinite [1]. Conical intersections are ubiquitous in dynamics involving excited states. Extra diff-
ficulties arise at these geometries: i) the electronic states acquire a geometric phase (also named Berry phase) upon encircling the conical intersections [2], and ii) a non-integrable intrastate (diagonal) term appear [3].

In this talk, I will first give numerical examples of failure in the Born-Oppenheimer representation. Then, I will present an alternative representation that handles the mentioned difficulties.

1 Limitations of the Born-Oppenheimer representation

Since electronic states are parameterized by the nuclear positions, the nuclear kinetic energy action on the electronic states gives rise to the so-called non-adiabatic couplings. These non-adiabatic couplings can be intra- or interstate couplings.

A first difficulty comes from the fact that inter and intrastate couplings diverge at conical intersections. In particular, the intrastate terms are not integrable [3]. These must necessarily be excluded from the equation to obtain a finite solution. The second difficulty comes from the appearance of a geometric phase attached to electronic states when they are transported on a closed loop around the conical intersection in the nuclear coordinate space [2]. Thus, electronic states are double-valued functions of the nuclear coordinates and so must be the nuclear components $\chi_n(R,t)$. Imposing double-valued boundary conditions on the latter is impossible without prior knowledge of the conical intersections positions. Therefore, not accounting for this double-valuedness is another common necessary approximation. These arbitrary approximations can lead to significant changes in the dynamics of molecular systems. I will expose these issues on numerical examples employing simple vibronic models [4].

2 A new representation for direct molecular quantum dynamics

Choosing the adiabatic representation greatly reduces the many-electron Hilbert space to only $N_v$ number of important electronic states in Eq. (3). Regarding the nuclear components, one can also avoid exponential scaling by employing a time-dependent basis that adapts along the dynamics. Gaussian functions $g(R,q_k[t])$ with time evolving centers $q_k[t]$ are commonly chosen in order to employ local approximate models and simplify space integrations. Then, the nuclear components read

$$\chi_n(R,t) = \sum_{k=1}^{N_v} C_{kn}(t) g(R,q_k[t]),$$

(4)

where $\{C_{kn}(t)\}$ are time-dependent complex coefficients. Nevertheless, Gaussian functions are not double-valued functions and have no specific cusp behavior that can avoid non-integrability of the intrastate terms.

To resolve this difficulty, we adopt a new type of electronic wavefunctions that are solutions of Eq. (2) only at the Gaussians’ centers:

$$\hat{H}_e(q_k[t])|\varphi_n(q_k[t])\rangle = \varepsilon_n(q_k[t])|\varphi_n(q_k[t])\rangle.$$ (5)

This small change removes the parametric dependence of the electronic states on the nuclear coordinates, such that the resulting states are not double-valued and do not give rise to any non-integrable term. I will present numerical simulations to support these findings [5].

References


Computing Spectral Properties of Topological Insulators with Disorder

Matthew J. Colbrook, Andrew Horning, Kyle Thicke, Alex Watson

Abstract

We develop new numerical methods to compute spectral properties of tight-binding Hamiltonians for disordered and defective topological insulators, which characterize their remarkable electronic behavior. Our approach extends a recent framework that uses rational filters to probe the continuous spectrum of infinite-dimensional operators [Colbrook et al., SIAM Rev. 2021].

Keywords: topological insulators, tight-binding models, computational spectral theory

1 Introduction

Topological insulators (TIs) are renowned for their remarkable electronic properties. They exhibit quantised bulk Hall and edge conductances and support electronic transport along edges and interfaces, features that persist even when material defects and disorder are present. These physical characteristics can be understood and quantified through spectral properties of tight-binding Hamiltonian models.

Computing the relevant spectral properties of tight-binding models for disordered and defective TIs in a principled manner poses a significant challenge for two reasons:

1. Transport in the bulk and edge is mediated by a continuum of generalized (non-normalizable) eigenstates associated with bands of continuous spectrum. In general, the tight-binding Hamiltonian’s spectrum may contain an exotic mix of continuous and discrete spectral types.

2. Periodic approximations and other artificial truncations of the computational domain may introduce spectral artifacts and, in general, fail to rigorously approximate continuous spectral properties of the Hamiltonian.

Here, we develop numerical methods that overcome both challenges by working within a framework recently proposed to compute discrete and continuous spectral properties of infinite-dimensional operators [1–4]. We compute spectra, approximate eigenstates, spectral measures, spectral projections, transport properties, and conductances of the tight-binding Hamiltonian. Numerical examples are given for the Haldane model, and the techniques extend easily to other TIs in two and three dimensions.

2 The resolvent framework

Let \( \mathcal{A} : \mathcal{D}(\mathcal{A}) \to \mathcal{H} \) be a self-adjoint operator on a Hilbert space \( \mathcal{H} \) with domain \( \mathcal{D}(\mathcal{L}) \). \( \mathcal{A} \) has the spectral decomposition

\[
\mathcal{A} = \int_{\Lambda(\mathcal{A})} \lambda \, d\mathcal{E}(\lambda),
\]

where \( \Lambda(\mathcal{A}) \) is the spectrum of \( \mathcal{A} \) and \( \mathcal{E} \) is the projection-valued spectral measure. That is, for each measurable set \( \Omega \subset \Lambda(\mathcal{A}) \), the spectral projection onto \( \Omega \) is given by \( \mathcal{E}(\Omega) = \int_{\Omega} d\mathcal{E}(\lambda) \).

The resolvent framework for infinite-dimensional spectral computations uses samples of the resolvent operator,

\[
\mathcal{R}(\mathcal{A}, z) = (\mathcal{A} - z\mathcal{I})^{-1}
\]

at points \( z_1, \ldots, z_\ell \in \mathbb{C} \) in the complex plane to construct rigorous approximations to both discrete and continuous spectral properties of \( \mathcal{A} \).

In practice, this means solving shifted linear equations of the form

\[
(\mathcal{A} - z_k\mathcal{I})u_k = f, \quad k = 1, \ldots, \ell.
\]

For certain spectral properties, one must also compute inner products in \( \mathcal{H} \).
2.1 Spectrum and eigenstates

The spectrum $\Lambda(A)$ can be computed with error control [1] by using localization properties of the $\epsilon$-pseudospectrum, i.e., the $\epsilon^{-1}$ level sets of

$$\|R(A, z)\|_H = \sup_{f \in \mathcal{H}} \sqrt{\langle R(A, z)f, f \rangle_{\mathcal{H}}}$$

in the complex $z$-plane. A sequence of maximizing functions $f_k \in \mathcal{H}$ (e.g., generated by shifted power iterations with $A$) provide approximating pseudo-eigenstates.

2.2 Spectral measures

We show how to construct spectrally smoothed approximations of the projection-valued spectral measure $\mathcal{E}([a, b])$ using analogs of Stone’s theorem:

$$\frac{1}{2\pi i} \lim_{\epsilon \to 0^+} \int_a^b (R(A, \lambda + i \epsilon) - R(A, \lambda - i \epsilon)) \, d\lambda = \mathcal{E}([a, b]) - \frac{1}{2} (\mathcal{E}([a]) - \mathcal{E}([b])).$$

In particular, we remove the endpoint contributions and prove an extension of Stone’s theorem to higher-order smoothing kernels that achieve rapid convergence as the smoothing parameter $\epsilon \to 0^+$. We also demonstrate why careful deformations of the integration contour on the left can accelerate the computation of $\mathcal{E}([a, b])$ by orders of magnitude. This work is best understood as an extension of the recent framework for computing smoothed densities of scalar spectral measures $\mu_f = d\mathcal{E}(\lambda)f, f \rangle_{\mathcal{H}}$ [3].

2.3 Functional calculus

In a spirit similar to the projection-valued spectral measure approximations, one can approximate the functional calculus of $A$ via

$$f(A) = \int f(\lambda) \, d\mathcal{E}(\lambda), \quad (4)$$

coupled with suitable analogs of Stone’s theorem and careful contour deformations into the complex $\lambda$-plane [4]. Of particular interest is the time evolution operator for tight-binding Hamiltonians, corresponding to $f_t(\lambda) = \exp(-iA t)$.

3 Haldane model experiments

The Haldane model describes electrons hopping on a two-dimensional honeycomb lattice in the presence of a periodic magnetic field with zero net flux. When the lattice is pristine (without defects), the infinite-dimensional Hamiltonian’s spectral properties can be studied analytically by using Bloch’s theorem for periodic media. When the lattice contains edges, defects, or disorder, periodic and truncated approximations are still applied heuristically. However, these may introduce spectral artifacts such as spectral pollution in the gap of the Bloch Hamiltonian.

In place of periodic or truncated approximations of the Haldane Hamiltonian $A$, we rigorously approximate the action of $R(A, z)$ on $\mathcal{H}$ by using rectangular sections of a banded infinite-dimensional representation of $A$ [2]. Applying the resolvent framework for infinite-dimensional spectral computations allows us to rigorously approximate the spectral properties discussed in section 2.

In particular, we use spectral projections to compute bulk and edge conductances of $A$ and confirm that these are quantized in the presence of weak global disorder, even in the exotic mobility gap regime. The corresponding topological phase diagrams of the Haldane model are computed and wave-packet approximations are constructed to probe generalized eigenstates mediating bulk and edge transport. The functional calculus is applied to compute the time evolution of topologically protected edge states.

References


Computation of resonances in locally perturbed periodic quantum systems

Eloïse Letournel\textsuperscript{1,}\textsuperscript{*}, Antoine Levitt\textsuperscript{2}, Ivan Duchemin\textsuperscript{3}, Luigi Genovese\textsuperscript{4}, Simon Ruget\textsuperscript{5}

\textsuperscript{1}Inria Paris, CERMICS (ENPC), Champs sur Marne, France
\textsuperscript{2}Inria Paris, CERMICS (ENPC), Champs sur Marne, France
\textsuperscript{3}CEA, Grenoble, France
\textsuperscript{4}CEA, Grenoble, France
\textsuperscript{5}ENPC

\textsuperscript{*}Email: eloise.letournel@polytechnique.edu

Abstract

We introduce a new numerical method to compute resonances induced by localized defects in crystals. This method solves an integral equation in the defect zone to compute analytic continuations of resolvents. Such an approach enables one to express the resonance in terms of a localized, compact-supported function. The kernel of the integral equation is the Green function of the undefective region, which is extended by a complex deformation of the Brillouin zone, thereby generalizing in reciprocal space the concept of complex coordinate transformations.

Keywords: Resonances, Green function, defect in a solid, complex scaling.

1 Introduction

We consider a one-body (possibly mean-field) Hamiltonian $H$, describing for instance a molecule or a defect in a solid. The motivation and the expected applications come from mean-field models such as time-dependent density functional theory (TDDFT). Knowledge of the resolvent $R(z)$ of the Hamiltonian close to the real axis is of interest to calculate the density of states, or for time-dependent response properties for instance. When the Hamiltonian is a small perturbation of a reference Hamiltonian that has both bound and continuous states at the same energy $E$, the coupling between these states typically results in a bump of $R$ at $E$. This corresponds to a resonance, which can be formally defined as a pole in the analytic continuation of the resolvent of the system from the upper complex plane into the lower, through the essential spectrum of $H$. This extension of the resolvent makes sense only if we consider $R(z)$ applied on localized functions, which we will always do.

However, the truncation of $H$ to a finite region of space will discretize the energy spectrum, not allowing for this extension. This is related to qualitative differences in wave propagation described by the full and truncated Hamiltonians. Quantities on the real axis can be obtained by approximating $R(\omega)$ by $R(\omega + i\eta)$ for some finite artificial dissipation $\eta > 0$, but it does not allow to reach the resonances below the real axis.

We propose a method to express the continuation of resolvent on and below the real spectrum for Hamiltonians of the form $H = H_0 + V$, where $H_0$ is periodic on an infinite domain, and $V$ is localized.

2 Method

We reformulate the problem as an integral equation posed in the region of the defect, similar to the Lippman-Schwinger method used in scattering problems. It allows to write the resolvent as $R(z) = R_0(z)(1 - VR_0(z))^{-1}$. $VR_0$ being localized, the essential of the work consists in computing $R_0$, the resolvent of the periodic part $H_0$ of the Hamiltonian, possibly extended the lower complex plane of energies $z$. Resonances can then be found with a Newton method applied to the determinant of $1 - VR_0(z)$.

The resolvent for a crystal Hamiltonian can be expressed as an integral on $k$ over the Brillouin zone, which we deform using a multi-dimensional generalization of the Cauchy integral formula. We choose the deformation function $k_i : k \mapsto k + ik_i(k)$ so that the singularities of the integrand get pushed down into the lower complex plane for $z$, extending the domain of validity of the integral formula below the essential spectrum. An analogy can be drawn with the complex scaling method, which is a deformation in the real space rather than the reciprocal space.

This new method is based on ideas that have been used for theoretical studies [1–3] and recently been used as a numerical method in 1D.
scattering problems [4]. The resulting scheme only requires unit cell computations.

3 Resolvent for a graphene lattice

We apply our method on a graphene tight-binding model (discrete Schrödinger operator). We will first compute the resolvent of the unperturbed Hamiltonian $H_0$ and extend it below the real axis.

The Bloch-Floquet transform of $H_0$ is a $2 \times 2$ complex matrix $H_k$. We plot Figure 1 the eigenvalues $\varepsilon_{nk}$ of this matrix over the Brillouin zone $B$.

At a given energy $z$, the points $k$ of the Brillouin zone at which the $\varepsilon_{nk}$ are equal to $z$ will cause a singularity, since the integral is:

$$ R_0(R, R'; z) = \frac{1}{|B|} \int_{B} \sum_{n=1}^{N} \frac{|u_{nk}\rangle\langle u_{nk}|}{z - \varepsilon_{nk}} d\mathbf{k}. $$

Using a generalization of the Cauchy integral theorem, we deform the integration path by adding an imaginary part $i\mathbf{k}(\mathbf{k})$ to $k$ around those points. Choosing $\mathbf{k}_i$ in the opposite direction to the gradient of the eigenvalue, we ensure that points $z$ at which the integrand of the resolvent is singular are pushed downwards the real axis at first order. The deformation $\mathbf{k}_i$ over the Brillouin zone is shown Figure 1.

This provides an extension of $R_0$ below the real axis as shown Figure 2.

4 Perturbation of the lattice with an adatom

We now add a single adatom on the lattice, linked to one site of the lattice with hopping constant $\epsilon$, and with an energy $E$. We use the $R_0$ computed as above to look for the zeros of the determinant of $(1 - VR_0(z))$ (see Figure 3) with a Newton descent. These zeros are resonances of the system. We show Figure 4 the resonant state of the system $\psi = R_0(z_{res})\phi$, where $\phi$ is the localized state associated to the eigenvalue 0 for $(1 - VR_0(z_{res}))$.

References


Contributed talks
Monday, July 25, Morning Session
Three types of quasi-Trefftz functions for the 3D convected Helmholtz equation: construction and theoretical approximation properties

Lise-Marie Imbert-Gérard\textsuperscript{1,*}, Guillaume Sylvand\textsuperscript{2}

\textsuperscript{1}Department of Mathematics, University of Arizona, Tucson, USA
\textsuperscript{2}Airbus Central R&T, France
*Email: lmig@math.arizona.edu

Abstract
Trefftz methods are numerical methods for the approximation of solutions to boundary and/or initial value problems. They are Galerkin methods with particular test and trial functions, which solve locally the governing partial differential equation (PDE). This property is called the Trefftz property. Quasi-Trefftz methods were introduced to leverage the advantages of Trefftz methods for problems governed by variable coefficient PDEs, by relaxing the Trefftz property into a so-called quasi-Trefftz property: test and trial functions are not exact solutions but rather local approximate solutions to the governing PDE.

In this presentation we will tackle the question of the definition, construction and approximation properties of three families of quasi-Trefftz functions for 3D scalar PDEs: two based on generalizations on plane wave solutions, and one polynomial.

Keywords: quasi-Trefftz bases, best approximation properties

1 Introduction
In the general context of wave propagation, the application of Trefftz methods in their standard form to problems of propagation through inhomogeneous media is limited since exact solutions are not known for most variable-coefficient equations. Quasi-Trefftz methods, relying on approximate solutions - called quasi-Trefftz functions - rather than exact solutions to the governing equation, were introduced to extend Trefftz methods to problems governed by variable-coefficient equations. They were first introduced in [3] under the name of Generalized Plane Wave (GPW) methods for 2D problems governed by the Helmholtz equation and their approximation properties were studied in [1]. The original idea behind the GPW concept was to retain the oscillating behavior of a plane wave (PW) while allowing for some extra degrees of freedom to be adapted to the varying PDE coefficient, and this is where their name came from. Initially this was performed via the introduction of Higher Order Terms (HOT) in the phase of a PW as follows:

\[
\begin{align*}
\quad \left\{ \begin{array}{l}
\phi(x) = \exp(i\hat{k} \cdot x + \text{HOT}) \\
[-\Delta - \kappa^2\epsilon(x)] \phi(x) \approx 0,
\end{array} \right. \\
\text{instead of:} \\
\quad \left\{ \begin{array}{l}
\phi(x) = \exp(ik \cdot x) \\
[-\Delta - \kappa^2] \phi = 0, \quad \forall \text{ unit vector } k \in \mathbb{R}^3,
\end{array} \right.
\end{align*}
\]

where \( \kappa \) is the wavenumber of the PW while \( \hat{k} \) can be interpreted as the local wavenumber of the GPW. Moreover the quasi-Trefftz property (being an approximated solution to the governing PDE) was defined as a local property thanks to Taylor expansion: given a desired order \( q \) and a point \( x_C \), a quasi-Trefftz function is a function \( \phi \) satisfying: \( \forall x \in \mathbb{R}^2 \) near \( x_C \),

\[
[-\Delta - \kappa^2\epsilon(x)] \phi(x) = O(||x - x_C||^q)
\]

This presentation, based on [5], focuses on three types of quasi-Trefftz functions for a set of second order PDEs in 3D including the convected Helmholtz equation.

2 Three families of quasi-Trefftz functions
Inspired by classical PWs \( \exp \Lambda \cdot (x - x_C) \), we will focus on three different families of quasi-Trefftz functions:

- phase-based GPWs, following the original ansatz proposed in [3] via the introduction of higher order terms in the phase of a PW, see (1),
- amplitude-based GPWs, following the ansatz proposed in [2] via the introduction of higher order terms in the amplitude of a PW,
- purely polynomial quasi-Trefftz functions, which so far we have only used for time-dependent wave propagation in [4].
Each of these is uniquely defined by a polynomial, either the phase polynomial, the amplitude polynomial, or the function itself in the polynomial case. Constructing such functions is then equivalent to constructing these polynomials, while imposing the quasi-Trefftz property yields a system whose unknowns are these polynomial’s coefficients. In each case a careful study of the corresponding system leads to the derivation of an algorithm to construct quasi-Trefftz function relying only on explicit formulas. Hence, on the one hand the existence of quasi-Trefftz functions is guaranteed for each of the three families, and on the other hand the computational cost for their construction is limited.

We will describe these algorithms, emphasizing the common structure that relies on the second order derivatives in the governing PDE.

3 Local approximation properties of quasi-Trefftz spaces

Both Trefftz and quasi-Trefftz spaces depend on the governing PDE. When comparing approximation properties of Trefftz spaces with standard polynomial spaces, there are two important differences: (1) to reach a given (high) order of approximation, Trefftz spaces require less degrees of freedom than polynomial spaces, (2) Trefftz spaces have high order approximation properties (as polynomial spaces) but only to approximate solutions to the governing PDE. The situation is the same for Quasi-Trefftz spaces, and their approximation properties can be expressed as follows.

**Theorem 1** Consider a desired order of approximation $n \in \mathbb{N}$, a point $x_C \in \mathbb{R}^3$, and a second order partial differential operator $\mathcal{L}_C$ (see [5] for precise hypothesis). Consider three quasi-Trefftz spaces associated to partial differential operator $\mathcal{L}_C$, defined as the spaces spanned by each of the three following sets:

- the set of amplitude-based GPWs,
- the set of phase-based GPWs,
- the set of polynomial functions,

each of them constructed with $q = \max(n-1, 1)$ and $p = (n + 1)^2$ functions. Then there exist a choice of functions such that any of these three spaces, denoted $\Psi_h^G$, satisfies the following approximation property:

$$\forall x \in C^{\max(2, n)}(\Omega) \text{ satisfying } \mathcal{L}_C u = 0, \exists u_a \in \Psi_h^G, \exists C \in \mathbb{R} \text{ s.t. } \forall x \in \Omega, |u(x) - u_a(x)| \leq C \|x - x_C\|^{n+1},$$

(2)

The constant $C$ here depends on the domain $\Omega$, on the desired order $n$, on the PDE solution $u$ to be approximated, as well as on the PDE coefficients $c$.

We will highlight the most important steps of the theorem’s proof, emphasizing the crucial role played by free parameters introduced in the construction algorithms to (i) construct a family of linearly independent quasi-Trefftz functions, and (ii) leverage the explicit formulas from the algorithms.

References


Iterative Trefftz Method For Three-dimensional Electromagnetic Waves Simulation.

Sébastien Pernet, Margot Sirdey, Sébastien Tordeux

1ONERA, Toulouse, France  
2INRIA - EPC MAKUTU, ONERA, E2S UPPA, CNRS  
3INRIA - EPC MAKUTU, Pau, France  

*Email: margot.sirdey@inria.fr

Abstract

The simulation of time-harmonic electromagnetic waves requires a matrix inversion whose cost, especially in three-dimensional cases, increases quickly with the size of the computational domain. This is a major issue regarding memory consumption. Iterative Trefftz methods [3] can overcome this problem when resorting to a GMRES type solver [2]. They can simulate electromagnetic waves in large domains by avoiding the storage of the LU factorization of the matrix.

Keywords: Trefftz method, Electromagnetic waves, Domain Decomposition

1 Maxwell problem

The studied adimensional Maxwell problem is

\[
\begin{align*}
\nabla \times \mathbf{H} &= ik \mathbf{E}, \\
\nabla \times \mathbf{E} &= -ik \mathbf{H},
\end{align*}
\]

on \( \Omega \), (1)

where \( \Omega \subset \mathbb{R}^3 \), \( k \) is the wavenumber, \( \mathbf{E} \) and \( \mathbf{H} \) are respectively the three-dimensional electric and magnetic fields. We impose an impedance boundary condition, see (3), on the boundary of the domain, denoted by \( \partial \Omega \).

The domain \( \Omega \) is meshed into a set of elements \( T \). It is also decomposed into a set of interior faces \( F_{\text{int}} \) and a set of exterior faces \( F_{\text{ext}} \). We define in each element \( T \in T \) the electromagnetic field \( \mathbf{E}^T := (\mathbf{E}^T, \mathbf{H}^T) \) whose tangential electric and magnetic traces are defined as \( \gamma_d \mathbf{E}^T = (\mathbf{n}_T \times \mathbf{E}^T) \times \mathbf{n}_T \) and \( \gamma_d \mathbf{H}^T = \mathbf{n}_T \times \mathbf{H}^T \), with \( \mathbf{n}_T \) the outward unit normal to \( T \).

2 Ultra-Weak Variational Formulation

Cessenat and Després developed in [1] the Ultra-Weak Variational Formulation (UWVF) method based on incoming and outgoing trace operators respectively defined as following

\[
\begin{align*}
\gamma_{\text{in}} \mathbf{E}^T &= \gamma_i \mathbf{E}^T + \gamma_s \mathbf{H}^T, \\
\gamma_{\text{out}} \mathbf{E}^T &= \gamma_i \mathbf{E}^T - \gamma_s \mathbf{H}^T.
\end{align*}
\]

The boundary condition can be written as

\[
\gamma_{\text{in}} \mathbf{E}^T = R \gamma_{\text{out}} \mathbf{E}^T + \mathbf{f} \quad \text{on} \quad \partial \Omega \cap \partial T, \quad (3)
\]

with \( \mathbf{f} \in L^2(\partial \Omega) \) a tangential field and \( R \) the reflexion coefficient.

A Trefftz method is defined by a Trefftz space \( \mathbb{X}_T \) and an ultra-weak energy conservation property. The Trefftz space is made of local solutions of (1) which are taken as analytical [3] plane waves [4] in our work. The energy property is given by

\[
\sum_{T \in \mathcal{T}} \int_{\partial T} \gamma_{\text{out}} \mathbf{E}^T \cdot \gamma_{\text{out}} \mathbf{E}^T = \sum_{T \in \mathcal{T}} \int_{\partial T} \gamma_{\text{in}} \mathbf{E}^T \cdot \gamma_{\text{in}} \mathbf{E}^T.
\]

Hence, the UWVF is Find \( \mathbf{E} \in \mathbb{X}_T \) such that

\[
a(\mathbf{E}, \mathbf{E}') = \ell(\mathbf{E}') \quad \forall \mathbf{E}' \in \mathbb{X}_T, \quad (4)
\]

where

\[
\begin{align*}
a(\mathbf{E}, \mathbf{E}') &= \sum_{T \in \mathcal{T}} (a^T(\mathbf{E}, \mathbf{E}') - b^T(\mathbf{E}, \mathbf{E}')), \\
a^T(\mathbf{E}, \mathbf{E}') &= \int_{\partial T} \gamma_{\text{out}} \mathbf{E}^T \cdot \gamma_{\text{out}} \mathbf{E}'^T, \\
b^T(\mathbf{E}, \mathbf{E}') &= \int_{\partial T} \gamma_{\text{in}} \mathbf{E}^T \cdot \gamma_{\text{in}} \mathbf{E}'^T, \\
\ell(\mathbf{E}') &= \sum_{T \in \mathcal{T}} \int_{\partial T \cap \partial \Omega} \mathbf{f} \cdot \gamma_{\text{in}} \mathbf{E}'^T.
\end{align*}
\]

The numerical flux \( \gamma_{\text{in}} \mathbf{E}^T \) ensures the consistency of the method. It imposes the continuity on interior faces and the impedance boundary condition (3) on exterior faces

\[
\gamma_{\text{in}} \mathbf{E}^T = \begin{cases}
\gamma_{\text{K}} \mathbf{E}^K & \text{on} \quad \partial T \cap \partial K \in F_{\text{int}}, \\
R \gamma_{\text{out}} \mathbf{E}^T & \text{on} \quad \partial \Omega \cap \partial T \in F_{\text{ext}}.
\end{cases}
\]

3 Iterative Trefftz method

Problem (4) is written into the matricial form

\[
(M + N)X = F, \quad (6)
\]
where $M$ is the matrix associated to (5b), $N$ is the matrix associated to (5c) and $F$ is the vector associated to (5d). Classically, (6) is solved by the Cessenat and Desprès fixed point algorithm

$$X^{n+1} = M^{-1}NX^n + F, \quad X^0 = 0, \quad (7)$$

which converges since $M^{-1}N$ is contractant, see Fig. 1 and [1]. However, eigenvalues close to the unit circle tend to slow down the convergence. A GMRES solver [2] performs better but still has difficulties to deal with small eigenvalues (in red in Fig. 1). Consequently, a new global pre-conditioner has been developed to accelerate the convergence of the iterative process, see Fig. 1.

Another major issue of UWVF method is related to rounding errors. The matrix $M^{-1}N$ is ill-conditioned since the plane waves Galerkin basis functions are numerically linearly-dependant. We present a new basis reduction inspired from [4] improving the local conditioning. Indeed, when considering 196 plane waves for a domain with size $\lambda$ and a mesh of size $h = \frac{\lambda}{4}$, the sparse solver MUMPS can even not invert the matrix without reduction due to a poor conditioning. When lurching the GMRES solver, the improvement when using reduction is clear, see Fig. 2. It leads to a robust iterative method and to a computational cost reduction.

4 Numerical results

In the presentation, we will focus on the memory cost, used to compute the numerical solution of (1), for different numerical methods when the domain size increases with respect to the wavelength $\lambda$, see Fig. 3. Namely, we will compare a Low and High Order Nédélec Finite Elements method, a LU Trefftz method and a GMRES Trefftz method using Cessenat and Desprès decomposition. These numerical results clearly show the potential of such iterative method.

Figure 1: Cessenat and Desprès preconditioner (left) and global preconditioner (right).

Figure 2: Conditioning gain when using reduction in GMRES solver for $\lambda = 1$ and $h = 0.25$.

Figure 3: Memory cost for solving (1) for different methods with 1% accuracy error.

References


Stable approximation of Helmholtz solutions with evanescent plane waves

Emile Parolin$^{1,*}$, Daan Huybrechs$^2$, Andrea Moiola$^1$

$^1$Università degli studi di Pavia, Pavia, Italy
$^2$KU Leuven, Leuven, Belgium

$^*$Email: emile.parolin@unipv.it

Abstract
Helmholtz solutions are known to be well approximated by a suitable finite superposition of (propagative) plane waves, leading to successful Trefftz methods. Yet, when too many plane waves are used, the computation of the approximation is known to be numerically unstable. This comes from the presence of (exponentially) large coefficients in the expansion.

We show that any Helmholtz solution on a disk can be exactly represented by a continuous superposition of plane waves, provided that evanescent ones (with a complex-valued propagation direction) are included. This generalizes the standard Herglotz representation. Besides, the operator mapping the Helmholtz solution to its extended Herglotz density is invertible and continuous. While the result holds at the continuous level, such a property paves the way for accurate discrete approximation expansions that are moreover stable.

Keywords: Helmholtz equation, Evanescent plane waves, Stable approximation

1 Introduction
We consider the numerical approximation of solutions $u$ of the homogeneous Helmholtz equation $-\Delta u - \kappa^2 u = 0$ with wavenumber $\kappa > 0$. As a model problem, the domain of propagation is the unit disk $B_1$.

A well-studied way to represent Helmholtz solutions is to approximate them with linear combinations of propagative plane waves (PPW) $x \mapsto e^{i\mathbf{d} \cdot \mathbf{x}}$, for different propagation directions $\mathbf{d}(\varphi) := (\cos \varphi, \sin \varphi) \in \mathbb{R}^2$ parametrized by the angle $\varphi \in [0, 2\pi]$. The main reason is that PPW offer better accuracy for less degrees of freedom in comparison to polynomial spaces and their simple exponential expressions allow very cheap implementations, in comparison to other particular solutions [3]. In 2D, isotropic approximations are obtained by using equispaced angles: for some $M \in \mathbb{N}$, $\varphi_m := \frac{2\pi m}{M}$, $1 \leq m \leq M$.

Explicit $hp$-estimates in suitable Sobolev semi-norms are available for general domains ensuring exponential convergence (with respect to the number of PPW used) of the approximation of homogeneous Helmholtz solutions [3, §3.2]. Therefore, at least in principle, PPW are well-suited for Trefftz approximations.

2 Propagative plane waves are unstable
The computation of PPW expansions is known to be numerically unstable when increasing the size of the approximation space [3, §4.3] and this is perhaps the main reason that prevented a widespread use of plane-wave based Trefftz schemes. The issue is often understood as an effect of the ill-conditioning of the underlying linear system, which necessarily arises from the almost linear dependence of propagative plane waves with similar directions of propagation. Some recent advances [1] in the general setting of Frame Theory have demonstrated that ill-conditioning arising from such redundancy can be successfully overcome using regularization techniques, provided (this is the key point) there exist accurate approximations in the form of expansions with bounded coefficients. It turns out that PPW approximations with bounded coefficients do not always exist.

To explain this, let us introduce the circular waves $b_p(x) := \beta_p J_p(\kappa r) e^{ip \theta}$, for $x = (r, \theta) \in B_1$ and $p \in \mathbb{Z}$, which are the bounded solutions that are separable in polar coordinates. The normalization coefficients $\beta_p$, computed e.g. for a $H^1(B_1)$-norm, grow super-exponentially with $|p|$ and allow to make the family $\{b_p\}_p$ a Hilbert basis for the space of Helmholtz solutions in the unit disk. It can be shown that an approximation $\tilde{b}_p$ of $b_p$ consisting in a finite sum of PPW with a vector of coefficients denoted $\mu$, that is accurate, namely $\|b_p - \tilde{b}_p\| \leq \eta$ for some tolerance $1 \geq \eta > 0$, has necessarily coefficients that satisfy $\|\mu\|_{L^1} \geq (1 - \eta)\beta_p$. Owing to the super-exponential growth of $\beta_p$ with $|p|$, this is a clear example of how accuracy and stability...
properties (in the sense of bounded coefficients) are sometimes mutually exclusive.

This issue can be understood (and proved) from the Jacobi–Anger identity: for any \( x \in B_1 \) and \( \varphi \in [0, 2\pi) \),

\[
e^{i\varphi \cdot \beta} = \sum_{p \in \mathbb{Z}} (p^e - i \varphi \cdot \beta_p^{-1}) b_p(x).
\]

The modulus of the coefficients in the above modal expansion as a function of \( p \) is reported in Figure 1 (case \( \zeta = 0 \)). This quantity, which is independent of \( \varphi \), decays super-exponentially away from the ‘propagative’ modes \( |p| \leq \kappa \). The direct implication is that PPW superpositions need cancellation (i.e. subtraction of values numerically close to each other) and large coefficients to approximate Helmholtz solutions with a high-frequency modal content (large \( |p| \)).

![Figure 1: Modulus of the coefficients of the modal expansion in the basis \( \{b_p\}_{p \in \mathbb{Z}} \) of various plane waves for \( \kappa = 16 \).](image)

### 3 Evanescent plane waves

To obtain accurate expansions with bounded coefficients, we enrich the PPW set with some evanescent plane waves (EPW), a technique already used in the Wave Based Method [3]. EPW are characterized by complex-valued direction vector \( \mathbf{d}(\varphi, \zeta) := (\cos(\varphi + i\zeta), \sin(\varphi + i\zeta)) \in \mathbb{C}^2 \), where we introduced the evanescence parameter \( \zeta \in \mathbb{R} \). The Helmholtz equation is still satisfied since \( \mathbf{d} \cdot \mathbf{d} = 1 \). The Jacobi–Anger expansion (1) extends to complex \( \mathbf{d} \): for any \( x \in B_1 \) and \( (\varphi, \zeta) \in [0, 2\pi) \times \mathbb{R} \),

\[
e^{i\varphi \cdot \beta} = \sum_{p \in \mathbb{Z}} (p^e - i \varphi \cdot \beta_p^{-1}) b_p(x).
\]

The modulus of the coefficients in the above modal expansion are reported (with a convenient normalization depending only on \( \zeta \)) in Figure 1 as a function of \( p \). We see that by tuning the evanescence parameter \( \zeta \) we are able to shift the modal content of the plane waves to higher frequency regimes. As a result, we expect the EPW to be able to capture well the high-frequency modes of Helmholtz solutions.

The main theoretical result that highlights the benefit of EPW is the following.

**Theorem 1** Let \( w(\zeta) := e^{-\kappa \sin \| \zeta \| / 4} \). For any Helmholtz solution \( u \) in the unit disk there exists a unique Herglotz density \( v \) that belongs to a proper subspace of the \( w^2 \)-weighted \( L^2 \)-space on \([0, 2\pi) \times \mathbb{R} \) such that: for any \( x \in B_1 \),

\[
u(x) = \int_{-\infty}^{+\infty} \int_{0}^{2\pi} v(\varphi, \zeta) e^{i\varphi \cdot \beta} \times w^2(\zeta) d\varphi d\zeta.
\]

Moreover, the operator that maps \( u \) to \( v \) is invertible and continuous.

This integral representation (that uses EPW) can be seen as a generalization of the classical Herglotz representation (that uses only PPW). While only very regular Helmholtz solutions admit a standard Herglotz representation (with density in \( L^2([0, 2\pi]) \)), the generalized Herglotz representation of Theorem 1 holds for any solution. The price to pay for this result is the need for a two-dimensional parameter domain in place of a one-dimensional one. In view of practical implementations, the difficulty is then to construct discrete counterparts of such continuous representations. We propose a procedure to construct suitable finite sets of EPW, that are reasonable in size, using sampling strategies in the parametric domain [2]. Numerical evidence shows that the resulting discrete expansions are both controllably accurate and with bounded coefficients, hence numerically stable. The proof of Theorem 1 and more details can be found in arXiv:2202.05658. The extension to other geometries is challenging and ongoing.

### References


A Hausdorff-measure boundary element method for scattering by fractal screens

I: Numerical Analysis

A. M. Caetano¹, S. N. Chandler-Wilde²*, A. Gibbs³, D. P. Hewett³, A. Moiola⁴
¹Departamento de Matemática, Universidade de Aveiro, Aveiro, Portugal
²Department of Mathematics and Statistics, University of Reading, Reading, UK
³Department of Mathematics, University College London, London, United Kingdom
⁴Dipartimento di Matematica “F. Casorati”, Università degli studi di Pavia, Pavia, Italy
*Email: s.n.chandler-wilde@reading.ac.uk

Abstract

Sound-soft fractal screens can scatter acoustic waves even when they have zero surface measure. To solve such problems we make what appears to be the first application of the boundary element method (BEM) where each BEM basis function is supported in a fractal set, and the integration is with respect to a Hausdorff measure rather than (Lebesgue) surface measure. We prove convergence rates for the Galerkin version of this “Hausdorff BEM” when the scatterer is a flat screen that is the attractor of an iterated function system. 2D numerical experiments confirm the sharpness of our theory.

Keywords: BEM, fractal, scattering

1 Introduction

Scattering in \( \mathbb{R}^{n+1} \) \( (n = 1 \text{ or } 2) \) by an infinitesimally thin flat screen \( \Gamma \) that is a bounded subset of \( \mathbb{R}^n \times \{0\} \) is a classical wave scattering problem, but usually \( \Gamma \) is assumed to be a relatively open subset of the hyperplane \( \Gamma_\infty := \mathbb{R}^n \times \{0\} \) that is Lipschitz or smoother. The study of screens that have a fractal structure is relevant in both naturally-occurring and engineered contexts. Recently it has been shown [1], for the time harmonic acoustic case, that well-posed boundary value problems (BVPs) and associated boundary integral equations (BIEs) can be formulated without any constraint on the geometry of \( \Gamma \), in particular when \( \Gamma \) is fractal with fractal dimension \( d < n \) and so has zero surface measure. In the case of sound-soft boundary conditions such screens are still visible to (i.e. scatter) acoustic waves if they have Hausdorff dimension \( d > n - 1 \) [1].

A natural methodology for numerical computation of scattering by a fractal screen \( \Gamma \) is to approximate \( \Gamma \) by a sequence of prefractal screens \( \Gamma_\ell \) which converge to \( \Gamma \) and which each have positive surface measure so that standard BEM can be applied. Conditions on the sequence \( \Gamma_\ell \) and on the BEM meshsize \( h_\ell \) on \( \Gamma_\ell \) that ensure convergence have recently been established in [2]. However, the Mosco convergence arguments in [2] do not lead to convergence rates.

In this talk we take a different approach which applies in the special case that \( \Gamma \) is a \( d \)-set for some \( d \in (n - 1, n) \). (For the definition see, e.g., [2], but roughly speaking this means that every part of \( \Gamma \) has finite positive \( d \)-Hausdorff measure and Hausdorff dimension that is precisely \( d \); if \( \Gamma \) is a Lipschitz domain it is a \( d \)-set with \( d = n \).) This approach is to use a Galerkin BEM with an approximation space that consists of piecewise constants restricted to finite elements of \( \Gamma \).

2 The fractal geometry, scattering problem, and boundary integral equation

Identifying \( \Gamma_\infty \) with \( \mathbb{R}^n \), consider the case when \( \Gamma \subset \Gamma_\infty \cong \mathbb{R}^n \) is the attractor of an iterated function system (IFS) of contracting similarities \( \{s_1, s_2, \ldots, s_M\} \), for some \( M \geq 2 \), that satisfies the standard open set condition [3]. Then \( \Gamma \) is a \( d \)-set, for some \( d \in (0, n] \). We assume throughout that \( d \) lies in the interesting range \( (n - 1, n) \).

The sound-soft scattering problem we wish to solve is: given an incident plane wave \( u' \), find \( u \in \dot{H}^1_{\text{loc}}(\mathbb{R}^{n+1} \setminus \Gamma) \) (the total field) such that 

$$
\Delta u + k^2 u = 0 \text{ in } \mathbb{R}^{n+1} \setminus \Gamma,
$$

and \( u^s := u - u' \) (the scattered field) satisfies the standard Sommerfeld radiation condition. By standard arguments this problem is well-posed. Moreover [1] \( u = -S\phi \), where \( S\phi \) is a single-layer potential with density \( \phi \in H^{-1/2}_\Gamma := \{ \psi \in H^{-1/2}(\Gamma_\infty) : \text{supp}(\psi) \subset \Gamma \} \) and \( \phi \) satisfies the boundary integral equation

$$
S\phi = Pu'\mid_{\Gamma_\infty},
$$

(1)
where $S : H_{Γ}^{-1/2} \to (H_{Γ}^{-1/2})^*$ is the single-layer potential operator, $(H_{Γ}^{-1/2})^*$ is a realisation of the dual space of $H_{Γ}^{-1/2}$ as a closed subspace of $H^{1/2}(Γ_∞)$, and $P$ is orthogonal projection onto that subspace.

Let $L_2(Γ)$ be the Hilbert space of functions on $Γ$ that are square-integrable with respect to $d$-dimensional Hausdorff measure restricted to $Γ$. A key result is that the trace operator $\text{tr}_Γ : C_0^∞(Γ_∞) \to C(Γ)$ extends to a continuous operator $H^s(Γ_∞) \to L_2(Γ)$ for $s > (n - d)/2$ (in particular for $s = 1/2$) with adjoint $\text{tr}_Γ^* : L_2(Γ) \to H^{-s}(Γ_∞)$ whose action is given, for $ψ ∈ L_2(Γ)$ and $φ ∈ H^s(Γ_∞)$, explicitly by

$$\langle \text{tr}_Γ^* ψ, φ \rangle_{H^{-s}(Γ_∞) \times H^s(Γ_∞)} = \int_Γ χ(x) dH^d(x) \chi(y) dH^d(y) = \int_Γ u(x) dH^d,$$

that satisfies $\langle \text{tr}_Γ^* ψ, φ \rangle_{H^{-s}(Γ_∞) \times H^s(Γ_∞)} = \int_Γ ψ(x) dH^d(x) φ(x) dH^d(x)$, as an integral with respect to $d$-dimensional Hausdorff measure.

3 The Hausdorff BEM

Let us assume now that each similarity $s_m$ has the same contraction factor $α ∈ (0, 1)$, in which case $d = \log(1/M)/\log(α)$, and that $Γ$ is disjoint, meaning that $s_m(Γ) \cap s_{m'}(Γ) = \emptyset$, for $m \neq m'$. $Γ$ is the unique non-empty compact set satisfying $Γ = \bigcup_{m=1}^M s_m(Γ)$. Given $ℓ ∈ \mathbb{N}$, divide $Γ$ up into $M^ℓ$ disjoint congruent components $T$, each given by $T = s_{m_1} \circ s_{m_2} \circ \cdots \circ s_{m_ℓ}(Γ)$, for some integer sequence $(m_1, \ldots, m_ℓ) ∈ \{1, \ldots, M\}^ℓ$, and let $V_ℓ$ denote the subspace of $L_2(Γ)$ consisting of those functions that are constant on each $T$. Let $V_0$ denote the subspace of $L_2(Γ)$ consisting of functions constant on $Γ$. Thus, for $ℓ ∈ \mathbb{N}_0 = \mathbb{N} \cup \{0\}$, $V_ℓ$ is finite-dimensional with dimension $N = M^ℓ$. For $ℓ ∈ \mathbb{N}_0$, let $V_ℓ := \text{tr}_Γ^* (V_ℓ) \subset H_{Γ}^{-1/2}$, and let $φ_ℓ ∈ V_ℓ$ denote the Galerkin solution of (1), given explicitly by $φ_ℓ = \text{tr}_Γ^* ψ_ℓ$ where $ψ_ℓ ∈ V_ℓ$ satisfies

$$\int_Γ \int_Γ Φ(x, y) ψ_ℓ(y) χ(x) dH^d(x) H^d(y) = \int_Γ u(x) χ dH^d,$$

for all $χ ∈ V_ℓ$, where $Φ(x, y)$, the kernel of $S$, is the fundamental solution of the Helmholtz equation. We can show the following theorem:

**Theorem 1** For each $ℓ ∈ \mathbb{N}_0$ the Galerkin solution $φ_ℓ ∈ V_ℓ$ is well-defined and satisfies, for some constant $c > 0$ independent of $ℓ$ and $φ$, that

$$\|φ - φ_ℓ\|_{H_{Γ}^{-1/2}} \leq c(ℓ+1/2)\|φ\|_{H_{Γ}^s},$$

if $φ ∈ H_{Γ}^s$ for some $-1/2 < s < -(n - d)/2$.

If, as we conjecture, $φ ∈ H_{Γ}^s$ for all $s < -(n - d)/2$, then this estimate implies, in the 2D case ($n = 1$) that, for every $ε > 0$, $\|φ - φ_ℓ\|_{H_{Γ}^{-1/2}} = O(M^{-ℓ/2}) = O(N^{ε/ℓ-1/2})$ as $ℓ \to ∞$. This convergence rate (with $ε = 0$) is observed in Figure 1 in which $n = 1$, $M = 2$, $s_1(t) = αt$, $s_2(t) = 1 - α + αt$, for $ℓ ∈ Γ_∞ \cong \mathbb{R}$, with $α ∈ (0, 1/2)$, so that $Γ$ is a Cantor set.

**References**


A Hausdorff-Measure Boundary Element Method for Scattering by Fractal Screens II: Numerical Quadrature

Andrew Gibbs\textsuperscript{1,*}, David Hewett\textsuperscript{1}, Andrea Moiola\textsuperscript{2}

\textsuperscript{1}Department of Mathematics, University College London, UK
\textsuperscript{2}Dipartimento di Matematica, Università degli Studi di Pavia, Italy

*Email: andrew.gibbs@ucl.ac.uk

Abstract

In a related talk [1], the Boundary Element Method (BEM) is generalised to the case of scattering by fractal obstacles. Implementation requires evaluating integrals of singular Green’s kernels over fractal domains, with respect to Hausdorff measure. This motivated the development of new quadrature rules, which are discussed here.

Keywords: Quadrature, BEM, Fractals

1 Introduction

We will study numerical quadrature rules for the evaluation of integrals of the form

\[ I_{\Gamma,\Gamma'}[\Phi] := \int_{\Gamma'} \int_{\Gamma} \Phi(x,y)d\mathcal{H}^d(y)d\mathcal{H}^d(x), \quad (1) \]

where \( \Gamma \) and \( \Gamma' \) are compact subsets of \( \mathbb{R}^2 \) of Hausdorff dimension \( d > 0 \) and \( d' > 0 \) respectively, \( \mathcal{H}^d \) and \( \mathcal{H}^{d'} \) are the corresponding Hausdorff measures, and \( \Phi(x,y) = \frac{\Phi(x-y)}{x-y} \) is the fundamental solution for the Helmholtz equation with wavenumber \( k > 0 \) in \( \mathbb{R}^3 \). (In what follows, similar results hold for the analogous problem posed in \( \mathbb{R}^d \).

Our motivation for approximating (1) is the Hausdorff BEM, which is introduced and analysed in the talk [1]. Such BEMs can model scattering by planar screens with non-integer (fractal) dimension, i.e. \( d \in (1, 2) \).

2 Attractors of Iterated Function Systems

Now we describe in detail the class of fractal scatterers that we consider. An iterated function system (IFS) is a set of \( 2 \leq M \in \mathbb{N} \) contracting similarities \( s_m(x) = \rho_m A_m x + \delta_m \), with contraction factors \( \rho_m \in (0,1) \), rotation matrices \( A_m \in \mathbb{R}^{n \times n} \) and translations \( \delta_m \in \mathbb{R}^n \), for \( m = 1, \ldots, M \). Saying that \( \Gamma \) is the attractor of the IFS means that \( \Gamma \) is the unique non-empty compact set satisfying \( \Gamma = s(\Gamma) \), where \( s(E) := \bigcup_{m=1}^{M} s_m(E), \quad E \subset \mathbb{R}^n \).

Our quadrature rules are based on splitting \( \Gamma \) into sub-components, using the IFS structure.

To describe these sub-components we adopt vector index notation. For \( \ell \in \mathbb{N} \) let \( I_{\ell} := \{1, \ldots, M\}^\ell \). Then for \( E \subset \mathbb{R}^n \) let \( E_0 := E \), and for \( m = (m_1, \ldots, m_{\ell}) \in I_{\ell} \) define \( E_m := s_m(E) \) and \( s_m := s_{m_1} \circ \cdots \circ s_{m_{\ell}} \). For an illustration of this notation in the case of the middle-third Cantor dust see Figure 1. We say \( \Gamma \) is \textit{hull-disjoint} if

\[ \mathcal{R} := \min_{m \neq m'} \{ \text{dist}(\text{Hull}(\Gamma_m), \text{Hull}(\Gamma_{m'})) \} > 0. \]

A key ingredient is the set of vector indices

\[ L_h(\Gamma) := \{m = (m_1, \ldots, m_{\ell}) \in \bigcup_{\ell \in \mathbb{N}} I_{\ell} : \text{diam}(\Gamma_m) \leq h \text{ and } \text{diam}(\Gamma_{(m_1, \ldots, m_{\ell-1})}) > h \}. \]

Heuristically, these indices correspond to a partition of \( \Gamma \), where we have subdivided \textit{just enough} so that all components have diameter no more than \( h \). This is depicted in Figure 2.

3 The barycentre rule

We define the barycentre rule for double integrals:

\[ Q_{\Gamma,\Gamma'}^{\mathcal{H}}[f] := \sum_{m \in L_h(\Gamma)} \sum_{m' \in L_h(\Gamma')} w_m w_{m'} f(x_m, x_{m'}), \quad (2) \]
where the weights and nodes are given by $w_m := \mathcal{H}^d(\Gamma_m)$ and $x_m := \int_{\Gamma_m} x \, d\mathcal{H}^d(x)/\mathcal{H}^d(\Gamma_m)$ for $m \in L_b(\Gamma)$, with analogous definitions for $\Gamma'$. The weights and nodes can be easily computed in terms of the IFS parameters, see [2, (27-29)]. For the single integral version of (2), see [2, §3.1]. In all estimates that follow, $C$ denotes a constant which depends only on $\Gamma$.

**Theorem 1 (Lipschitz integrands)** [2, Theorem 3.7] If $L_0[f]$ and $L_1[f]$ are the Lipschitz constants of $f$ and $\nabla f$ respectively in $\text{Hull}(\Gamma) \times \text{Hull}(\Gamma')$, then

$$|I_{\Gamma, \Gamma'}[f] - Q^h_{\Gamma, \Gamma'}[f]| \leq CL_p[f]h^{p+1} \quad \text{for } p \in \{0, 1\}.$$ 

A result for non-diagonal entries of Hausdorff BEM matrices follows immediately:

**Corollary 2 (Smooth Galerkin integrals)** [2, Proposition 5.2] If $R := \text{dist}(\text{Hull}(\Gamma), \text{Hull}(\Gamma')) > 0$, then

$$|I_{\Gamma, \Gamma'}[\Phi] - Q^h_{\Gamma, \Gamma'}[\Phi]| \leq C h^2 \frac{1 + (kR)^{n+2}}{R^{n+1}}.$$ 

**5 Approximating (1)**

Noting the decomposition (3), Theorem 3 states that $I_{\Gamma, \Gamma'}[\Phi_\ast]$ can be estimated with $O(h^2)$ error, provided $\Gamma$ is hull-disjoint.

Since $\Phi_\ast \in C^{0,1}(\mathbb{R}^3) \setminus C^{1,1}(\mathbb{R}^3)$, Theorem 1 suggests $|I_{\Gamma, \Gamma'}[\Phi_\ast] - Q^h_{\Gamma, \Gamma'}[\Phi_\ast]| = O(h)$. With further work it can be shown that this is actually $O(h^2)$, when (i) $\Gamma$ is hull-disjoint and (ii) $\rho_0 = \cdots = \rho_M$. Hence using (3) we can approximate $I_{\Gamma, \Gamma'}[\Phi_\ast]$ with $O(h^2)$ accuracy (see [2, §5] for details).

Furthermore, numerical experiments [2, §6] suggest $O(h^2)$ convergence for fractals which violate either or both of the conditions (i)-(ii).

**References**


A new theory for acoustic transmission problems with variable coefficients modeled as stable integral equations

Francesco Florian\(^1\), Ralf Hiptmair\(^2\), Stefan Sauter\(^1\)

\(^1\)Institut für Mathematik, Universität Zürich, Zürich, Switzerland
\(^2\)Seminar für Angewandte Mathematik, ETH Zürich, Zürich, Switzerland

Email: francesco.florian@math.uzh.ch

Abstract

In this paper we consider transmission problems in either the full space or a subset and solve the heterogeneous Helmholtz equation. By using tools from harmonic analysis we construct the layer potentials in an abstract way, so as solution of certain transmission problem, not using a representation via Green’s functions. We derive a formulation as boundary integral equations, which is coercive, self-dual and continuous, hence well posed.

Keywords: Boundary element methods, layer potentials, frequency-domain wave equation

1 Introduction

We consider the domain \( \Omega \subseteq \mathbb{R}^3 \) with (possibly empty) boundary \( \Gamma \); it is partitioned in \( n_\Omega \) subdomains \( \Omega_j, 1 \leq j \leq n_\Omega \). We define the skeleton \( \Sigma := \bigcup_{1 \leq j \leq n_\Omega} \Gamma_j \). We analyze the Helmholtz transmission problem: for \( Re s > 0 \)

\[
\begin{cases}
p^2 s^2 u - \text{div}(A \nabla u) = 0 & \text{in } \Omega_j, 1 \leq j \leq n_\Omega, \\
[u]_{\partial \Omega_j} = 0 & \text{on } \Gamma_j, 1 \leq j \leq n_\Omega, \\
[u]_{N_j} = g_j & \text{on } \Gamma_j, 1 \leq j \leq n_\Omega,
\end{cases}
\]

where \([ \cdot ]_{\partial \Omega_j} \), \([ \cdot ]_{N_j} \) denote the jump and co-normal jump at \( \Gamma_j := \partial \Omega_j \).

For simplicity \( g_j = 0 \), except possibly on some closed boundary \( \Gamma_j \).

We allow for general coefficients \( A, p \), i.e:

\[
A \in L^\infty(\Omega, \mathbb{R}^{3\times3}_{\text{sym}}), \quad p \in L^\infty(\Omega, \mathbb{R});
\]

moreover it is assumed that \( p \) is positive, and \( A \) is uniformly positive definite.

2 Layer Potentials

The layer potentials are defined for each subdomain \( \Omega_j \) separately. They are introduced in an abstract way, by PDE techniques, and not relying on the Green’s function [2].
V_j(s) := \{ \{ S_j(s) \} \}_{D;j},
K_j(s) := \{ \{ D_j(s) \} \}_{D;j},
K'_j(s) := \{ \{ S_j(s) \} \}_{N;j},
W_j(s) := -\{ \{ D_j(s) \} \}_{N;j},

where \( \{ \cdot \}_{D;j} \), \( \{ \cdot \}_{N;j} \) denote the mean of the Dirichlet and Neumann traces.

The Calderón operators are first constructed for a single domain in the usual way:

\[
C_j(s) := \begin{bmatrix}
-K_j(s) & V_j(s) \\
W_j(s) & K'_j(s)
\end{bmatrix} - \frac{1}{2} \text{Id};
\]

they are then collected in the block-diagonal operator \( C(s) := \text{diag}_{1 \leq j \leq n_0} C_j(s) \) having the trace data on the full skeleton as domain.

We incorporate homogeneous transmission conditions into the function space where the solution is sought by using the single trace space. Homogeneous boundary conditions are also incorporated in the function space. Inhomogeneities are treated with suitable offset functions, which modify the right-hand side. We refer to [3, 5] for details.

At this point we are able to prove our main theorem, namely the stability of the sesquilinear form associated to the boundary integral operators.

**Theorem 1.** The operator \( C(s) \) is continuous. Let \( \sigma := \frac{s}{|s|} \), and denote with \( \langle \cdot, \cdot \rangle_X \) the natural scalar product in the product trace space; then the following coercivity estimate holds for all \( \Phi \) in the single trace space which satisfy the homogeneous boundary conditions on \( \Gamma \):

\[
\text{Re} \langle C\Phi, \sigma \Phi \rangle_X \geq C \min \{ 1, |s|^2 \} \frac{\text{Re} s}{|s|} \| \Phi \|_X^2,
\]

for some \( C > 0 \) which does not depend on \( s \).

It follows that the resulting problem in weak form is well-posed [1, 3, 4].

From the implementation point of view the single trace space is enforced by only keeping one pair of traces at each interface, adding the contributions from both domains in order to apply the discretized operator.

4 Conclusions

- We present a general method to transform acoustic transmission problems with mixed boundary conditions to a system of non-local Calderón operators on the skeleton, without relying on the explicit knowledge of the Green’s function. The resulting skeleton operators are coercive, self-dual and continuous.
- If the Green’s function is explicitly known, the Calderón operators admit a representation as skeleton integrals, which allow for a standard discretization by conforming Galerkin BEM.

References


Inverse problem for the Helmholtz equation and singular sources in the divergence form

L. Baratchart\textsuperscript{1}, H. Haddar\textsuperscript{2}, C. Villalobos Guillén\textsuperscript{1,*}
\textsuperscript{1}INRIA d’Université Côte d’Azur, Sophia Antipolis, France
\textsuperscript{2}INRIA Saclay & ENSTA Paris Tech, Palaiseau, France
*Email: cristobal.villalobos-guillen@inria.fr

Abstract
We shall discuss an inverse problem where the underlying model is related to sources generated by currents on an anisotropic layer. This problem is a generalization of another motivated by the recovering of magnetization distribution in a rock sample from outer measurements of the generated static magnetic field. The original problem can be formulated as inverse source problem for the Laplace equation \cite{1,2} with sources \( M \) and \( H \) regularized schemes adapted to these assumptions. We then present some validating experiments and some related open questions.

Keywords: Helmholtz equation, Divergence free, Inverse problems, Magnetization

1 Introduction
Let \( k \geq 0, \Omega \subset \mathbb{R}^3 \) be a bounded Lipschitz domain, \( S \subset \partial \Omega \) be compact, and \( G(x) = \frac{e^{ik|x|}}{4\pi|x|} \), a Green function for the Helmholtz equation. Let \( H^s(\partial \Omega) \) denote the Bessel potential space of order \( s \) and \( H^s(\partial \Omega) \), the space of \( 1 \)-forms on \( \partial \Omega \) with coefficients in \( H^s(\partial \Omega) \).

Given a \( M \in L^2(\partial \Omega)^3 \), with support contained in \( S \), define \( J(M) := G \ast \nabla \cdot (M \sigma) \), where \( \sigma \) denotes the surface measure on \( \partial \Omega \). It follows that \( J(M) \) is analytic on \( \mathbb{R}^3 \setminus S \) and locally integrable. Then, for \( w = J(M) \),

\[ \Delta w + k^2 w = \nabla \cdot (M \sigma). \] (1)

Note that this implies that the kernel of \( J \) consist precisely of all \( M \) such that \( \nabla \cdot (M \sigma) = 0 \). Also, \( w = J(M) \) satisfies the Sommerfeld radiation condition:

\[ \lim_{|x| \to \infty} \frac{1}{|x|} \left( \frac{\partial}{\partial |x|} - ik \right) w(x) = 0. \] (2)

If we let \( \nu \) denote the normal vector to \( \partial \Omega \), we can write \( M = \nu M_\nu + M_T \), with \( M_\nu := M \cdot \nu \) and \( M_T := M - \nu M_\nu \). Note that in this case \( M_T(x) \) is tangent to \( \partial \Omega \) for \( \sigma \)-a.e. \( x \in \partial \Omega \) and we can define tangential divergence \( \nabla_T \cdot M_T \) weakly. We will denote by \( M_T^\nu \) the \( 1 \)-form that is the flat of \( M_T \), i.e., for every \( p \in \partial \Omega \) and \( v \) tangent to \( \partial \Omega \) at \( p \), \( M_T^\nu(p)(v) = M_T(p) \cdot v \).

We will restrict ourselves to the case when \( M_\nu \in H^{1/2}(\partial \Omega) \) and \( \nabla_T \cdot M_T \in H^{-1/2}(\partial \Omega) \). Notice that, if \( M_T^\nu \in H^{1/2}(\partial \Omega) \) then \( \nabla_T \cdot M_T \in H^{1/2}(\partial \Omega) \), we will represent a source as a pair \( (M_T^\nu, M_\nu) \in M := H^{1/2}(\partial \Omega) \times H^{1/2}(\partial \Omega) \) with a slight abuse of notation we will identify \( M \) with the pair \( (M_T^\nu, M_\nu) \), and think of \( M \) as a subspace of \( L^2(\partial \Omega)^3 \).

Let \( SL \) and \( DL \) denote the single and double layer potentials associated to (1). That is, for \( x \in \mathbb{R}^3 \setminus \partial \Omega \), \( \psi \in H^{-1/2}(\partial \Omega) \) and \( \phi \in H^{1/2}(\partial \Omega) \),

\[ SL\psi(x) := \int_{\partial \Omega} G(x - y) \psi(y) d\sigma(y), \]
\[ DL\phi(x) := \int_{\partial \Omega} \partial_{\nu,y} G(x - y) \phi(y) d\sigma(y), \]
where \( \partial_{\nu,y} \) is the normal derivative with respect to the variable \( y \). Then we have that \( J(M) = -DL(M_\nu) + SL(\nabla_T \cdot M_T) \).

The following result shows the limitations for the theoretical inverse problem. Given \( Q \subset \mathbb{R}^3 \setminus S \) compact and a measure \( \rho \) supported on \( Q \), define \( A_Q : M \to L^2(\mathbb{Q}, \rho) \) as \( A_Q(M) = J(M)|_Q \).

\textbf{Theorem 1} Take \( D \) a Lipschitz domain containing \( S \) with unbounded complement, and \( Q \subset \mathbb{R}^3 \setminus S \) compact. If \( \mathbb{R}^3 \setminus S \) is connected and either

1. \( \partial D \) is an analytic surface and \( \overline{Q} \cap \partial D \) has Hausdorff dimension \( > 1 \),
2. or \( \partial D \subset \overline{Q} \),
then, \( M \) belong to the kernel of \( A_Q \) if and only if \( M_\nu = 0 \) and \( \nabla_T \cdot M_T = 0 \).
2 Full Bounded Lipschitz Domain

In what follows we will assume that $S = \partial \Omega$. Let $j(\phi, \psi) = -DL(\phi) + SL(\psi)$, for $(\phi, \psi) \in H^{1/2}(\partial \Omega) \times H^{-1/2}(\partial \Omega)$, and define for $\phi \in H^{1/2}(\partial \Omega)$ and $\psi \in H^{-1/2}(\partial \Omega)$:

$$S\psi(x) := \text{p.v.} \int_{\partial \Omega} G(x - y)\psi(y)d\sigma(y),$$

$$K\phi(x) := \text{p.v.} \int_{\partial \Omega} \delta_{\nu,y}G(x - y)\phi(y)d\sigma(y),$$

$$T\phi := (\partial_\nu D\phi)|_{\partial \Omega}.$$  

Next, let $P_+, P_- : H^{1/2}(\partial \Omega) \times H^{-1/2}(\partial \Omega) \to H^{1/2}(\partial \Omega) \times H^{-1/2}(\partial \Omega)$ be defined by matrix multiplication as

$$P_+(\phi, \psi) := \left( \begin{array}{cc} 1/2 I_d - K & -1/2 I_d + K' \\ -T & 1/2 I_d + K' \end{array} \right) \left( \begin{array}{c} \phi \\ \psi \end{array} \right),$$

$$P_-(\phi, \psi) := \left( \begin{array}{cc} 1/2 I_d + K & 1/2 I_d - K' \\ T & -1/2 I_d - K' \end{array} \right) \left( \begin{array}{c} \phi \\ \psi \end{array} \right).$$

Then $P_+$ and $P_-$ are Calderón projections [4], they satisfy $P_+ P_+ = P_+ I_d - P_-$, and we obtain the following result:

Theorem 2 Let $w = J(M)$. Then, $w|_{\partial \Omega} = 0$ if and only if $P_+(M_{0\nu}, \nabla_T \cdot M_T) = 0$, and $w|_\Omega = 0$ if and only if $P_-(M_{0\nu}, \nabla_T \cdot M_T) = 0$.

3 Decomposition of $M$

Let $\omega \in H^1_{loc}(\mathbb{R}^3 \setminus \Omega)$ satisfy (2) and

$$\Delta \omega + k^2 \omega = 0 \text{ on } \mathbb{R}^3 \setminus \Omega,$$

$$\omega = \left( K + \frac{1}{2} I_d \right) 1_{\partial \Omega} |_{\partial \Omega},$$

where $1_{\partial \Omega}$ is the constant function with value 1 in $\partial \Omega$, and let $f = \overline{\nu} \omega$. Then we can define the following subspaces of $M$:

$${\mathcal M}_0 = \{ M \in \mathcal M : (M_{0\nu}, \nabla_T \cdot M_T) = (0, 0) \},$$

$${\mathcal M}_+ = \{ M \in \mathcal M_0 \cap \mathcal M : P_+(M_{0\nu}, \nabla_T \cdot M_T) = (0, 0) \},$$

$${\mathcal M}_- = \{ M \in \mathcal M_0 \cap \mathcal M : P_-(M_{0\nu}, \nabla_T \cdot M_T) = (0, 0) \},$$

where $\mathcal M_0$ is taken in $L_2(\partial \Omega)^3$. Also, there exists a $\mathcal M_0$ that satisfies for every $M \in H^{1/2}(\partial \Omega)^3$,

$$(M_0, M)_{H^{1/2}(\partial \Omega)} = (f, M \cdot \nu)_{H^{-1/2}(\partial \Omega), H^{1/2}(\partial \Omega)} = \left( \int_{\partial \Omega} \nabla_T \cdot M_T \right)_{H^{1/2}(\partial \Omega), H^{-1/2}(\partial \Omega)},$$

which allows us to define $\mathcal M = \text{vec}(\{ \mathcal M_0 \})$.

Let us observe for instance that when $\Omega$ is a ball then $\mathcal M_0 = c\nu$ where $c$ is a constant.

Theorem 3 $\mathcal M_0, \mathcal M_+ \oplus \mathcal M_- \text{ and } \mathcal M_H$ are pairwise orthogonal as subspaces of $\mathcal M$ and

$$\mathcal M = \mathcal M_0 \oplus \mathcal M_+ \oplus \mathcal M_- \oplus \mathcal M_H.$$  

Furthermore, when $k^2$ is a Neumann eigenvalue for $-\Delta$ in $\Omega$ and the trace of one eigenfunction on $\partial \Omega$ coincides with $1_{\partial \Omega}$, then $\mathcal M_0 = 0$, and hence $\mathcal M = \mathcal M_0 \oplus (\mathcal M_+ + \mathcal M_-)$.

4 Partial inversion of the problem

Using the above decomposition it is now clear that the problem of recovering sources when measurements are only done outside of the sample is only solvable up to an element of $\mathcal M_0 \oplus \mathcal M_+$.

Given an original source $M$, let $\tilde{M}$ denote the unique element of $\mathcal M_+ \oplus \mathcal M_H$ which generates the same potential as $M$ outside of $\Omega$. We will now give a rough description of a way to obtain $\tilde{M}$. Let $Q \subset \mathbb{R}^3 \setminus \Omega$ be such that for every $w \in \mathcal J(\mathcal M)$, $w|_Q = 0$ implies $w|_{\partial \Omega} = 0$ (for example, a dense subset of some type of analytic surface). Since, $\mathcal J(\mathcal M)|_{\partial \Omega} = 0$ implies $P_+(M_{0\nu}, \nabla_T \cdot M_T) = 0$, then the linear operator $B$, defined from $H^{1/2}(\partial \Omega) \times H^{-1/2}(\partial \Omega)$ to $H^{1/2}(\partial \Omega) \times H^{-1/2}(\partial \Omega)$, sends $\tilde{(\phi, \psi)}$ to $(P_-(\phi, \psi), j(\phi, \psi)|_Q)$, is injective. Letting $\omega = \mathcal J(M)$, then $B^{-1}(0, \omega)$ is well defined and such that $P_+(B^{-1}(0, \omega) - (M_{0\nu}, \nabla_T \cdot M_T)) = 0$. Hence, using the definition of $\mathcal M_0$ and the above results, we can recover $\tilde{M}$.

References


A reconstruction method for the inverse gravimetric problem

GERBER-ROTH Anthony$^{1,*}$, MUNNIER Alexandre$^1$, RAMDANI Karim$^1$

$^1$Université de Lorraine, CNRS, Inria, IECL, F-54000 Nancy, France
*$^*$Email: anthony.gerber-roth@univ-lorraine.fr

Abstract
We consider an inverse source problem for the 2D Laplace operator, for sources of the form $\mathbb{1}_\omega$. The reconstruction method is based on the computation of the harmonic moments of $\omega$. Although not directly related to wave propagation, this problem can be used to handle by perturbation techniques source inverse problems for Helmholtz equation at low frequencies, and can possibly be adapted to tackle wave problems by replacing harmonic functions by plane waves.

Keywords: Inverse gravimetric problem, Quadrature domains, Harmonic moments.

1 Problem setting
Let $\omega$ be an open set included in the unit disk and $\Gamma$ be the unit circle. Denote by $U_\omega$ the solution of

$$-\Delta U_\omega = \mathbb{1}_\omega \quad \text{on} \quad \mathbb{R}^2,$$

such that $U_\omega(x) = O(\ln |x|)$ at infinity. The function $U_\omega$ can be thought of as the gravitational field generated by a uniform mass distribution in $\omega$ and is given by the Newtonian potential $U_\omega(x) = (G * \mathbb{1}_\omega)(x) = \int_{\omega} G(x-y)dy$, where $G(x):=-1/2\pi \ln |x|$ is the fundamental solution of the Laplacian in $\mathbb{R}^2$. The inverse problem we are interested in consists in reconstructing $\omega$ from the knowledge of $\nabla U_\omega$ on $\Gamma$.

The problem is known to be ill-posed, as uniqueness is not guaranteed in general. However, under either of the two following properties:

(S) $\omega$ is star-shaped with respect to its center of gravity.

(C) $\omega$ is convex in $x_1$, i.e. the intersection of any straight line parallel to the $x_1$-axis with $\omega$ is an interval.

uniqueness and stability results can be proved (see [4]). More precisely, we have:

Theorem 1 Assume that $\omega_1, \omega_2$ are two domains both satisfying either (S) or (C). If $\nabla U_{\omega_1} = \nabla U_{\omega_2}$ on $\Gamma$, then $\omega_1 = \omega_2$.

In addition, if the domains $\omega_1, \omega_2$ satisfy property (S) and admit a representation of the form $\omega_l = \{r < d_l(\sigma)\}$ (in polar coordinates associated to their centers of gravity), then the following logarithmic-type stability estimate holds:

$$\|d_1 - d_2\|_{L^\infty} \leq \kappa |\ln \varepsilon|^{-1/\kappa} \quad (\kappa > 0),$$

provided $\|\nabla U_{\omega_1} - \nabla U_{\omega_2}\|_{L^\infty(\Gamma)} \leq \varepsilon$.

2 Reconstruction method
From now on, we assume that $\omega$ satisfies property (S). We shall reconstruct $\omega$ by generating a sequence of domains $(\omega_N)_N$ satisfying (S) and such that $\|\nabla (U_{\omega_1} - U_{\omega_N})\|_{L^2(\Gamma)}$ tends to 0.

We first observe that Green’s formula leads to the equality:

$$\int_{\Gamma} \partial_n U_\omega \partial_n v = \int_\omega v,$$ (2)

for all harmonic functions $v$ on the unit disk.

Since the knowledge of $\nabla U_\omega$ on $\Gamma$ allows deducing the values of $U_\omega$ on $\Gamma$ (recall that $U_\omega$ is harmonic outside $\Gamma$), our inverse problem can be rephrased as a shape-from-moments problem:

How to reconstruct a domain $\omega$ from the knowledge of its harmonic moments $\int_\omega z^\ell$? This can be done by choosing a positive integer $N$ and:

(i) computing the weights $c_1, ..., c_N \in \mathbb{C}$ and the nodes $z_1, ..., z_N \in \mathbb{C}$ such that:

$$\forall 0 \leq \ell \leq 2N-1, \quad \int_\omega z^\ell = \sum_{k=1}^N c_k z_k.$$

(ii) constructing a domain $\omega_N$ which actually satisfies these identities for all $\ell \geq 0$ (such a domain does exist and is called a harmonic quadrature domain, as described in the next Section).

As a result we have therefore:

$$\forall 0 \leq \ell \leq 2N-1, \quad \int_\omega z^\ell = \int_{\omega_N} z^\ell,$$

from which we can prove that $\|\nabla (U_\omega - U_{\omega_N})\|_{L^2(\Gamma)} \to 0$ as $N \to +\infty$. 
3 Quadrature domains

A bounded domain \( \Omega \) in the complex plane is called a harmonic quadrature domain if there exists a finite number of weights \((c_k)_{1 \leq k \leq N}\) and nodes \((x_k)_{1 \leq k \leq N}\) in \( \Omega \) such that for all harmonic integrable function \( v \):

\[
\int_{\Omega} v = \sum_{k=1}^{N} c_k v(x_k).
\]

We refer the interested reader to [3] for details on this notion. Unfortunately, in general, a quadrature domain is not uniquely determined by solely the quadrature nodes \( x_k \) and weights \( c_k \).

An important subclass of harmonic quadrature domains, for which this uniqueness is ensured, is that of subharmonic quadrature domains. This class is defined as the domains satisfying \( \int_{\Omega} v \geq \sum_{k=1}^{N} c_k v(x_k) \) for all integrable subharmonic functions \( v \) in \( \Omega \), with \( c_k \geq 0 \). In addition, for a subharmonic quadrature domain \( \Omega \), the function \( U_{\Omega} = G * 1_{\Omega} \) satisfies the following properties:

\[
-\Delta U_{\Omega} \leq 1 \quad \text{in } \mathbb{R}^2 \quad (3a)
\]
\[
U_{\Omega} = U_N \quad \text{in } \mathbb{R}^2 \setminus \Omega \quad (3b)
\]
\[
U_{\Omega} \leq U_N \quad \text{in } \mathbb{R}^2, \quad (3c)
\]

where \( U_N = \sum_{k=1}^{N} c_k G(\cdot - x_k) \). Notice that we can recover \( \Omega \) from \( U_{\Omega} \) since \(-\Delta U_{\Omega} = 1_{\Omega}\).

4 Reconstruction algorithm

We fix some integer \( N \geq 1 \) and:

1. We compute \( \int_{\omega} z^\ell \), for \( 0 \leq \ell \leq 2N - 1 \).
2. We compute \( c_k \in \mathbb{R}^+ \) and \( z_k \in \mathbb{C} \) such that

\[
\forall 0 \leq \ell \leq 2N - 1, \quad \sum_{k=1}^{N} c_k z_k^\ell = \int_{\omega} z^\ell \quad (4)
\]

3. We determine \( \omega_N \), the unique subharmonic quadrature domain \( \Omega \) solving system (3).

The harmonic moments \( \int_{\omega} z^\ell \) are computed from the boundary data using (2). System (4) is solved by Prony’s method (see [2]), while the differential inequality (3) is solved using FEM (see [1]). We can prove the following convergence results.

Theorem 2 If \( \omega \) is a subharmonic quadrature domain, there exists \( N \geq 1 \) such that \( \omega = \omega_N \).

If \( \omega \) is a domain satisfying (S), and if the domains \( \omega_N \) also satisfies property (S), then the sequence \( \omega_N \) converges to \( \omega \) in the sense of (1).

5 Numerical results

We compute \( 1_{\Omega} = -\Delta U_{\Omega} \) using FreeFEM++. Figure 1 shows the results for exact (left) and noisy (right) moments with 3 % noise.

Figure 1: Star-shaped domain with \( N = 16 \).

Figure 2: Domain satisfying (C) with \( N = 18 \).

References


A layer potential approach to functional and clinical brain imaging

Masimba Nemaire$^{1,2,*}$, Paul Asensio$^{2}$, Jean-Michel Badier$^{3}$, Juliette Leblond$^{2}$, Jean-Paul Marmorat$^{4}$

$^{1}$Institut de Mathématiques de Bordeaux, Université de Bordeaux, Talence, France
$^{2}$FACTAS, Inria Sophia Antipolis-Méditerranée, Valbonne, France
$^{3}$Institut de Neurosciences des Systèmes, Aix-Marseille Université, Marseille, France
$^{4}$Center of Applied Mathematics, Ecole des Mines ParisTech, Sophia Antipolis, France

*Email: masimba.nemaire@inria.fr

Abstract
We study the inverse problems of source recovery and cortical mapping for sEEG, EEG and MEG under the quasi-static approximation of Maxwell’s equations. These problems are known to be ill-posed due to the existence of silent source, i.e., those non-zero sources that generate null field. In addition the collected data are corrupted with noise that has to be regularized so to solve the problem. We make use of single and double layer potentials to express the electromagnetic (EM) fields associated with a source which allows to simultaneously solve the source recovery and cortical mapping problems for a particular modality or coupled data. The expression of the electro-magnetic fields we use make the different couplings of sEEG, EEG and MEG data direct and complementary. Numerical results of experiments performed using meshes of realistic head geometries will be presented.

Keywords: Electroencephalography (EEG), stereo-EEG, magnetoencephalography (MEG), inverse problems, brain imaging, cortical mapping

1 Introduction
We model the head as a layered conductor with different electric conductivities between layers which are constant in each layer. These homogeneous layers are the brain, skull and scalp, with the brain subdivided into the grey and white matter regions. Brain activity is modelled as vector-fields (sources) $\mu_0 \in [\mathcal{M}(\Sigma_0)]^3$, $\mathcal{M}(\Sigma_0)$ being a Banach space whose elements are supported on grey/white matter interface, the surface $\Sigma_0$. Let $\Sigma_i$ be the closed surfaces on which the electric conductivity is discontinuous, $\sigma_i^-$ and $\sigma_i^+$ are the electric conductivities inside and outside $\Sigma_i$, respectively, and $\mathcal{H}_i$ is the Hausdorff measure on $\Sigma_i$ then the electric potential associated with $\mu_0$ at $x \in \mathbb{R}^3$ is:

$$\sigma(x) \phi(x) = \frac{1}{4\pi} \int \frac{(x - y) \cdot d\mu_0(y)}{|x - y|^3} - \frac{1}{4\pi} \sum_{i=1}^{n+1} \sigma_i^- - \sigma_i^+ \int_{\Sigma_i} \phi(y) \nu(y) \cdot \frac{(x - y)}{|x - y|^3} d\mathcal{H}_i(y).$$

(1)

The magnetic flux density associated with $\mu_0$ at $x \in \mathbb{R}^3$ is:

$$B(x) = \frac{\mu}{4\pi} \int \frac{(x - y)}{|x - y|^3} \times d\mu_0(y) - \frac{\mu}{4\pi} \sum_{i=1}^{n+1} \sigma_i^- - \sigma_i^+ \int_{\Sigma_i} \nu(y) \times \frac{(x - y)}{|x - y|^3} \phi(y) d\mathcal{H}_i(y),$$

(2)

where the $\phi \in L^2(\Sigma_i)$ are as computed in (1).

2 Inverse Problems
We aim to solve problems of the following form with measurement in $D_1 \subset \mathbb{R}^3$ depending on the modalities:

**Problem 1** Given data $f \in L^2(D_1)$ and parameters $\lambda, \lambda_i > 0$, $i = 1, 2, \ldots, n + 1$, find

$$\arg\inf_{(\mu_0, \phi_1, \phi_2, \ldots, \phi_{n+1}) \in S} T_{f, \lambda}(\mu_0, \phi_1, \phi_2, \ldots, \phi_{n+1}),$$

where

$$T_{f, \lambda} := ||\mathcal{F}_1(\mu_0, \phi_1, \phi_2, \ldots, \phi_{n+1}) - f||_{L^2(D_1)} + \sum_{i=1}^{n+1} \lambda_i ||\phi_i||_{L^2(\Sigma_i)}^2 + \lambda ||\mu_0||_{TV}$$

$$+ \lambda \sum_{i=1}^{n+1} \lambda_i ||\phi_i||_{L^2(\Sigma_i)}^2,$$

where $\mathcal{F}_1$ corresponds to the EM data, $\mathcal{F}_2$ to the cortical mapping, $D_2$ is the Hilbert space $L^2(\Sigma_1) \times \cdots \times L^2(\Sigma_n) \times L^2(\Sigma_{n+1})$ which corresponds to the electric potential on the interfaces $\Sigma_i$, $i = 1, 2, \ldots, n + 1$ and $S$ is the product Banach space $[\mathcal{M}(\Sigma_0)]^3 \times L^2(\Sigma_2) \times \cdots \times L^2(\Sigma_n) \times L^2(\Sigma_{n+1})$.  

[10]
We propose to use an alternating minimisation procedure generating a sequence of solutions
\[
\left\{ (\mu_0^{(k)}, \phi_1^{(k)}, \phi_2^{(k)}, \ldots, \phi_{n+1}^{(k)}) \right\}_{k \in \mathbb{N}}
\]
with some initial guess for \( k = 0 \) by solving the problems
\[
\mu_0^{(k+1)} = \arg \inf_{\mu_0 \in [M(\Sigma_0)]^3} \mathcal{T}_{f,\lambda}(\mu_0, \phi_1^{(k)}, \ldots, \phi_{n+1}^{(k)})
\]
\[
(\phi_1^{(k+1)}, \phi_2^{(k+1)}, \ldots, \phi_{n+1}^{(k+1)}) = \arg \inf_{(\phi_1, \ldots, \phi_{n+1}) \in D_{2}} \mathcal{T}_{f,\lambda}(\mu_0, \phi_1, \ldots, \phi_{n+1})
\]
to achieve a minimiser of \( \mathcal{T}_{f,\lambda} \). Using the results of [1,2] we conclude in both the continuous and discrete versions of Problem 1 that the sequence generated above converges to a minimiser of \( \mathcal{T}_{f,\lambda} \) with the functional \( \mathcal{T}_{f,\lambda} \) converging to its minimum linearly.

3 Numerical Experiments

We require triangular meshes of the grey/white matter interface, cortex, skull and scalp. Note that (1) and (2) contain boundary integral operators that are defined on the cortex, skull and scalp. From [3] these boundary integrals can be computed exactly for triangular meshes and piecewise linear \( \phi \)'s. When \( M(\Sigma_0) \) is the Banach space of Borel measures, we approximate \( \mu_0 \) by a collection of dipoles. If the possible dipoles locations are \textit{apriori} known and fixed, we use a FISTA algorithm with \( \ell_1 \) penalisation to recover the dipole moments, see Figure 1 for EEG with \( D_1 \subseteq \Sigma_{n+1} \). Whereas if the dipoles locations are allowed to be arbitrarily located on \( \Sigma_0 \), we use the algorithm in [4]. If \( M(\Sigma_0) = L^2(\Sigma_0) \) with \( \mu_0 \) being normally oriented to \( \Sigma_0 \), we model the magnitude and orientation of the vector-field as a piecewise linear \( L^2(\Sigma_0) \)-function which results in Problem 1 being a least-squares problem. In this case a least-squares solution based on the Moore-Penrose pseudo-inverse can be obtained to solve the source recovery and cortical mapping problem together. The source is interpreted to be located in a neighbourhood of the extrema of the \( L^2(\Sigma_0) \) function.

References


On corner matrices for high order DDMs

Bruno Després1,∗, Anouk Nicolopoulos2, Bertrand Thierry3

1LJLL, Sorbonne university, Paris, France
2University of Zurich, Zurich, Switzerland
3Somewhere in the States

Email: bruno.despres@sorbonne-universite.fr

Abstract
Our problem concerns the construction of domain decomposition methods (DDM) for the model Helmholtz equation with high order transmission conditions (2nd order TC in our case) and cross-points. A compatibility condition is formulated for cross-points matrices so that the DDM is proved to be convergent under general conditions. The proof is based on a new global energy formulated on the skeleton of the DDM decomposition. The equivalence of the new energy with the $H^1$ norm on the skeleton of the DDM decomposition is shown. The extension at any order is briefly discussed.

Keywords: DDM, second-order TC, cross-points.

1 Introduction
We consider a general family of domain decomposition iterative processes:

- Initialize $u_i^0 \in H^1(\Omega_i)$ for all $i$.
- For $p \in \mathbb{N}$, compute $u_i^{p+1} \in H^1(\Omega_i)$ for all $i$

\[
\begin{align*}
(\Delta + \omega^2) u_i^{p+1} &= f \text{ in } \Omega_i, \forall i, \\
(\partial_n - \omega T) u_i^{p+1} &= - (\Pi \delta_{ii} + \omega T \Pi) u_i^p, \\
(\partial_n - \omega) u_i^{p+1} &= 0 \text{ on } \Gamma,
\end{align*}
\]

where the second equation denotes a possibly global transmission condition on the skeleton $\Sigma$ of the DDM. The operator $\Pi$ denotes the natural exchange operator on $\Sigma$.

We report hereafter on recent advances [5] (to compare with [1–3]) where the operator $T$ comes from a second order approximation of transparent condition on a flat boundary in 2D. That is we desire that the transmission equation $T$ on $\Sigma$ in (1) models

\[
\begin{align*}
(1 - \frac{1}{2\pi} \partial_{i,j}^{x}) \partial_{n,k} u_i^{p+1} - \omega u_i^{p+1} &= - \frac{1}{2\pi} \partial_{i,j} \partial_{n,k} u_i^{p+1} - \omega u_i^{p+1} \text{ on } \Sigma_{ij},
\end{align*}
\]

where $\Sigma_{ij} = \Sigma_{ji}$ is the part of $\Sigma$ in between $\Omega_i$ and $\Omega_j$. Such a requirement is algorithmically natural since second order transmission operators are already implemented in [4]. One notices that we have selected a second order operator which has some positivity property since the principal symbol is $1 - \frac{1}{2\pi} \partial_{tt} \geq 0$ which is formally non negative.

We propose to focus on combinations of Neumann traces and Dirichlet traces under the form

\[
\partial_{x_{ij}} \varphi_{ij}(x_r) + \sum_{(k,l) \in \mathcal{E}_r} \alpha_{ij,kl}^r \varphi_{kl}(x_r) = 0, \forall (ij) \in \mathcal{E}_r,
\]

where $\mathcal{E}_r$ denotes the set of edges around the node/vertex $x_r$. $\tau_{ij}$ denotes a tangential derivation and $\varphi_{ij}$ denotes with simpler notations a linear rescaling of $\partial_{n,ij} u_{ij}$. All quantities (3) which concern Neumann traces and Dirichlet traces around the same node/vertex $x_r$ are gathered in two vectors, one for the Neumann traces and one for the Dirichlet traces. One obtains

\[
\partial_{x_r} \varphi_r + A^r \varphi_r = 0,
\]

with the matrix $A^r \in \mathcal{M}_{2d \times (C)}$ contains the unknowns coefficients $(\alpha_{ij,kl})_{ij,kl}$.

2 Definition of $T$ and other considerations
We model/introduce the above considerations by defining the bilinear form $a(\cdot, \cdot)$ on the skeleton: for all $\varphi, \psi \in H^1_{br}(\Sigma)$

\[
a(\varphi, \psi) = \sum_{ij} \int_{\Sigma_{ij}} \left( \partial_{ij} \partial_{ij} \varphi \psi + \frac{1}{2\pi} \partial_{ij} \varphi \partial_{ij} \psi \right) d\sigma
\]

\[
+ \frac{1}{\omega^2} \sum_{r=1}^{N_r} \left( A^r \varphi_r, \psi_r \right)_{C_{2d_r}}.
\]

We make the assumption that $A^r$ has pure imaginary coefficients and that it is skew-hermitian $A^r = iH^r$ where $H^r = (H^r)^T \in \mathcal{M}_{2d_r}(R)$. Since $a$ is coercive (in particular because the transmission operator is symmetric non negative), one can define

\[
\begin{align*}
\{ \text{Find } \varphi \in H^1_{br}(\Sigma) \text{ such that } \\
a(\varphi, \psi) = (v, \psi)_{L^2(\Sigma)}, \forall \psi \in H^1_{br}(\Sigma). \}
\end{align*}
\]
This problem is well posed, there exists a unique solution $\varphi \in H^1_{\text{br}}(\Sigma)$, which denotes the skeleton endowed with the natural broken $H^1$ norm.

**Definition 1** Let $T: L^2(\Sigma) \to L^2(\Sigma)$ be the operator such that $Tv = \varphi$, where $\varphi$ is the solution to the problem (6) for $v \in L^2(\Sigma)$.

The symmetric part of $T$ admits a spectral decomposition. Let $(u_n)_{n \in \mathbb{N}} \subset H^1_{\text{br}}(\Sigma)$ be the Hilbertian basis such that $(\mathcal{T} + T)^{-1} u_n = \lambda_n u_n$, $\langle u_n, u_m \rangle_{L^2(\Sigma)} = \delta_{nm}$ and $\text{span}\{u_n\}_{n \in \mathbb{N}} = L^2(\Sigma)$. The eigenvalues satisfy $1 \geq \lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \ldots \geq 0$ and $\lambda_n$ converges towards zero as $n$ goes to infinity. This leads to the definition of the operator $(\mathcal{T} + T)^{-1}: L^2(\Sigma) \to L^2(\Sigma)$ such that $(\mathcal{T} + T)^{-1} u = \lambda_1 u$, and the space $H^1_1(\Sigma) = \{ u \in L^2(\Sigma), \| u \| < \infty \}$, endowed with the norm $\| \cdot \|$ defined as

$$\| u \| := \left( \sum_{n \geq 0} \left( \frac{\| u_n \|_{L^2(\Sigma)}^2}{\lambda_n} \right)^2 \right)^{1/2}, \quad \forall u \in L^2(\Sigma).$$

The hermitian scalar product in $H^1_1(\Sigma)$ is denoted $\langle u, v \rangle := \sum_{n \geq 0} \frac{1}{\lambda_n} \langle u_n, u_n \rangle_{L^2(\Sigma)}$. \(\mathcal{T} + T\) $L^2(\Sigma) \mapsto L^2(\Sigma)$ is a Hilbert space. One of our main mathematical result is that $H^1_1(\Sigma) = H^1_{\text{br}}(\Sigma)$ with equivalence of norms.

**Definition 2** We say that operator $T$ is compatible if $\Pi^H T = T^*$.

Under the compatibility assumption, DDM (1) can be rewritten as

$$\begin{align*}
\left\{ \begin{array}{l}
(\Delta + \omega^2) u_{\text{E}+1}^p &= f \text{ for all } i, \\
(\partial_n - i\omega T) u_{\text{E}+1}^p &= -\Pi (\partial_n + i\omega T^*) u_{\text{E}+2}, \\
(\partial_n - i\omega) u_{\text{P}+1}^p &= 0 \text{ on } \Gamma.
\end{array} \right.
\end{align*}$$

Define $E^p := \| (\partial_n - i\omega T) u_{\text{E}+1}^p \|^2$.

**Lemma 3** Assume that $T$ verifies the compatibility condition from Definition 2, and that at each stage of the algorithm (7) $u^p \in \oplus_i H^1(\Omega_i)$ and $\partial_n u^p \in H^1_{\text{br}}(\Sigma)$. Then, algorithm (7) is stable (and finally convergent) in the sense that its energy is decreasing: $E^{p+1} = E^p - 4\omega^2 \| u^p \|^2_{L^2(\Gamma)}$.

### 3 Extension to higher order transmission conditions

A natural question for our methodology is to model transmission conditions at higher order. Let us consider a plane wave

$$u(x) = e^{i\omega (\cos \theta x + \sin \theta y)},$$

One considers the exact outgoing condition on a flat boundary $\{ x = 0 \}$ such that $\partial_n = \partial_x$: $\partial_{\text{t}} u - i\omega u = 0$. For $|\sin \theta| < 1$, one has the convergent expansion

$$\frac{1}{1 - \sin \theta} = (1 - \sin^2 \theta)^{-1/2} = 1 + \frac{\sin^2 \theta}{2} + \frac{3\sin^4 \theta}{8} + \frac{5\sin^6 \theta}{16} + \frac{35\sin^8 \theta}{128} + \ldots$$

All coefficients are positive. Then a truncation at any order yields a transparent boundary condition of the corresponding order. For example, an expansion at order 6 writes

$$1 + \frac{\sin^2 \theta}{2} + \frac{3\sin^4 \theta}{8} + \frac{5\sin^6 \theta}{16} \partial_{\text{t}} u - i\omega u = 0.$$ One has formally $i\omega \sin \theta = \partial_y = \partial_k$. One obtains the artificial condition

$$\left(1 - \frac{\partial^2_{uu}}{2\omega^2} + 3\frac{\partial^4_{tttt}}{8\omega^4} - \frac{5\partial^6_{ttttt}}{16\omega^6}\right) \partial_{\text{t}} u - i\omega u = 0.$$

By construction, the operator $A = 1 - \frac{\partial^2_{uu}}{2\omega^2} + 3\frac{\partial^4_{tttt}}{8\omega^4} - \frac{5\partial^6_{ttttt}}{16\omega^6}$ is formally symmetric non negative. For such an operator one can defines generalized Neumann traces $(\partial_{\text{n}}^\# \varphi)$ and Dirichlet traces $(\partial_{\text{t}}^\# \varphi)$ for $r = 3, 4, 5$ and it is possible to define a new bilinear form (5) with generalized corner matrices. The properties of this new bilinear and of the corresponding new transmission operator is left for further studies.

### References


Advances in overlapping-domain framework for wave propagation in heterogeneous and unbounded regions

Victor Domínguez\textsuperscript{1,*}, Mahadevan Ganesh\textsuperscript{2}, Stuart C. Hawkins\textsuperscript{3}

\textsuperscript{1}Departamento de Estadística, Informática y Matemáticas, Universidad Pública de Navarra, Tudela, Spain.
\textsuperscript{2}Department of Applied Mathematics & Statistics, Colorado School of Mines, Golden, Colorado, USA.
\textsuperscript{3}School of Mathematical and Physical Sciences, Macquarie University, Sydney, Australia

*Email: victor.dominguez@unavarra.es

Abstract

Simulation of absorbed- and scattered-fields induced by an incident wave impinging on bounded heterogeneous configurations is fundamental for numerous applications. Scalar absorbed-and scattered-fields can be modeled by the Helmholtz partial differential equation (PDE) defined inside and exterior to the configuration, respectively. Finite element and boundary element methods (FEM and BEM), respectively, provide efficient tools for simulations of the Helmholtz PDE in the interior (varying wave speed) bounded domain and in its complement (constant wave speed) exterior medium. A novel coupled overlapping FEM-BEM framework was introduced for the interior-exterior Helmholtz model in [2] and for the 2D framework, FEM-BEM numerical analysis was developed in [3]. The main aim of the present work is on the advancement of the framework with numerical analysis for the 3D model.

Keywords: Helmholtz, heterogeneous, unboundedness, scattering, FEM-BEM

1 Heterogeneous and unbounded model

We consider the heterogeneous Helmholtz wave propagation problem for the total field $u$: \[ \Delta u + k^2 n^2 u = 0, \text{ in } \mathbb{R}^3, \] with the Sommerfeld radiation condition (SRC) [1] for the scattered field $u^{\text{sc}}$. In (1), $k > 0$ is a constant wavenumber and $n$ is the spatially varying refractive index function with the variable wave speed restricted to a compact domain $\Omega_0$. That is, $n$ is a piecewise-continuous function with $n|_{\Omega_0} \equiv 1$. The unknown of the problem is the total field $u := u^{\text{inc}} + u^{\text{sc}}$, where typically $u^{\text{inc}} = \exp(ikd \cdot x)$ is an incident plane wave.

The majority of computational wave modeling approaches over the last five decades (see [6] and references therein) are restricted to either the FEM or BEM. This is because the literature is dominated by either truncating the above model to a bounded absorbing medium (and hence not satisfying the SRC exactly) or not allowing for practically important spatially varying wave speeds occurring inside a domain, say, $\Omega_0 \subset \mathbb{R}^d$ by assuming constant wave speeds [1]. Computational models that satisfy the SRC exactly facilitate accurate simulation of the far-field using high-order algorithms. Far fields are important for quantities of interests such as differential scattering cross sections (DSCS) [7]; and also for solving inverse wave propagation problems [1]. Our overlapping FEM-BEM algorithm satisfies the SRC exactly and also allow for heterogeneous refractive index in the Helmholtz model, consequently leading to simulations of the 3D heterogeneous media DSCS.

2 Overlapping-domain equivalent model

For practically incorporating both heterogeneity and unboundedness (H-U) in the full space $\mathbb{R}^d$ model, we developed and analyzed an equivalent continuous overlapping-domain equivalent model in both two and three dimensional settings. Our mathematically established equivalent continuous model approach in [2] is entirely different from the continuous (and discrete) models investigated using non-overlapping framework with a single interface coupling, for which several open challenging analysis problems remain to be solved (see [5, 8] and references therein). Advances in computational and numerical analysis counterpart of the full equivalent continuous model in [2] has been the aim of our recent and ongoing work. Below, we briefly introduce the continuous and a discrete framework. The focus of our present work is on algorithm, numerical analysis, and implementa-
tion using high-order discretization of the H-U overlapping construction for the 3D case. The continuous H-U framework in [2] was based on introducing two, free to choose, artificial boundaries: a smooth closed surface surrounding \( \Omega_0 \), with an exterior free-space, and a further outer simple polyhedral boundary Indeed, let \( Q \) be a polyhedron with \( \Omega_0 \subset Q \) and let \( S \subset Q \setminus \Omega_0 \) be the smooth closed surface. Thus, \( Q \) includes the full model heterogeneity and intersects with a bounded region exterior to \( S \), and the unbounded exterior to the boundary \( S \) is a constant wave speed medium. Hence, in our computational framework, we can apply high-order FEM for the total wave \( u \) in the interior heterogeneous problem in \( Q \), and use spectrally accurate BEM for the exterior model [1,4], that are specially designed for curved boundaries for the scattered field \( u^{sc} \) and that exactly satisfies the SRC in the BEM model as well.

3 The FEM-BEM coupling procedure

We conclude by briefly describing our algorithm. For the interior problem, we seek approximations in \( V_h \), a continuous high-order FEM space on triangulated conformal meshes of \( Q \). Let

\[
V_h^H = \{u_h \in V_h : \Delta_h u_h + k^2 n^2 u_h = h 0 \}
\]

(i.e. elements of \( V_h \) which are FE solutions of the Helmholtz equation). Then we have

\[
V_h^H \ni u_h \approx u|_Q
\]

simply by demanding the trace relation:

\[
\gamma_{\Sigma} u_h = \gamma_{\Sigma,h} = \gamma_{\Sigma} u^{sc} + \gamma_{\Sigma,h} u^{inc}, \tag{2}
\]

with \( \Sigma = \partial Q \), the boundary of \( Q \) and \( \gamma_{\Sigma,h} \) above being the result of interpolation of \( \gamma_{\Sigma} u \), the trace of \( u \) on \( \Sigma \).

On the other hand, we seek spectrally accurate scattered field BEM solutions in \( T_N \), a discrete space of smooth functions on \( S \) with a maximum degree parameter \( N [1,4] \) such that

\[
T_N \ni \varphi_N \text{ s.t. } \mathcal{L}_{k,N} \varphi_N \approx u^{sc}.
\]

In the expression above, \( \mathcal{L}_{k,N} \) is a (discrete evaluation of a) robust layer potential representation of radiation solutions of Helmholtz equation and \( \varphi_N \) a suitable density determined by

\[
\gamma_{S,N}(\mathcal{L}_{k,N} \varphi_N - u^{sc}) = 0. \tag{3}
\]

That is, \( \varphi_N \) is the spectrally accurate surface density solution of a BIE.

Gathering (2)-(3), we conclude that \( (\varphi_N, \gamma_{\Sigma} u_h) \), the ultimate true unknowns of our computational framework, is solution of

\[
\begin{align*}
\gamma_{\Sigma} u_h - \gamma_{\Sigma,h}(\mathcal{L}_{k,N} \varphi_N) &= \gamma_{\Sigma,h} u^{inc}, \\
\gamma_{S,N} u_h - \gamma_{S,N}(\mathcal{L}_{k,N} \varphi_N) &= -\gamma_{S,N} u^{inc}.
\end{align*}
\]

References


A comparison between Hierarchical Poincaré-Steklov approaches for the 3D Helmholtz equation with variable coefficients.

José Pablo Lucero Lorca\textsuperscript{1,*}, Adrianna Gillman\textsuperscript{1}
\textsuperscript{1}Department of Applied Mathematics, University of Colorado at Boulder, Boulder, USA
*Email: pablo.lucero@colorado.edu

Abstract

We present two solvers for the Hierarchical Poincaré-Steklov (HPS) discretization of 3D variable coefficient Helmholtz problems. An iterative approach uses a GMRES solver coupled with a leaf-wise block-Jacobi preconditioner. The preconditioner is built using two nested local solvers accelerated by local homogenization. Both the operator and preconditioner are implemented in a matrix-free fashion and with distributed memory. The solver can tackle problems approximately 50 wavelengths in each direction requiring more than a billion unknowns to get approximately 7 digits of accuracy in less than an hour.

We compare with an extension to 3D of the direct solver shown in [1,2]. Iterative local solvers, matrix compression and a modified discretization accelerate the solution and reduce memory footprint. We test both approaches and their performance with application examples.

Keywords: Helmholtz, Domain-Decomposition, Poincaré-Steklov

1 Introduction

We consider the variable coefficient Helmholtz problem with impedance boundary conditions given below

\[-\Delta u(x) - \kappa^2 (1 - b(x)) u(x) = s(x), \quad x \in \Omega, \]
\[\frac{\partial u}{\partial n} + i\eta u(x) = t(x), \quad x \in \partial \Omega. \]

(1)

\[\Omega = (0,1)^3, \quad u(x) \text{ is the complex unknown solution, } \kappa \in \mathbb{R} \text{ is the wave number, } b(x) \text{ is a given smooth scattering potential and } n \text{ is the outward normal unit vector to the boundary of the domain.} \]

The functions \(s(x)\) and \(t(x)\) are assumed to be smooth complex functions.

We discretize the geometry into a collection of disjoint patches or leaves. Leaves are sized so that a local boundary value problem can be solved to high accuracy via a high degree Chebyshev spectral collocation method. Impedance-to-impedance (ItI) constraints are required between neighboring leaves. By using this operator for the coupling of elements, the HPS discretization is able to avoid artificial resonances and does not appear to observe the so-called pollution effect [1].

The iterative technique relies on the fact that the matrix that results from HPS is block sparse, where all non-zero blocks are also sparse and can be applied matrix-free. To solve the linear system we utilize a leaf-wise block-Jacobi preconditioned GMRES solver. The proposed block-Jacobi preconditioner and the system matrix are applied via matrix-free operations and exploit the tensor product nature of the element wise discretization matrices. The local nature of the blocks and the preconditioner make the solution technique naturally parallelizable in a distributed memory model. Numerical tests show that the solution technique is efficient and capable of tackling problems with a billion degrees of freedom (DoFs) in less than forty minutes in parallel (see Table 1).

The direct technique is an extension of [1,2] to 3D, it consists of two main steps after local spectral discretization:

- Approximate boundary (Poincaré–Steklov) and solution operators are constructed for each patch, starting with the leaves.
- In a hierarchical fashion, using Schur com-

\begin{table}[h]
\centering
\begin{tabular}{|c|c|}
\hline
Problem size in leaves & \(64 \times 64 \times 64\) \\
\hline
MPI distributed memory procs & 4096 \\
Degrees of Freedom & 1027M \\
GMRES time (1114 iterations) & 2206s \\
\hline
\end{tabular}
\caption{Performance for 50 wavelengths across, \(10^{-8}\) residual reduction, Chebyshev degree 16.}
\end{table}

Figure 1: Merging subdomains in 3D
implements obtain new patches by “glueing” patches together two at a time by enforcing ITL conditions via the Poincaré-Steklov operators on the boundaries of each patch. The procedure is illustrated in Figure 1. For each merged patch, corresponding boundary and solution operators are constructed.

2 Leaf discretization and solver

Let $\tau$ be a leaf, we seek to approximate the solution to (1) on $\Omega^\tau$ using classical spectral collocation. Discretizing this way we obtain the matrix $A^\tau_c := -D^\tau_x - D^\tau_y - D^\tau_z - C^\tau$. $C^\tau$ is a diagonal matrix with entries $\{\kappa^2 (1 - b(x_k))\}_{k=1}^N$, $D^\tau_x$, $D^\tau_y$ and $D^\tau_z$ are Chebyshev differentiation matrices with corner and edge interaction entries removed.

The incoming and outgoing impedance operators in eq. (1) are approximated using the matrices $F^\tau = N + inI$ and $G^\tau = N - inI$. $I$ is the identity matrix and $N$ approximates the derivative at the boundary and is composed of submatrices of $D_x$, $D_y$ and $D_z$.

Let $A^\tau := \begin{pmatrix} A^\tau_i & A^\tau_b \\ F^\tau_{bi} & F^\tau_{bb} \end{pmatrix}$, where $I^\tau_i$ are the interior node indices and $I^\tau_b$ are the indices for all nodes. Reordering we obtain a leaf system of the form

$$A^\tau \begin{pmatrix} u^\tau_i \\ u^\tau_b \end{pmatrix} = RHS^\tau,$$

(2)

where the subscript $i$ stands for “interior” and $b$ for “boundary” nodes of the leaf. The matrix $A^\tau_i$ is sparse can be applied rapidly thanks to its Kronecker product structure and $A^\tau_{ib}$, $F^\tau_{bi}$, $F^\tau_{bb}$ are also sparse.

When $b(x)$ varies slowly, we solve this system by using the $2 \times 2$ block-matrix inversion formula. The formula needs the inverse of the Schur complement $S^\tau$ and $A^\tau_i$ which we apply iteratively using two nested GMRES solvers preconditioned with the inverses of homogenized versions of $A^\tau_i$ and $S^\tau$. Given their structure, such homogenized inverses are relatively cheap to calculate.

3 Iterative method

The efficient leaf solver discussed in section 2 makes a leaf-wise block-Jacobi preconditioner a natural choice for the GMRES global solver. Thus we use a total of 3 nested GMRES solvers for leaves and global systems. Further details are given in [3] and some performance results are given in Table 1.

The solver can efficiently tackle very big problems to obtain a single solution. Inverse problems involving solving for several body loads and boundary conditions are better addressed with a direct method as we explain hereafter.

4 Direct method

The direct technique used in [1, 2] demonstrated an excellent performance in 2D. We extend the technique to 3D overcoming many dimensionality challenges.

Increased dimensionality requires a large amount of DoFs in each leaf. We accelerate inversion using a modified spectral discretization. Leaf matrices being sparse, we apply a local iterative technique from section 3 when possible.

Operators for merging patches are significantly larger in 3D. However, large patch operators are rank-deficient up to the desired accuracy, especially for high frequency. Interpolative compression is used to reduce memory footprint. Linear algebra is parallelized with distributed memory akin to multifrontal solvers.

For inverse problems where the solution for many body loads and boundary conditions is needed, a direct technique outperforms an iterative solution. We study and compare both techniques with application examples including seismic inversion.

5 References

References


dGFEM-BEM mortar coupling for the Helmholtz problem in three dimensions

Ch. Erath1, L. Mascotto2, J. M. Melenk3, I. Perugia4, A. Rieder5,∗
1University College of Teacher Education Vorarlberg, 6800 Feldkirch, Austria
2Dipartimento di Matematica e Applicazioni, University of Milano-Bicocca, 20125 Milano, Italy
3Institut für Analysis und Scientific Computing, TU Wien, 1040 Vienna, Austria
4Fakultät für Mathematik, Universität Wien, 1090 Vienna, Austria
5Institut für Analysis und Scientific Computing, TU Wien, 1040 Vienna, Austria
∗Email: alexander.rieder@tuwien.ac.at

Abstract
We present a way of coupling an interior penalty discontinuous Galerkin method with a boundary element method for the Helmholtz equation in 3d. The coupling is realized with a mortar variable related to an impedance trace. We prove quasi-optimality of the h- and p-versions of the scheme, under a threshold condition on the approximation properties of the discrete spaces.

Keywords: discontinuous Galerkin method; boundary element method; mortar coupling; Helmholtz equation;

1 Model Problem
Consider a bounded domain Ω ⊆ R³ with analytic boundary Γ. Fix a characteristic wave speed k > 0 and let n : R³ → R be a smooth function with n(x) > 0 and n(x) = 1 outside of Ω. Assume that the right-hand side f is analytic and satisfies supp(f) ⊆ Ω.

We aim to approximate solutions to the Helmholtz problem

\[-Δu - (kn)^2 u = f \text{ in } R³\]  

\[\lim_{|x|→∞} |x| (\partial_\nu u - iku) = 0.\]  

Most of the details to this talk can be found in the preprint [1].

2 Mortar coupling
We introduce two auxiliary variables on the boundary m := ∂Ω⁻ u + ikγ⁻ u and uext := γ⁺ u where γ⁻ and ∂Ω⁻ are the interior trace and normal derivative. γ⁺ correspondingly is the exterior trace. This gives the coupled problem:

\[-Δu - (kn)^2 u = f \text{ in } Ω,\]
\[\partial_\nu u + iku = m \text{ on } Γ,\]
\[uext = P_{H^1} m,\]
\[γ⁻ u = (\frac{1}{2} + K_k) uext - V_k (m - ikuext).\]  

For discretization, we use an interior penalty dG discretization [3] for the equation posed on Ω based on a piecewise polynomial space Vh. For the boundary integrals, we use a combined-field type representation for the Impedance-to-Dirichlet operator and BEM spaces Wh ⊆ H⁻¹/2(Γ) and Zh ⊆ H¹/2(Γ) for the approximation of m and uext respectively.

3 Analysis
We use two different norms:

\[\|(v, λ, vext)\|_{dG}^2 := \|\nabla_h v\|^2_{0,Ω} + \|k v\|^2_{0,Ω} + k^{-1}\|\beta/2 \|\nabla_h v\|^2_{0,Γ}\]
\[+ k^{-1}\|\alpha/2 \|v\|^2_{0,Γ} + k\|\alpha/2 \|v\|^2_{0,Γ} + \|\lambda\|^2_{-1/2,Γ} + \|vext\|^2_{1/2,Γ},\]

and

\[\|(v, λ, vext)\|_{dG}^2 := \|(v, m, vext)\|_{dG}^2 + k^{-1}\|\alpha/2 \|\nabla_h v\|^2_{0,Γ} + \|h^{1/2} p^{-1} λ\|^2_{0,Γ},\]

where \[\|\cdot\|_{0,Γ}^2\] denotes the sum of the L²-norms over all interior facets, \[\|\cdot\|_{Γ}\] denote the jump and mean across facets respectively. α, β and δ are stabilization parameters that need to be chosen appropriately.

We denote the sesquilinear form obtained by Galerkin discretization of (2) by \[\mathcal{T}(\cdot, \cdot).\] This form satisfies a Gårding inequality in the dG-norm, i.e., there exists ε > 0, c > 0 such that

\[(Re + ε Im)\mathcal{T}(v, λ, vext), (v, λ, vext)) ≥ c\|\|v, λ, vext\|\|^2_{dG} - Ω(v, λ, vext),\]

with \[Ω(v, λ, vext)\] a compact perturbation. Stability holds in the stronger dG⁺-norm. By carefully designing the discretization scheme, we can ensure adjoint consistency, i.e., the transpose of the discretization matrix is the dG-discretization of a natural adjoint problem to (2). This enables the use of the powerful Schatz argument.
4 Reconstruction operator

The main obstacle when trying to prove Gårding inequality and stability of the bilinear form is that while the dG approximation $u_h$ in the interior has jumps across the faces, the boundary integral operators require functions which are $H^{1/2}(\Gamma)$-conforming. Our solution: a novel reconstruction operator $\mathcal{P}$ in the spirit of [2], which maps piecewise $H^1$ functions to globally continuous functions.

**Theorem 1** Let $\mathcal{T}$ be a shape-regular mesh of size $h$ on $\Omega$. Then, for each $p \in \mathbb{N}$ there exists a linear operator $\mathcal{P} : H^1_{pw}(\Omega_h) \to H^1(\Omega)$ that satisfies, for all $v \in H^1_{pw}(\Omega_h)$,

$$
\|\nabla P v\|_{0,\Omega} \lesssim \|\nabla_h v\|_{0,\Omega} + \|h^{-1/2} p[v]\|_{0,\mathcal{F}_h},
$$

$$
\|P v\|_{0,\Omega} \lesssim \|h^{-p} \nabla_h v\|_{0,\Omega} + \|v\|_{0,\Omega} + \|h^{1/2} p^{-1}[v]\|_{0,\mathcal{F}_h},
$$

as well as the approximation property

$$
\|h^{-1/2} p(I-P)v\|_{0,\Gamma} \lesssim \|\nabla_h v\|_{0,\Omega} + \|h^{-1/2} p[v]\|_{0,\mathcal{F}_h}.
$$

The construction of Theorem 1 is such that we first use a quasi-interpolation into piecewise linear functions on an artificial mesh of size $O(h^{-2})$. There, we use the “averaging of degrees of freedom” operator from [2]. This gives robust stability and approximation estimates for piecewise polynomials of degree $p$. The price is that the operator does not map into the space $Z_h$ of piecewise polynomials on the original triangulation. Instead, it maps to the space of piecewise linears on an artificial refined grid.

5 Main Theorem

Using all these ingredients, we can derive a quasi-optimality result.

**Theorem 2** Let the solution $(u, m, u^{ext})$ to (2) be in $H^{3/2}(\Omega) \times L^2(\Gamma) \times H^{1/2}(\Gamma)$ for some $t > 0$, and let $(u_h, m_h, u_h^{ext}) \in V_h \times W_h \times Z_h$ be the discrete solution. Assume that the adjoint problem can be approximated sufficiently well. Then:

$$
\|u - u_h, m - m_h, u^{ext} - u_h^{ext}\|_{h} \lesssim \inf_{v_h, \lambda_h, v_h^{ext}} \|u - v_h, m - \lambda_h, u^{ext} - v_h^{ext}\|_{h},
$$

where the infimum is taken over all $(v_h, \lambda_h, v_h^{ext}) \in V_h \times W_h \times Z_h$.

The analysis of [1] is not explicit in $k$. We will briefly discuss how to address this issue.

6 Numerical results

We performed numerical simulations in which we compared the numerical approximations of our scheme to a known exact smooth solution. Namely, we used the domain $\Omega := (-1, 1)^3$, the coefficient $n = 1$ and set

$$
u(x, y, z) := \begin{cases} 
\sin(k x) \cos(k y) & (x, y, z) \in \Omega \\
\frac{c_k \sqrt{x^2 + y^2 + z^2}}{\sqrt{x^2 + y^2 + z^2}} & \text{otherwise}. 
\end{cases}
$$

Note that this solution is discontinuous across $\Gamma$, and thus does not strictly fit (1). One can easily modify the right-hand sides of the scheme to account for given jumps across $\Gamma$.

We observe in Figure 1 that the method performs as expected when refining the mesh, i.e. the error is $O(h^p)$ where $p$ denotes the order of the polynomials employed.

![Figure 1: Convergence of the $h$-version for $k = 2\sqrt{3}$.](image)

References


Rational-based MOR methods for Helmholtz frequency response problems with adaptive finite element snapshots

Francesca Bonizzoni\textsuperscript{1,*}, Davide Pradovera\textsuperscript{2}, Michele Ruggeri\textsuperscript{3}

\textsuperscript{1}Department of Mathematics, University of Augsburg, Augsburg, Germany
\textsuperscript{2}CSQI, EPFL, Lausanne, Switzerland
\textsuperscript{3}Department of Mathematics and Statistics, University of Strathclyde, Glasgow, United Kingdom

\textsuperscript{*}Email: francesca.bonizzoni@math.uni-augsburg.de

Abstract
We introduce several spatially adaptive model order reduction approaches tailored to parametric-in-frequency Helmholtz problems. The offline information is computed by means of adaptive finite elements, so that each snapshot lives on a grid adjusted to the considered frequency value. A rational surrogate is then assembled adopting either a least-squares or an interpolatory approach. Numerical experiments are performed to compare the proposed methodologies.

Keywords: model order reduction, rational approximation, parametric Helmholtz equation, frequency response, adaptive mesh refinement

1 Introduction
The present talk, based on [3], deals with numerical approximation of solutions to time-harmonic wave propagation problems over a range of frequencies. In particular, given any \( k \) in the interval of interest \( K = [k_{\text{min}}, k_{\text{max}}] \), we look for the solution to the interior or scattering Helmholtz problem

\[
\begin{aligned}
&-\Delta u - k^2 u = f \quad \text{in } \Omega, \\
&u = 0 \quad \text{on } \Gamma_D, \\
&\partial_\nu u = g_N \quad \text{on } \Gamma_N, \\
&\partial_\nu u - iku = g_R \quad \text{on } \Gamma_R,
\end{aligned}
\]

where \( f \in L^2(\Omega) \), \( g_N \in L^2(\Gamma_N) \) and \( g_R \in L^2(\Gamma_R) \), with \( \Gamma_D, \Gamma_N, \Gamma_R \) forming a partition of \( \partial \Omega \).

Due to oscillations in the analytical solutions, accurate finite element (FE) approximations are computationally expensive and time-consuming, already for moderate frequencies. Therefore, in the multi-query context, when responses at many frequencies are of interest, their direct computation is unaffordable.

Model order reduction (MOR) methods aim at alleviating the computational cost by producing an approximation of (some functional of) the frequency response map. The produced approximation (the so-called \textit{surrogate}) has to be close to the quantity of interest (QoI) and, at the same time, cheap to evaluate.

MOR methods rely on a two-phase procedure. The accurate computation of the offline information often requires a considerable computational effort. However, it is performed only once, and then it is stored for later use during the online phase, when the surrogate is evaluated (in real-time) at any new frequency value of interest.

2 Offline phase
The offline phase consists in two operations: (i) the sampling, namely numerical evaluation of the frequency response map for a set of frequency values (the sample points); and (ii) the surrogate assembling.

2.1 Sampling strategy
In standard MOR techniques, the snapshots are all computed on one grid of the considered physical domain. In the specific framework we are handling, this might represent a big drawback. Indeed, the analytical solution of the Helmholtz equation oscillates (the more so as the frequency increases), and it may exhibit local features or local resonance-type behavior, depending on the shape of the domain and the considered frequency values.

In constrast, the presented spatially adaptive MOR technology performs the sampling by means of the adaptive FE method. As a result, each snapshot is taken on a mesh adapted to the local features at the given parameter, and it belongs to a problem-adapted FE space.

2.2 Surrogate assembling
In [1, 2] the authors have proved that the frequency-to-solution map \( u: \mathbb{C} \to H_{1,0}^1(\Omega) \) is a mero-
morphic map. It is therefore sensible to look for its surrogate in the class of rational $H^1$-valued maps. In the present talk, we consider several techniques delivering a rational surrogate, namely the standard rational interpolation (SRI) method, which computes the rational approximant my minimizing the linearized interpolation error at the sample points, and the multipoint rational interpolation (MRI) method, which improves the SRI with the objective of reducing the number of snapshots needed to achieve a rational approximant of a certain order.

3 Discussion on $h$-adaptive MOR methods

The use of $h$-adaptive FE snapshots, each living on a different mesh of the domain, allows to save computational resources. On the other hand, it implies intrinsic difficulties: even linear combinations of snapshots cannot be easily computed. In principle, to circumvent this issue, one could express all the snapshots as elements of some common FE space. However, this calls for the construction of the so-called global mesh overlay, which entails a prohibitive computational effort and goes against the main purpose of $h$-adaptivity. Therefore, in all the algorithms that we propose, we never construct the global mesh overlay, but only require the evaluation of scalar products of pairs of snapshots, which is equivalent to building overlays of pairs of meshes.

4 A numerical example

Consider problem (1) with triangular domain $\Omega = \{x \in \mathbb{R}^2, 0 < x_2 < x_1 < \frac{\pi}{2}\}$, $f = 1$, $g_N = 0$, $\Gamma_D = (0, \frac{\pi}{2}) \times \{0\}$, $\Gamma_N = \partial \Omega \setminus \Gamma_D$ and $\Gamma_R = \emptyset$. Given $k^2 = 51$, we first present the computation of a snapshot using the $h$-adaptive FE driven by the classical residual-based error estimator $\eta_s$. In Figure 1, we show the evolution of $\eta_s$ and the true error $\epsilon(z) = \|\nabla(u_s(z) - u(z))\|_{L^2(\Omega)}$ as the mesh gets adaptively refined. Several peaks - caused by resonances of the discrete problem - appear before the asymptotic convergence regime is reached. To ensure accuracy, it is then crucial that the adaptive algorithm stops once the asymptotic convergence regime is achieved, namely, after all the peaks.

We now introduce the QoI $y(z) = \int_{\Gamma} u(z)$, with $\Gamma = \{\frac{\pi}{2}\} \times (0, \frac{\pi}{2})$ and the interval of interest $K = [1, 100]$. We construct the surrogate of the QoI by means of the SRI method, the MRI method and, for the sake of comparison, a projection-based method (POD). Building the latter two reduced models requires only 15 snapshots, as opposed to the 29 needed for SRI. We take such snapshots uniformly spaced in $K$. We show the results of the approximation in Figure 2. We see that the approximations yielded by the three approaches are quite similar. Moreover, we highlight that building the SRI and MRI surrogates is about 20% faster than POD.

References


Solvability of Discrete Helmholtz Equations

Stefan Sauter, Maximilian Bernkopf, Céline Torres, Alexander Veit

1 Institute für Mathematik, Universität Zürich, Switzerland
2 Institute for Analysis and Scientific Computing, TU Wien, Austria
3 Harvard Medical School, Boston, USA

Abstract

We study the unique solvability of the discretized Helmholtz problem with Robin boundary conditions using a conforming Galerkin hp-finite element method.

Instead of employing the classical compact perturbation argument by Schatz (1974) we will introduce a new and more direct approach to prove discrete solvability by mimicking the tools for proving well-posedness of the continuous problem directly on the discrete level. In this way, a computable criterion is derived which certifies discrete well-posedness without relying on an asymptotic perturbation argument. By using this novel approach we obtain a) new existence and uniqueness results for the hp-FEM for the Helmholtz problem b) examples for meshes such that the discretization becomes unstable (stiffness matrix is singular), and c) a simple checking Algorithm MOTZ “marching-of-the-zeros” which guarantees in an a posteriori way that a given mesh is certified for a well-posed Helmholtz discretization.

Keywords: Helmholtz equation at high wave number; adaptive mesh generation; pre-asymptotic stability; hp-finite elements; a posteriori stability

1 Setting

In this paper, we consider the numerical discretization of the Helmholtz problem for modeling acoustic wave propagation in a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2$, with boundary $\Gamma := \partial \Omega$. Robin boundary conditions are imposed on $\Gamma$ and the strong form is given by

$$\begin{aligned}
-\Delta u - k^2 u &= f \quad \text{in } \Omega, \\
\frac{\partial u}{\partial n} - iku &= g \quad \text{on } \Gamma,
\end{aligned}$$

(1)

where $n$ denotes the outer normal vector and $k \in \mathbb{R} \setminus \{0\}$ is the wavenumber.

The well-posedness of this problem follows from Fredholm’s alternative by proving that the homogeneous problem has only the trivial solution. This follows from the unique continuation principle.

We consider the discretization of this equation (in variational form) by a conforming Galerkin method. The established proof of well-posedness for this discretization goes back to [2] and is based on a perturbation argument: the subspace which defines the Galerkin discretization has to be sufficiently “rich” in the sense that a certain adjoint approximation property holds. However, this adjoint approximation property contains a constant which is a priori unknown.

The existing analysis gives insights into how the parameters defining the Galerkin space should be chosen asymptotically but does not answer the question whether, for a concrete finite dimensional space, the corresponding Galerkin discretization has a unique solution.

In this paper, we study whether the conforming Galerkin discretization of the Helmholtz problem with Robin boundary conditions can lead to a system matrix which is singular and how to define a computable criterion to guarantee that for a given mesh the conforming Galerkin discretization is well posed.

As a prelude, we start off with some general remarks. Let $\Omega$ be a finite interval (in 1D) or a bounded polygonal domain (in 2D). We denote the $L^2(\Omega)$ scalar product by $(\cdot, \cdot)$ and the $L^2(\Gamma)$ scalar product by $(\cdot, \cdot)_{\Gamma}$. $H^1(\Omega)$ is the usual Sobolev space consisting of $L^2(\Omega)$ functions whose gradients exist in a weak sense and belong to $L^2$. The weak form of (1) is given by:

$$\begin{aligned}
\text{find } u \in H^1(\Omega) \text{ s.t. } a_k(u,v) &= F(v) \quad \forall v \in H^1(\Omega), \\
\text{where } a_{0,k}(u,v) &:= (\nabla u, \nabla v) - k^2 (u,v), \quad b_k(u,v) := -ik (u,v)_{\Gamma}, \quad a_k = a_{0,k} + b_k, \quad \text{and } F(v) = (f,v) + (g,v)_{\Gamma}.
\end{aligned}$$

(2)

Let $T = \{\tau_i : 1 \leq i \leq N\}$ denote a simplicial finite element mesh for the domain $\Omega$ and for $p \in \mathbb{N}$, let

$$S_T^p := \{ u \in C^0(\Omega) \mid \forall \tau \in T \quad u|_\tau \in P_p \}.$$
The usual nodal basis for $S^p_T$ is denoted by $b_i$, $1 \leq i \leq n$, where $n := \dim S^p_T$. The conforming $hp$ finite element discretization of (1) is given by

$$\text{find } u \in S^p_T \text{ s.t. } a_k(u, v) = F(v) \quad \forall v \in S^p_T. \quad (3)$$

The equivalent matrix formulation is

$$A_k u = F \quad (4)$$

with the matrix $A_k = (\alpha_{r,s})^n_{r,s=1} \in \mathbb{C}^{n \times n}$ and the right-hand side $F = (f_r)^n_{r=1} \in \mathbb{C}^n$ given by

$$\alpha_{r,s} = a_k(b_s, b_r) \quad \text{and} \quad f_r = F(b_r).$$

It is well known that the sesquilinear form $a_k(\cdot, \cdot)$ satisfies a Gårding inequality in $H^1(\Omega)$ as well as in $S^p_T$ and Fredholm’s alternative tells us that well-posedness of (2) and (3) follow from uniqueness. Hence, (3) is well posed if the following implication holds:

$$a_k(u, v) = 0 \quad \forall v \in S^p_T \quad (5)$$

$$\implies u = 0. \quad (6)$$

We note that if we choose $v = u$ in (5) and consider the imaginary part, we get

$$0 = \text{Im} a_k(u, u) = -k^2 ||u||_T^2 \implies ||u||_T = 0.$$

2 Main Results

In this section, we present the main results and refer for the proofs to [1]

**Theorem 1** Let $\Omega \subset \mathbb{R}$ be a bounded interval and consider the Galerkin discretization (3) of (2) with conforming $hp$ finite elements. Then, for any $k \in \mathbb{R} \setminus \{0\}$ the matrix $A_k$ in (4) is regular.

In two spatial dimensions, an analogue of Theorem 1 does not hold in that generality as can be seen from the following example.

**Lemma 2** Let $\alpha \in (0, 1)$ and the triangulation $T(\alpha)$ as depicted in Figure 1. Let

$$k_\alpha := \sqrt{\frac{6(2-\alpha)}{\alpha(1-\alpha)}}$$

Then for any $k \in \mathbb{R} \setminus \{0\}$ the Galerkin discretization (3) of (2) with conforming piecewise linear elements $S^p_T(\alpha)$ is well posed if $k \neq \pm k_\alpha$. For $k = \pm k_\alpha$, the system matrix $A_k$ is singular and its kernel has dimension one.

This lemma shows that there exists finite element meshes for two-dimensional domains such that the discrete Helmholtz problem is not well posed. In our presentation, we describe an algorithm MOTZ (marching of the zeroes) which is based on a discrete unique continuation principle, which takes as an input the finite element mesh and gives the result “certified” if the discretization (3) leads to a well posed linear system. Otherwise the algorithm returns the output “critical”.

References


Monday, July 25, First Afternoon Session
Decay Theory and Numerical Analysis for Hybrid Frequency/Time Methods in Long-Time Transient Wave Scattering

Thomas G. Anderson$^{1,*}$, Oscar P. Bruno$^{2}$

$^{1}$Mathematics, University of Michigan, Ann Arbor, MI USA
$^{2}$Applied & Computational Mathematics, California Institute of Technology, Pasadena, CA USA
$^{*}$Email: tganders@umich.edu

Abstract

Frequency/time hybrid integral-equation methods [1] for transient wave scattering have been demonstrated to provide a highly efficient and accurate, trivially parallelizable means to compute solutions to time-domain scattering problems. We discuss further enhancements for high-fidelity simulation of scattering of long wave-trains via connection to newly-developed results in time-domain scattering theory. The new theory impacts on several long-standing problems in scattering theory, resolving open questions relating to “domain-of-dependence” and decay for problems of wave scattering by bounded, possibly trapping, obstacles. In particular, we present the first rapid decay estimates for connected trapping obstacles and provide norm-bounds on physical surface quantities in terms of measurements over a finite history of time. The theory leads to efficient sum-truncation numerical analysis results for hybrid wave scattering methods that justify an $O(1)$ asymptotic cost for producing solutions at arbitrarily large times.

Keywords: transient wave propagation, integral equations, decay theory, domain-of-dependence bounds

1 Introduction

Frequency-time hybrid methods [1] for the obstacle scattering problem

$$
\frac{\partial^2 u}{\partial t^2}(\mathbf{r}, t) - c^2 \Delta u(\mathbf{r}, t) = 0, \quad \mathbf{r} \in \Omega^c, \quad (1a)
$$
$$
u(\mathbf{r}, 0) = \frac{\partial u}{\partial t}(\mathbf{r}, 0) = 0, \quad (1b)
$$
$$
u(\mathbf{r}, t) = b(\mathbf{r}, t) \quad (\mathbf{r}, t) \in \Gamma \times [0, T^{inc}], \quad (1c)
$$

with Lipschitz boundary $\Gamma = \partial \Omega$, rely on Fourier time transformation of the incident wavefield $b$ in conjunction with certain time-partitioning and windowing techniques which serve to allow solutions at all times $t$ to be computed on the basis of solutions to a fixed set of frequency-domain problems. Briefly, the method uses well-spaced time-window centers $s_k \in [0, T^{inc}]$ and smooth compactly-supported window functions $w_k(t) = w(t - s_k)$ to expand $b$ in a partition of unity representation $b(\mathbf{r}, t) = \sum_{k=1}^{K} b_k(\mathbf{r}, t)$, where the functions $b_k$ are temporally-localized “wave packets” that also solve (1a) and serve as boundary data for solutions $u_k$ to (1). The solution results by reconstruction via the sum $u(\mathbf{r}, t) = \sum_{k=1}^{K} u_k(\mathbf{r}, t)$.

We will present efficient means to produce solutions $u_k$ at arbitrary times $t$ at $O(1)$ cost. Furthermore, it is important to note that since $K = O(T^{inc})$ the sum-representation of $u$ in principle involves an increasing number of solutions $u_k$—an issue that we resolve in what follows on the basis of solution decay.

2 3D decay and sum-truncation

In our surface-scattering context, we use the representation formula,

$$
u(\mathbf{r}, t) = (S \psi_k)(\mathbf{r}, t), \quad \psi_k = \partial_n u_k^{tot},
$$

where $S$ the time-domain single layer potential, from which it follows that if bounds on $\psi_k$ can be established, then the contribution of $u_k$ to the full solution $u$ on certain space-time regions $\mathcal{R} \times \mathcal{T}$ can be neglected with provably small error:

**Lemma.** Let $\mathcal{R} \subset \Omega^c$ satisfy $\text{dist}(\mathcal{R}, \Gamma) > 0$, and denote by $T_0$ a given observation time. Then there exists a (known) constant $C(\mathcal{R})$ such that

$$
sup_{t > T_0 + r_{\text{max}}/c} |u_k(\mathbf{r}, t)| \leq C \sup_{t > T_0} ||\psi_k(\cdot, t)||_{L^2(\mathcal{T})},
$$

where $r_{\text{max}} = \max_{\mathbf{r} \in \mathcal{R}, \mathbf{r}' \in \Gamma} |\mathbf{r} - \mathbf{r}'|$. We develop a novel class of time-domain estimates: “domain-of-dependence” estimates that bound $\psi_k$ in terms of its values over a finite time-history of length about $\text{diam}(\Omega)/c$.

We show more, that in fact solutions decay: the decay theorem applies to obstacles satisfying a certain $q$-growth condition, known to be satisfied by a variety of obstacles.
Theorem ([2]). Let $\Gamma$ be the boundary of an obstacle $\Omega \subset \mathbb{R}^3$ satisfying a $q$-growth condition and assume that the incident wavefield packet $b_k$ is sufficiently smooth. Let $I_{T_0}$ be any time interval (with upper limit $T_0$) with length exceeding $\text{diam}(\Omega)/c$ and laying after the incident packet ceases on $\Omega$. Then for each positive integer $n$ there exists a $C > 0$ independent of $b_k$ and of $T_0$ such that $\psi_k$ satisfies

$$
\|\psi_k(\cdot, t)\|_{L^2(\Gamma)} \leq C(t - T_0)^{1/2 - n} \|\psi_k\|_{H^{(q+1)+1}(I_{T_0};L^2(\Gamma))} \quad \text{for all } t > T_0.
$$

Figure 1: Deep rectangular cavity that satisfies a $q$-growth condition.

Definition ($q$-growth condition). A Lipschitz obstacle $\Omega$ satisfies a $q$-growth condition if there exists a $C > 0$ such that for a non-negative $q$ the frequency-domain combined-field operator $A_\omega$ satisfies

$$
\|A_\omega^{-1}\|_{L^2(\Gamma) \rightarrow L^2(\Gamma)} \leq C\omega^q \quad \text{as } \omega \rightarrow \infty.
$$

The decay theorem above enables the following numerical analysis result for hybrid frequency/time methods, showing that only an $O(1)$ number of solutions $u_k$ need to be computed for approximation (within some tolerance $\varepsilon_{\text{tol}}$) of the solution $u$.

Theorem ([3]). Let $\Gamma$ be the boundary of an obstacle that satisfies a $q$-growth condition. For smooth incident data, a region of space $\mathcal{R}$ of diameter $D_r$ and a time interval $\mathcal{T}$ of length $D_t$, there exist for every $\varepsilon_{\text{tol}} > 0$ an integer $M(\varepsilon_{\text{tol}}, D_r, D_t)$ and certain integers $M_l$ and $M_f$ satisfying $M_f - M_l = M$ so that for all incident wavefields

$$
\sup_{t \in \mathcal{T}} \left| u(r, t) - \sum_{k=M_l}^{M_l-1} u_k(r, t) \right| \leq C(\Gamma, D_r, D_t)\varepsilon_{\text{tol}}.
$$

Numerical experiments confirm the guarantees of this theorem for problems with incident wavetrains of many thousands of wavelengths in duration (Figure 2).

3 Classical Scattering Theory

Our primary decay theorem is a result of independent interest in the field of scattering theory, as it is the first decay result not based on the classical Lax-Phillips approach which has not been used to establish wave decay for any of the known trapping obstacles that have resonances lying arbitrarily close to the real axis (i.e. when wave solutions cannot be exponentially decaying). Our techniques are based on real-axis estimates (based on the $q$-growth condition) and use integration by parts as well as frequency-differentiated boundary integral densities, resulting in the first rapid decay estimates (a) in connected-trapping contexts and (b) In contexts where trapped orbits span the full volume of a physical cube (Figure 1).

References


Long time behaviour for electromagnetic waves in dissipative Lorentz media

Maxence CASSIER¹, Patrick JOLY², Alejandro ROSAS²

¹Aix Marseille Univ, CNRS, Centrale Marseille, Institut Fresnel, Marseille, France
²POEMS, ENSTA Paris, Institut Polytechnique de Paris, 91120 Palaiseau, France

Abstract
A very general class of models for describing the propagation of waves in dispersive electromagnetic media is provided by generalized Lorentz models [1]. In this work, we study the long time behaviour of the solutions of the dissipative version of these models.

1 Introduction

We are interested in Maxwell’s equations

\[
\begin{align*}
\varepsilon_0 \partial_t \mathbf{E} - \nabla \times \mathbf{H} + \varepsilon_0 \partial_t \mathbf{P} &= 0, \\
\mu_0 \partial_t \mathbf{H} + \nabla \times \mathbf{E} + \mu_0 \partial_t \mathbf{M} &= 0,
\end{align*}
\]

where \(\mathbf{E}\) and \(\mathbf{H}\) are, respectively, the electric and magnetic fields, while \(\mathbf{P}\) (resp. \(\mathbf{M}\)) is the electric polarization (resp. magnetization). In generalized dissipative Lorentz media, these are related to the electromagnetic field via a system of ODE’s (the constitutive laws of the medium)

\[
\begin{align*}
P &= \sum_{j=1}^{N_e} \Omega_{e,j}^2 P_j, \\ M &= \sum_{l=1}^{N_m} \Omega_{m,l}^2 M_l, \\
\partial_t^2 P_j + \alpha_{e,j} \partial_t P_j + \omega_{e,j}^2 P_j &= \mathbf{E}, \\
\partial_t^2 M_l + \alpha_{m,l} \partial_t M_l + \omega_{m,l}^2 M_l &= \mathbf{H},
\end{align*}
\]

where \((P_j, \partial_t P_j, M_l, \partial_t M_l)\) vanish at \(t = 0\). In (1.2), \((\Omega_{e,j}, \Omega_{m,l}) > 0\) while \((\alpha_{e,j}, \alpha_{m,l}) \geq 0\) and \((\omega_{e,j}, \omega_{m,l}) > 0\). Our goal is to analyze the long time behaviour of the solution of the Cauchy problem associated to (1.1, 1.2) and any initial data \((\mathbf{E}_0, \mathbf{H}_0)\) under the so-called weak dissipative assumption

\[
\sum_{j=1}^{N_e} \alpha_{e,j} + \sum_{l=1}^{N_m} \alpha_{m,l} > 0.
\]

2 Main results

In what follows \(f \lesssim g\) means \(f \leq C g\), for some constant \(C > 0\) independent of \(x, t, \mathbf{E}_0, \mathbf{H}_0\).

Let \(\mathcal{E}(t)\) be the electromagnetic energy

\[
\mathcal{E}(t) = \frac{1}{2} \int_{\mathbb{R}^3} (\varepsilon_0 |\mathbf{E}|^2 + \mu_0 |\mathbf{H}|^2)(x, t) \, dx
\]

The generic result (cf. Remark 3) is as follows

**Theorem 1** For \(\mathbf{E}_0\) and \(\mathbf{H}_0\) in \(L^2(\mathbb{R}^3)^3\) such that \(\nabla \cdot \mathbf{E}_0 = \nabla \cdot \mathbf{H}_0 = 0\), the energy \(\mathcal{E}(t)\) tends to 0 when \(t \to +\infty\). Moreover if for some integers \(m \geq 0\) and \(p \geq 0\),

\[
(\mathbf{E}_0, \mathbf{H}_0) \in H^m(\mathbb{R}^3)^3 \times H^m(\mathbb{R}^3)^3,
\]

\[
|x|^p (\mathbf{E}_0, \mathbf{H}_0) \in L^1(\mathbb{R}^3)^3 \times L^1(\mathbb{R}^3)^3,
\]

\[
\int_{\mathbb{R}^3} x^\alpha \mathbf{E}_0 \, dx = 0, \quad \int_{\mathbb{R}^3} x^\alpha \mathbf{H}_0 \, dx = 0, \quad \forall |\alpha| < p
\]

one has a polynomial decay rate

\[
\mathcal{E}(t) \leq C_p^m(\mathbf{E}_0, \mathbf{H}_0) \frac{t^{-m}}{t^{-\frac{1}{2}}} + \frac{C_1^p(\mathbf{E}_0, \mathbf{H}_0)}{t^{rac{1}{2}}}
\]

where the above constants satisfy

\[
C_p^m(\mathbf{E}_0, \mathbf{H}_0) \leq \|\mathbf{E}_0\|^2_{H^m(\mathbb{R}^3)} + \|\mathbf{H}_0\|^2_{H^m(\mathbb{R}^3)},
\]

\[
C_1^p(\mathbf{E}_0, \mathbf{H}_0) \leq \|\mathbf{E}_0\|^2_{L^1(\mathbb{R}^3)} + \|\mathbf{H}_0\|^2_{L^1(\mathbb{R}^3)}
\]

and \(\|u\|_{L^1(\mathbb{R}^3)} := \left\|(1 + |x|^p) u\right\|_{L^1(\mathbb{R}^3)}\).

**Remark 2** The upper bounds in (2.3) are sharp in the sense that similar lower bounds can be obtained for well chosen initial data.

**Remark 3** The statement of the theorem has to be slightly modified if one of the \(\alpha_{e,j}\) vanishes while \(\alpha_{e,m} = 0\) for all \(m\) (or vice versa). More precisely, with the same assumptions, one has to replace in the estimate (2.3) \(t^{-m}\) by \(t^{-m/2}\).

3 Comparison with the literature

The law (1.2) enters a more general class of non local (in time) constitutive laws of the form

\[
\begin{align*}
P(x, \cdot) &= \chi_e \ast \mathbf{E}(x, \cdot), \\
M(x, \cdot) &= \chi_m \ast \mathbf{H}(x, \cdot)
\end{align*}
\]
where \((\chi_e, \chi_m)\) are time convolution causal kernels. The long time behavior of solutions of (1.1, 3.1) has been investigated in many papers such as in [2] for bounded domains of propagation (using abstract results from semi-group theory). In these works, polynomial stability, i.e. time decay estimates of the type
\[
\mathcal{E}(t) \leq (1 + t)^{-p}, \quad \text{for some } p > 0, \quad (3.2)
\]
is proven under direct assumptions on the kernels \((\chi_e, \chi_m)\). In the case of Lorentz media, the assumptions used in [2] are satisfied only under the strong dissipativity assumption, i.e.
\[
a_{e,j}, a_{m,\ell} > 0, \quad \forall \ j, \ell, \quad (3.3)
\]
Another major difference is in the method of proof: we use here a more physically oriented method based on a modal/spectral approach.

4 Method of proof

One first writes the problem as a generalized Schrödinger equation of the form
\[
\frac{dU}{dt} + i\mathcal{A}(\nabla)U = 0 \quad (4.1)
\]
where \(U := (E, H, P_j, \partial_t P_j, M_t, \partial_t M_t) \in \mathbb{R}^N\) with \(N = 3(2 + 2N_e + 2N_m)\) and \(\mathcal{A}(\nabla)\) is a first order differential operator in space. We apply the space Fourier transform
\[
U(x, t) \longrightarrow U(k, t),
\]
so that \(U(k, t)\) satisfies
\[
\frac{dU}{dt}(k, t) + i\mathcal{A}(k)U(k, t) = 0, \quad (4.2)
\]
where \(\mathcal{A}(k), k \in \mathbb{R}^3\) is a family of non-normal \(N \times N\) matrices. We next derive a priori estimates for \(U(k, t)\) before coming back to space domain via Plancherel’s theorem.

We have developed two approaches to obtain estimates in the \(k\)-space.

(I) Via frequency dependent Lyapunov functions.

This approach is more direct but limited to the strict dissipativity assumption (3.3).

We construct a \(|k|\)-dependent and positive quadratic functional \(\mathcal{L}_{m,p}(|k|; U)\) such that
\[
\frac{d}{dt} \mathcal{L}_{m,p}(|k|; U) + \Phi(|k|) \mathcal{L}_{m,p}(|k|; U) \leq 0,
\]
for some function \(\Phi(r) > 0\) \((r \in \mathbb{R}_+^+)\). Then combining Grönwall’s lemma with a careful examination of the behaviour of \(\Phi(|k|)\) for small and large values of \(|k|\) leads to (2.3).

(II) Via spectral decomposition.

We use the spectrum \(\{\omega_n(k)\}\) of \(\mathcal{A}(k)\) which is made of the solutions of a dispersion relation that satisfy \(\Im \omega_n(k) < 0\). We then use the associated spectral decomposition of \(\mathcal{A}(k)\) to represent the solution \(U(k, t)\) of (4.2) as
\[
U(k, t) = \sum e^{-i\omega_n(k)t} P_n(k, t) U_0(k), \quad (4.3)
\]
where the operators \(P_n(k, t)\) are directly related to the spectral projectors of \(\mathcal{A}(k)\). We then split the analysis in three parts:

(i) estimates for low (space) frequencies \(|k| < m,\)
(ii) estimates for high frequencies \(|k| > M,\)
(iii) estimates for mid-frequencies \(m \leq |k| < M.\)

While step (iii) provides a uniform (in \(k\)) exponential decay, the polynomial decay results from the estimates (i) and (ii) which rely on

(a) the asymptotic behaviour of each \(\omega_n(k)\) for small and large values of \(|k|,\)
(b) uniform bounds for the operators \(P_n(k, t).\)

For the above, we use the implicit function theorem and the holomorphic functional calculus.

References

Bi-Parametric Operator Preconditioning and Applications

Carlos Jerez-Hanckes1,∗, Paul Escapil-Inchauspé1
1Faculty of Engineering and Sciences, Universidad Adolfo Ibáñez, Santiago, Chile
∗Email: carlos.jerez@uai.cl

Abstract
We extend the operator preconditioning framework [1] to Petrov-Galerkin methods while accounting for parameter-dependent perturbations of both variational forms and their preconditioners, as occurs when performing numerical approximations. By considering different perturbation parameters for the original form and its preconditioner, our bi-parametric abstract setting leads to robust and controlled schemes. For Hilbert spaces, we derive exhaustive linear and super-linear convergence estimates for iterative solvers, such as h-independent convergence bounds, when preconditioning with low accuracy or, equivalently, with highly compressed approximations.

Keywords: Operator preconditioning, Galerkin methods, Numerical approximation, Iterative linear solvers

1 Introduction
In this note, we extend the framework of operator preconditioning (OP) from Bubnov-Galerkin to general Petrov-Galerkin methods (OP-PG) as well as analyze the effects of numerical perturbations in iterative solvers. In this regard, we provide estimates for spectral and Euclidean condition numbers with details found in [2]. Next, we consider parameter-dependent perturbed problems and introduce the bi-parametric OP paradigm used, for example, for fast Calderón preconditioning [3,6]. This allows for explicit bounds on spectral and Euclidean condition numbers with respect to perturbations. We further deduce linear convergence results for GMRES(m) when working on Hilbert spaces.

2 Bi-parametric Operator Preconditioning
Let X, Y, V and W be reflexive Banach spaces and let a ∈ L(X × Y; C) be a continuous complex sesqui-linear form, with induced operator A and norm ∥a∥. Similarly for c ∈ L(V × W; C), n ∈ L(V × Y; C), m ∈ L(X × W; C). For a linear form b ∈ Y′, the weak continuous problem is: seek u ∈ X such that
\[ a(u, v) = b(v), \quad \forall \ v \in Y. \] (1)

Given an index h > 0, we introduce finite-dimensional conforming spaces, i.e. X_h ⊂ X and Y_h ⊂ Y, and assume that dim(X_h) = dim(Y_h) = N, with N → ∞ as h → 0. Same occurs for V_h ⊂ V and W_h ⊂ W. The counterpart of (1) is the weak discrete problem: find u_h ∈ X_h such that
\[ a(u_h, v_h) = b(v_h), \quad \forall \ v_h \in Y_h. \] (2)

We build the stiffness Galerkin matrix and right-hand side
\[ A := (a(ϕ_j, ϕ_ι))_{i,j=1}^N, \quad b := (b_ι(ϕ_i))_{i=1}^N, \]
\[ \text{span}\{ϕ_j\}_{j=1}^N = X_h, \text{span}\{ϕ_ι\}_{ι=1}^N = Y_h. \]
\[ \text{span}\{ψ_i\}_{i=1}^N = V_h, \text{span}\{ξ_ι\}_{ι=1}^N = W_h, \]
\[ c := (a(ψ_j, ξ_i))_{ι,j=1}^N, \quad n := (n(ϕ_j, ϕ_ι))_{ι,j=1}^N \]
and M := (n(ϕ_j, ϕ_ι))_{ι,j=1}^N.

We are ready to give a notion of admissible perturbations needed for the ensuing analysis.

Definition 1 ((h, ν)-perturbation) Let ν ∈ [0,1] and h > 0 be given. We say that a_ν ∈ L(X × Y; C) is a (h, ν)-perturbation of a if it belongs to the set Φ_{h,ν}(a):
\[ a_ν ∈ Φ_{h,ν}(a) \iff γ^{-1}_ν[a(u_h, v_h) - a_ν(u_h, v_h)] ≤ ν\|u_h\|_X\|v_h\|_Y, \]
\[ ∀ u_h ∈ X_h, \forall v_h ∈ Y_h. \]
Likewise, we define b_ν ∈ Y′ as being a (h, ν)-perturbation of b.

Inspired by [1], we state the preconditioned version of the operator equation for PG Galerkin: seek u ∈ X such that
\[ ((CA)) : \quad PAu = Pb, \quad \text{with} \quad P := M^{-1}CN^{-1}. \]
Its perturbed matrix version reads: find u_ν ∈ C^N such that
\[ ((CA))_{h,ν} : \quad P_νA_νu_ν = P_νb_ν, \]
with P_ν := M^{-1}C_νN^{-1}. 

Theorem 2 (Bi-Parametric OP-PG [2]) For
the perturbed problem \(((\text{CA}))_{\mu,\nu}\) for \(\mu,\nu \in [0,1]\)
and \(h > 0\), the spectral condition number is bounded as
\[
\kappa_S(P_{\mu}A_{\nu}) \leq K_\star \left(\frac{1 + \mu}{1 - \mu}\right) \left(\frac{1 + \nu}{1 - \nu}\right) =: K_{\star,\mu,\nu}.
\]
with \(K_\star\) the original estimate for OP in [1].

3 Iterative Solvers Performance: Hilbert space setting
Consider \(X \equiv H\) with \(H\) being a Hilbert space
with inner product \((\cdot,\cdot)_H\) and \(\|\cdot\|_H = \sqrt{(\cdot,\cdot)_H}\).
We introduce the \(H\)-field of values \(V_H(\cdot)\) [4].

Assumption 1 For \(((\text{CA}))_{\mu,\nu}\) with \(X := H\)
being a Hilbert space, assume that there holds that
\[
\gamma_{C_\mu} \gamma_{A_\nu} \frac{\|m\|_H}{\|n\|_H} \leq \mathcal{V}_H(P_{h,\mu}A_{h,\nu}) \quad \text{and}
\gamma_{M} \gamma_{N} \frac{\|c_{\mu}\|_H}{\|a_{\nu}\|_H} \leq \mathcal{V}_H((P_{h,\mu}A_{h,\nu})^{-1}).
\]
With this, we can apply the linear convergence results for GMRES to \(((\text{CA}))_{\mu,\nu}\) [2].

Theorem 3 Consider \(((\text{CA}))_{\mu,\nu}\) along with Assumption 1. Then, the numerical radius for the
weighted GMRES\((m)\) for \(1 \leq k, m \leq N\) is bounded as
\[
\rho_k^{(m)} \leq \left(1 - \frac{1}{K_{\star,\mu,\nu}}\right)^{\frac{1}{2}}.
\]

4 Fast Calderón Preconditioning
We test our ideas by using the bi-parametric framework to the Calderón preconditioned EFIE [5] for a complex shape [6]. Rough approximations are implied by the \(H\)-matrix tolerance and
quadrature rules. Besides providing similar convergence results for the Euclidean GMRES\((m)\) (see Fig. 1), one also observes significant gains in computational time and memory usage.

5 Conclusion
For general Petrov-Galerkin methods, we considered their operator preconditioning and
introduced the novel bi-parametric framework. Several results were derived including bounds in
Euclidean norm for the convergence of iterative solvers when preconditioning, with GMRES as a reference. These results pave the way toward new paradigms for preconditioning, as they allow to craft robust preconditioners, better understand the efficiency of existing ones and relate them to experimental results.

References
An OSRC Preconditioner for the EFIE

Ignacia Fierro-Piccardo\textsuperscript{1,*}, Timo Betcke\textsuperscript{1,2}

\textsuperscript{1}Department of Mathematics, University College London, London, United Kingdom
\textsuperscript{2}Department of Mathematics, University College London, London, United Kingdom

*Email: ucahmib@ucl.ac.uk

Abstract

In this research we demonstrate the preconditioning properties of an approximation of the Magnetic-to-Electric operator applied to the EFIE (Electric Field Integral Equation) when solving electromagnetic scattering problems. For this we use a Bempp implementation and show a number of numerical comparisons against other preconditioning techniques like the Calderón Preconditioner.

Keywords: Preconditioner, OSRC approximation, Electric Field Integral Equation.

1 Introduction

When modelling electromagnetic scattering of PEC objects we resort to Maxwell’s Equations. There are many numerical methods to solve this problem, but specifically when modelling scattering in unbounded domains, we resort to Boundary Elements Methods to solve them, where the electromagnetic field can be calculated from the representation formula:

\[ e(x) := -\mathcal{T}([\gamma_{\nu}]_{\Gamma} e(x) - \mathcal{K}([\gamma_{\nu}]_{\Gamma} e(x)) \]

\[ \mathcal{T}(p)(x) := ik \int_{\Gamma} p(y) G(x,y) \]

\[ - \frac{1}{ik} \nabla_x \int_{\Gamma} G(x,y) \text{Div}_y p(y) d\Gamma(y), \]

\[ \mathcal{K}(p)(x) := \text{curl}_x \int_{\Gamma} G(x,y) p(y) d\Gamma(y) \]

and

\[ \gamma^+_{\nu} p := \lim_{\Omega^{\pm} \ni x' \to x \in \Gamma} p(x') \times \nu(x) \]

\[ \gamma^\pm_{\nu} w := \lim_{\Omega^{\pm} \ni x' \to x \in \Gamma} w(x') \cdot \nu(x) \]

To find \( e(x) \) we can often use the Electric Field Integral Equation that comes from applying traces to (1):

\[ -S_{\kappa} \gamma^+_{\nu} e = \left( C_{\kappa} + \frac{I}{2} \right) \gamma^+_{\nu} u \]

However, the EFIE being a First Kind Fredholm operator, needs a regulariser, namely \( R \):

\[ RS_{\kappa} \gamma^+_{\nu} e = -R \left( \frac{I}{2} + C_{\kappa} \right) \gamma^+_{\nu} e^{inc} \]

One if the most known preconditioners for the EFIE is the so-called Calderón Preconditioner [2], which is the very same EFIE operator and has the property of transforming the EFIE into a Second Kind Fredholm operator:

\[ S^2_{\kappa} = C_{\kappa} - \frac{I}{4} \]

which is very effective and robust, but has the disadvantage of needing from a barycentric discretisation of the mesh. Hence, the main objective of this research is to propose and test an alternative preconditioner that does not require mesh refinements and keeps the Calderón Preconditioner robustness.

2 MtE Preconditioner for the EFIE

A good alternative for a regulariser \( R \) is the exact Magnetic-to-Electric (MtE) operator:

\[ V^{-1} = -\left( \frac{I}{2} + C_{\kappa} \right)^{-1} S_{\kappa} \]

which can be easily seen to result in a Second Kind Fredholm operator when applied to \( S_{\kappa} \):

\[ V^{-1} S_{\kappa} \equiv \left( \frac{I}{2} - C_{\kappa} \right). \]

However, the application of the MtE is not practical as its computation is as expensive as the solution of the EFIE itself. In [1] a local surface approximation of the MtE for time-harmonic Maxwell’s equations was developed. In particular, the authors propose the following approximation operator to the MtE:
\[ \gamma_N^+ u = \Lambda^{ex} (\nu \times \gamma_N^+ u) \text{ on } \Gamma, \]

where
\[ \Lambda^{ex} := (I + J)^{-1/2} \left( I - \frac{1}{\kappa_\varepsilon^2 \text{opt}} \text{curl} I \right), \]

\[ J := \text{Grad} \frac{1}{\kappa_\varepsilon^2} \text{Div} \Gamma - \text{curl} \frac{1}{\kappa_\varepsilon^2} \text{curl} I. \]

In [1] the authors propose a Padé approximation of \((I + J)^{1/2}\) which we have adapted in [3] to build an effective EFIE preconditioner. The discrete form of the preconditioned system takes the form

\[ -\Lambda_{2,\varepsilon,h}^{-1} \left( R_0 I_h - I_h \sum_{j=1}^{Np} A_j B_j \Pi_{j,\varepsilon,h}^{-1} S_{k,h} y = \text{rhs}_h, \right. \]

where \(\Pi_{j,\varepsilon,h}\) involves Schur complements of sparse operators. In this talk we describe how this can be solved efficiently and used as a highly effective preconditioner that is almost as cheap to evaluate as the unpreconditioned system but provides similar efficiency to expensive Calderón preconditioners.

### 3 Numerical Results

In the following we demonstrate some results on the unit sphere obtained by implementing the preconditioner in the boundary element software package Bempp. Figure 1 demonstrates the iteration counts of variants of the MtE preconditioner compared to standard Calderón preconditioning \((S_{2,h})\) and no preconditioning \((S_{k,h})\), showing that performance is similar to Calderón preconditioning. Tables 1 and 2 show that the cost of the MtE preconditioner is much lower than that of a Calderón preconditioner and only little more than no preconditioning at all. Details of the implementation of our preconditioner can be found in [3].

### References


<table>
<thead>
<tr>
<th>Formulation</th>
<th>(\kappa = 3\pi)</th>
<th>(\kappa = 4\pi)</th>
<th>(\kappa = 5\pi)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(S_{k,h})</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
</tr>
<tr>
<td>(S_2^{h})</td>
<td>19.273</td>
<td>15.738</td>
<td>16.612</td>
</tr>
<tr>
<td>(V_{z,h,1.1} S_{k,h})</td>
<td>1.148</td>
<td>1.180</td>
<td>2.571</td>
</tr>
<tr>
<td>(V_{z,h,1.2} S_{k,h})</td>
<td>1.265</td>
<td>1.339</td>
<td>1.194</td>
</tr>
<tr>
<td>(V_{z,h,2.1} S_{k,h})</td>
<td>1.010</td>
<td>1.012</td>
<td>1.067</td>
</tr>
<tr>
<td>(V_{z,h,2.2} S_{k,h})</td>
<td>1.010</td>
<td>1.012</td>
<td>1.025</td>
</tr>
</tbody>
</table>

Table 1: \(T(R S_{k,h}) / T(S_{k,h})\) assembly time ratios comparison between different EFIE formulations on a grid with constant relation \(\kappa \cdot h\).

![Figure 1: Iterations comparison between different EFIE formulations on a grid with varying \(h\).](image)

<table>
<thead>
<tr>
<th>Formulation</th>
<th>(h = 0.037)</th>
<th>(h = 0.056)</th>
<th>(h = 0.074)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(S_{k,h})</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
</tr>
<tr>
<td>(S_2^{h})</td>
<td>22.122</td>
<td>20.792</td>
<td>18.179</td>
</tr>
<tr>
<td>(V_{z,h,1.1} S_{k,h})</td>
<td>1.128</td>
<td>1.098</td>
<td>1.088</td>
</tr>
<tr>
<td>(V_{z,h,1.2} S_{k,h})</td>
<td>1.282</td>
<td>1.218</td>
<td>1.198</td>
</tr>
<tr>
<td>(V_{z,h,2.1} S_{k,h})</td>
<td>1.012</td>
<td>1.010</td>
<td>1.010</td>
</tr>
<tr>
<td>(V_{z,h,2.2} S_{k,h})</td>
<td>1.012</td>
<td>1.010</td>
<td>1.010</td>
</tr>
</tbody>
</table>

Table 2: \(T(R S_{k,h}) / T(S_{k,h})\) assembly time ratios comparison between different EFIE formulations on a grid with varying \(h\).
Probabilistic Wave Inversion Using Gibbs Posteriors: Application in Ultrasound Vibrometry

Youngsoo Baek¹, Wilkins Aquino²*, Sayan Mukherjee¹

¹Department of Statistics, Duke University, Durham, USA
²Department of Mechanical Engineering, Duke University, Durham, USA
*Email: wilkins.aquino@duke.edu

Abstract
We propose a general framework for solving probabilistic wave inversion with applications in dispersion-based ultrasound vibrometry. Bayesian methods, while attractive, are often unable to handle the lack of a likelihood function due to the presence of nonlinear operators in the model. We adopt a loss-based framework [1] to estimate the parameter and summarize our confidence through Gibbs posteriors. Gibbs posteriors are derived as a solution to the variational problem on the space of distributional estimators of the parameter. We develop a cross-validation strategy that allows us to draw samples from the Gibbs posterior, tune the free parameter, and make pairwise comparisons between many models for practical inversion workflow. We support the merits of our method through simulated dispersion-based wave inversions that arise in the characterization of arterial vessels using ultrasound vibrometry.

Keywords: Uncertainty quantification, inverse problems, wave inversion, stochastic inversion

1 Introduction
The majority of Bayesian methods for inverse problems rely on an exact noise model, typically assumed to be i.i.d. Gaussian, to perform inference. It is desirable to extend such inference to more general settings where a noise model is unavailable or modeling the data generating mechanism is challenging. For instance, in arterial ultrasound vibrometry [2], space-time data is transformed to dispersion curves in the frequency domain through nonlinear operations. Then, these curves are used to invert for elastic or viscoelastic parameters. Even if the noise generating mechanisms are known in the space-time data, postulating closed-form likelihoods using dispersion curves becomes a very difficult (often impossible) task. The Gibbs posterior provides a way to update belief distributions in a general setting without the need of an explicit likelihood function [1]. Instead, the Gibbs posterior is applicable where the unknown parameters are only connected to the data through a loss function. Our contributions are: 1) the development of a principled approach to calibrating a Gibbs posterior that generalizes the Bayes posterior, and 2) the application of this framework to the inversion of geometric and material parameters in waveguides using dispersion data.

2 Incorporating Gibbs Posteriors to Inversion
Our interest is in solving an inverse problem for finite-dimensional parameter \( \theta \in \Theta \subset \mathbb{R}^p \). Suppose we define a forward model through the following equation:

\[
\mathcal{M}(\mathcal{F}(\theta), \theta) = 0. \tag{1}
\]

\( \mathcal{M} \) can be thought of as a PDE for an elastic medium, which implicitly defines the forward operator \( \mathcal{F} \) that maps \( \theta \) to a solution field of PDE. In practice, we solve the discretized equation model \( \mathcal{M} \) and compute a discretized solution field, \( \hat{\mathcal{F}} : \Theta \rightarrow \mathbb{R}^D \times \mathbb{R}^T \). We assume observing an \( n \)-ensemble model (possibly \( n > 1 \)) contaminated with an i.i.d. noise as

\[
x_i(u, t) = \hat{\mathcal{F}}(\theta) + \epsilon_i, \quad \epsilon_i \sim P, \quad i = 1, \ldots, n. \tag{2}
\]

We consider waveguide problems in the frequency domain. In this context, space-time states are transformed to dispersion curves in the frequency domain. Thus, we have the following observation model in \( \mathbb{R}^d \):

\[
y_i(\omega) = \hat{\mathcal{G}}(\hat{\mathcal{F}}(\theta) + \epsilon_i). \tag{3}
\]

where \( \hat{\mathcal{G}} \) is a nonlinear operator that maps space-time data to dispersion curves. We notice that the pushforward through \( \hat{\mathcal{G}} \) complicates the simple linear noise model in 2.

The abstract model (3) usually has a nonlinear, non-smooth form, which leads to an intractable likelihood of the sample dispersion curves
and a challenge to Bayesian methods. We instead assume an access to a loss function $l : \Theta \times \mathbb{R}^d \rightarrow \mathbb{R}$ quantifying discrepancy between the exact solution field $F_d(\theta)$ and noisy samples $y_i$'s. Then, we posit the following variational problem on the space of probability distributions for $\theta$ [1]:

$$\hat{\rho}(d\theta) = \arg\min_{\rho \ll \rho_0} \mathcal{L}(\rho),$$

$$\mathcal{L}(\rho) = W \sum_{i=1}^n \int l(\theta, y_i) \rho(d\theta) + D_{KL}(\rho|\rho_0).$$

(5)

The variational framework naturally extends the Tikhonov regularization in linear inverse problems, with $W$ playing the role of a regularization parameter. The solution of the problem is the following Gibbs posterior for $\theta$:

$$\hat{\rho}(d\theta) \equiv \frac{\exp(-W \sum_{i=1}^n l(\theta, y_i) \rho_0(d\theta))}{\int_\Theta \exp(-W \sum_{i=1}^n l(\theta, y_i) \rho_0(d\theta))}.$$  

(6)

When a true likelihood model can be exactly specified, we can match $W$ and loss function to that of a Bayesian posterior.

3 Computation and Simulation Studies

To develop a principled inversion workflow, we develop a cross-validation framework that simultaneously allows for drawing samples from a sequence of Gibbs posteriors and tuning $W$, using ideas from stochastic gradient descent (SGD) and sequential Monte Carlo (SMC). Furthermore, we show that a slight extension of the variational problem 6 and our calibration strategy allows for between-model comparison: for distinct loss functions, we can estimate their predictive optimality in the sample space $Y$ using cross-validation.

We apply our methods to simulated data that mimic dispersion curves arising in dispersion-based wave inversions. The goal is confidence statement about the material and geometric parameters of arterial vessels using ultrasound vibrometry. Fig.1 shows that our Gibbs posterior estimate covers the truth used to simulate the data, with its shape capturing the correlation between the parameters due to the model structure. Fig.2 compares different Gibbs posterior samples obtained by using different loss functions. In this example, $L^1$ loss is similarly accurate as $L^2$ loss in covering the truth, but leads to a narrower confidence region estimate and better predictive performance.

4 References

References


Damage Identification in Fiber Metal Laminates with Guided Ultrasonic Wave using Bayesian Inference and Model Order Reduction

Nanda Kishore Bellam Muralidhar$^{1,*}$, Natalie Rauter$^{2,2}$, Andrey Mikhailenko$^{2}$, Rolf Lammering$^{2}$, Dirk A. Lorenz$^{1}$

$^1$Institute of Analysis and Algebra, Technische Universität Braunschweig, Braunschweig, Germany
$^2$Institute of Mechanics, Helmut-Schmidt-University Hamburg, Hamburg, Germany

*Email: n.bellam-muralidhar@tu-braunschweig.de

Abstract

Structural health monitoring using guided ultrasonic wave (GUW) in fiber metal laminate (FML) seeks to precisely identify the damage with minimal use of sensors. In this research work, it is accomplished through Bayesian inference method that utilizes the sensor measured data and an accurate finite element model of GUW propagation in FML. The results are found to be promising when detecting and characterizing the damage.

Keywords: Guided ultrasonic wave, Fiber metal laminates, Model-order reduction, Bayesian inference

1 Introduction

Vibration-based structural health monitoring with guided ultrasonic waves (GUW) is one of the eminent techniques for damage identification in layered laminates, as their propagation behavior changes when interacting with a damage [1]. A Bayesian inference via Markov chain Monte Carlo (MCMC) method not only identifies the damage parameters from the measurements but also quantifies their uncertainties. However, the inference problem in a stochastic framework requires a very large number of forward simulations of the process which drastically rises the computational effort. Therefore, this research focuses on two key aspects: (a) generating a low-cost but accurate model through model-order reduction (MOR); (b) employing the produced global reduced-order model (ROM) with Bayesian inference to localize and characterize the damage.

2 Numerical Model of Lamb Wave Propagation

Numerical modeling and analysis of anti-symmetric lamb wave mode ($A_0$) propagation as well as its interaction with the defect in FML were studied using the FEM on COMSOL-Multiphysics© software. A 16-layered two dimensional carbon fiber reinforced plastic (CFRP)-steel laminate model was considered for further analysis. The excitation was realized by a five-cycle Hanning window with sinusoidal burst of 120 kHz central frequency, applied on the top and bottom left node of the model as shown in Figure 1. The damage was modeled as the loss of stiffness in a localized area within the steel lamina.

![Figure 1: 2D-Model setup in COMSOL®](image1)

Although COMSOL implicit solver was used, time step and mesh sizes were calculated using a Courant–Friedrichs–Lewy condition. The finite element simulated GUW signal measured by the sensor embedded in the FML model is plotted in Figure 2. The simulation time for a solve using this high-fidelity (HiFi) numerical model was 66.29 s.

![Figure 2: Displacement signal at sensor location](image2)
3 Parametric Model Order Reduction

In real-time operation, the construction of ROMs should be robust to parameter changes and needs to be fast such that the precomputed reduced model can be adapted to new sets of modeling parameters. In this research, parametric model-order reduction (PMOR) along with a surrogate model based on [2] was adapted to generate the global ROM. An adaptive POD-greedy algorithm was applied to train the ROM of GUW propagation in the FML. The training was carried out on a 3D parametric space, defined by Young’s modulus, position on the x-axis and length of the damage. The comparison of the out-of-plane displacement of FML obtained by the HiFi model and reduced-order model is shown in Figure 3. A detailed methodology of its application on GUW propagation in FML can be found in [3].

![Comparison of HiFi and reduced-order solution](image)

Figure 3: Comparison of HiFi and reduced-order solution

Using the adaptive POD-greedy approach, a speedup factor of 33.82 is achieved. This substantial decrease in the computational effort is very much appreciated in inverse problem analysis for the localization and characterization of the defect in the FML.

4 Damage Identification by Bayesian Inference

Bayesian inference for damage characterization was informed by the ROM instead of the high-fidelity model. A random walk procedure, MCMC method, was performed to draw the samples from the posterior distribution concerning the damage parameters: stiffness, x-position and length of the damage element in the FML. The synthetic measurement data is obtained by adding a zero mean Gaussian-type errors to the model output. Figure 4 and Figure 5 represents the histograms of the samples drawn to characterize the damage with parameters. It can be clearly seen that the true values of different parameters lie close to the bin corresponding to the maximum number of samples in the histogram.

![Histogram for stiffness of the damage](image)

Figure 4: Histogram for stiffness of the damage

![Histogram for the x-position and length of the damage](image)

Figure 5: Histogram for the x-position and length of the damage

References


Modal approximation for plasmonic resonators in the time domain

Pierre Millien$^{1,*}$, Lorenzo Baldassari$^2$, Alice Vanel

$^1$Institut Langevin, Espci, Paris, France
$^2$Department of Mathematics, ETH Zürich, Rämistrasse 101, 8092 Zurich, Switzerland

Email: pierre.millien@espci.fr

Abstract

We study the electromagnetic field scattered by a metallic nanoparticle with dispersive material parameters in a resonant regime. We consider the particle placed in a homogeneous medium in a low-frequency regime. We define modes for the non-Hermitian problem as perturbations of electro-static modes, and obtain a modal approximation of the scattered field in the frequency domain. The poles of the expansion correspond to the eigenvalues of a singular boundary integral operator and are shown to lie in a bounded region near the origin of the lower-half complex plane. Finally, we show that this modal representation gives a very good approximation of the field in the time domain. We present numerical simulations in two dimensions to corroborate our results.

Keywords: Plasmonic resonance · Time-domain modal expansion · Subwavelength resonators · Quasi-normal modes

Main results

The starting point is the Electric Field Integral Equation (or Lippman-Schwinger equation) in the scatterer $D$:

$$(I - \gamma^{-1}(\omega) T^{\omega}) E = E^{in} \quad \text{in } D, \quad (1)$$

where $T^{\omega}$ is a singular integral operator and $\gamma$ is a non-linear function of $\omega$ that depends on the permittivity model for the scatterer $D$. We assume $D$ has characteristic size $\delta$ with $\frac{\delta}{c} \ll 1$ where $c$ is the speed of light in the background. Building on the previous spectral analysis of $T$ [3] and classic results on the compact symmetrisable Neumann-Poincaré operator, we exhibit a complete modal basis for the static transmission problem.

Theorem 1 When $\omega \delta c^{-1} \to 0$, the electric field inside the particle converges to:

$$E^0 = \sum_{n=0}^{\infty} \frac{\gamma(\omega)}{\gamma(\omega) - \gamma_n} \langle E^{in}, e_n \rangle_{L^2(D,\mathbb{R}^3)} e_n \quad \text{in } D, \quad (2)$$

where $(e_n)_{n \in \mathbb{N}}$ is an orthonormal basis of $W(D)$ for the usual $L^2(D,\mathbb{R}^3)$ scalar product, eigenvectors of $T^\omega$ associated with the eigenvalue $\gamma_n$. The space $W(D)$ is the space of gradients of harmonic $H^1$ fields on $D$.

We show that, under the assumption that the particle is strictly convex, the excitation coefficients of the eigenfunctions exhibit superpolynomial decay with the order of the mode, and therefore the field can be well approximated by a finite number of modes. Using elementary perturbative analysis, we then show in Proposition 2 that the resolvent for the dynamic problem ($\omega \neq 0$) can be approximated by a perturbed resolvent of a finite-dimensional operator (the truncated static operator):

Proposition 2 There exists a sequence with superpolynomial decay $(\epsilon_N(E^{in}))_{N \in \mathbb{N}}$ depending only on $E^{in}$ and $B$, and a sequence of open complex neighbourhood of the origin $\mathcal{V}(N) \ni 0$ such that for $\omega \delta c^{-1} \in \mathcal{V}(N) \cap \mathbb{R}$ the electric field solution of (1) satisfies:

$$E = \sum_{n=0}^{N} \frac{\gamma(\omega)}{\gamma(\omega) - \gamma_n(\frac{\omega}{c})} e_n + O\left(\epsilon_N(E^{in}) \left(\left[\gamma(\omega) - \tilde{C}_D(\omega \delta c^{-1})\right]\right)ight),$$

in $D$ and $f(x) := xe^{x^2}$ and $\gamma_n(\frac{\omega}{c})$ are eigenvalues of $T^\omega_D$ obtained via classic perturbative spectral theory applied to $T^\omega_D$.

Next, using Rouché’s theorem, we prove the existence of poles for this approximated resolvent and give a resonance-like expansion for the electric field inside the particle:

Theorem 3 For a given $E^{in}$ there exists $N$ (depending on $E^{in}$), $\delta_{max}(N)$ such that for all $\delta < \delta_{max}(N)$, there exists $\omega_{max} = \mathcal{O}(\delta^{-1})$ such that for all $\omega \in \mathbb{R}$ satisfying $|\omega| < \omega_{max}$ the
following holds:

\[ E = \sum_{n=0}^{N} \frac{\gamma(\omega) - \gamma_n(\Omega_n(\delta))}{\gamma(\omega) - \gamma_n(\Omega_n(\delta))} \langle E_n, e_n \rangle_{L^2(D, \mathbb{R}^3)} e_n \]

+ \epsilon_{int} \text{ in } D,

and

\[ E(x) - E_n(x) = \sum_{n=0}^{N} \frac{\langle E_n, e_n \rangle_{L^2(D, \mathbb{R}^3)}}{\gamma(\omega) - \gamma_n(\Omega_n(\delta))} \left( \frac{\omega}{c} \right)^2 \int_D \Gamma^\pi(x, y)e_n(y)dy + \epsilon_{ext}(x) \text{ in } \mathbb{R}^3 \setminus D, \]

and \( \gamma_n(\Omega_n(\delta)) \) are the eigenvalues of \( T_D^\pi \) at the dynamic plasmonic resonant frequency \( \omega = \Omega_n(\delta) \) on \( W(D) \) associated with the eigenvectors \( e_n \), and \( \Gamma^\pi(x, y) \) the outgoing Green function associated with Maxwell’s equation in \( \mathbb{R}^3 \). The error terms \( \epsilon_{int} \) and \( \epsilon_{ext} \) depend mainly on the incident wave and the number of modes considered.

From this expansion we construct the so-called quasi-normal modes found in the physics literature. Finally, using elementary complex analysis tools, we give an expansion for the low-frequency part of the electromagnetic field in the time domain and we show that the truncated inverse Fourier transform (low frequency only, \( \omega < \rho \)) has the form:

\[ P_n[E^{\text{REM}}](x, t) = \sum_{n=1}^{N} C_n E_n(x)e^{-i\Omega_n(\delta)t} + \epsilon(x, t) \]

for \( t \geq t^n_0 \) where

\[ t^n_0(s, x) := \frac{1}{c} (|s - z| + |x - z| \pm 2\delta), \]

is the time it takes to the signal to reach first the scatterer from source point \( s \) and then observation point \( x \), and \( E_0 \) the generalised (exponentially diverging) eigenvectors, the so-called quasi normal modes. The error term \( \epsilon(x, t) \) can be analyzed precisely. By doing so, we show that in the time domain causality ensures that the electromagnetic field does not diverge exponentially in space. Similar results were obtained in [4] for a non-dispersive dielectric spherical scatterer in any frequency range.

In the scalar case, we numerically study the quality of the approximation in a two dimensional setting for different shapes of scatterers.

The real part of the field scattered by the ellipse and observed at some fixed observation point is the superposition of two dipole modes:

We also show that the approximation is valid well outside of the restrictive theoretical hypotheses from the paper, for example the approximation seems to be valid for non convex scatterers.

References


Asymptotic models for time-domain scattering by small particles

Maryna Kachanovska

1POEMS, CNRS, INRIA, ENSTA Paris, Institut Polytechnique de Paris, 91120 Palaiseau, France

Abstract

We propose a new asymptotic model for two-dimensional sound-soft scattering by small circular particles in the time domain. It generalizes existing Foldy-Lax models, enjoys uniform stability properties, and is second-order accurate.

Keywords: sound-soft scattering, asymptotic models, time domain

1 Introduction

We consider the problem of time-domain sound-soft scattering by small circular particles, in the regime when the size of the particles tends to zero. For the moment only very few related works exist in the time domain, see e.g. [1, 3].

2 Problem setting

Let \( N \in \mathbb{N}^* \), and \( R_j > 0 \), \( j = 1, \ldots, N \). We denote by \( B(a,r) := \{ x : \| x - a \| < r \} \), and consider the system of \( N \) circles, parametrized by a small parameter \( \varepsilon > 0 \),

\[
\Omega^\varepsilon = \bigcup_{j=1}^N B(c_j, \varepsilon R_j), \quad c_j \in \mathbb{R}^2, \quad j = 1, \ldots, N.
\]

Let \( \Omega^\varepsilon = \mathbb{R}^2 \setminus \overline{\Omega}^\varepsilon \), and

\[
\Gamma_j^\varepsilon = \partial B(c_j, \varepsilon R_j), \quad \Gamma^\varepsilon = \bigcup_j \Gamma_j^\varepsilon.
\]

We look for \( u^\varepsilon : \mathbb{R}^+ \times \Omega^\varepsilon \rightarrow \mathbb{R} \) solving

\[
\begin{align*}
\partial_t^2 u^\varepsilon - \Delta u^\varepsilon &= 0, & \text{in} \quad \mathbb{R}^+ \times \Omega^\varepsilon, \\
\gamma_0 u^\varepsilon(t) &= -\gamma_0 u^{inc}(t), & t \in \mathbb{R}^+,
\end{align*}
\]

(1)

where \( u^{inc} : \mathbb{R}^+ \times \mathbb{R}^2 \rightarrow \mathbb{R} \) is a known solution of the homogeneous wave equation in \( \mathbb{R}^2 \). Evidently, \( \lim_{\varepsilon \to 0} \| u^\varepsilon(t) \|_{L^2(\Omega^\varepsilon)} = 0 \), and it can be demonstrated that there exist \( u^{inc} \) and \( t > 0 \), s.t. \( \| u^\varepsilon(t) \|_{L^2(\Omega^\varepsilon)} \approx \log^{-1} \varepsilon^{-1} \); thus, approximating the field by zero leads to an error of \( O(\log^{-1} \varepsilon) \). Our goal is to find a higher-order approximation \( u_{app}^\varepsilon \) to \( u^\varepsilon \).

3 Motivation: one Foldy-Lax model

Since the problem (1) had been rather extensively studied in the frequency domain, it is natural to ask whether time-domain counterparts of the available Foldy-Lax models are of practical interest. We would like to illustrate that such models may be not robust. For this we consider the model [2], which is \( O(\varepsilon \log^{-1} \varepsilon) \)-accurate. The time-domain counterpart of the Foldy-Lax model of [2] approximates the field \( u^\varepsilon \) by the superposition of the point sources

\[
u^FL(t,x) = \sum_{k=1}^N G_t(\|x - c_k\|) * \mu_{\varepsilon,k},
\]

where \( \mu_{\varepsilon,k} \) and \( \gamma_0 \) are the unknown point densities and the unknown point source densities, \( \mu_{\varepsilon,k} : \mathbb{R}^+ \rightarrow \mathbb{R} \) solve

\[
\begin{align*}
u^inc(c_k,t) &= \frac{1}{2\pi \sqrt{r^2 - d^2}} \mu_{\varepsilon,k}(t), \quad t \in \mathbb{R}^+,
\end{align*}
\]

Unfortunately, this model may exhibit instabilities for some geometric configurations, when the particles are close to each other.

Lemma 1 Let \( N = 3 \), and \( R_k = 1 \), \( \forall i \). Let \( \varepsilon > 0 \) and \( \| c_i - c_j \| = c > 0 \) for all \( i \neq j \) and \( c/\varepsilon < 4 \). Then there exist \( u^{inc} \in C_\infty(\mathbb{R}^3) \) such that \( u^{inc} \notin C_\infty(\mathbb{R}^3) \) and \( A > 0 \) s.t. \( \lim_{t \to +\infty} \| e^{-At} u^FL(t) \|_{L^2(\mathbb{R}^3)} \geq \alpha \).

Let us remark that we observed this phenomenon in the numerical simulations as well. To cope with it, we propose an improved model*.

4 Galerkin Foldy-Lax model

4.1 Main idea and derivation

The solution to (1) can be represented as a single-layer potential of the unknown density \( \lambda^\varepsilon \):

\[
u^\varepsilon(t, x) = \int_0^t \int_{\Gamma^\varepsilon} G_{t-t'}(\|x - y\|) \lambda^\varepsilon(t', y) d\Gamma_y d\tau.
\]

The continuity of the trace of the single-layer potential yields the following boundary-integral equation for the density \( \lambda^\varepsilon \): for \( x \in \Gamma^\varepsilon, \ t \in \mathbb{R}^+ ,

\[
\gamma_0 u^{inc}(t, x) = \int_0^t \int_{\Gamma^\varepsilon} G_{t-t'}(\|x - y\|) \lambda^\varepsilon(t', y) d\Gamma_y d\tau.
\]

* I am grateful to Patrick Joly (POEMS) for the suggestion of the name of the new model.
Because the functional framework associated to the above problem is somewhat subtle, we rewrite it in the frequency domain. With \( b(\omega) \) denoting the Fourier-Laplace transform of \( b(t) \), i.e. \( \hat{b} = \mathcal{F}b \), the above integral equation can be rewritten as: find \( \hat{x}_\varepsilon \in H^{-1/2}(\Gamma^c) \), s.t.
\[
-\gamma_0 \hat{u}^{inc}(\omega, x) = \frac{i}{\lambda} \int_{\Gamma^c} H_0^1(\omega) \hat{x}_\varepsilon(\omega, y) d\Gamma y.
\]
Rewriting the above as: for all \( \phi \in H^{-1/2}(\Gamma^c) \),
\[
-\langle \gamma_0 \hat{u}^{inc}(\omega), \phi \rangle = \langle S(\omega) \hat{x}_\varepsilon, \phi \rangle \tag{2}
\]
we remark that the sesquilinear form in the right-hand side is coercive for each \( \omega \in \mathbb{C} : \Im \omega > 0 \). The respective continuity estimates on \( \hat{x}_\varepsilon \) can be made explicit in \( \omega \) and \( \Re \omega \); this allows to translate them into the time domain as stability estimates for \( \hat{x}_\varepsilon \). The coercivity of (2) translates straightforwardly to its conforming discretization, and thus automatically yields the stability of the corresponding discretization. Let
\[
S_0(\Gamma_k^c) := \{ \phi \in H^{-1/2}(\Gamma_k^c) : \phi = \text{const} \},
\]
\[
S_k^c := \prod_{k=1}^N S_0(\Gamma_k^c).
\]
We discretize (2) on this space: we look for \( \hat{x}_{\varepsilon,k}^{app} \in S_0^c \), which solves
\[
-\langle \gamma_0 \hat{u}^{inc}(\omega), \phi \rangle = \langle S(\omega) \hat{x}_{\varepsilon,k}^{app}, \phi \rangle, \quad \forall \phi \in S_0^c. \tag{3}
\]
The time-domain counterpart of (3) is then called the Galerkin Foldy-Lax model. Denoting by \( \hat{x}_{\varepsilon,k}^{app} = \hat{x}_{\varepsilon,k}^{app} \big|_{\Gamma_k^c} \), we obtain the following convolutional system of equations for unknown functions \( \lambda_{\varepsilon,k}^{app} \):
\[
-\int_{\Gamma_k^c} \hat{u}^{inc}(t, x) d\Gamma_x = \sum_{n=0}^N \int_0^t \sum_{\lambda_{\varepsilon,n}^{app}}(t-\tau) d\Gamma y. \tag{4}
\]
Knowing the densities \( \lambda_{\varepsilon,k}^{app} \) allows to compute \( u_{\varepsilon,k}^{app} \) according to the following rule:
\[
u_{\varepsilon,k}^{app}(x) = \sum_{\lambda_{\varepsilon,n}^{app}} \int_0^t \left( \int_{\Gamma_k^c} G_{\varepsilon,n}(x - y) d\Gamma y \right) \times \lambda_{\varepsilon,n}^{app}(t) d\tau.
\]

4.2 Circular particles
While the above procedure works for particles of arbitrary shape, for the circles the Galerkin Foldy-Lax densities solve the equation of a particularly simple form (in the frequency domain):
\[
-\int_{\Gamma_k^c} \hat{u}^{inc}(\omega) d\Gamma_x = \left( \omega r_k \right) \sum_{\lambda_{\varepsilon,n}^{app}} H_0^1(\omega r_k) J_0(\omega r_k) \hat{x}_{\varepsilon,n}^{app}.
\]
Surprisingly, with a suitable change of variables, the model of [2] can also be rewritten in the above form, modulo the term \( J_0(\omega r_n) \) in the last sum: this term is responsible for the instabilities in the time domain.

4.3 Convergence
We can show the following convergence result.

**Theorem 2** Let \( K \) be compact, \( \text{dist}(K, \Omega^{\text{co-c}}) > 0 \) for some \( \varepsilon_0 > 0 \). As \( \varepsilon \to 0 \),
\[
\| u_{\varepsilon,k}^{app} - u_{\varepsilon,k}^{app} \|_{L^\infty(0,T;L^\infty(\Omega))} \leq \varepsilon^2 \times C\| u^{inc} \|_{H^p(0,T;H^3(\mathbb{R}^2))},
\]
with \( C > 0 \) depending polynomially on \( T, N, \) inverse distance between particles, \( \min R_j, \max R_j \).

5 Prospectives
We plan to consider the method for more general particle shapes, as well as study the case of closely located particles.

References
Radiation Conditions for Periodic Waveguides

Andreas Kirsch\textsuperscript{1,*}, Guanghui Hu\textsuperscript{1,2}

\textsuperscript{1}Department of Mathematics, Karlsruhe Institute of Technology, Karlsruhe, Germany
\textsuperscript{2}School of Mathematical Sciences and LPMC, Nankai University, Tianjin, China
\*Email: andreas.kirsch@kit.edu

Abstract

In this talk we consider scattering problems for periodic open or closed waveguide problems for equations of Helmholtz type and different kind of periodic boundary conditions which allow the existence of propagating modes. By a general approach we show that many radiation conditions lead to well posed problems. Among them there exist some which follow from the Limiting Absorption Principle applied to the parameter of the problem and, therefore, are physically meaningful. At the end we sketch the case of locally perturbed periodic media.

Keywords: Helmholtz equation, periodic structure, radiation condition, Limiting Absorption Principle

1 Introduction

\begin{figure}[h]
\centering
\begin{tikzpicture}
\draw[->] (0,0) -- (4,0) node[anchor=north west] {$x_1$};
\draw[->] (0,0) -- (0,2) node[anchor=south east] {$x_2$};
\draw[fill=white] (0,0) rectangle (4,2);
\draw[thick] (0,0) -- (0,1) node[anchor=south east] {$D$};
\draw[thick] (4,0) -- (4,2) node[anchor=south west] {$D$};
\draw[thick] (0,1) -- (4,1) node[anchor=south] {$D$};
\draw[thick] (0,0) -- (0,1) node[anchor=south] {$\pi$};
\end{tikzpicture}
\caption{Two possible configurations}
\end{figure}

Let $k > 0$ be the wavenumber, $D \subset \mathbb{R}^2$ the waveguide which is $2\pi$-periodic with respect to $x_1$, see Figure 1. For simplicity in the presentation we consider the case on the left; that is, $\{x \in \mathbb{R}^2 : x_2 > H\} \subset D \subset \{x : x_2 > 0\}$. Let $A \in L^{\infty}(D, \mathbb{R}^{2 \times 2}_{\text{sym}})$ and $n \in L^{\infty}(D)$ be bounded below by positive constants and $2\pi$-periodic with respect to $x_1$. Furthermore, let $A = I$ and $n = 1$ for $x_2 > H$ and $f \in L^2(D)$ have compact support in the cell $Q := \{x \in D : 0 < x_1 < 2\pi, x_2 < H\}$. It is the aim to solve

\begin{equation}
\nabla(A \nabla u) + k^2 n u = -f \quad \text{in } D, \tag{1}
\end{equation}

complemented by the boundary condition

\begin{equation}
\partial_\nu u = 0 \quad \text{on } \partial \Omega, \tag{2}
\end{equation}

and a suitable radiating condition stated below.

\begin{definition}
$\alpha \in (-1/2, 1/2]$ is called a propagative wave number (or quasi-momentum or Floquet spectral value) if there exists a non-trivial $\alpha$-quasi-periodic $\phi \in H^{1}_{\text{loc}}(D)$ such that $\phi$ solves

\begin{equation}
\nabla(A \nabla \phi) + k^2 n \phi = 0 \quad \text{in } D, \tag{3}
\end{equation}

the boundary condition (2), and the Rayleigh expansion

\begin{equation}
\phi(x) = \sum_{\ell \in \mathbb{Z}} \phi_{\ell} e^{i\beta_{\ell} x_2 + i(\alpha + \ell \pi)x_1} \tag{4}
\end{equation}

for $x_2 > H$. Here, $\beta_{\ell} = \sqrt{k^2 - (\ell + \alpha)^2}$. The functions $\phi$ are called propagating (or guided) modes.

We make the assumption that the cut-off values $\{k + \ell : \ell \in \mathbb{Z}\}$ are no propagative wave numbers. Under this assumption there exists at most a finite number of propagative wave numbers in $[-1/2, 1/2]$ which can be numerated as $\{\alpha_j : j \in J\}$ where $J \subset \mathbb{Z}$. Furthermore, it is known that every eigenspace

\begin{equation}
\hat{X}_j := \{\phi \in H^{1}_{\text{loc}}(D) : \phi \text{ satisfies (2)-(4)}\}
\end{equation}

is finite dimensional with some dimension $m_j > 0$. In every $\hat{X}_j$ we choose a basis $\{\phi_{\ell,j} : \ell = 1, \ldots, m_j\}$ which is orthogonal with respect to the sesqui-linear form $E(u,v) := -i \int_{Q} [\nabla \alpha^{(1)} \cdot \nabla u - u \alpha^{(1)} \cdot \nabla \nu] \, dx$ for $u, v \in H^{1}(Q^{\infty})$ where $Q^{\infty} = \{x \in D : 0 < x_1 < 2\pi\}$ and $\alpha^{(1)} = (A_{11}, A_{12})^T$; that is, $E(\phi_{\ell,j}, \phi_{\ell',j'}) = 0$ for all $\ell \neq \ell'$ and $j \neq j'$. We note that the basis is not unique if $m_j > 1$.

We assume that $E$ is non-degenerated on every $X_j$; that is, $E(\phi_{\ell,j}, \phi_{\ell,j}) \neq 0$ for every $\ell, j$.

2 A Class of Radiation Conditions

To formulate radiation conditions we choose a function $\rho \in C^{\infty}(\mathbb{R})$ with $\rho(x_1) = 1$ for $x_1 \geq \sigma_0$ (for some $\sigma_0 > 2\pi + 1$) and $\rho(x_1) = 0$ for $x_1 \leq \sigma_0 - 1$. 
Definition 2 For every $j \in J$ we decompose
\[ \{1, \ldots, m_j\} = L^+_j \cup L^-_j \] (disjoint) in a fixed, but arbitrary way.

A solution $u \in H^1_{\text{loc}}(D)$ of (1) and (2) satisfies the open waveguide radiation condition with respect to $\{\hat{\phi}_{\ell,j} : \ell = 1, \ldots, m_j\}$ and $L^+_j \cup L^-_j$ if $u$ has a decomposition into $u = u_{\text{rad}} + u_{\text{prop}}$ with a radiating part $u_{\text{rad}} \in H^1(W_b)$ for all $b > 0$ (where $W_b := \{x \in D : x_2 < b\}$) and a propagating part $u_{\text{prop}}$ of the form
\[
u_{\text{prop}}(x) = \sum_{j \in J} \sum_{\sigma \in \{+,-\}} \rho(\sigma x_1) \sum_{\ell \in L^\sigma_j} \alpha_{\ell,j} \hat{\phi}_{\ell,j}(x)
\]
for $x \in D$ and some $\alpha_{\ell,j} \in \mathbb{C}$. Furthermore, $u_{\text{rad}}$ satisfies the angular spectrum radiation condition, see [2].

Transforming the differential equation for the radiating part $u_{\text{rad}}$ with the Floquet-Bloch transform into the space $H^1_1(D)$ of $\alpha$-quasi-periodic functions and using the quasi-periodic Dirichlet-Neumann map we are able to show:

Theorem 3 Under the assumptions formulated above there exists a unique solution of the source problem for every $f \in L^2(D)$, and the solution depends continuously on $f$.

By replacing $A$ or $n$ by the boundary condition by $A + i\varepsilon B$ or $n + i\varepsilon p$ or $\partial_n u + i\varepsilon q u$, respectively, with $\varepsilon > 0$ and periodic and non-negative functions $B \in L^\infty(D, \mathbb{R}^{n^2}_{\text{sym}})$ or $p \in L^\infty(D)$ or $q \in L^\infty(\partial D)$, respectively, such that $B = 0$ and $p = 0$ for $x_2 > H$ we can prove the Limiting Absorption Principle: that is, convergence as $\varepsilon \to 0$. These cases lead to different basis functions $\hat{\phi}_{\ell,j}$ in the case where $m_j > 1$ and to the decomposition $\{1, \ldots, m_j\} = L^+_j \cup L^-_j$ with $L^\pm_j = \{\ell : E(\hat{\phi}_{\ell,j}, \hat{\phi}_{\ell,j}) \geq 0\}$. These are physical meaningful radiation conditions because of the physical interpretation of $E(u, u)$ as an energy flux. Other decompositions of $\{1, \ldots, m_j\}$ lead to purely mathematical conditions.

3 Local Perturbations

In the last part we mention briefly the cases where $n$ or $D$ are perturbed on compact sets. With the same radiation conditions the assertions of Theorem 3 hold (for the particular choices of $L^\pm_j$) under the additional assumption that no bound states exist. A local perturbation with respect to $n$ leads to a compact perturbation of the solution operator $f \mapsto u|Q$ from $L^2(Q)$ into itself of the unperturbed problem and yields existence by the Fredholm theory. For the case of a local perturbation $\hat{D}$ of $D$ (see Figure 2) the proof is more complicated because not necessarily $\hat{D} \subset D$. In this case we choose a bounded region $K$ such that $\hat{D} \setminus D \subset K$ and $D \setminus \hat{D} \subset K$ and construct the Dirichlet-Neumann operator $\varphi \mapsto \partial_n v$ on $C := \partial K \cap D$ for the region $\Sigma := D \setminus K$ with homogeneous boundary data on $\partial D \setminus K$. The problem is then reduced to the bounded domain $\hat{D} \cap K$.

![Figure 2: A local perturbation $\hat{D}$ of $D$.](image)

References


Energy method approach to existence results for the Helmholtz equation in periodic wave-guides

Ben Schweizer\(^1\,*\)

\(^1\)Department of Mathematics, TU Dortmund, Dortmund, Germany
*Email: ben.schweizer@tu-dortmund.de

Abstract
We consider the Helmholtz equation in an unbounded wave-guide and derive an existence result for non-singular frequencies. Proofs of such results exist, our emphasis is that our proof uses only energy methods. The flexibility of the new method allows to study also the case that two different media are used in the two unbounded directions.

Keywords: Helmholtz equation, existence result, energy methods

1 Introduction
We study the Helmholtz equation
\[-\nabla \cdot (a \nabla u) = \omega^2 u + f (H)\]
in the wave-guide geometry \(\Omega := \mathbb{R} \times S\) with \(S \subset \mathbb{R}^{d-1}\) bounded Lipschitz. The coefficient of the operator is given by a function \(a : \Omega \rightarrow \mathbb{R}\) which is strictly positive and 1-periodic in \(x_1\). We impose a Neumann condition on \(\partial \Omega\). The given data are a source term \(f \in L^2(\Omega)\) with compact support and a frequency \(\omega \in \mathbb{R}\); below we will assume some non-singularity assumption on \(\omega\).

Our solution concept demands \(u \in H^1_{\text{loc}}(\Omega)\) and:

(i) \(u\) solves \((H)\) in \(\Omega\) in the weak sense

(ii) \(\sup_{t \in \mathbb{Z}} \|u\|_{L^2((r,r+1) \times S)} < \infty\)

(iii) a radiation condition is satisfied

The precise definition of the radiation condition (iii) is given below. Loosely speaking, (iii) on the right is demanding: There exist finitely many quasiperiodic homogeneous solutions \(\varphi_j\) of \((H)\) with positive energy-flux and corresponding coefficients \(\alpha_j\) such that \(u - \sum \alpha_j \varphi_j \rightarrow 0\) as \(x_1 \rightarrow \infty\). For further details on this condition and for an existence proof with other methods we refer to \([1, 2]\).

Some further notation: We use the elliptic operator \(Au := -\nabla \cdot (a \nabla u)\). Important bounded subsets of \(\Omega\) are the cylinders \(W_r := (r, r+1) \times S\), defined for arbitrary \(r \in \mathbb{R}\). These cylinders allow, in particular, to introduce the norm \(\|u\|_{sL} := \sup_{t \in \mathbb{Z}} \|u\|_{L^2(W_r)}\). To formulate our assumption on \(\omega\) and to define below the radiation condition, we introduce the space of homogeneous solutions of the Helmholtz equation,
\[X := \{u|_{W_0} \mid u \in H^1_{\text{loc}}(\Omega), \|u\|_{sL} < \infty, Au = \omega^2 u\text{ in }\Omega\}.

We can now specify our assumption on the frequency.

Definition 1 (Non-singular frequency) \(\omega > 0\) is called a non-singular frequency for the coefficient \(a\) if:

(a) Finite dimension: The space \(X\) has a basis \((\varphi_j)_{1 \leq j \leq M}\) with quasimoments \(\xi_j \in [0, 2\pi]\) such that each \(\varphi_j\) possesses a \(\xi_j\)-quasiperiodic extension satisfying \(A\varphi_j = \omega^2 \varphi_j\) in \(\Omega\).

(b) Non-vanishing flux: For every quasiperiodic function \(u \in H^1_{\text{loc}}(\Omega)\) with \(Au = \omega^2 u\), the restriction \(\varphi = u|_{W_0} \in X\) has the property that the flux is non-vanishing:
\[\Im \int_{W_0} a \nabla \varphi \cdot e_1 \varphi \neq 0.\]

The basis \((\varphi_j)_{1 \leq j \leq M}\) can be improved to another basis \((\phi_j^+)^{1 \leq j \leq N}\) with \(2N = M\) and some orthogonality properties and with the property that the flux of \(\phi_j^+\) is positive and negative, respectively. Since we have a basis of \(X\), every \(u \in X\) can be written as \(u = \sum_{j=1}^N \alpha_j \phi_j^+ + \sum_{j=1}^N \beta_j \phi_j^-\) with appropriate factors \(\alpha_j, \beta_j \in \mathbb{C}\).

This allows to define projections, e.g., \(\Pi_{X^+} : u \mapsto \sum_{j=1}^N \alpha_j \phi_j^+\) onto right-going waves. Together with the orthogonal \(L^2(W_0)\)-projection we can define projections onto right- and left-going waves
\[\Pi_{\pm} : L^2(W_0) \rightarrow X_{\pm} \subset L^2(W_0).\]

These projections allow to extract, from an arbitrary function \(u \in L^2(W_0)\) the right-going part and the left-going part. The projections also allow to make the radiation condition precise. Our definition turns out to be equivalent with more classical definitions; our definition is useful since our proofs imply the radiation condition in this form.
**Definition 2 (Radiation condition)** Let $\omega$ be non-singular and $\Pi_{\pm}$ the above projections. We say that $u : \Omega \to \mathbb{C}$ with $\|u\|_{L^2} < \infty$ satisfies the radiation condition if

$$\Pi_-(u|_{W_r}) \to 0 \text{ and } \Pi_+(u|_{W_{-r}}) \to 0 \text{ as } r \to \infty.$$  

We identify a function on $W_r$ with a function on $W_0$ via a shift.

**2 Main results**

As announced earlier, our results are based on energy methods. Loosely speaking, this means that we use only $L^2$-based function spaces and that our proof relies on testing procedures. A multiplication of the equation $Au = \omega^2u$ with $u$ or, more precisely, with the complex conjugate of $u$, and an integration over the domain $\{ \rho < x_1 < r \}$ for arbitrary $-\infty < \rho < r < \infty$, we obtain

$$\Im \int_{\{ \rho \} \times S} a \nabla u \cdot e_1 \, \bar{u} = \Im \int_{\{ r \} \times S} a \nabla u \cdot e_1 \, \bar{u}.$$  

The quantity on the left is the flux of $u$ at position $\rho$, more precisely, it is the right-going energy flux. The above equality therefore expresses energy conservation: the total (energy-) flux into the domain $\{ \rho < x_1 < r \}$ is vanishing.

Our results are based on energy conservation principles. Let us turn to the results.

**Theorem 3 (Periodic media)** Let the data $\Omega$, $f$, $\omega$, $a$ be as described, in particular, with the periodicity $a(x + e_1) = a(x)$ $\forall x \in \Omega$ and with the frequency $\omega$ being non-singular. Then there exists one and only one solution $u$ to the radiation problem (i)-(iii).

The method of proof decouples the problem on the left and on the right hand side. Because of this, we can also treat media that are periodic on the left and periodic on the right, but these could be two different periodic media. Our assumption on the medium can also be formulated as follows: There are two periodic fields $a^{\text{left}}, a^{\text{right}} : \Omega \to \mathbb{R}^{d \times d}$, $a^{\text{left}}(x + e_1) = a^{\text{left}}(x)$ and $a^{\text{right}}(x + e_1) = a^{\text{right}}(x)$ for every $x \in \Omega$. The coefficient $a$ is of class $L^\infty(\Omega)$, it is pointwise symmetric and positive and has the ellipticity bounds $\Lambda > \lambda > 0$. It satisfies, for some $R_0 > 0$:

$$a(x) = a^{\text{left}}(x) \quad \text{if } x_1 < -R_0,$$

$$a(x) = a^{\text{right}}(x) \quad \text{if } x_1 > R_0.$$  

We obtain the following result, which takes the form of a Fredholm alternative.

**Theorem 4 (Non-periodic media)** Let $\Omega$ be as above, let $a : \Omega \to \mathbb{R}^{d \times d}$ be periodic outside a compact set: For some $R_0 > 0$ holds

$$a(x + e_1) = a(x)$$  

for every $x \in \Omega$ with $|x_1| > R_0$. Let $\omega > 0$ be a non-singular frequency for the left and the right medium. If (i)-(iii) with $f = 0$ possesses only the trivial solution, then there is a unique solution $u$ for arbitrary $f \in H^{-1}(\Omega)$ with compact support.

The proof for the above two theorems can be found in the preprint [3]. The principal idea is to solve a Helmholtz problem in a truncated domain $\{-R < x_1 < R\}$. This is done with a technique that was first used in [4], the solution $u = u_R$ is found with an application of the Lax-Milgram theorem. The energy method is used to derive uniform bounds for the sequence $(u_R)_R$. The limit $R \to \infty$ provides the desired solution $u$ of the radiation problem.

**References**


Monday, July 25, Second Afternoon Session
EM-WaveHoltz: A time-domain frequency-domain solver for Maxwell’s equations

Daniel Appelö\textsuperscript{1,*}, Zhichao Peng\textsuperscript{1}

\textsuperscript{1}Michigan State University, East Lansing, USA

*Email: appeloda@msu.edu

Abstract

The EM-WaveHoltz method for computing time-harmonic solutions of Maxwell’s equations by time-domain simulations is presented. Numerical examples illustrating the properties of EM-WaveHoltz are given.

Keywords: Maxwell’s equations, frequency-domain, time-domain, positive definite.

1 The WaveHoltz iteration for Maxwell

Maxwell’s frequency-domain equations closed by boundary conditions corresponding to either a perfect electric conductor or to an unbounded domain take the form

\begin{align}
\imath \omega \epsilon \mathbf{E} &= \nabla \times \mathbf{H} - \mathbf{J}, \\
\imath \omega \mu \mathbf{H} &= -\nabla \times \mathbf{E}.
\end{align}

(1a) (1b)

Here \( \mathbf{E} \) and \( \mathbf{H} \) are the complex valued electric and magnetic fields, \( \epsilon, \mu \) are real valued permittivity and permeability and \( \mathbf{J} \) is the real valued current source.

Let \( T = 2\pi/\omega \)-periodic fields \( \hat{\mathbf{E}} = \hat{\mathbf{E}}_0 \cos(\omega t) + \hat{\mathbf{E}}_1 \sin(\omega t), \hat{\mathbf{H}} = \hat{\mathbf{H}}_0 \cos(\omega t) + \hat{\mathbf{H}}_1 \sin(\omega t) \), be solutions of the time-domain equations

\begin{align}
\imath \omega \hat{\mathbf{E}} &= \nabla \times \hat{\mathbf{H}} - \imath \omega \mathbf{J}, \\
\imath \omega \mu \hat{\mathbf{H}} &= -\nabla \times \hat{\mathbf{E}}.
\end{align}

(2a) (2b)

Then \( \Re\{\mathbf{E}\} = \hat{\mathbf{E}}_0, \Re\{\mathbf{H}\} = \hat{\mathbf{H}}_0, \Im\{\mathbf{E}\} = \hat{\mathbf{E}}_1 = \frac{1}{\imath} \nabla \times \hat{\mathbf{H}}_0, \) and \( \Re\{\mathbf{H}\} = \hat{\mathbf{H}}_1 = -\frac{1}{\mu} \nabla \times \hat{\mathbf{E}}_0 \).

Building on the ideas introduced in [1] our EM-WaveHoltz method finds the periodic solutions by iteratively determining the initial data to (2). Let \( \nu = (\nu_E, \nu_H)^T \) be initial conditions to (2). Then the filter operator, \( \Pi \), is defined

\[ \Pi \nu = \Pi \left( \begin{array}{c} \nu_E \\ \nu_H \end{array} \right) = \frac{2}{T} \int_0^T \left( \cos(\omega t) - \frac{1}{4} \right) \left( \hat{\mathbf{E}}_\nu \right) \left( \hat{\mathbf{H}}_\nu \right)^T dt. \]

Here \( T = 2\pi/\omega \) and \( \hat{\mathbf{E}}_\nu, \hat{\mathbf{H}}_\nu \) are the solution to (2) with initial conditions \( \nu = (\nu_E, \nu_H)^T \). The operator \( \Pi \) is contractive and can be used to define the EM-WaveHoltz iteration

\[ \nu^{n+1} = \Pi \nu^n, \quad \text{with} \quad \nu^0 = (\nu_E^0, \nu_H^0)^T = 0. \]

(3)

The EM-WaveHoltz iteration converges to the imaginary parts of the solution to the frequency-domain equation

\[ \lim_{n \to \infty} \nu^n = \lim_{n \to \infty} (\nu_E^n, \nu_H^n)^T = (\Im\{\mathbf{E}\}, \Im\{\mathbf{H}\})^T, \]

and the real parts can be recovered via the expressions above.

It is easy to rewrite the fixed point problem as a positive definite linear system that can be efficiently solved by a Krylov subspace method. To see this define \( S \nu \equiv \Pi \nu - \Pi \mathbf{0} \). We can then write \( \Pi \nu = S \nu + \Pi \mathbf{0} \), thus finding the fix point of \( \Pi \): \( \Pi \nu = \nu \) is equivalent to solving the equation \((I - S) \nu = \Pi \mathbf{0}\). To obtain the right hand side \( \Pi \mathbf{0} \), we first solve, (using your favourite Maxwell solver) the time-domain problem (2) with zero initial conditions \( \nu = \mathbf{0} \) from \( t = 0 \) to \( t = T = 2\pi/\omega \) once. The filter is computed using the trapezoidal rule. Similarly the cost to compute one Krylov vector is that of a wave solve with initial data. In our method we can choose to make the Krylov subspace smaller by noting that although we are looking for a \( T = \frac{2\pi}{\omega} \)-periodic solution, there is nothing in the method that prevents us from changing the filtering to extend over a longer time, say, \( T = N_{\text{periods}} \frac{2\pi}{\omega} \). As we show in the numerical examples below, for moderate \( N_{\text{periods}} \) this reduces the number of iterations by a factor of roughly \( N_{\text{periods}} \) so that the overall computational cost is almost the same, but the memory consumption is \( N_{\text{periods}} \) times smaller.

2 Numerical Examples

2.1 Comparison with MEEP

We fist compare our method with the iterative Yee-FDFD solver of the open source C++ package MEEP [2]. Our code is implemented by combining EM-WaveHoltz with the Yee scheme of the C library RBCpack [3]. Our code uses GMRES without restart. The FDFD solver of MEEP uses the BICG-Stab(l) method.

Following MEEP package’s benchmark example for the FDFD code we consider a ring
resonator and the 2D TM model. The computational domain is $[-6,6]^2$ with nonreflecting boundary conditions, [3]. A ring resonator with $\varepsilon_r = 3.4^2$ is located at $\{(x, y) : 1 \leq \sqrt{x^2 + y^2} \leq 1\}$. The permittivity outside the ring is $\varepsilon = 1$, and the permeability $\mu = 1$ in the whole computational domain. Two point sources are placed at $(1.1,0)$ with magnitude 1 and $(-1.1,0)$ with magnitude $-1$. We consider $\omega = \omega_0, 2.24\omega_0$ and $2.7\omega_0$, with $\omega_0 = 0.118 \times 2\pi$. The relative tolerance is $10^{-7}$. We use $l = 10$ in the MEEP BICG-Stab-(l) FDFD solver. In the results displayed in Figure 1, we observe that the EM-WaveHoltz and MEEP solutions agree well. Table 1 presents the computational time needed ($N$ is the number of gridpoints in each dimension). The Yee-EM-WaveHoltz method is almost always faster and its advantage increases as the solution is more accurate when the frequency is increased. We sweep $\omega \in [2\omega_0, 3.8\omega_0]$ with step size 0.2. The number of grid points per wavelength is fixed. We use $l = 20$ in the BICG-Stab-(l) and a relative tolerance $10^{-5}$. The bottom right figure of Figure 1 shows the scaling of the two solvers.

![Figure 1](image1.png)

**Figure 1:** The real part of the $E_z$ field (normalized) for $\omega = \omega_0, 2.24\omega_0, 2.7\omega_0$. Left part of the figures is Yee-EM-WaveHoltz, and MEEP’s FDFD solver is to the right.

![Figure 2](image2.png)

**Figure 2:** Unscaled (top) and scaled (bottom) number of iterations as a function of frequency for different filtering time. Left: 2D open problem. Right: 3D open problem.

### 2.2 Smaller Krylov Subspaces

As mentioned, we can filter over multiple periods. We consider $T = N_p/\omega$ with $N_p = 1, 3, 5$ for 2D and 3D open domain problems (same EM-WaveHoltz solver as above). We scan over different frequencies and apply the GMRES accelerated Yee-EM-WaveHoltz. The total number of iteration allowed is set as 200 in 2D and 100 in 3D. In Figure 2, we present the number of iterations as a function of the frequency. We also scale the number of iterations by $N_p$ and present the result in the same Figure. Note that for $N_p = 3$ and $N_p = 5$ the scaled curves visually collapse, implying that the the total computational time is approximately the same but with 3 and 5 times smaller memory footprint.

### References


A controllability method for Maxwell’s equations

T. Chaumont-Frelet\textsuperscript{1,*}, M.J. Gröte\textsuperscript{2}, S. Lanteri\textsuperscript{1}, J.H. Tang\textsuperscript{2}

\textsuperscript{1}Inria Université Côte d’Azur
\textsuperscript{2}University of Basel
\textsuperscript{*}Email: theophile.chaumont@inria.fr

Abstract

We propose a novel “controllability” method coupled with a conjugate gradient iteration to solve time-harmonic Maxwell’s equations. As opposed to traditional “frequency-domain” approaches, controllability methods seek a periodic solution by employing a “time-domain” discretization method. The periodicity condition is applied weakly by minimizing an “energy functional” with a conjugate gradient iteration. We show that up to an inexpensive filtering procedure, our method always converges toward the correct time-harmonic solution. Besides, we provide several numerical experiments suggesting that the controllability approach converges much faster than the naive “limiting amplitude principle” in the presence of trapping.

Keywords: Maxwell’s equations; High-frequency problems; discontinuous Galerkin; iterative solver

1 Introduction

Solving high-frequency Maxwell problems is an arduous task. In particular, the linear systems resulting from discretization by finite difference or finite element methods is sparse, but very large and indefinite. The design of efficient preconditioners, which are required to practically solve the problem, is currently the subject of extensive research, and recent developments include domain decomposition [2,6], shifted-laplacian [3], and sweeping [8] preconditioners. Still, the efficient solution of 3D time-harmonic Maxwell’s equations with heterogeneous coefficients remains to this day a formidable challenge, especially in the high-frequency regime.

In this contribution, we propose an novel approach to iteratively solve time-harmonic Maxwell’s equations using a controllability method, coupled with a conjugate gradient iteration (CMCG). This approach has been previously applied to the (simpler) scalar Helmholtz equation [1, 4, 5, 7], and we extend this idea to electromagnetic applications here.

2 Model problem

We consider time-harmonic Maxwell’s equations at the angular frequency $\omega > 0$, in a domain $\Omega \subset \mathbb{R}^3$. Given a current density $j : \Omega \to \mathbb{C}^3$, we seek two vector fields $e, h : \Omega \to \mathbb{C}^3$ such that

$$\begin{cases}
\begin{align*}
i\omega e + \sigma e + \nabla \times h &= j, \\
i\omega h - \nabla \times e &= 0,
\end{align*}
\end{cases}$$

inside the computational domain $\Omega$, where the first-order tensors $\varepsilon, \sigma$ and $\mu$ are the permittivity, conductivity and permeability of the medium in $\Omega$. At the boundary $\partial \Omega$ of $\Omega$, divided into two disjoint sets $\Gamma_P$ and $\Gamma_I$, we impose the boundary conditions

$$\begin{cases}
e \times n = 0 \quad &\text{on } \Gamma_P, \\
e \times n + Z h_r = g \quad &\text{on } \Gamma_I,
\end{cases}$$

where $n$ stands for the outward unit normal to $\partial \Omega$ and $h_r := n \times (h \times n)$. Here, the first-order tensor $Z$, defined on $\Gamma_I$, describes a surface impedance while $g : \Gamma_I \to \mathbb{C}^3$ typically represents incident electromagnetic field.

3 The CMCG algorithm

In the CMCG approach, we look for a periodic solution to the time-domain equation. Specifically, we seek initial conditions $(E_0, H_0)$ such that the time-domain fields $(E, H)$ satisfying

$$\begin{cases}
\varepsilon \dot{E} + \sigma E + \nabla \times H &= J \quad &\text{in } \mathbb{R}_+ \times \Omega, \\
\mu \dot{H} - \nabla \times E &= 0 \quad &\text{in } \mathbb{R}_+ \times \Omega, \\
E \times n &= 0 \quad &\text{on } \mathbb{R}_+ \times \Gamma_P, \\
E \times n + Z H_r &= G \quad &\text{on } \mathbb{R}_+ \times \Gamma_I,
\end{cases}$$

with time-harmonic forcing $J(t, x) := \text{Re}\{j(x)e^{i\omega t}\}$, $G(t, x) := \text{Re}\{g(x)e^{i\omega t}\}$, and initial conditions $E|_{t=0} = E_0$ and $H|_{t=0} = H_0$, are periodic, i.e. $(E(T), H(T)) = (E_0, H_0)$, where $T = 2\pi/\omega$.

To solve this problem, we introduce an “energy” functional

$$\mathcal{J}(E_0, H_0) = \|E(T) - E_0\|^2_{\mu, \Omega} + \|H(T) - H_0\|^2_{\varepsilon, \Omega}.$$
that we minimize using the conjugate gradient iteration, and our key theoretical results are threefold.

First, we show that the gradient $J'$ of the functional is efficiently computing by solving the forward and backward time-domain equation over one period, leading to an efficient algorithm.

Second, although the minimizer of the functional may not be unique, we show that simple filtering procedure post-processing

$$F(E_0, H_0) := 2T \int_0^T (E(t), H(t)) e^{-i\omega t} dt,$$

Finally, we rigorously establish the convergence of the conjugate gradient iteration toward a minimizer of the functional.

4 Numerical examples

We also provide numerical examples where the time-domain equations are discretized with a discontinuous Galerkin method coupled with Runge-Kutta time-integration schemes. We present a series of numerical experiments indicating that the proposed methodology converges faster than “naively” letting the time-domain solver run for “long enough” with a periodic forcing, especially when the computational domain features trap rays.

A particular example of a Gaussian source in a trapping obstacle is presented on on Figures 1 and 2.

References

A time-domain preconditioner for the Helmholtz equation: Analysis and performance on GPUs

Christiaan C. Stolk

1Korteweg-de Vries Institute for Mathematics, University of Amsterdam, Amsterdam, The Netherlands

*Email: C.C.Stolk@uva.nl

Abstract

Several methods in the literature determine solutions to the Helmholtz equation by solving instances of a discrete time-domain wave equation. In this work we study a new method of this type. Given an indefinite linear system, a matrix recurrence relation is constructed, such that in the limit of infinitely many time steps the exact discrete solution is obtained, i.e. unaffected by time-discretization errors. Using a large, finite number of time steps, an approximate solution is obtained. To improve the convergence, the process is used as a preconditioner for GMRES, and the time-harmonic forcing term is multiplied by a smooth window function. We study the convergence of the method analytically and numerically, and conclude with some initial results about the performance on the GPUs.

Keywords: Helmholtz equation, fast solvers, wave equation, parallel computing

1 Introduction

High-frequency Helmholtz equations, i.e. when a large number of wave lengths fit inside the domain, are still difficult to solve, even though a large number of approaches has been studied.

The cost of these different methods may be of different forms. Domain decomposition methods typically require the factorization of sparse matrices from discretized Helmholtz equation on the subdomains. Such factorizations require large amounts of memory and are often for larger problems not so easy to parallelize. Other methods, including time-domain Helmholtz solvers, generally require many applications of sparse matrices like those from a discrete Helmholtz or time-domain wave equation. While requiring many computations, these methods can be much less memory intensive.

In all cases, the question is how to optimally make use of modern hardware such as Graphics Processing Units (GPUs). GPUs have many compute cores (1000s per GPU unit), a large memory bandwidth (between compute cores and GPU memory) and are suitable to execute structured and “local” computations with high efficiency. Relatively few works study how to exploit these capabilities. Our study of time-domain Helmholtz solvers is motivated by the possibilities of such modern hardware, see also [2,3].

2 Method

The method takes as a starting point a linear system

\[ HU = F, \]

where \( H \) is a complex \( N \times N \) matrix, such that \( \text{Re} H \) is symmetric and \( \text{Im} H \) is symmetric positive semidefinite. For simplicity we also assume \( \text{Im} H \) is diagonal. This is written in the form

\[ (-\omega^2 I + i\omega B + A)U = F. \]

where \( A, B \in \mathbb{R}^{N \times N} \) and \( \omega \in \mathbb{R} \) are such that \( H = -\omega^2 I + i\omega B + A \) (here \( \omega \) is a frequency parameter, but need not be equal to the physical frequency).

Equation (2) is related to an ordinary differential equation (ODE) via the substitution \( \frac{d}{dt} \leftarrow i\omega \). This scheme will be solved with a time-harmonic forcing term \( f_n \). To obtain exact time-harmonic solutions at the choice of frequency \( \omega \), the ODE is discretized using a modified leap frog scheme

\[ \frac{1}{\Delta t^2} (u_{n+1} - 2u_n + u_{n-1}) + \frac{1}{2\Delta t} \tilde{B} (u_{n+1} - u_{n-1}) + \tilde{A} u_n = \alpha^{-1} f_n, \]

where \( \tilde{A} = \alpha^{-1} A, \tilde{B} = \alpha^{-1} \beta B \), with

\[ \alpha = \frac{(\Delta t \omega)^2}{2 - 2 \cos(\omega \Delta t)}, \]

\[ \beta = \frac{\omega \Delta t}{\sin(\omega \Delta t)}. \]

The choice of \( A \) and \( B \), \( \omega \) and the time-step \( \Delta t \) can be made such that (3) is a stable scheme.
To approximate the solution $U$ to (1) one can solve (3) for $u_n$, during a long time interval $[0, T]$, with $n$ up to $T/\Delta t$ and with

$$f_n = \chi(n\Delta t)e^{i\omega n \Delta t} F$$

(5)

with $\chi$ a suitable window function. Then

$$U \approx e^{-i\omega T}u_{T/\Delta t} =: P_T(F).$$

(6)

The resulting map from $F$ to the result of (6) is called a time-domain preconditioner and denoted $P_T(F)$.

3 Results and discussion

Theoretical and numerical results were obtained, to be summarized here. Some of the results have been published in [5].

The convergence was studied theoretically and indeed the approximate solution $P_T(F) \to H^{-1}F$ as $T \to \infty$.

The cost of this approach depends strongly on the size of the eigenvalues, e.g. on the “gap” defined by

$$\text{gap} = \min\{ |\lambda_1|, \ldots, |\lambda_N| \}.$$  

(7)

A study of the speed of convergence reveals that the error from a preconditioned iterative method can be estimated by

$$\text{error} < Ce^{-(\#\text{timesteps}) \cdot \text{gap}}.$$  

(8)

(The idea of studying the dependence on the gap was taken from [1].)

Numerical results obtained so far are encouraging. For example, a 3-D problem with about $2.54 \times 10^7$ degrees of freedom (the SEG/EAGE salt model, discretized using the method of [4] using 6 points per wavelength) was solved in 601 seconds on Macbook Pro (2019) with 16 GB of memory. Numerical results for different discretizations and using GPUs are forthcoming.

Overall, the numerical examples show good results for finite-difference discretized Helmholtz equations. For finite-element discretizations, both this method and alternative methods will be more costly and further research is necessary to analyse the benefits in this case.

References


Fast boundary element method for fault mechanics and earthquake control

Laura Bagur$^{1,*}$, Stéphanie Chaillat$^1$, Jean-François Semblat$^2$, Ioannis Stefanou$^3$

$^1$Laboratoire POEMS, CNRS - ENSTA-Paris - INRIA Institut Polytechnique de Paris (IP-Paris)
$^2$Laboratoire IMSIA, CNRS - EDF - CEA - ENSTA Paris IP-Paris
$^3$Laboratoire GEM, Centrale Nantes - Université de Nantes - CNRS

*Email: laura.bagur@ensta-paris.fr

Abstract

This work focuses on the simulation of sequences of seismic and aseismic slip events using Fast boundary element methods (BEMs). An algorithm based on FFT-accelerated BEMs is first considered, validated and results are shown for a basic problem in crustal faulting. These developments target the formulation of efficient computational tools for studying human-induced seismicity and to investigate its control numerically. A first multi-physics case using accelerated BEMs to solve the previous crustal faulting problem with fluid injection is considered.

Keywords: (Fast) Boundary element methods, Fault mechanics, Seismic control, Induced seismicity.

1 Motivations: Assessment of earthquake control strategies by fluid injection

Earthquakes due to either natural or anthropogenic sources cause important human and material damage. This justifies the development of efficient numerical tools for modeling the earthquake instability. Particularly, we aim at simulating problems in unbounded domains incorporating seismic and aseismic time scales (1 s and 1 yr respectively). Here, we propose to introduce Fast BEM formulations [1] to meet the expectations of a multi-physic large-scale robust model required for modeling earthquake processes, human-induced seismicity and their control [4]. These methods are known to be efficient for solving elastodynamic problems in large-scale unbounded domains. The challenge of this work is thus to enhance the capabilities of Fast BEMs to model large crustal faulting problems incorporating thermo-hydro-mechanical couplings.

2 Existing methods for fault mechanics

BEMs already allow to solve basic problems in crustal faulting. In order to assess their ability to simulate these problems, we use a well-known method consisting in BEMs accelerated by FFT for 2D antiplane problems. Let us consider a 1D planar vertical strike-slip fault, embedded in a 2D homogeneous, linear elastic infinite space (Figure 1). The antiplane shear movement assumed in the $x$ direction leads to a displacement on either side of the fault independent of the $x$ coordinate. BEMs applied to the equilibrium combined with Hooke’s law, leads to a relation between the jump in displacement denoted $\delta$ across the fault and the shear stress $f$ due to quasi-static deformation:

$$f(x,t) = \frac{\mu}{2\pi} \int_\Gamma \frac{1}{z-z'} \frac{\partial \delta}{\partial z'}(z',t)dz'$$

which simplifies in the Fourier space:

$$F(\xi,t) = \frac{\mu|k|}{2}D(\xi,t), \quad k = 2\pi \xi.$$

This technique is only valid for planar faults. The fault is obeying an empirical rate-and-state friction law:

$$\tau(z,t) = \tau(\sigma_n(z)) = h(z)\sinh^{-1}\left[V(z,t)\exp\left\{\frac{f_0+f(z)\ln(V(z,t)/\sqrt{\sigma_n(z)})}{n}\right]\right].$$

completed by the aging law:

$$\frac{\partial \theta}{\partial \tau} = 1 - \frac{V(z,t)\theta(z,t)}{L(z)}.$$

Where $\tau = \tau^0 + f - \eta V$ is the sum of the pre-stress, the shear stress due to quasi-static deformation, and the radiation damping approximation to inertia, where $\eta = \mu/(2c_n)$ is half the shear-wave impedance for shear wave velocity $c_n = \sqrt{\mu/\rho}$. $V = \partial \delta/\partial t$ is the slip rate, and $\theta$ is the state variable. $\sigma_n$ is the effective normal stress on the fault. The algorithm used to solve this problem is based on the prediction-correction method in the spirit of a second-order Runge-Kutta procedure proposed by [2]. The unknowns are $\delta, V, \tau, \theta$. We verify this approach considering the case where the slip rate is constant in time equal to $V_p$, which leads to have the unknowns equal to their initial values.
3 1D planar vertical strike-slip fault, embedded in a 2D homogeneous, linear elastic half-space

Figure 1: Representation of the 1D antiplane problem

In this case the equations at stake are the same and the free surface condition is taken into account using the image method. Figure 2 shows sequences of seismic and aseismic phases (which last about $108 \, s$ and $84 \, yrs$ in average respectively).

Figure 2: Maximal slip rate at depth evolution with respect to time

4 Perspectives

The objective is now to explore the advantages and limitations of novel strategies of earthquake control using fluid injection to drive the fault from an unstable state of high potential energy to a stable state of lower potential energy [4]. Ongoing work concerns the use of Fast BEMs to solve more realistic problems in crustal faulting. The main challenge is the extension of accelerated BEMs from single physic problems to incorporate thermo-hydro-mechanical couplings due to fluid injection. Some works have already shown that poroelasticity can be modeled with BEMs [3] but these methods have never been used in elastodynamics and multi-physics. We will first apply Fast BEMs to the previous antiplane - shear case incorporating fluid injection. We will validate this formulation on the quasi-dynamic and fully dynamic version of the previous problem. The BEM used in this ongoing work will be accelerated using Hierarchical Matrices. Increasing pore fluid pressure induces variations in the effective normal stress on the fault. The modeling assumptions of which poroelastodynamic framework we will use will depend on the specific problem we are solving. Fast BEMs will be considered to calculate both shear and normal stresses which contain similar terms. Our final goal is to develop an efficient formulation of this multi-physics problem and show that fluid injection can induce a controllable aseismic slip numerically.

Acknowledgement

This work is supported by a Contrat Doctoral Spécifique Normalien (CDSN) and forms part of the ERC project CoQuake (Controlling earthQuakes, www.coquake.eu), funded by the European Research Council (ERC, https://erc.europa.eu/) under the European Union’s Horizon 2020 research and innovation program (Grant agreement n° 757848 CoQuake).

References


Quadrature by Parity Asymptotic eXpansions (QPAX) for light scattering by high aspect ratio plasmonic particle

Camille Carvalho 2,1,∗, Arnold D. Kim 2, Zoës Moitier 3
1Univ Lyon, INSA Lyon, UJM, UCBL, ECL, CNRS UMR 5208, ICJ, F-69621, France
2Department of Applied Mathematics, UC Merced, Merced, USA
3Institute for Analysis, Karlsruhe Institute of Technology, Karlsruhe, Germany
∗Email: camille.carvalho@insa-lyon.fr

Abstract
The study of scattering by a high aspect ratio particle has important applications in sensing and plasmonic imaging. To illustrate the effect of particle’s narrowness (that can be related to parity properties) and the need for adapted methods (in the context of boundary integral methods), we consider the scattering by a penetrable, high aspect ratio ellipse. This problem highlights the main challenge and provides valuable insights to tackle general high aspect ratio particles. We find that boundary integral operators are nearly singular due to the collapsing geometry to a line segment. We show that these nearly singular behaviors lead to qualitatively different asymptotic behaviors for solutions with different parities. Without explicitly taking this into account, computed solutions incur large errors. We introduce the Quadrature by Parity Asymptotic eXpansions (QPAX) that effectively and efficiently addresses these issues. We demonstrate the effectiveness of QPAX through several numerical examples.

Keywords: Boundary integral methods; asymptotic analysis; numerical quadrature; scattering.

1 Problem setting
Consider a penetrable high aspect ratio ellipse $D$ characterized by some material property $\varepsilon - \in \mathbb{C}$. Typically, the plasmonic case corresponds to $\Re(\varepsilon) < 0$, where $\varepsilon -$ represents the inverse of the dielectric permittivity of the particle made of a noble metal such as gold or silver. The ellipse is surrounded by vacuum (characterized by $\varepsilon_+ = 1$). The associated scattering problem is given by the transmission problem: Find $u_+ \in \mathcal{C}^2(E := \mathbb{R}^2 \setminus D) \cup \mathcal{C}^1(\mathbb{R}^2 \setminus D)$ such that $u_- \in \mathcal{C}^2(D) \cup \mathcal{C}^1(D)$ such that, $\Delta u_+ + k_+^2 u_+ = 0$ in $E$, $\Delta u_- + k_-^2 u_- = 0$ in $D$, $u_+ = u_-$ and $\varepsilon_+ \partial_n u_+ = \varepsilon_- \partial_n u_-$ on $\partial D$. We denote $u_\pm = u^n_\pm + u^s_\pm$ the total fields, $u^s_\pm$ the scattered fields, $u^n$ is the incident field, $\partial_n$ is the normal derivative. Consider a wavenumber $k > 0$, we define $k_\pm = k/\sqrt{\varepsilon_\pm}$. We also require $u^n_\pm$ to satisfy the Sommerfeld radiation condition, and we assume that $(\varepsilon_-, \varepsilon_+)$ are such that the problem is well-posed. Using the representation formula [1] and the transmission conditions on $\partial D$, we write

$$u_+ = u^n_+ + \mathcal{K}^H_+ [u_+] - \mathcal{S}^H_+ [\partial_n u_+] \quad \text{in } E,$$

$$u_- = -\mathcal{K}^H_- [u_-] + \mathcal{S}^H_- [\partial_n u_-] \quad \text{in } D,$$

where $\mathcal{K}^H_\pm, \mathcal{S}^H_\pm$, are the double-layer potentials, single-layer potentials, associated to the considered Helmholtz equations, respectively. To study scattering by a high aspect ratio particle, we consider the ellipse defined according to $y(t) = (\varepsilon \cos(t), \sin(t))$, $t \in \mathbb{T} := \mathbb{R}/2\pi\mathbb{Z}$, with $0 < \varepsilon \ll 1$, and we study the asymptotic limit $\varepsilon \to 0^+$. Given $x \in \mathbb{R}^2 \setminus \partial D$, we denote $x^b \in \partial D$ the closest point on the boundary, and we write $x^b = y(s)$ for $s \in \mathbb{T}$ (see Fig. 1). When $y = y(s)$ for $s \in \mathbb{T}$, we find that the unknown fields on the boundary, $(u_+(s), v_+(s)) := (u_+(y(s)), \partial_n u_+(y(s)))$, satisfy the system

$$\begin{bmatrix} \frac{1}{2} - \mathcal{K}^H_+ & \mathcal{S}^H_+ \\ \frac{1}{2} + \mathcal{K}^H_- & -\mathcal{S}^H_- \end{bmatrix} \begin{bmatrix} u_+ \\ v_+ \end{bmatrix} = \begin{bmatrix} u^n_+ \\ 0 \end{bmatrix},$$

with $\mathcal{K}^H_\pm [v](s) = \frac{1}{4} \int_\mathbb{T} \mathcal{H}_0^{(1)}(r^\pm_\varepsilon(t), r(t)) dt$, $\mathcal{S}^H_\pm [u](s) = \frac{i\pi k^\pm_\varepsilon}{2} \int_\mathbb{T} r^\pm_\varepsilon(t) \mathcal{H}_1^{(1)}(k^\pm_\varepsilon r^\pm_\varepsilon(t))dt$, $K^L_\varepsilon(s, t) u(t) dt$, with $r^\pm_\varepsilon(t) = |y(s) - y(t)|$, $\mathcal{H}_m^{(1)}$ the Hankel function of the first kind of order $m$, and $K^L_\varepsilon$ the Laplace’s double-layer potential kernel

$$K^L_\varepsilon(s, t) = \frac{1}{2\pi} \frac{1 + \varepsilon^2 + (1 - \varepsilon^2)\cos(s + t)}{1 + \varepsilon^2 + (1 - \varepsilon^2)\cos(s + t)}.$$

The kernel $K^L_\varepsilon$ is sharply peaked at the reflection-points along the semi-major axis of the ellipse, $s + t \equiv \pi [2\pi]$: $K^L_\varepsilon(s, t) = -\frac{1}{4\varepsilon^2}$. This peak is enhanced as the ellipse collapses ($\varepsilon \to 0$).
This sharp peak leads to nearly singular integral operators in the boundary integral equation system (1). Not addressing this behavior gives large errors when using standard quadrature rules such as Kress’ Product Quadrature Rule (PQR), as plotted in Fig. 1.

![Figure 1](image.png)

**Figure 1:** (Top left) Sketch and notations of the problem. (Top right) Error with respect to $\varepsilon$ when approximating the solution $(u_+, v_+)$ of (1) using PQR, QPAX (leading order), $k = 2$, $(\varepsilon, \varepsilon_+)(1, 4)$, and $N = 128$ quadrature points. The analytic solution is computed using Mathieu functions [2]. (Bottom) Error for $(u_+, v_+)$ for various $\varepsilon, N$.

2 Parity asymptotic expansions

We rewrite system (1) as $A_\varepsilon U_\varepsilon = F_\varepsilon$, we perform an asymptotic expansion about $\varepsilon = 0$. The leading order gives us

$$A_\varepsilon = \begin{bmatrix} \Pi_{ev} & S_0^T \\ \Pi_{od} & -\frac{\varepsilon}{\pi}\varepsilon_0 S_0 \end{bmatrix} + O(\varepsilon),$$

$$U_\varepsilon = \begin{bmatrix} u_0 \\ v_0 \end{bmatrix} + O(\varepsilon),\quad F_\varepsilon = \begin{bmatrix} u_0^{in}(0, \sin(s)) \\ 0 \end{bmatrix} + O(\varepsilon).$$

where $S_0^T$ are integral operators that can be found following [2, Section 4] (along with order 1 terms). Above, $\Pi_{ev}$, $\Pi_{od}$, denotes the projection onto even, odd function with respect to the semi-major axis of the ellipse, respectively: $\Pi_{ev}[\mu](s) = \mu(s) + \mu(s - \pi) = \left(\frac{\mu(s) - \mu(\pi - s)}{2}\right)$.

Quadratures such as PQR are well adapted to treat weakly singular integrals involved in (1) (e.g., [1]), but do not treat the parity or the close evaluation problem. To address these, we introduce the Quadrature by Parity Asymptotic eXpansions (QPAX) [2], a modification of PQR as follows: split the fields and the operators obtained from the previous linear system into their even and odd parts, discretize the systems obtained with asymptotic expansions (accuracy depends on the expansions truncation’s order), use PQR on weakly singular integrals involved in the systems, and spectral methods on the rest. Considering an $O(\varepsilon)$ expansion, we expect the error to decrease linearly as $\varepsilon \to 0$, for any number of quadrature points. To validate the method we plot in Figure 1 the errors in log obtained with PQR (• line) and QPAX (+ line), for a classical penetrable ellipse ($\zeta_+ > 0$) where one can compute an analytic solution (codes available on GitHub). Results show that QPAX approximation effectively addresses the inherent parity in the nearly singular behaviors associated with this high aspect ratio ellipse. QPAX efficiently computes near-fields in plasmonic cases as well (but no analytic solution is available).

3 Future work

The above approach can be carried out for more general high aspect ratio particles where two distinct asymptotic behaviors along reflection-points must be addressed carefully. Extensions to three-dimensional high aspect ratio particles are considered, starting with axisymmetric high aspect ratio particles.

**Acknowledgment.** This research was funded by the National Science Foundations Grants DMS-1819052, DMS-1840265, and by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) Project-ID 258734477 – SFB 1173.

**References**


A High-order Density-Interpolation-Based Nyström Method for Three-Dimensional Electromagnetic Boundary Integral Equations

Rodrigo Arrieta¹, Luiz M. Faria², Carlos Pérez-Arancibia³*, Catalin Turc⁴

¹Department of Electrical Engineering, Pontificia Universidad Católica de Chile, Santiago, Chile
²POEMS Team, ENSTA Paris, Palaiseau, France
³Department of Applied Mathematics, University of Twente, Enschede, The Netherlands
⁴Department of Mathematical Sciences, New Jersey Institute of Technology, Newark, United States

Email: c.a.perezarancibia@utwente.nl

Abstract

This work presents a novel high-order Nyström method for the numerical solution of electromagnetic boundary integral equations. Our method is based on the construction of suitable surface current interpolants as linear combination of electric dipole fields. Relying on Stratton-Chu formula applied to the density interpolants, we recast standard electromagnetic boundary integral equations, such as the classical EFIE, MFIE, and CFIE, in terms of smooth (at least bounded) surface integrands that can be accurately and inexpensively integrated over curved triangular or quadrilateral surface discretizations by means of elementary quadrature rules. Several numerical examples demonstrate the accuracy of the proposed approach.

Keywords: Maxwell equations, Nyström method, singularity

1 Introduction

We consider the kernel regularization of electromagnetic surface integral operators of the form

\[ C_{\alpha,\beta} \varphi(x) = \alpha K \varphi(x) + \beta T [n \times \varphi](x) \] (1)

for \( x \in \Gamma \), where \( \alpha, \beta \in \mathbb{C} \) and \( n \) denotes the outward unit normal to the smooth closed surface \( \Gamma = \partial \Omega \). Here,

\[ (T \varphi)(x) = n(x) \times \int_{\Gamma} G(x, y) \varphi(y) \, ds(y) \] (2)

\[ (K \varphi)(x) = n(x) \times \int_{\Gamma} \text{curl}_x G(x, y) \varphi(y) \, ds(y) \] (3)

are the electric and magnetic field integral operators at \( x \in \Gamma \), \( \varphi : \Gamma \to \mathbb{C}^3 \) is a vector field tangential to \( \Gamma \), and

\[ G(x, y) = \left( I + \frac{\nabla_x \nabla_y}{k^2} \right) \frac{e^{ik|x-y|}}{4\pi|x-y|} \] (4)

is the Maxwell free-space dyadic Green’s function [3]. The operators \( T \) and \( K \) can be retrieved as \( T = C_{0,-1} \circ n \times \) and \( K = C_{1,0} \). \( C_{1,0} \) with \( \eta > 0 \), on the other hand, is the indirect combined field integral operator. The operators \( K \) and \( T \) feature singular integrands that behave like \( O(|x-y|^{-1}) \) and \( O(|x-y|^{-3}) \) as \( \Gamma \ni y \to x \in \Gamma \), respectively, which pose significant challenges to the accurate implementation of Nyström methods. Existing Nyström methods for electromagnetics [2] rely on rather involved singular integration techniques.

2 Density interpolation method

Our approach relies on recasting \( C_{\alpha,\beta} \) in terms of smooth integrands. To do so, we introduce a high-order density interpolant that is constructed by means of a simple collocation procedure using points within a neighborhood of the target (singular) point \( x \in \Gamma \). In detail, for a given point \( x \in \Gamma \) we consider a finite set of distinct neighboring points \( \{y_j\}_{j=1}^p \subset \Gamma_h(x) \), where \( \Gamma_h(x) \) is a small subset of \( \Gamma \) containing \( x \) and satisfying \( \sup_{y \in \Gamma_h(x)} |x-y| < h \) for some \( h > 0 \). \( \Gamma_h(x) \) is selected as the surface element to which \( x \) belongs, \( h \) is the characteristic element diameter, and the neighboring points are chosen as the interior quadrature nodes used for numerical integration over that element.

We then seek interpolants of \( \varphi \) at \( x \in \Gamma \) of the form

\[ \Phi(r; x) = \sum_{\ell=1}^L G(r, z_\ell) c_{\ell}(x) \] (5)

for \( r \in \mathbb{R}^3 \), where \( \{c_{\ell}(x)\}_{\ell=1}^L \subset \mathbb{C}^3 \) is a set of coefficients to be determined by enforcing suitable interpolation conditions. The set of dipole source point locations \( \{z_\ell\}_{\ell=1}^L \subset \mathbb{R}^3 \backslash \Omega \) is chosen placed in the exterior of \( \Omega \) so that \( E = \Phi(\cdot; x) \) satisfies Maxwell equations in its interior. Applying then Stratton-Chu formula [3] to \( \Phi(\cdot; x) \) and evaluating \( n(x) \times \Phi(x; x) \) for \( x \in \Gamma \) (taking
the limit from inside $\Omega$), and combining it with $C_{\alpha,\beta}$ we obtain
\[
C_{\alpha,\beta}[\phi](x) = K\left[\alpha \phi - \gamma_0^\alpha \Phi(\cdot; x)\right](x) +
T\left[\beta n \cdot \phi - \gamma_1^\beta \Phi(\cdot; x)\right](x) - \frac{1}{5} \gamma_0^\alpha \Phi(x; x) \tag{6}
\]
where we have employed the notations $\gamma_0^\alpha F(x) = \lim_{h \to 0} n(x) \times F(x \pm \delta n(x))$ and $\gamma_1^\beta F(x) = \lim_{h \to 0} n(x) \times \nabla F(x \pm \delta n(x))$ for the traces.

To find the coefficients $\{c_i(x)\}_{i=1}^L$ in (5) we impose:
\[
\gamma_0^\alpha \Phi(y_j; x) = \alpha \phi(y_j) \quad (7a)
\]
\[
\gamma_1^\beta \Phi(y_j; x) = \beta n(y_j) \times \phi(y_j) \quad (7b)
\]
at all neighboring points $\{y_j\}_{j=1}^P \subset \Gamma_h(x)$. The conditions (7) give rise to a total of $6P$ linear equations for the $3L$ unknown coefficients $\{c_i\}_{i=1}^L$, which can be solved by means of the Moore-Penrose pseudoinverse of the associated matrix provided $L \geq 2P$. In practice, efficiency is gained by using the fact that the same interpolant can be used for all the quadrature points belonging to $\Gamma_h(x)$.

Under reasonable assumptions, the conditions (7) yield
\[
\left|\partial_\theta^\beta \left[\gamma_0^\alpha \Phi(\cdot; x) - \phi(\cdot; x)\right]\right| \lesssim h^{p-|\theta|} \tag{8a}
\]
\[
\left|\partial_\theta^\beta \left[\gamma_1^\alpha \Phi(\cdot; x) - \beta n(\cdot) \times \phi(\cdot; x)\right]\right| \lesssim h^{p-|\theta|} \tag{8b}
\]
which hold uniformly for $y \in \Gamma_h(x)$, where $p$ scales like $\sqrt{P}$ and the symbol $\partial_\theta^\beta$ with $\theta = (\theta_1, \theta_2)$ denotes the tangential derivatives of or-der $|\theta| = \theta_1 + \theta_2$.

In order to avoid the kernel singularity in (1) altogether and in view of (8), we use the following approximate regularized integral operator:
\[
\tilde{C}_{\alpha,\beta}[\phi](x) = n(x) \times \int_{\Gamma_h(x)} \nabla \Phi(x, y) \{\alpha \phi(y) - \gamma_0^\alpha \Phi(y; x)\} ds(y) + n(x) \times \int_{\Gamma_h(x)} \Phi(x, y) \{\beta n(y) \times \phi(y) - \gamma_1^\beta \Phi(y; x)\} ds(y) - \frac{\gamma_0^\alpha \Phi(x; x)}{2} \tag{9}
\]
Assuming that the density interpolant (5) satisfies the error estimates (8), it holds that the approximate regularized operator satisfies
\[
\left|\tilde{C}_{\alpha,\beta}[\phi] - C_{\alpha,\beta}[\phi]\right| \lesssim h^{p-1}. \tag{10}
\]

Our Nyström method is based on the direct application of standard surface discretizations and quadrature rules to the approximate regularized operator (9).

3 Numerical Results
To validate the proposed Nyström method, we take $\Gamma$ as the unit sphere centered at the origin and we discretize it using quadrilateral patches. We then construct an exact Maxwell’s equation solution by taking $E(x) = G(x, 0)[1, -1, 1]^T$ for $x \in \mathbb{R}^3 \setminus \Omega$ and $k = \pi$. Applying Stratton-Chu formula to $E$ and taking $\gamma_0^\alpha$ we obtain
\[
\frac{\gamma_0^\alpha E(x)}{2} = T [\gamma_1^\alpha E(\cdot)](x) + K [\gamma_0^\alpha E(\cdot)](x) \tag{11}
\]
for $x \in \Gamma$. This relation is used to measure the numerical integration error $\max_j |\gamma_0^\alpha E(x_j) - 2(\tilde{T} [\gamma_1^\alpha E(\cdot)](x_j) + \tilde{K} [\gamma_0^\alpha E(\cdot)](x_j))/\max_j |\gamma_0^\alpha E(x_j)|$, where $x_j \in \Gamma, j = 1, \ldots, N$, are the discretization points, and $\tilde{K}$ and $\tilde{T}$ are the regularized operators produced by the proposed approach.

Figure 1: Numerical errors for various values of $\sqrt{N} \propto h$ ($N$ being the total number of discretization points) in the numerical approximation of $T [\gamma_1^\alpha E(\cdot)] + K [\gamma_0^\alpha E(\cdot)]$ using $P = p^2$ interpolation points per patch. The dashed lines correspond to the expected converge orders in (10).

References
Eddy-current asymptotics of the Maxwell PMCHWT formulation: the multi-body case

Edouard Demaldent$^{1,*}$, Marc Bonnet$^{2}$

$^{1}$Université Paris-Saclay, CEA, List, F-9120, Palaiseau, France
$^{2}$POEMS, ENSTA Paris, 91120 Palaiseau, France

*Email: edouard.demaldent@cea.fr

Abstract. A low-frequency, high-conductivity asymptotic approximation of the Maxwell transmission problem for configurations with highly-conducting, moderately-conducting, and non-conducting bodies, motivated by eddy current testing applications, is proposed and validated.

Keywords: Maxwell equations, PMCHWT formulation, eddy currents, asymptotic expansion

Introduction In eddy current (EC) testing applications, ECs $\sigma \mathbf{E}$ ($\mathbf{E}$: electric field, $\sigma$: conductivity) are induced in tested metal parts by a low-frequency ($\omega$) source idealized as a closed current loop in air. The EC model corresponds to the magneto-quasi-static approximation of the Maxwell problem, which neglects the displacement current. In presence of highly conductive (HC) media, the boundary integral equation (BIE) of the first kind under the magneto-quasi-static approximation proposed in [4] was shown in [2] to coincide with the leading order of an asymptotic expansion of the Maxwell BIE in a small parameter $\gamma$ reflecting both LF and HC assumptions. Here, we extend [2] and derive a low-$\gamma$ asymptotic approximation for configurations involving multiple moderately-conducting ($\mathcal{MC}$, $\sigma = O(1)$) or non-conducting ($\mathcal{NC}$) objects in addition to HC objects, which may be multiplyconnected and nested.

Setting We consider the time-harmonic electromagnetic transmission problem whereby $M$ objects with conductivity $\sigma_a$, complex permeabilities $\varepsilon_a := \varepsilon_a \sigma_a = \varepsilon_a^0 + i \sigma_a / \omega$ and permeabilities $\mu_a = \mu_0 \mu_a$ ($1 \leq a \leq M$), which occupy the bounded Lipschitz domains $\Omega_a \subset \mathbb{R}^3$, are surrounded by vacuum $\Omega_0 := \mathbb{R}^3 \setminus (\bigcup_{a=1}^M \Omega_a)$ (Fig. 2). The objects are excited by fields created by a given current density $\mathbf{J}_s$ with compact support in $\Omega_0$. The electric field $\mathbf{E}$ thus solves the transmission problem

\[
\begin{align*}
\mathbf{E} &= \mathbf{E} \quad \text{in} \; \Omega_0, \\
\n\mathbf{E} &= \mathbf{E} \quad \text{in} \; \Omega_a, \\
\gamma_0^a E_n - \gamma_N^a E = 0 \quad \text{on} \; \Gamma_a, \quad (1)
\end{align*}
\]

wherein $\kappa_0^a = \varepsilon_a \mu_0 \omega^2$, $\kappa_N^a = \kappa_0^a (\varepsilon_a^0 \mu_a + i \sigma_a / \omega) \mu_a$ are the wavenumbers in $\Omega_a$, and the trace operators $\gamma_0^a$, $\gamma_N^a$ are defined by $\gamma_0^a \mathbf{u} := \gamma_0^{a \perp} \mathbf{u} \times \mathbf{n}$ and $\gamma_N^a \mathbf{u} := \gamma_N^{a \perp} \mathbf{u}$. The asymptotic expansion of the PMCHWT system for configurations with highly-conducting, moderately-conducting and non-conducting bodies, motivated by eddy current testing applications, is proposed and validated.

Keywords: Maxwell equations, PMCHWT formulation, eddy currents, asymptotic expansion

Figure 1: Scattering by multiple objects.

Expansion of the PMCHWT system We introduce the dimensionless parameter $\gamma := \varepsilon_0 L / \lambda$, with $L$ a characteristic length. Each object $\Omega_a$ is taken as either NC (i.e. $\sigma_a = 0$), MC (i.e. $\sigma_a = \varepsilon_a \sigma_{\text{ref}}$) or HC (i.e. $\sigma_a = \gamma^{-1} \varepsilon_a \sigma_{\text{ref}}$), each dimensionless factor $\varepsilon_a$ being fixed (i.e. independent on $\gamma$) and with $\sigma_{\text{ref}} := L^{-1} \varepsilon_0 \mu_0$. In particular, the HC bodies are in the eddy current regime. Our general aim is to define ap-
proximate solutions of (2) for low values of $\gamma$ by seeking an expansion in powers of $\gamma$ of $X$. For the surface current densities on each $\Gamma_a$, we obtain formal expansions of the form

$$
\begin{align*}
J^a_L &= J^a_{L,0} + \gamma J^a_{L,1} + \gamma^{3/2} J^a_{L,3/2} + O(\gamma^2), \\
\gamma^{-2} J^a_T &= J^a_{T,0} + \gamma J^a_{T,1} + \gamma^{3/2} J^a_{T,3/2} + O(\gamma^2), \\
M^a_L &= M^a_{L,0} + \gamma M^a_{L,1} + \gamma^{3/2} M^a_{L,3/2} + O(\gamma^2), \\
M^a_T &= M^a_{T,0} + \gamma M^a_{T,1} + \gamma^{3/2} M^a_{T,3/2} + O(\gamma^2),
\end{align*}
$$

with all coefficients $J^a_{L,0}$ defined as solutions of integral problems arising from the expansion of problem (2). This in turn results in expansions

$$
\begin{align*}
E &= \gamma \left( E_0 + \gamma E_1 + \gamma^{3/2} E_{3/2} + O(\gamma^2) \right), \\
H &= H_0 + \gamma H_1 + \gamma^{3/2} H_{3/2} + O(\gamma^2), \\
\Delta Z &= \gamma \left( \Delta Z_0 + \gamma \Delta Z_1 + \gamma^{3/2} \Delta Z_{3/2} + O(\gamma^2) \right),
\end{align*}
$$

with all coefficients well-defined in terms of those of (3), for the electromagnetic fields $E, H$ in $\Omega_0$ and in each $\Omega_a$ and the impedance variation $\Delta Z$ (see [2, eq. 27], of main interest in EC testing).

**Remarks and extensions** The leading-order operator matrix $\Xi_0$ arising from the expansion of problem (2) has some zero block entries, such that any system of the form $\Xi_0 X = \Xi$ can be solved blockwise in three stages, with computational benefits. Stage I yields $(J^a_{L,0}, M^a_{L,0}, M^a_{T,0})_{a \in HC}$ and $(\hat{J}^a_{L,0}, \hat{M}^a_{L,0})_{a \in NC, MC}$ at any order and often suffices in practice as it provides at order $\gamma^0$ the correct leading-order approximations of $\Delta Z$, of $H$ everywhere, and of $E$ in the HC bodies.

Moreover, the operator submatrix for Stage I is found to not depend on $\sigma_a$ in the MC bodies, if any. Treating the latter as NC thus produces the same Stage-I solutions, and hence all the correct leading-order approximations obtainable from Stage I at order $\gamma^0$ alone.

In the absence of MC bodies, all terms of orders 1 and 3/2 vanish in (3) and (4), so that (for example) we have $\Delta Z = \gamma \left( \Delta Z_0 + O(\gamma^2) \right)$.

The asymptotic formulation outlined above for homogeneous and simply-connected objects has in addition been extended for also catering to (i) bi-material objects of different conductivity classes (e.g. a HC object embedded in a MC object) and (ii) multiply connected objects (setting the global loop functions apart due to their distinct behavior under integral operators). Both cases required significant modifications of the asymptotic expansion.

**Numerical example** We validate the asymptotic approximations (3), (4) on an example involving two objects (one bi-material, one homogeneous), the embedded object being multiply connected (Figure 2). The predicted convergence orders are confirmed. Other examples of this type, as well as applications to EC testing configurations, will be presented.

**References**


Maximizing the electromagnetic chirality for metallic nanowires in the visible spectrum

Marvin Knöller1,*
1Department of Mathematics, Karlsruhe Institute of Technology, Karlsruhe, Germany
*Email: marvin.knoeller@kit.edu

Abstract

Electromagnetic chirality describes differences in the interaction of scattering objects with electromagnetic fields of different helicity. If the scattering behavior of an object with respect to incident waves of one helicity cannot be reproduced with incident fields of the opposite helicity, then the object is said to be electromagnetically chiral (em-chiral), otherwise it is called em-achiral. Em-chirality can be quantified by chirality measures that attain the value 0 for an em-achiral object and the value 1 for a maximally em-chiral object. We investigate a shape optimization problem, where the goal is to construct thin metallic nanowires that exhibit large measures of em-chirality at a given frequency. We present a gradient based optimization method, based on an asymptotic representation formula for approximating scattered fields due to thin metallic scattering objects.

Keywords: Electromagnetic chirality, shape optimization, asymptotic representation formula

1 Scattering from metallic wires

Let \( \omega > 0 \) denote the angular frequency and let \( \varepsilon_0, \mu_0 > 0 \) denote the electric permittivity and magnetic permeability in free space. We define the wave number \( k > 0 \) in free space to be \( k = \omega \sqrt{\varepsilon_0 \mu_0} > 0 \). Let the pair of incident fields \((E^i, H^i)\) be entire solutions of time harmonic Maxwell’s equation in homogeneous space, i.e.

\[
\begin{align*}
\text{curl } E^i - i \omega \mu_0 H^i &= 0 \quad \text{in } \mathbb{R}^3, \\
\text{curl } H^i + i \omega \varepsilon_0 E^i &= 0 \quad \text{in } \mathbb{R}^3.
\end{align*}
\]

We assume that the incident field is scattered by a non-magnetic scattering object \( D \), for which we assume a constant electric permittivity \( \varepsilon_1 \in \mathbb{C} \) with \( \text{Re}(\varepsilon_1) < 0 \) and \( \text{Im}(\varepsilon_1) > 0 \). These electric permittivities are observed in the study of metallic scattering objects like silver and gold, especially for wavelengths in the visible electromagnetic spectrum. We define the permittivity distribution \( \varepsilon = \varepsilon_1 \chi_D + \varepsilon_0 \chi_{\mathbb{R}^3 \setminus \overline{D}} \) and consider the scattering problem in full space, which is to find the total fields

\[
(E, H) = (E^i + E^a, H^i + H^a)
\]

satisfying

\[
\begin{align*}
\text{curl } E - i \omega \mu_0 H &= 0 \quad \text{in } \mathbb{R}^3, \\
\text{curl } H + i \omega \varepsilon_0 E &= 0 \quad \text{in } \mathbb{R}^3,
\end{align*}
\]

together with the Silver-Müller radiation condition (SMR). The scattered field \( E^a \) satisfies a far field expansion, which reads

\[
E^a(x) = \frac{e^{ik|x|}}{4\pi|x|} \left( E^\infty(\hat{x}) + O(|x|^{-1}) \right)
\]

as \( |x| \to \infty \) uniformly with respect to all directions \( \hat{x} = x/|x| \in S^2 \).

In this talk we focus on thin tubular scattering objects \( D_\rho \), having an elliptical cross section that possibly rotates around the center curve \( \Gamma \). Here, the parameter \( \rho > 0 \) represents the radius of the elliptical cross section. The space of admissible parametrizations is denoted by \( \mathcal{U}_\text{ad} \).

The rotation function is further denoted by \( \theta \). In our work (see [3]) we establish an asymptotic representation formula for electric fields scattered by \( D_\rho \).

Theorem 1 For a thin tubular scatterer with elliptical cross section with semiaxes lengths \( a = \rho \bar{a} \) and \( b = \rho \bar{b} \), the far field of \( E_\rho^a \) satisfies

\[
E_\rho^\infty(\hat{x}) = a b k^2 \pi \int_{\Gamma} (\varepsilon_1 - 1) e^{-ik\hat{x} \cdot y} (\hat{x} \times \hat{e}_3) \times \hat{x} M_\rho(y) E^i(y) \, ds(y) + o(|D_\rho|)
\]

as \( \rho \to 0 \). The matrix valued function

\( M_\rho \in L^2(\Gamma, \mathbb{C}^{3 \times 3}) \)

is the so-called electric polarization tensor.

2 Maximizing electromagnetic chirality

We define the far field operator

\[
(\mathcal{F}_D A)(\hat{x}) = \int_{S^2} E^\infty(\hat{x}, d, A(d)) \, ds(d).
\]

Electromagnetic chirality describes the interaction of a scattering object \( D \) with fields of different helicities. As shown in [2], helicity of either
an incident Herglotz field $E^i[A]$ or the corresponding scattered field $E^s[A]$ can be characterized by the assignment of the representative field $A \in L^2(S^2, \mathbb{C}^3)$ to spaces $V^+$ or $V^-$ with $V^+ \oplus V^- = L^2(S^2, \mathbb{C}^3)$ where

$$V^\pm = \{ A \pm \epsilon A : A \in L^2(S^2, \mathbb{C}^3) \}$$

and $(\epsilon A)(\theta) = i \theta \times A(\theta)$ for $\theta \in S^2$. Using orthogonal projections, it is possible to derive a decomposition of the far field operator

$$F_D = F^{++} + F^{+-} + F^{-+} + F^--,$$  \tag{1}

where $F^{pq}$ characterizes the helicity contribution of the $p$ incident field to the $q$ scattered field for $p, q \in \{+, -\}$. For a thin scatterer $D_\rho$ we employ theorem 1 to approximate the far field operator. Introducing the operator

$$(T_{D_\rho}(A))(\hat{x}) := abk^2 \pi \int_{\Gamma} (\epsilon_\rho - 1) e^{-ik\hat{x}y} (\hat{x} \times \hat{y}) \times \hat{x} M_{\rho}(y) E^s[A](y) \, ds(y)$$

consequently gives that $F_D = T_{D_\rho} + o((k\rho)^2)$ as $\rho \to 0$ and the term $o((k\rho)^2)$ is such that $\|o((k\rho)^2)\|_{HS}/(k\rho^2)$ converges to zero. Here, $\| \cdot \|_{HS}$ denotes the Hilbert-Schmidt norm. We define the nonlinear operator

$$T_\rho(\Gamma, \theta) = T_{D_\rho},$$  \tag{2}

where $D_\rho$ is the thin tubular scatterer characterized by the center curve $\Gamma$ and the rotation function $\theta$. The operators $T_\rho(\Gamma, \theta)^{pq}$ for $p, q \in \{+, -\}$ are defined analogously to $F^{pq}$ and constitute a decomposition of $T_\rho$, equally to (1). These operators are now used to approximate the relative chirality measure introduced in [4]. In our setting, this approximation is denoted by

$$J_2 : L^2(S^2, \mathbb{C}^3) \to [0, 1]$$

with

$$J_2 = \sqrt{\frac{\|\sigma_{++}^- - (\sigma_{--}^+)\|^2_{L^2} + \|\sigma_{+-}^- - (\sigma_{-+}^+)\|^2_{L^2}}{\|T_\rho\|^2_{HS}}}$$

where $(\sigma_{pq}^\rho)$ denote the singular values of $F^{pq}$. The functional $J_2$ takes the value 1 for a maximally em-chiral object and the value 0 for an em-achiral object. Since the function $J_2$ is not smooth, we consider a smooth relaxation of $J_2$, denoted by $J_{\text{HS}}$. Moreover, we introduce penalty terms and regularization parameters, denoted by $\Lambda$ and $\alpha$, respectively, in order to stabilize the optimization functional. Thus, we define the regularized functional

$$F(\Gamma, \theta) = J_{\text{HS}}(\Gamma, \theta) - \alpha \Lambda(\Gamma, \theta),$$

that we aim to maximize with respect to the center curve $\Gamma$ and the rotation $\theta$ of the elliptical cross section around $\Gamma$. For this purpose, we apply the BFGS method to $F$. The far field operator approximation in (2) allows an explicit computation of the Fréchet derivative of $F$ with respect to $\Gamma$ and $\theta$, resulting in an efficient optimization scheme. An example of such an optimization can be found in Figure 1. The initial guess on the left, a 4 turn helix with an elliptical cross section, is iteratively deformed by the optimization scheme. An example of such an optimization can be found in Figure 1. The initial guess on the left, a 4 turn helix with an elliptical cross section, is iteratively deformed by the optimization scheme. An example of such an optimization can be found in Figure 1. The initial guess on the left, a 4 turn helix with an elliptical cross section, is iteratively deformed by the optimization scheme. An example of such an optimization can be found in Figure 1. The initial guess on the left, a 4 turn helix with an elliptical cross section, is iteratively deformed by the optimization scheme.

In Figure 1, the optimization functional is presented by $J_{\text{HS}}(\Gamma, \theta) = \alpha \Lambda(\Gamma, \theta)$, that we aim to maximize with respect to the center curve $\Gamma$ and the rotation $\theta$ of the elliptical cross section around $\Gamma$. For this purpose, we apply the BFGS method to $F$. The far field operator approximation in (2) allows an explicit computation of the Fréchet derivative of $F$ with respect to $\Gamma$ and $\theta$, resulting in an efficient optimization scheme. An example of such an optimization can be found in Figure 1. The initial guess on the left, a 4 turn helix with an elliptical cross section, is iteratively deformed by the optimization scheme. An example of such an optimization can be found in Figure 1. The initial guess on the left, a 4 turn helix with an elliptical cross section, is iteratively deformed by the optimization scheme. An example of such an optimization can be found in Figure 1. The initial guess on the left, a 4 turn helix with an elliptical cross section, is iteratively deformed by the optimization scheme. An example of such an optimization can be found in Figure 1. The initial guess on the left, a 4 turn helix with an elliptical cross section, is iteratively deformed by the optimization scheme. An example of such an optimization can be found in Figure 1. The initial guess on the left, a 4 turn helix with an elliptical cross section, is iteratively deformed by the optimization scheme.

References


Angle-dependent SIBC model of metamaterial in FDTD method

Samuel Gaucher1,∗, Christophe Guiffaut2, Alain Reineix2, Olivier Cessenat1

1CEA CESTA, Le barp, France
2XLIM laboratory, Limoges, France
∗Email: samuel.gaucher@xlim.fr

Abstract
To control the diffraction of a target illuminated by a RADAR wave, one technique is to consider metamaterials. Simulating their behaviour can be complex especially when they are applied as thin heterogeneous layers on the surface of the target. This can be achieved, by first determining an angle-dependent surface impedance model, that is after implemented in a 3D FDTD solver.

Keywords: SIBC, metamaterial, FDTD

1 Introduction
The interest of using a surface impedance model (SIBC) is multiple. First, it avoids meshing a complex geometry covering some parts of the target. Then, the spatial mesh can be released. Indeed, it is supposed to be small enough to capture the field variations inside the thin layer of metamaterials. Since the latter is replaced by a SIBC model, the chosen spatial mesh can be larger because it is not governed anymore by the thin layer thickness. As a result, the computational volume is reduced as $R^3$ and the computational time by $R^4$ where $R$ is the factor of relaxed meshing.

For this purpose, both the wideband and efficiency finite-difference time-domain (FDTD) method is used to compute the electromagnetic fields. In a first step, the surface impedances are calculated with the Spectral FDTD (SFDTD) scheme [1] for all incidence angles and for the TE and TM modes. SFDTD method is a good candidate because no additional constraint is needed on the CFL criterion. Thus, periodic Floquet boundary conditions (PBC) are applied around the elementary pattern of the periodic metamaterial. In a second step, the frequency-angle-polarization-dependent SIBC model is decomposed by the vector fitting (VF) technique [2] and the Leontovich relation is used to introduce the metamaterial on the target surface [3]. This approach allows a simple and efficient calculation of the tangential electric field at the metamaterial surface. Moreover, the VF decomposition avoids the processing of a convolution product in the time domain.

2 SIBC model construction
Let $k$ be the unit vector along the incident axis. For each cell containing an interface with a metamaterial, we identify the local coordinates reference $(u, v, n)$ where $n$ is the normal outgoing unit vector and $(u, v)$ are the unit tangential vectors on the surface of the metamaterial. The local elevation angle $\theta_n$ and azimuth $\varphi_{u,v}$ defined on the figure 1 are deduced as

$$\theta_n = \arccos k_n, \quad \varphi_{u,v} = \arctan \frac{k_v}{k_u}.$$  \hspace{1cm} (1)

where $(k_u, k_v, k_n)$ are the components of vector $k$ in the local benchmark. The electric field components in the cylindrical coordinates $(\rho, \phi)$ are then calculated by the Leontovich relation

$$\begin{bmatrix} E_\rho \\ E_\phi \end{bmatrix} = \begin{bmatrix} 0 & -Z_\rho(\omega, \theta_n, \varphi_{u,v}) \\ Z_\phi(\omega, \theta_n, \varphi_{u,v}) & 0 \end{bmatrix} \begin{bmatrix} H_\rho \\ H_\phi \end{bmatrix}.$$  \hspace{1cm} (2)

Note that the metamaterial surface impedances $Z_\rho$ and $Z_\phi$ in (2) are known as they have been previously computed by the SFDTD method. Let $\mathcal{M}$ be the transform matrix between the cylindrical basis and the local cartesian basis. The local components $(E_u, E_v)$ read

$$\begin{bmatrix} E_u \\ E_v \end{bmatrix} = \mathcal{M}^{-1}(\varphi) \begin{bmatrix} 0 & -Z_\rho \\ Z_\phi & 0 \end{bmatrix} \mathcal{M}(\varphi) \begin{bmatrix} H_u \\ H_v \end{bmatrix}.$$  \hspace{1cm} (3)
To solve (3), the impedances are decomposed using the VF technique to make time domain processing easier

$$Z_{\rho,\phi}(\omega) = r_0 + \sum_{n=1}^{N} \frac{k_n}{j\omega - \omega_n}, \quad (4)$$

where $r_0$ is the resistance, $k_n$ the residues et $\omega_n$ the poles. The poles number should be at least $N = 3$ for a sufficient accuracy. Then, $N = 6$ poles are used in the simulation of section 3.

3 Numerical results

The problem consists in a perfectly conducting (PEC) cube covered with patterns on its three $xOy$ inf, $yOz$ inf and $xOz$ inf faces. Fig. 2 represents the elementary pattern geometry of an arbitrary and non-absorbing periodic structure which has been previously simulated by the SFDTD method for several incident angles, for the TE and TM modes and on the $0^\circ - 15$ GHz frequency band. The cube is submitted to an incident plane wave at incidence $\theta_i = 60^\circ$, $\varphi = 30^\circ$ (see Fig. 3). The three faces covered with patterns are in direct visibility of the incident rays. We compare the SIBC model with the reference FDTD scheme and the case where the cube is only a PEC to note the material effect. The PEC cube side length is $L = 37.5$ mm. Spatial discretization steps are all set to $\Delta = 0.125$ mm for the FDTD reference and 3.22 times bigger $\Delta = 0.4025$ mm for the SIBC case. Then, CFL = 0.99. Note that the three sides are covered with a patch of $20 \times 20$ patterns. The radar cross section (RCS) is computed in the direction $\varphi = 30^\circ$ for all $\theta$ angles and for the TM mode. Fig. 4 shows the good agreement between the SIBC model and the standard FDTD scheme for the chosen frequency $f = 5$ GHz.

References


Localization landscape for interacting Bose gases in one-dimensional speckle potentials

Filippo Stellin$^{1,*}$, Marcel Filoche$^2$, Frédéric Dias$^{1,3}$

$^1$Centre de Borelli, École Normale Supérieure Paris-Saclay, Gif-sur-Yvette, France
$^2$Laboratoire de Physique de la Matière Condensée, École Polytechnique, Palaiseau, France
$^3$School of Mathematics and Statistics, University College Dublin, Belfield, Ireland

Email: filippo.stellin@ens-paris-saclay.fr

Abstract

Using the localization-landscape theory [1], we investigate the properties and the shape of the ground state (GS) of a gas of ultracold bosons in one-dimensional (1D) speckle potentials, starting from the Gross-Pitaevskii equation (GPE). For attractive interactions, we find approximate relations holding between the localization length and the disorder parameter as well as between the former quantity and the nonlinear coefficient. For weakly repulsive interactions, we prove that the ground state $\psi_0$ of the GPE can be understood as a superposition of a finite number of single-particle (SP) states. We show numerically that, for intermediate repulsive interactions, $\psi_0$ follows the modulations of the effective potential. We further prove that, for given parameters of the SP Hamiltonian, there exists a value of the nonlinear coefficient at which $\psi_0$ is well predicted by the normalized localization landscape.

Keywords: Nonlinear waves, Atomic gases, Random and disordered media

1 Introduction

We consider ultracold dilute Bose gases in a geometry with a 1D random potential along the $x$ axis and a two-dimensional harmonic potential with frequency $\omega_x$ in the $(y, z)$ plane. The level spacing between two neighboring eigenstates of the SP 1D problem along $x$ is assumed to be smaller than zero-point energy $E_x := \hbar \omega_x$ of the harmonic oscillator (HO), so the GS can be factorized into the one of the two-dimensional (2D) HO and that of a one-dimensional GPE. After integrating out the transverse-plane wave-functions, the GPE along the $x$ axis reads [2]:

\[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_R(x) + \hbar \omega_x + \frac{2\hbar \omega_x a_s (N-1)|\psi_0(x)|^2}{m g} \psi_0(x) = \mu \psi_0(x), \quad (1)\]

where $V_R$ denotes the random potential, $H^{\text{sp}}$ the SP Hamiltonian, $g$ labels the nonlinear coupling and $a_s$ represents the s-wave scattering length. The random potential treated here is a correlated speckle potential, whose probability distribution in the space obeys the Rayleigh law,

\[P(V_R) = \frac{\Theta_H(V_R V_0)}{V_0 e^{-V_R/V_0}}, \quad (2)\]

where $\Theta_H(x)$ is Heaviside’s step function and $V_0$ the disorder parameter. The spatial correlation profile $C(x)$ of the potential is chosen to be Gaussian:

\[C(x) := |V_R(0) - V_0| |V_R(x) - V_0| = V_0^2 e^{-\frac{x^2}{\sigma^2}}, \quad (3)\]

in which $\sigma$ denotes the correlation length, whereas $\bar{\lambda}$ indicates the average over the configurations of the disordered potential.

2 The localization landscape

From the one-dimensional problem found in Eq. (1), a localization landscape (LL) function $u(x)$ can be defined in analogy to the one introduced in Ref. [1],

\[H^{\text{sp}}(x)u(x) = 1, \quad (4)\]

satisfying the boundary conditions $u(x)|_{x=\pm L} = 0$, where $L$ is the length of the 1D domain. Similarly to the procedure carried out in Ref. [1], the solution $\psi$ can be expressed as a product of the landscape function $u$ and the auxiliary function $\varphi$. Equation (1) can be thus recast as:

\[-\frac{\hbar^2}{2m} \left[ \frac{1}{u^2} \frac{\partial}{\partial x} \left( u^2 \frac{\partial \varphi}{\partial x} \right) \right] + \frac{\varphi}{u} + \frac{g(N-1)|u|^2|\varphi|^2}{u} \varphi = \mu \varphi, \quad (5)\]

which is a GP-like equation with a different elliptic differential operator and a space-dependent coefficient of the nonlinear interaction term. The effective random potential is now given by $W(x) := u(x)^{-1}$, as proven in the SP case [3].

3 Attractive interactions

We numerically computed ground state $\psi_0$ of the GPE using the split-step Crank-Nicolson method [4], which is based on imaginary-time evolution. In the case of attractive interactions, the wavefunction is localized and its asymptotical behaviour can be well approximated as:

\[\psi_0(x) \approx \sqrt{\frac{2}{\lambda_L + \lambda_R}} \begin{cases} e^{\frac{-(x-x_0)}{\lambda_L}} & x < x_0 \\ e^{\frac{-(x-x_0)}{\lambda_R}} & x > x_0 \end{cases}, \quad (6)\]

where $\lambda_L$ and $\lambda_R$ represent the left and the right localization lengths respectively. The latter quantities
appear to shrink as $|g(N−1)|$ is increased. By computing the localization lengths for variable nonlinear coefficients and performing nonlinear regressions, we find that the following relations hold:
\[
\tilde{\lambda}_n = \frac{a_n}{\tilde{g}(N−1) + b_n} + c_n, \quad (7)
\]
where $\tilde{\lambda}_n := \lambda_n/l_\perp$ with $l_\perp := \sqrt{\frac{\hbar}{m\omega}}$ and $n = L, R$, whereas $\tilde{g} = g/(E_n l_\perp)$. By proceeding with an analogous method, we numerically assessed the validity of the following relation with the disorder mean value:
\[
\tilde{\lambda}_n = \frac{A_n}{(\tilde{V}_0 + B_n)^2} + C_n, \quad (8)
\]
where $\tilde{V}_0 := V_0/E_n$, which is also consistent with the known result in the absence of interactions [5].

4 Repulsive interactions

For weak repulsive interactions ($\mu \sim E_0$), we prove that $\psi_0(x)$ can be expressed as a superposition of the $N_x$ lowest-lying SP eigenstates of $H^{\text{pp}}$:
\[
\psi_0^{\text{pp}}(x) = \sum_{j=0}^{N_x-1} c_j \psi_j^{\text{sp}}(x), \quad (9)
\]
where the coefficients $\{c_j\}$ must satisfy $\sum_{j=0}^{N_x-1} |c_j|^2 = 1$. $N_x$ can be reckoned as $N_x \approx n^{\text{sp}}(E_0^{(0)})$, which is the number of SP states whose energy lies below $E_0^{(0)}$, i.e., the integrated density of states (IDoS), evaluated at $E_0^{(0)}$. The latter quantity is defined as:
\[
E_0^{(0)} := E_0^{\text{pp}} + \frac{g(N−1)}{2} \int_{-L/2}^{L/2} |\psi_0^{\text{pp}}(x)|^4 \, dx. \quad (10)
\]

In the presence of repulsive interactions, in contrast with the attractive case, the wavefunction $\psi_0(x)$ gets increasingly delocalized (with decreasing oscillation amplitude) as the nonlinearity coefficient is raised. For intermediate repulsive interactions, when the healing length $\xi := \sqrt{\frac{\hbar \sqrt{2m\mu}}{\mu^{\text{pp}}}}$ satisfies $\xi \geq \sigma$ and $\xi \ll L$, we introduce the following approximation scheme based on the the effective potential $W(x)$:
\[
|\psi_0^{\text{TF}}(x)| \approx \begin{cases} 
\psi_0^{\text{TF}}(x) & \mu \geq W(x) \\
0 & \mu < W(x)
\end{cases}, \quad (11)
\]
where $\psi_0^{\text{TF}}$ denotes the normalization constant. In Panels (c)-(f) of Fig. 1, $|\psi_0^{\text{TF}}(x)|$ is compared against the perturbative approximation, $\psi_0^{\text{sp}}$ proposed in Ref. [6]. We further prove that, for given parameters of $H^{\text{pp}}$, there exists a value of $g(N−1)$ at which $\psi_0$ is well predicted by the normalized localization landscape:
\[
\psi_i(x) = \frac{u(x)}{\int_{-L/2}^{L/2} |u(x)|^2 \, dx}. \quad (12)
\]

For strong repulsive interactions ($\xi \ll \sigma$), the kinetic energy term in the GPE can be neglected and the wavefunction follows the modulations of the original potential $V(x)$, thus is well described by the Thomas-Fermi approximation [6].

Figure 1: Approximations of $|\psi_0| := |\psi_0^{\text{pp}}|^{1/2}$ plotted as functions of $\tilde{x} := x/l_\perp$ for different values of the nonlinear coefficient.

References

Complex Effective Wavenumbers of Isotropic Particulate Materials

Aristeidis Karnezis\(^1\),*, Artur L. Gower\(^1\)

\(^1\)Department of Mechanical Engineering, The University of Sheffield, Sheffield, UK
*Email: akarnezis1@sheffield.ac.uk

Abstract

A key assumption used to describe scalar waves in a random particulate material is that the average field satisfies a wave equation with a unique effective wavenumber \(k_\ast\). By average wave we mean to ensemble average over all possible configurations of particles. As the medium is homogeneous and isotropic - because the particles have no specific orientation and are evenly distributed - it seems reasonable to assume that there is only one effective wavenumber. However, recently two different theoretical models have predicted that there exist at least two (complex) effective wavenumbers for one fixed frequency [1], [3]. A phenomenon normally observed only in anisotropic media. Our goal is to find clear evidence of these complex effective wavenumbers by using a Monte Carlo approach based on high fidelity simulations. To achieve this, we place a mix of random particles inside a very large plate geometry. In conclusion, we find evidence for two effective wavenumbers and even discover an effective wavenumber with a negative real part, which implies there is an average transmitted wave going backwards, i.e the opposite direction of the incident wave.

Keywords: wave propagation, random media, multiple scattering, ensemble averaging

1 Introduction

Particulate materials consisting of particles that are randomly distributed within some homogeneous media are frequently used across many research disciplines and industries. For instance, these materials are used as contrast agents in medical ultrasound and other imaging fields. This is why accurate models of waves in these materials are of great importance.

When using light or sound waves to sense the particulates, it is necessary to understand how each particle scatters waves. In other words, it is important to consider that both particle properties and particle positions affect the total scattered waves, as shown in Figure (1). Although it is usually impossible to know both particle properties and positions, there are specific types of average measurements that can help us obtain reliable measurements for the total average wave \(\langle u(x)\rangle\). These measurements are based on the ensemble averaging technique, which can both simplify the calculations and devise measurements that do not depend on the positions of the particles.

![Figure 1: Scattering from one specific configuration of particles due to an incident plane wave striking a very large plate geometry filled with randomly distributed particles.](image)

The process of calculating the ensemble average relates the speed of the effective wave \(c_\ast\) and the rate of attenuation \(\alpha\) with the particles. The combination of those two measurables, forms the complex effective wavenumbers:

\[
k_\ast = \frac{\omega}{c_\ast} + i\alpha
\]

where \(\omega\) is the frequency.

In this paper, we look to design a computational experiment investigating the simplest case that shows the existence of at least two of these effective wavenumbers.

2 Why does it matter?

Two different theoretical models have predicted that there exist at least two (complex) effective wavenumbers for one fixed frequency [1]. These two wavenumbers would make a significant difference in the reflection and transmission [2].
The theoretical models would predict the number of effective waves $P$ described by the complex effective wavenumbers. This will allow us to obtain more accurate predictions for the overall average wave and by extension, the reflection and transmission coefficients. Hence, our objective is to verify these predictions using a robust numerical method based on high fidelity Monte Carlo simulations.

3 Theoretical and Numerical Predictions

Let us consider a plate filled with particles that are randomly distributed and a plane wave source that emits the incoming waves (Fig.1). As a result, the average transmitted wave inside the homogeneous, isotropic particulate material takes the form

$$\langle u(x) \rangle = \sum_{p=1}^{P} A_p e^{i k_p x - i \omega t}. \quad (1)$$

In this expression, $A_p$ represent the average transmission coefficient, $k_p$ are the complex effective wavenumbers and $x$ is a position vector inside the material. The factor $e^{i \omega t}$ is omitted for our convenience since it carries information about the incident wave emitted by the source.

Our goal is to approximate the $A_p$ and $k_p$ terms of the effective waves.

Recent studies show that in most cases, these effective waves are highly attenuating, meaning that the lower the attenuation $\text{Im} \, k_p$, the greater the resulting amplitude of the effective wave and therefore the more it contributes to the overall average wave $\langle u(x) \rangle$.

Following our study case, we will use simpler methods to approximate only the first two coefficients $A_1$ and $A_2$ in equation (1) along with the incident plane-wave. Applying the asymptotic approximations, we get that

$$\langle u(x) \rangle = A_1 e^{i k_1 x} + A_2 e^{i k_2 x} + A_n e^{i k_n x} + \epsilon(x), \quad (2)$$

where $\epsilon(x)$ rapidly decays with $x$.

To extract the amplitude and the complex effective wavenumber of each effective wave forming equation (2), we employ the nonlinear least-square fitting, as shown in Figure (2). Data generated from high fidelity Monte Carlo simulations are fitted to a function that looks like equation (2). This leads to the desired coefficients $A_1, A_2, k_1, k_2$. At this point, we even discovered an effective wavenumber with a negative real part. In this peculiar case, the average transmitted wave propagates backwards, i.e. in the opposite direction to the incident wave.

Predicting the existence of more than one effective wavenumbers, increases the number of effective waves $P$. Hence, to produce more accurate results for the reflection and transmission, we need to generate phase diagrams that would indicate the essential number of effective waves.

In this talk, I will present a comparison between the fitted wavenumbers and the wavenumbers predicted by the Monte Carlo simulations. I will also discuss the necessity of the phase diagrams and the importance of calculating the wavenumbers for a wide range of frequencies, volume fractions and particle properties.

References


Speckle statistics in stochastic homogenization regime

Quentin Goepfert\textsuperscript{1,∗}, Josselin Garnier\textsuperscript{2,2}, Laure Giovangigli\textsuperscript{1}, Pierre Milien\textsuperscript{3,3}

\textsuperscript{1}UMA Poems ENSTA, Palaiseau, France
\textsuperscript{2}CMAP Ecole Polytechnique, Palaiseau, France
\textsuperscript{3}Institut Langevin, Paris, France

\textsuperscript{∗}Email: quentin.goepfert@ensta-paris.fr

Abstract

We aim at describing the statistics of the acoustic wavefield backscattered by a randomly heterogeneous penetrable medium in the homogenization regime.

Keywords: stochastic homogenization, wave equation

1 Introduction

In biological ultrasound imaging, the measured quantity is the backscattered wave generated by a large number of unresolved subwavelength scatterers. These scatterers can be modeled as inhomogeneities in density and compressibility. In the Born approximation, the backscattered field is well understood, but the assumption does not hold when the number of scatterers becomes very large, which is the case in many situations. Stochastic homogenization techniques do not rely on single diffusion approximation and can be an accurate model to describe the backscattered field.

2 Framework

Here $d$ denotes the dimension, $d = 1, 2$ or $3$. Let $(\Omega, \mathcal{F}, \mathbb{P})$ be the probability space and let $\mathcal{M} \subset \mathbb{R}^d$ be the medium in which lie small randomly placed inhomogeneities of size $\epsilon > 0$. We denote by $a_\epsilon \in C^\infty(\mathbb{R}^d, \mathbb{R}^d \times \mathbb{R}^d)$ the density and $n_\epsilon \in C^\infty(\mathbb{R}^d)$ the compressibility. We suppose that the outer medium $\mathbb{R}^d \setminus \mathcal{M}$ is homogeneous of parameters $(I, 1)$. The inhomogeneities $(\epsilon S^\omega_i)_{i \in \mathbb{N}_\ast}$ have constant parameters denoted by $(a^S_{\omega_i})_{i \in \mathbb{N}_\ast}$ and $(n^S_{\omega_i})_{i \in \mathbb{N}_\ast}$ and lie in a homogeneous background with properties $(a_m, n_m)$.

For all $x \in \mathbb{R}^d$ and a.e. $\omega \in \Omega$, the density and compressibility are therefore modeled by:

\[
\begin{align*}
\{a_\epsilon(x) &:= a_m(1 + \eta_a(x/\epsilon, \omega))\chi_M(x) + (1 - \chi_M(x))I \\
n_\epsilon(x) &:= n_m(1 + \eta_n(x/\epsilon, \omega))\chi_M(x) + (1 - \chi_M(x))1
\end{align*}
\]

with

\[
\begin{align*}
\eta_a(x, \omega) &= \sum_{i \in \mathbb{N}_\ast} \left(\frac{a^{-1}_{\omega_i}a^S_{\omega_i}}{n_{\omega_i}} - 1\right) \chi_{S^\omega_i}(x) \\
\eta_n(x, \omega) &= \sum_{i \in \mathbb{N}_\ast} \left(\frac{n^S_{\omega_i}}{n_{\omega_i}} - 1\right) \chi_{S^\omega_i}(x)
\end{align*}
\]

The medium contains around $\epsilon^{-d}$ particles, spaced from each other by a distance of order $\epsilon$, so that we are in the homogenization regime. Furthermore we assume that the distribution of the center of the particles $(S^\omega_i)_{i \in \mathbb{N}_\ast}$ of size 1, is a stationary and ergodic process. Therefore $\eta_a$ and $\eta_n$ are stationary and ergodic processes. Moreover, $a_\epsilon$ and $n_\epsilon$ are supposed to be bounded both below and above, by respectively strictly positive matrices or constants independent of the randomness.

We excite the medium by a time-harmonic plane wave $u^0$. An example is shown on figure 1.

\[
\begin{align*}
\Delta u_\epsilon + k^2 u_\epsilon &= 0 & \text{in } \mathbb{R}^d \setminus \mathcal{M} \\
\nabla \cdot (a_\epsilon \nabla u_\epsilon) + k^2 n_\epsilon u_\epsilon &= 0 & \text{in } \mathcal{M} \\
(u_\epsilon + u^0) &= u_\epsilon & \text{on } \partial \mathcal{M} \\
\nabla (u_\epsilon + u^0) \cdot \nu &= a_\epsilon \nabla u_\epsilon \cdot \nu & \text{on } \partial \mathcal{M}
\end{align*}
\]
along with the Sommerfeld radiation condition on the scattered wave field \( u_0^s \).
This problem has already been treated in [3] in the periodic case.

Under the stationary and ergodic assumption, it can be shown [1] that the solution \( u_0 \) converges in almost surely weakly in \( H^1_{\text{loc}}(\mathbb{R}^d) \) towards a homogenized field \( u_0 = u^i + u_0^s \) solution of:

\[
\begin{align*}
\{ & \Delta u_0^s + k^2 u_0^s = 0 & \text{in } \mathbb{R}^d \setminus \overline{\mathcal{M}} \ \\
\n\n\{ & \nabla \cdot (a^s \nabla u_0) + k^2 n^s u_0 = 0 & \text{in } \mathcal{M} \\
\n\n\{ & (u_0^s + u^i) = u_0 & \text{on } \partial \mathcal{M} \\
\n\n\{ & \nabla (u_0^s + u^i) \cdot \nu = a^s \nabla u_0 \cdot \nu & \text{on } \partial \mathcal{M}
\end{align*}
\]

complemented with the radiation condition on \( u_0^s \), for some positive definite and constant tensor \( a^* \) and positive constant \( n^* \).

We will present our estimates of the error in the Hilbert space \( \mathcal{L} := L^2(\Omega, L^2_{\text{loc}}(\mathbb{R}^d \setminus \overline{\mathcal{M}})) \) in several situations.

Though, in order to get quantitative results, we need to strengthen our hypotheses and assume a quantitative mixing condition [2] such as a Log Sobolev Inequality. Numerous processes satisfy all these conditions such as the type-2 Matérn process which match our model and satisfy a weighted Log-Sobolev Inequality.

3 Case \( a_c \) constant

We will first present the case where \( a_c \) is constant. Indeed, in this case the equation is simpler and we can find a far field expansion, involving the homogenized Green function \( G_0 \), solution for \( y \in \mathbb{R}^d \) of:

\[
\begin{align*}
\{ & \Delta G_0(\cdot, y) + k^2 G_0(\cdot, y) = -\delta_y & \text{in } \mathbb{R}^d \setminus \overline{\mathcal{M}} \\
\n\n\{ & \nabla \cdot (a^s \nabla G_0(\cdot, y)) + k^2 n^s G_0(\cdot, y) = -\delta_y & \text{in } \mathcal{M}
\end{align*}
\]

along with the usual transmission conditions and the Sommerfeld radiation condition.

Theorem 1. For \( x \in \mathbb{R}^d \setminus \overline{\mathcal{M}} \):

\[
u_c(x) = u_0(x) + k^2 \int_{\mathcal{M}} (n_c(y) - n^*)u_0(y) \times G_0(y, x) \, dy + O_\mathcal{L}(\epsilon^d)
\]

This result is a generalization of the Born expansion with the homogenized solution instead of the incident wave field. A corollary of Theorem 1 describes the statistics of the wave field \( e^{-d/2}u_c \) as a zero-mean Gaussian process with a covariance function that depends on the two-point statistics of the random process \( n_c \).

4 1D case

When \( d = 1 \), explicit formulae can be found and therefore, it is possible to get an asymptotic model in the general case and control all of the error terms.

Theorem 2. For \( x \in \mathbb{R} \setminus \overline{\mathcal{M}} \):

\[
u_c(x) = u_0(x) + \int_{\mathcal{M}} \left( \frac{a^*}{a_c(y)} - 1 \right) a^* u_0^s(y) \partial_x G_0(x, y) \, dy \\
+ k^2 \int_{\mathcal{M}} (n_c(y) - n^*)u_0(y)G_0(x, y) \, dy + O_\mathcal{L}(\epsilon)
\]

In dimension 1, we have explicit formulae for \( a^* \) and \( n^* \), that is:

\[
\begin{align*}
a^* &= \mathbb{E}(\frac{1}{a_c})^{-1} \\
n^* &= \mathbb{E}(n_c)
\end{align*}
\]

Using these formulae, we can also evaluate the two main terms in (5) which are both of mean zero and of size \( \epsilon^2 \) as expected.

5 Conclusion

We have described the behavior of the speckle field generated by a large number of compressibility inhomogeneities which results in an analogue to the Born approximation. The case when the inhomogeneities also present a density contrast shall be treated in forthcoming work.

References


A space–time Trefftz discontinuous Galerkin method for the linear Schrödinger equation

Sergio Gómez, Andrea Moiola

1 Dipartimento di Matematica “F. Casorati”, Università di Pavia, 27100 Pavia, Italy
*Email: sergio.gomez01@universitadipavia.it

Abstract
A space–time Trefftz discontinuous Galerkin method for the Schrödinger equation with piecewise-constant potential is presented. Trial and test spaces are spanned by non-polynomial complex wave functions that satisfy the Schrödinger equation locally on each element of the space–time mesh. We prove well-posedness and stability of the method, and optimal, high-order, h-convergence error estimates in a skeleton norm. We validate numerically our theoretical results presented.

Keywords: Linear Schrödinger equation, Trefftz method, discontinuous Galerkin method.

1 Introduction
In this work we consider the following initial boundary value problem for the homogeneous, time-dependent Schrödinger equation on a space–time cylinder $Q = \Omega \times I$, where $\Omega$ is an open and bounded domain in $\mathbb{R}^d$, $d \in \mathbb{N}$, with Lipschitz boundary $\partial \Omega$ and $I = (0, T)$, for some $T > 0$:

\begin{equation}
\label{eq:1.1a}
 i \partial_t \psi + \Delta \psi - V \psi = 0, \quad \text{in } Q,
\end{equation}

\begin{equation}
\label{eq:1.1b}
 \psi = g_0 \quad \text{on } \partial \Omega \times I,
\end{equation}

\begin{equation}
\label{eq:1.1c}
 \psi(x, 0) = \psi_0(x), \quad \text{on } \Omega.
\end{equation}

Here the Dirichlet boundary datum $g_0$ and the initial condition $\psi_0$ are given functions; $V : \Omega \to \mathbb{R}$ is a piecewise-constant potential and the Laplacian operator $\Delta$ refers to the space variable $x$ only.

The model (1.1) arises from a wide number of applications: it is the fundamental equation of quantum mechanics, in optics it is known as “paraxial wave equation” and approximates the Helmholtz equation when the optical field acts mostly along one specific axis (Fresnel’s approximation), while in underwater acoustics it is called “parabolic equation”.

We present the main details in the formulation and the analysis of the space–time Trefftz-DG method for the linear Schrödinger equation proposed in [2].

2 Trefftz-DG formulation
Let $\mathcal{T}_h(Q)$ be a space–time finite element mesh of $Q$, where each element $K \in \mathcal{T}_h(Q)$ has a tensor product structure $K = K_x \times I_n$ with $K_x$ being an element of a polytopic partition of $\Omega$ and $I_n$ is an interval in time.

The global Trefftz space $\mathbf{T}(\mathcal{T}_h)$ consists of functions whose restriction to each cell $K \in \mathcal{T}_h(Q)$ belongs to the following space:

\begin{equation}
\mathbf{T}(K) := \left\{ w \in H^1(I_n; L^2(K_x)) \cap L^2(I_n; H^2(K_x)) \mid s.t. \right. \quad \left. i \partial_t w + \Delta w - V w = 0 \quad \text{on } K = K_x \times I_n \right\}.
\end{equation}

We consider a finite-dimensional subspace $\mathbf{T}_p(\mathcal{T}_h) := \prod_{K \in \mathcal{T}_h} \mathbf{T}_p(K) \subset \mathbf{T}(\mathcal{T}_h)$ defined for each $K = K_x \times I_n \in \mathcal{T}_h(Q)$ and for $p \in \mathbb{N}$ as the following set of complex exponentials:

\begin{equation}
\mathbf{T}_p(K) := \left\{ \phi_\ell(x, t) \mid \ell = 1, \ldots, n_{d,p} \right\},
\end{equation}

where

\begin{equation}
\phi_\ell(x, t) := \text{exp} \left[ i \left( k_\ell \mathbf{d}_\ell \cdot \mathbf{x} - (k_\ell^2 + V|K|)t \right) \right]
\end{equation}

for $\ell = 1, \ldots, n_{d,p}$,

for some parameters $\{k_\ell\} \subset \mathbb{R}$ and directions $\{\mathbf{d}_\ell\} \subset \mathbb{R}^d$.

As numerical fluxes we use an upwind in time and classical average in space with an appropriate complex penalization. The Trefftz-DG variational formulation is: seek $\psi_{hp} \in \mathbf{T}_p(\mathcal{T}_h)$ such that $\mathbf{A}(\psi_{hp}; s_{hp}) = \ell(s_{hp})$, $\forall s_{hp} \in \mathbf{T}_p(\mathcal{T}_h)$, where

\begin{equation}
\mathbf{A}(\psi_{hp}; s_{hp}) := \int_{\mathcal{F}_h^0} (\nabla \psi_{hp} \cdot \mathbf{n}\bar{h} + i\alpha \psi_{hp}) \bar{s}_{hp} dS
\end{equation}

\begin{equation}
+ \int_{\mathcal{F}_h^{\text{time}}} \left( \{\nabla \psi_{hp}\} \cdot \bar{\mathbf{n}_{\mathbb{R}^2}} |\nabla \psi_{hp}|_N + i\beta \{\nabla \psi_{hp}\} \cdot \bar{\mathbf{n}_{\mathbb{R}^2}} |\nabla \psi_{hp}|_N \right) dS
\end{equation}

\begin{equation}
- \left\{\{\psi_{hp}\}\right\} \bar{\mathbf{n}_{\mathbb{R}^2}} |\nabla \psi_{hp}|_N + i\beta |\nabla \psi_{hp}|_N \bar{\mathbf{n}_{\mathbb{R}^2}} dS
\end{equation}

\begin{equation}
\int_{\mathcal{F}_h^{\text{space}}} i\psi_{hp} \bar{\mathbf{n}_{\mathbb{R}^2}} \mathbf{d}x + \int_{\mathcal{F}_h^{\text{time}}} i\psi_{hp} \bar{\mathbf{n}_{\mathbb{R}^2}} \mathbf{d}x,
\end{equation}

\begin{equation}
\ell(s_{hp}) := \int_{\mathcal{F}_h^{\text{time}}} i\psi_{hp} \bar{\mathbf{n}_{\mathbb{R}^2}} \mathbf{d}x
\end{equation}

\begin{equation}
+ \int_{\mathcal{F}_h^{\text{space}}} g_0 (\nabla \bar{s}_{hp} \cdot \mathbf{n}\bar{h} + i\alpha \bar{s}_{hp}) dS.
\end{equation}
As a result of the Trefftz property, the definitions of \( \mathcal{A}(\cdot; \cdot) \) and \( \ell(\cdot) \) in the variational formulation are independent of the potential \( V \), which has an effect only on the discrete space.

Well-posedness and a quasi-optimality estimate follow from the Lax–Milgram theorem and the coercivity and continuity of \( \mathcal{A}(\cdot; \cdot) \).

3 Approximation estimate

The key idea to establish convergence rates in the mesh size \( h \) was introduced by O. Cessenat and B. Després in the proof of [1, Thm.3.7] (in the case of the ultra weak variational formulation applied to the Helmholtz equation): if, given any smooth PDE solution \( \psi \), the local discrete space contains an element with the same degree-\( p \) Taylor polynomial of \( \psi \), then the space enjoys the same \( h \)-approximation properties of the space \( \mathbb{P}_p \) of degree-\( p \) polynomials. The following condition implies that for any sufficiently smooth Schrödinger solution \( \psi \) such an approximant exists in the local Trefftz space.

**Condition 1** Let \( B \subset K \) be a \((d+1)\)-dimensional ball such that \( K \) is star-shaped with respect to \( B \). Let \( \{\phi_1, \ldots, \phi_{n_{d,p}}\} \subset C^\infty(K) \) be a basis of \( \mathbb{T}_p(K) \). For every \( \psi \in \mathbb{T}(K) \cap H^{p+1}(K) \), there exists a complex vector-valued function \( a \in L^1(B)^{n_{d,p}} \) satisfying the following two conditions

For all \( |j| \leq p \) and a.e. \( (z, s) \in B \),

\[
D_j^j \psi(z, s) = \sum_{\ell=1}^{n_{d,p}} a_\ell(z, s) D_j^j \phi_\ell(z, s),
\]

\[
\||a_1|||_{L^1(B)} \leq C_s |K|^{1/2} \|\psi\|_{H^{p+1}(K)},
\]

where \( C_s > 0 \) might depend on \( d, p \), and \( \{\phi_\ell\} \) but is independent of \( K \) and \( \psi \).

Theorem 1 provides the error estimate for the Trefftz-DG approximation of (1.1) in the mesh skeleton norm \( ||| \cdot |||_{DG} \) (defined in [2]) assuming that Condition 1 holds true. A key ingredient in the proof consists of estimating the approximation properties of the discrete Trefftz function

\[
\Phi(x, t) := \frac{1}{|B|} \sum_{\ell=1}^{n_{d,p}} \left( \int_B a_\ell(z, s) dV(z, s) \right) \phi_\ell(x, t).
\]

**Theorem 1** Let \( p \in \mathbb{N} \). Let \( \psi \in \mathbb{T}(T_h) \cap H^{p+1}(T_h) \) be the exact solution of (1.1) and \( \psi_{hp} \in \mathbb{T}_p(T_h) \) be the Trefftz-DG solution with \( \mathbb{T}_p(T_h) \) satisfying Condition 1 for all \( K \in T_h(Q) \). Set the stabilization parameters \( \alpha \) and \( \beta \) as in [2], then there exists a constant \( C \) independent of the mesh size such that

\[
|||\psi - \psi_{hp}|||_{DG} \leq C \sum_{K \in T_h(Q)} h_K^p \|\psi\|_{H^{p+1}(K)},
\]

where \( h_K := \max\{h_K, h_h\} \).

In [2] we prove that Condition 1 is indeed true for the \((1+1)\) and \((2+1)\) dimensional cases under some restrictions of the tuning parameters \( k_\ell \) and \( d_\ell \) for our basis choice.

4 Numerical experiments

We consider the \((1+1)\)-dimensional Schrödinger equation (1.1) on \( Q = (-2, 2) \times (0, 1) \) with homogeneous Dirichlet boundary conditions and the following square-well potential:

\[
V(x) = \begin{cases} 0, & x \in (-1, 1), \\ V_* & x \in (-2, 2) \setminus (-1, 1), \end{cases}
\]

for some \( V_* > 0 \). The initial condition is taken as an eigenfunction of \( -\Delta_x + V \) on \((-2, 2)\). The solution of the corresponding initial boundary value problem (1.1) is \( \psi(x, t) = \psi_0(x) \exp(-ik_\xi t) \), where \( k_* \) is a real root of the function \( f(k) := \sqrt{V_* - k^2} - k \tan(h(\sqrt{V_* - k^2})) \).

In Fig.1 we plot the DG norm of the Galerkin error obtained for \( V_* = 20 \) and a sequence of space–time, uniform, Cartesian meshes.

![Figure 1: Trefftz-DG error for \( V_* = 20 \) and \( k_* \approx 3.7319 \).](image)

**References**


Implicit Filon Methods for Highly Oscillating Problems and Controlled Qubits

Spencer Lee$^{1,*}$, Daniel Appelö$^1$

$^1$Michigan State University, East Lansing, United States

$^*$Email: leespen1@msu.edu

Abstract
We present a numerical methods tailored for Schrödinger equations with time dependent Hamiltonians and rapidly oscillating solutions, such as those arising in the modeling of controlled qubits. Our method discretizes the Picard form of the ordinary differential equation (ODE) by Filon quadrature. The method is implicit but the size of the linear system is always the dimension of the ODE independent of order. We illustrate that the new method is superior to the classic RK4 method.

Keywords: Filon quadrature, highly oscillatory, quantum computing, qubit

1 Introduction
The Picard form of the ODE
\[ \frac{dv(t)}{dt} = F(t, v(t)), \quad v(0) = u_0, \quad 0 \leq t \leq \Delta t, \]
is
\[ v(t) = u_0 + \int_0^{\Delta t} F(t, v(t)) dt. \quad (1) \]

We assume that $f$ is smooth, and that the components in the right hand side will be highly oscillatory and best approximated by methods for integrals of the type
\[ I_\omega[f] = \int_{-1}^{1} f(x) e^{i\omega x} dx. \quad (2) \]

In particular our implicit Filon method approximates the solution $v(t_n)$ by replacing the integral in (1) by Filon quadrature, [1]. This results in schemes in the form
\[ u_{n+1} = u_n + \Delta t \sum_{k=0}^{m} b_k f(t_{n+k}, u_{n+k}). \]
The $\omega$ dependent weights of the Filon quadrature for (2) are found by insisting that the quadrature is exact for
\[ \mathcal{F}_{\omega}^m = \int_{-1}^{1} p(x)e^{i\omega x} dx, \]
where $p(x)$ is the unique degree $2m+1$ Hermite interpolation polynomial such that $p^{(i)}(\pm 1) = f^{(i)}(\pm 1)$, $l = 0, \ldots, m$.

Assuming $\omega \gg 1$, integration by parts
\[ \mathcal{F}_{\omega}^m[f] - I_\omega[f] = \int_{-1}^{1} (p(x) - f(x))e^{i\omega x} dx \]
\[ = - \sum_{k=0}^{\infty} \left[ (g^{(k)}(x) - f^{(k)}(x))e^{i\omega x} \right]_{-1}^{1} \]
\[ = \frac{1}{(-i\omega)^{m+1}} I_\omega[(p - f)^{(m+1)}] \]
reveals that the error of this method is $O(\omega^{-m-2})$.
As for all high frequency methods the error decreases as $\omega \to \infty$. But in the limit of $\omega \to 0$, spectacularly the approximation becomes $\mathcal{F}_{\omega}^m = \int_{-1}^{1} p(x) dx \approx \int_{-1}^{1} f(x) dx$, so that $\mathcal{F}_{\omega}^m$ becomes the Birkhoff-Hermite quadrature [2] and our implicit Filon methods resemble Hagstrom’s Hermite-in-time methods [3].

2 Examples of the Implicit Filon Method
Consider the ODE
\[ \frac{dv}{dt} = (\lambda + ig(t))v, \quad v(0) = u_0, \quad 0 \leq t \leq \Delta t, \quad (3) \]
where $\lambda \in \mathbb{C}$ and $g(t)$ is smooth. Generally $dv/dt$ is not in the form $f(t)e^{i\omega t}$, so we rewrite
\[ \frac{dv(t)}{dt} = f(t)e^{i\omega t}, \quad f(t, v(t)) \equiv (\lambda + ig(t))v(t)e^{-i\omega t}. \]

Here, the assumption is that $f$ oscillates over a larger timescale than $v$, and that it is easier to discretize $f$ than $v$. 

Figure 1: Comparison of implicit Filon method and the 4th order accurate RK method.
As \( f(t, v(t)) \) depends on \( v(t) \), the quantities \( f^{(l)}(t_{n+1}, u_{n+1}), l = 0, \ldots, m \) in the approximation are defined implicitly. If we set \( q(t) \equiv (\lambda + i\omega t) \), and \( r(t) \equiv e^{-i\omega t} \), so that \( f(t) = q(t)r(t)v(t) \), then the chain rule gives \( f'(t) = (q(t)r(t))'v(t) + (q(t)r(t))v'(t) \). Thus, this relation together with the ODE (3) recursively defines the derivatives of \( f \) in terms of \( u_{n+1} \) alone.

For example, if we consider the Dahlquist equation (when \( g(t) = 0 \)) the 4th order Filon method can be expressed as

\[
S_+(\omega, \Delta t, \lambda) u_{n+1} = S_-(\omega, \Delta t, \lambda) u_n,
\]

\[
S_+ = 1 - \frac{\Delta t}{2} e^{-i\frac{\omega t}{2}} \left( \lambda b_{2,0} + \frac{\Delta t}{2} (\lambda^2 - i\omega\lambda) b_{2,1} \right),
\]

\[
S_- = 1 + \frac{\Delta t}{2} e^{i\frac{\omega t}{2}} \left( \lambda b_{1,0} + \frac{\Delta t}{2} (\lambda^2 - i\omega\lambda) b_{1,1} \right).
\]

Note that here all the quadrature weights are evaluated at \( \omega \Delta t \).

The stability of the method is governed by the absolute value of \( Q = S_-/S_+ \). At the time of writing we have not been able to prove that this quantity is always less than unity in the left half of the complex plane but in Figure 2 we display contours of \( |Q| \) for \( \omega \Delta t/2 = 0 \) and 35. In both cases it appears that the method is A-stable. In addition, from [3] we know that the methods are A-stable in the limit \( \omega \to 0 \).

A comparison between solutions obtained with the 4th order implicit Filon and the classic fourth order Runge-Kutta method (RK4) for the case \( \lambda = i\omega = i10 \) and \( g(t) = \cos(t) \) is provided in Figure 1. The implicit Filon method achieves a relative error \( 6.1 \times 10^{-2} \) using five time steps, while RK4 does not achieve a single digit of precision using 50 time steps.

Figure 2: Contours for the stability function \( Q \) for \( \omega = 0 \) (black contours) and \( \omega \Delta t/2 = 35 \) (red contours). The \( x \) and \( y \) axis correspond to the real and imaginary parts of \( \Delta t \).

3 Application to Controlled Qubit

A controlled qubit can be modeled by the Schrödinger equation

\[
\frac{du(t)}{dt} = -i \left( \begin{array}{cc} 0 & 0 \\ 0 & \omega_A \end{array} \right) u(t) + g_c(t) \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) u(t),
\]

where \( u \) is the state vector and \( g_c(t) \) is the control. Here we can apply the Filon quadrature component-wise, using \( \omega = 0 \) in the first component and \( \omega = \omega_A \) in the second component. With these choices and with \( \omega_A = 10^6 \) and \( g_c(t) = \cos(t) \), we evolve the qubit until time \( 10 \times 2\pi/\omega_A \). In Figure 3 we display (in dashed lines) the errors at the final time as a function of the points per wavelength. We display results using \( \omega = \omega_A, 0.99\omega_A \), and 0.9\omega_A in the second component and, as a reference, we also display the errors using RK4. In the same figure in solid lines we display the errors for the scalar problem (3) with \( g(t) = g_c(t) \) and \( \lambda = i\omega_A \) and with the same choices of \( \omega \). The reference result for RK4 is also displayed. Clearly our method drastically outperforms RK4 in all cases.

References


Stable finite differences for the piecewise homogeneous dynamic beam equation

Gustav Eriksson1,*, Jonatan Werpers, David Niemelä, Niklas Wik, Valter Zethrin, Ken Mattsson

1Department of Information Technology, Uppsala University, Uppsala, Sweden
*Email: gustav.eriksson@it.uu.se

Abstract
The imposition of interface conditions for the piecewise homogeneous dynamic beam equation (DBE) is considered. Based on high order summation-by-parts finite differences, two novel energy stable methods are presented. Numerical experiments comparing the methods verify the theoretical convergence expectations and show that both methods are similar in terms of accuracy.

Keywords: dynamic beam equation, interface treatment, summation by parts, finite differences

1 Introduction
The dynamic beam equation (DBE) is a standard beam theory model describing the motion of free vibrations of an Euler-Bernoulli beam. Today it is used in construction of infrastructure involving beams such as buildings, bridges and railways.

The DBE is a dispersive wave equation for which the group velocity depends linearly on the wave number [1]. Consequently, the time step of any numerical method must scale as the square of the spatial step to resolve high frequency components of the solution. To keep the spatial step size small and still obtain an accurate solution, a high order finite difference method with summation-by-parts (SBP) properties is suggested. Together with either the projection method (SBP-P) or simultaneous approximation terms (SBP-SAT) to impose the interface conditions, the resulting numerical schemes can be proven stable using the energy method.

In this short paper novel SBP-P and SBP-SAT discretizations are presented and compared for the DBE with discontinuous material parameters. To save space, the proofs of energy conservation for the continuous and the two semi-discrete problems are omitted.

2 Continuous problem
The dynamic beam equation with a material discontinuity at \( x = 0 \) is given by

\[
\begin{align*}
\dot{b}^{(1)}u_{tt} &= -\alpha^{(1)}u_{xxxx}, & x \in [-1, 0], \\
\dot{b}^{(2)}v_{tt} &= -\alpha^{(2)}v_{xxxx}, & x \in [0, 1],
\end{align*}
\]

where \( \alpha^{(1,2)} \) and \( \dot{b}^{(1,2)} \) are positive constants incorporating the material parameters in each block and \( u \) and \( v \) denote the solutions in each block. The interface conditions at \( x = 0 \) ensuring energy conservation are given by

\[
\begin{align*}
u_t &= v_x, \\
u_x &= v_x, \\
\alpha^{(1)}u_{xx} &= \alpha^{(2)}v_{xx}, \\
\alpha^{(1)}u_{xxx} &= \alpha^{(2)}v_{xxx}.
\end{align*}
\]

3 Semi-discrete problem
The two blocks \([-1, 0]\) and \([0, 1]\) are discretized into equidistant grids with \( m \) grid points and step size \( h \). Let \( u \) and \( v \) denote the semi-discrete solution vectors. The spatial discretizations are done using SBP operators of 2nd-, 4th and 6th-order accuracy in the interior (see [1]) satisfying

\[
D_4 = H^{-1} \left( N + e_l d_{3,1}^T + e_r d_{5,1}^T + e_l d_{5,2}^T - d_{1,1}^T d_{1,1} - d_{2,1}^T d_{2,1} - d_{2,2}^T d_{2,2} - d_{3,1}^T d_{3,1} - d_{3,2}^T d_{3,2} - d_{3,3}^T d_{3,3} \right),
\]

where \( H = H^T > 0 \) is a diagonal matrix, \( N = N^T \geq 0, e_l \) and \( e_r \) are the first and last columns of the \( m \times m \) identity matrix and \( d_{1,1}, d_{1,2}, d_{2,1}, d_{2,2}, d_{3,1}, d_{3,2}, d_{3,3} \) are one-sided finite difference approximations of the first, second and third normal derivatives at the left and right boundary points. Furthermore, the matrix \( N \) can be decomposed as

\[
N = \tilde{N} + h \alpha_{II} \left( d_{2,1}^T d_{2,1} + d_{2,2}^T d_{2,2} \right) + h^3 \alpha_{III} \left( d_{3,1}^T d_{3,1} + d_{3,2}^T d_{3,2} \right),
\]

where \( \tilde{N} = \tilde{N}^T \geq 0 \) and \( \alpha_{II} \) and \( \alpha_{III} \) are positive constants not dependent on \( h \).
3.1 SBP-P discretization

A consistent and stable semi-discrete approximation of (1) with the interface conditions (2) imposed using the projection method [2] is given by

\[(B \otimes I_m)u_{tt} = -P(A \otimes D_1)Pw,\]  

(4)

where

\[w = \begin{bmatrix} u \\ v \end{bmatrix}, \quad B = \begin{bmatrix} b^{(1)} & 0 \\ 0 & b^{(2)} \end{bmatrix}, \quad A = \begin{bmatrix} a^{(1)} & 0 \\ 0 & a^{(2)} \end{bmatrix}.\]

The projection operator is given by

\[P = I_{2m} - H^{-1}L^T(LH^{-1}L^T)^{-1}L,\]

(5)

where \(I_{2m}\) is the \(2m \times 2m\) identity matrix and \(L\) is given by

\[L = \begin{bmatrix} e_r^T & -e_l^T \\ d_{1,r}^T & d_{1,l}^T \\ a^{(1)}d_{2,r}^T & a^{(2)}d_{2,l}^T \\ a^{(1)}d_{3,r}^T & a^{(2)}d_{3,l}^T \end{bmatrix}.\]

3.2 SBP-SAT discretization

A consistent and stable semi-discrete approximation of (1) with the interface conditions (2) imposed using the SAT method [1] is given by

\[b^{(1)}u_{tt} = a^{(1)}D_1u\]

\[-H^{-1}\frac{\tau}{h^2}e_r + \frac{a^{(1)}}{2}d_{3,r}(e_r^Tu - e_l^Tv)\]

\[-H^{-1}\frac{\sigma}{h}d_{1,r} - \frac{a^{(1)}}{2}(d_{2,r}u + d_{1,l}v)\]

\[-\frac{1}{2}H^{-1}d_{1,r}(a^{(1)}d_{2,r}u + a^{(2)}d_{2,l}v)\]

\[+ \frac{1}{2}H^{-1}e_r(a^{(1)}d_{3,r}u + a^{(2)}d_{3,l}v),\]

\[b^{(2)}v_{tt} = a^{(2)}D_2v\]

\[-H^{-1}\frac{\tau}{h^2}e_l + \frac{a^{(2)}}{2}d_{3,l}(e_l^Tv - e_r^Tu)\]

\[-H^{-1}\frac{\sigma}{h}d_{1,l} + \frac{a^{(2)}}{2}(d_{2,l}v + d_{1,r}u)\]

\[+ \frac{1}{2}H^{-1}d_{1,l}(a^{(2)}d_{2,l}v + a^{(1)}d_{2,r}u)\]

\[+ \frac{1}{2}H^{-1}e_l(a^{(2)}d_{3,l}v + a^{(1)}d_{3,r}u),\]

where

\[\tau = \frac{1}{4\alpha_{III}}(a^{(1)} + a^{(2)}), \quad \sigma = \frac{1}{4\alpha_{II}}(a^{(1)} + a^{(2)}),\]

and \(\alpha_{II}\) and \(\alpha_{III}\) are chosen so that \(\bar{N}\) is positive semi-definite.

4 Numerical results

The accuracies of the two methods are evaluated by an analytical solution derived using separation of variables with \(a^{(1)} = 1, a^{(2)} = 4\) and \(b^{(1,2)} = 1\). To isolate the influence of the interface the blocks are coupled at both ends, i.e. at \(x = 0\) and \(x = \pm 1\), resulting in a periodic problem. The second order ODE systems are integrated using a compact and explicit 4th order accurate finite difference time marching scheme [1]. The time step is chosen such that the spatial error dominates the temporal error.

In Figure 1 the error versus step size is plotted for the 2nd, 4th and 6th order operators with SBP-P and SBP-SAT. The results indicate that the theoretical convergence rates are obtained and that the methods are very similar in terms of accuracy.

5 Conclusions

Two novel and stable methods of imposing interface conditions for the piecewise homogeneous dynamic beam equation are presented. Numerical experiments demonstrate that both methods obtain the expected theoretical convergence rates.

References


Tuesday, July 26, Morning Session
Sound Propagation in Slowly-Varying Lined Ducts

Tom White1,∗, Raphael Assier1, William Parnell1
1Department of Mathematics, University of Manchester, United Kingdom
∗Email: thomas.white-4@manchester.ac.uk

Abstract
This talk will consider the modelling of sound propagation in slowly varying ducts. In straight cylindrical ducts, lined with a locally reacting material, sound transmission can be decomposed into a set of modal solutions. However, in practice, the ducts we wish to model have boundaries which vary slowly along the axial direction. In order to maintain semi-analytic modal solutions, the WKB (Wentzel-Kramers-Brillouin) approximation is adopted. The approximation assumes that the boundaries vary sufficiently slowly, that any propagating modes remain in the same eigenstate and do not experience any reflection. This allows for the introduction of a small parameter ϵ, related to the gradient of the duct boundaries, which allows for multiple scale asymptotics. The resulting solutions are slowly varying modes. Such modes have been studied extensively to leading order, however, in this talk we shall consider the first order behaviour in ϵ.

Keywords: aeroacoustics, multiple-scales, impedance

1 Introduction
The study of sound propagation in slowly-varying lined ducts is well established to leading order, with [1] and [2] considering the problem without flow, and in the presence of an axial mean flow respectively. In this talk we shall consider the case of extending the previous work on ducts without flow to higher order in ϵ, with a view to completing the analysis to include mean axial flow in the near future. The ducts are considered to be lined with a locally reacting acoustic material, such as an array of Helmholtz resonators, which can be modelled by a frequency dependent surface impedance. In order to preserve modal analysis, the WKB approximation is assumed, which is that if the geometry is sufficiently slowly varying, any propagating modes will remain in the same eigenstate and will not experience any reflection.

2 Definition of the Problem
Let us consider an axisymmetric annular duct, defined in polar co-ordinates \((r, \theta, x)\), with boundaries whose position’s vary in the axial direction. At both boundaries, the duct is lined with a locally reacting acoustic material. Then, we define a slowly varying parameter, \(\epsilon\), which is related to the rate of change of the duct boundaries. Here we take \(\epsilon\) to be the root mean square of the gradient of the boundaries in \(x\). Note, that \(\epsilon\) is not present in the final solutions, so can be chosen to be any measure of the speed of variance of the boundaries.

Figure 1: Sketch of an annular duct with slowly varying boundaries.

A slowly varying co-ordinate, \(X = \epsilon x\), is defined, which the slowly varying boundaries, \(r = a(X)\) and \(r = b(X)\), depend on. After assuming periodic solutions in time \(t\) and angle \(\theta\) and performing the multiple scales analysis outlined in [3], an ansatz of the following form is posed:

\[
P_m(r, X) = (\tilde{p}_{m,0}(r, X) + \epsilon \tilde{p}_{m,1}(r, X)) + \epsilon^2 \tilde{p}_{m,2}(r, X) \exp \left\{ -\frac{i}{\epsilon} \int^X k_0(X')dX' \right\}, \tag{1}
\]

where \(P_m(r, X)\) is a single time harmonic mode, \(m\) is the azimuthal order and the axial periodicity is governed by the slowly wavenumber \(k_0(X)\). Substituting (1) into the Helmholtz equation and collecting powers of \(\epsilon\) gives the hierarchy of equations:

\[
\mathcal{O}(1) : \mathcal{L}_0(\tilde{p}_{m,0}) = 0,
\]

\[
\mathcal{O}(\epsilon) : \mathcal{L}_0(\tilde{p}_{m,1}) = \mathcal{F}_0(\tilde{p}_{m,0}), \tag{2}
\]

\[
\mathcal{O}(\epsilon^2) : \mathcal{L}_0(\tilde{p}_{m,2}) = \mathcal{F}_0(\tilde{p}_{m,1}) + \mathcal{F}_1(\tilde{p}_{m,0}),
\]

where \(\mathcal{L}_0\) is the 2nd order linear differential operator for Bessel’s equation, and \(\mathcal{F}_{0,1}\) are known.
forcing terms. For the boundary condition, it is assumed that at \( r = a(X) \), \( b(X) \) the surface impedance are given by \( Z_a(\omega) \) and \( Z_b(\omega) \) respectively. This leads to the boundary conditions:

\[
\frac{\partial P_m}{\partial n_a,b} = \frac{\omega P_m}{iZ_{a,b}} \text{ at } r = a(X), \ b(X), \tag{3}
\]

where \( n_{a,b} \) is the normal pointing into the boundary. The hierarchy of equations for the boundary conditions are derived by expanding the normal at each boundary in powers of \( \epsilon \).

3 Finding Modal Solutions

The leading order solution is well established to be a weighted sum of Bessel functions of the first kind, multiplied by a slowly varying amplitude,

\[
\tilde{p}_{m,0} = A_0(X) (J_m(\alpha_0(X)r) + \Xi(X)Y_m(\alpha_0(X)r)), \tag{4}
\]

where \( \alpha_0(X) \) is the, slowly varying, radial wave number and \( \Xi(X) \) is known. In order to find the slowly varying amplitude \( A_0(X) \), the \( \mathcal{O}(\epsilon) \) governing equations must be considered. It is not necessary to consider the full solution to this problem, as we can apply a solvability condition, by considering Green’s second identity:

\[
\int_{a(X)}^{b(X)} \left( \tilde{p}_{m,0} \partial \tilde{p}_{m,1} - \tilde{p}_{m,1} \partial \tilde{p}_{m,0} \right) r' dr' = \left[ \tilde{p}_{m,0} \frac{\partial \tilde{p}_{m,1}}{\partial r} - \frac{\partial \tilde{p}_{m,0}}{\partial r} \tilde{p}_{m,1} \right]_{r=a(X)}. \tag{5}
\]

Upon substitution of the governing equations and boundary conditions, (5) can be reduced to find an explicit form of \( A_0(X) \). However, in the case considered, the full solution to the \( \mathcal{O}(\epsilon) \) equations is required. One way to find this solution is to apply the method of variation of parameters to the inhomogeneous ODE. By applying the boundary conditions we find \( A_0(X) \) to be the same as applying (5), but leaves a similar unknown slowly varying coefficient \( A_1(X) \) at first order. In order to solve for \( A_1(X) \) another solvability condition can be applied, this time on the \( \mathcal{O}(\epsilon^2) \) equations, which leads to an ODE to solve for \( A_1(X) \) of the form

\[
\mathfrak{A}(X) \frac{dA_1}{dX} + \mathfrak{B}(X)A_1(X) + \mathfrak{C}(X) = 0, \tag{6}
\]

where \( \mathfrak{A}(X) \), \( \mathfrak{B}(X) \) and \( \mathfrak{C}(X) \) are known functions.

4 Results and Comparisons

To demonstrate the improved accuracy of the first order solution, compared to the leading order, we consider the example of cylindrical duct with a cosine outer boundary. The boundary is chosen, such that \( \epsilon = 0.1 \). The angular frequency is \( \omega = 3 \), and \( m = 0 \), with surface impedance \( Z_b = 2 - i \).

Figure 2: The absolute error between the complex pressure fields for the leading and first order propagating modes, compared with numeric results.

Figure 2 shows the absolute error between the pressure fields, \( P_m(r, X) \), at \( \mathcal{O}(1) \) and \( \mathcal{O}(\epsilon) \) and numeric simulations performed using COMSOL. The numeric solution for a single mode is found by applying the mode shape as a boundary condition at \( x = 0 \). The geometry shown is an axis-symmetric slice in \( (r, x) \). Clearly it can be seen that the first order correction provides a significant reduction in error between the fields.

5 Flow Duct Extension

Depending on whether or not results are generated in time for the conference, the first order solution could also be presented for the case of axial mean flow, as this is the ultimate goal of the current work. The method of solution will be the same, however, the inhomogenous parts of the equations becomes more complex when flow is introduced, leading to greater computational complexity.

References


Scattering in a partially open waveguide: the forward problem

Laurent Bourgeois$^1$, Sonia Fliss$^1$, Jean-François Fritsch$^2$, Christophe Hazard$^1$, Arnaud Recoquillay$^2$

$^1$Laboratoire POEMS, ENSTA Paris, Palaiseau, France
$^2$Université Paris-Saclay, CEA, LIST, F-91120, Palaiseau, France

*Email: laurent.bourgeois@ensta.fr

Abstract
We consider an acoustic scattering problem in a two-dimensional partially open waveguide, in the sense that the left part of the waveguide is closed, that is with a bounded cross-section, while the right part is bounded in the transverse direction by some Perfectly Matched Layers that mimic the situation of an open waveguide, that is with an unbounded cross-section. We prove well-posedness of such scattering problem, then propose and justify artificial conditions in the longitudinal direction based on Dirichlet-to-Neumann maps.

Keywords: Open waveguide, PMLs, DtN operators, Kondratiev theory

1 Introduction
Let us introduce the domains $\Omega^- := (-\infty, 0) \times (-h, h)$, $\Omega^+ := (0, +\infty) \times (-h_{\text{out}}, h_{\text{out}})$ and $\Omega := \Omega^- \cup \Sigma_0 \cup \Omega^+$, with $\Sigma_0 := \{0\} \times (-h, h)$, as well as a bounded domain $O \subset (0, +\infty) \times (-h, h)$.

We consider the problem: find $u$ such that

$$\begin{cases}
P u &= 0 \quad \text{in } \Omega \setminus \Omega^+,
\partial_\nu u &= 0 \quad \text{on } \partial\Omega,
\psi &= 0 \quad \text{on } \partial\Omega,
\end{cases}$$

$$u - u^\text{out} \text{ is outgoing},$$

where $\nu$ is the outward unit normal vector to $\partial\Omega$, $u^\text{out}$ is a mode coming from the left waveguide, and the differential operator $P$ is defined by

$$P := -\partial_y (\alpha \mu \partial_y \cdot - \frac{\mu}{\alpha} \partial_x \cdot - k^2),$$

with $(\alpha, \mu, k) := (1, \mu_0, k_0)$ in $\mathbb{R} \times (-h, h)$ (blue zone), $(\alpha, \mu, k) := (1, \mu_\infty, k_\infty)$ in $(0, +\infty) \times ((-h_{\text{in}}, -h) \cup (h_{\text{in}}, h))$ (pink zone) and $(\alpha, \mu, k) := (\alpha_\infty, \mu_\infty, k_\infty)$ in $(0, +\infty) \times ((-h_{\text{out}}, -h_{\text{in}}) \cup (h_{\text{in}}, h_{\text{out}}))$ (brown zone), with $\alpha_\infty$ a complex constant such that $\arg(\alpha_\infty) = \frac{-\pi}{2} + 0$. We also assume that $k_0 < k_\infty$. The objective is to prove well-posedness of problem (1) in a appropriate functional space.

2 The uniform PML-waveguide
Let us consider the straight waveguide $\Omega_{\text{out}} := \mathbb{R} \times I_{\text{out}}$ with $I_{\text{out}} := (-h_{\text{out}}, h_{\text{out}})$, the coefficients of $P$ being those of $\Omega^+$. for a given $f$, find the outgoing solution $u$ to the problem

$$\begin{cases}
P u &= f \quad \text{in } \Omega_{\text{out}},
\partial_\nu u &= 0 \quad \text{on } \partial I_{\text{out}}.
\end{cases}$$

The solutions in the form $u(x, y) = e^{\lambda x} \varphi(y)$ to problem (2) for $f = 0$ are called the modes. To specify them, we introduce the operator $L(\lambda) : H^1(I_{\text{out}}) \rightarrow H^1(I_{\text{out}})^*$ defined by

$$\langle L(\lambda) \varphi, \psi \rangle_{H^1(I_{\text{out}})^*, H^1(I_{\text{out}})} := \int_{I_{\text{out}}} (\alpha \mu dy \varphi d_y \psi - \frac{\mu}{\alpha} \psi dy \varphi) dy,$$

for all $\varphi, \psi \in H^1(I_{\text{out}})$. We denote by $\Lambda$ the discrete set of $\lambda \in \mathbb{C}$ for which there exists a non zero eigenvector $\varphi \in H^1(I_{\text{out}})$ such that

$$L(\lambda) \varphi = 0.$$ 

We assume that any eigenvector $\varphi$ satisfies

$$\int_{I_{\text{out}}} \frac{\mu}{\alpha} \varphi^2 dy \neq 0,$$

which guarantees that the $\lambda_n$ are simple eigenvalues, both geometrically and algebraically. In addition, the fact that $k_0 < k_\infty$ enables us to write $\Lambda = \cup_{n=0}^{\infty} (-\lambda_n, \lambda_n)$ with

$$\cdots \leq \Re(\lambda_{n+1}) \leq \Re(\lambda_n) \leq \cdots \leq \Re(\lambda_{0}) < 0.$$ 

If the $\varphi_n$ satisfy (3) for $\lambda = \pm \lambda_n$, up to a rescaling we have the biorthogonality condition
\[ \int_{\Omega} \varphi_n \varphi_m \, dy = \delta_{mn}. \]

The modes (divided into leaky and PMLs modes) are given by \( w_n^\pm(x, y) = e^{\pm \beta x} \varphi_n(y) \) and are all evanescent. Since the transverse operator \( L \) is not self-adjoint, the \( \varphi_n \) do not form a complete orthonormal basis of \( L^2(\Omega_{\text{out}}) \): the classical projection method used for a closed uniform waveguide fails. This is why we used the Kondratiev theory (see [1] for details and references) as the main ingredient of the proofs of both following theorems.

We introduce the space \( W_1^1(\Omega_{\text{out}}) \) as the set of \( v \in \mathcal{D}'(\Omega_{\text{out}}) \) such that \( e^{-\beta|x|}v, e^{-\beta|x|}\partial_x v \) and \( e^{-\beta|x|}\partial_y v \) belong to \( L^2(\Omega_{\text{out}}) \).

**Theorem 1** For \( f \in H^1(\Omega_{\text{out}})^* \), the problem (2) has a unique solution \( u \in H^1(\Omega_{\text{out}}) \). Furthermore, if \( \beta > 0 \) is such that \( \Lambda \) has no intersection with the line \( \ell_{-\beta} := -\beta + i \mathbb{R} \) and \( f \in W_2^1(\Omega_{\text{out}})^* \), denoting \( \Lambda \cap \{ \lambda \in \mathbb{C}, -\beta < \Re \lambda < 0 \} = \{ \lambda_0, \lambda_1, \ldots, \lambda_{N_\beta-1} \} \), there exist some complex numbers \( a_n^+, a_n^- \) and a function \( \tilde{u} \in W_2^1(\Omega_{\text{out}}) \) such that

\[
 u = \chi^+ \sum_{n=0}^{N_\beta-1} a_n^+ w_n^+ + \chi^- \sum_{n=0}^{N_\beta-1} a_n^- w_n^- + \tilde{u},
\]

where \( \chi^\pm \in \mathcal{C}^\infty(\mathbb{R}) \), \( \chi^\pm = 1 \) for \( \pm x \geq 2L \) and \( \chi^\pm = 0 \) for \( \pm x \leq L \).

**Remark 2** Since \( k_0 < k_\infty \), the radiation condition simply consists here to search the solution in \( H^1(\Omega_{\text{out}}) \), which guarantees its uniqueness.

## 3 The scattering problem of interest

In order to analyze problem (1), we formulate an equivalent one set in the bounded domain \( D_M \), that is the domain \( \Omega \setminus \overline{\Omega} \) truncated by the sections \( \Sigma_0 \) and \( \Sigma_M := \{ M \} \times (-h_{\text{out}}, h_{\text{out}}) \). We introduce the DtN operator

\[
 T_0 : H^{1/2}(\Sigma_0) \to H^{1/2}(\Sigma_0)^*, \quad \varphi \mapsto T_0 \varphi = -\mu_0 \partial_x u^-|_{\Sigma_0},
\]

where \( u^- \) is the solution to the left half-waveguide problem with Dirichlet data \( \varphi \) on \( \Sigma_0 \), and the DtN operator with an overlap (\( M - L \))

\[
 T_{L,M} : H^{1/2}(\Sigma_L) \to H^{1/2}(\Sigma_M)^*, \quad \varphi \mapsto T_{L,M} \varphi = \frac{\mu}{\alpha} \partial_x u^+|_{\Sigma_M},
\]

where \( u^+ \) is the solution to the right half-waveguide problem with Dirichlet data \( \varphi \) on \( \Sigma_L \), with \( L \leq M \). That the operator \( T_0 \) is well-defined and has the form of a series is classical. Using the first part of the previous theorem and a symmetry argument, we prove that \( T_{L,M} \) is well-defined as well. Then we introduce the problem set in \( D_M \): find \( u \in H^1(D_M) \) such that

\[
 \begin{cases}
 Pu = 0 & \text{in } D_M, \\
 \partial_D u = 0 & \text{on } \Gamma_M, \\
 u = 0 & \text{on } \partial \Omega, \\
 -\mu_0 \partial_x u = T_0(u)|_{\Sigma_0} - 2\mu_0 \partial_x u^i & \text{on } \Sigma_0, \\
 \frac{\mu}{\alpha} \partial_x u = T_{L,M}(u)|_{\Sigma_L} & \text{on } \Sigma_M.
\end{cases}
\]

with \( \Gamma_M = \partial D_M \setminus (\Sigma_0 \cup \Sigma_M \cup \partial \Omega) \). Having in mind the numerical computation of the solution, we also introduce an operator which approximates the DtN operator \( T_{L,M} \) with the help of the eigenvalues and eigenfunctions \( (\lambda_n, \varphi_n) \) of the transverse operator \( L \), that is for a fixed \( \beta > 0 \), \( T_{L,M}(\varphi) \) is replaced for \( \varphi \in H^{1/2}(\Sigma_L) \) by

\[
 T_{L,M}^\beta(\varphi) = \sum_{n=0}^{N_\beta-1} \frac{\mu}{\alpha} \lambda_n e^{\lambda_n(M-L)} \left( \int_{\Sigma_L} \frac{\mu}{\alpha} \varphi_n \, dy \right) \varphi_n.
\]

**Theorem 3** Problems (1) and (4) are equivalent. Problem (4) has a unique solution \( u \in H^1(D_M) \) if the same problem for \( u^i \) has only the trivial solution. Moreover, using the same assumption on \( \beta \) and the same notation as in Theorem 1, then exist some complex numbers \( a_n^+ \) and a function \( \tilde{u} \in W^1_2(\Omega_{\text{out}}) \) such that \( \tilde{u}|_{\partial \Omega} = 0 \) satisfying in \( \Omega_{\text{out}} \setminus \overline{\Omega} \)

\[
 u = \chi^+ \sum_{n=0}^{N_\beta-1} a_n^+ w_n^+ + \tilde{u}.
\]

For a fixed \( L \) and \( M \) large enough, if problem (1) is well-posed, then the problem (4) with operator \( T_{L,M} \) replaced by \( T_{L,M}^\beta \) is well-posed as well. Moreover, denoting \( u_{L,M}^\beta \) the corresponding solution, there exists a constant \( C_\beta > 0 \) which is independent of \( M \) such that

\[
 \| u - u_{L,M}^\beta \|_{H^1(D_M)} \leq C_\beta e^{-\beta(M-L)} \| u \|_{H^1(\Omega_{\text{out}} \setminus \overline{\Omega})}.
\]

**References**

Scattering in a partially open waveguide: the inverse problem

Laurent Bourgeois\textsuperscript{1}, Jean-François Fritsch\textsuperscript{2,1,*}, Arnaud Recoquillay\textsuperscript{2}

\textsuperscript{1}POEMS (CNRS-INRIA-ENSTA Paris), Institut Polytechnique de Paris, Palaiseau, France
\textsuperscript{2}Université Paris-Saclay, CEA, List, F-91120, Palaiseau, France
\textsuperscript{*}Email: jean-francois.fritsch@cea.fr

Abstract

Guided waves can be used to perform nondestructive testing of partially buried elongated structures in various industrial sectors such as civil engineering or oil and gas. Such an inverse problem presents two main challenges: we can access to only one side of the zone to control, and the waves propagating in the structure partially leak in the surrounding medium. The buried part of the structure is truncated in the transverse direction with Perfectly Matched Layers (PMLs), which enable us to treat the domain as the junction of two closed waveguides with complex coefficients. The Linear Sampling Method (LSM) is adapted to this new configuration.

Keywords: Inverse scattering, Linear Sampling Method, buried waveguide, PML

1 Introduction

The closed part of the structure occupies the domain $\Omega^- := \mathbb{R}^- \times (-h, h)$ with $h > 0$ and its buried part the domain $\Omega_\infty^+ := \mathbb{R}^+ \times \mathbb{R}$. The shear modulus and the density are piecewise positive constants given by $(\mu, \rho) = (\mu_0, \rho_0)$ in $\mathbb{R} \times (-h, h)$ and $(\mu, \rho) = (\mu_\infty, \rho_\infty)$ in $\mathbb{R}^+ \times ((-\infty, h) \cup (h, +\infty))$. The speed and the wavenumber are respectively given by $c := \sqrt{\mu/\rho}$ and $k := \omega/c$ where $\omega$ is the angular frequency. The defect we want to identify occupies a smooth and bounded domain $O$ which lies either in the core $\mathbb{R}^+ \times (-h, h)$ of the buried part, or in its sheath $\mathbb{R}^+ \times ((-h_{in}, h) \cup (h, h_{in}))$ with $h_{in} > h$. The domain $\Omega_\infty^+$ is truncated in the transverse direction with a bounded PML occupying the domain $\mathbb{R}^+ \times ((-h_{out}, h_{in}) \cup (h_{in}, h_{out}))$ for $h_{out} > h_{in}$; the truncated domain is denoted by $\Omega^+ := \mathbb{R}^+ \times (-h_{out}, h_{out})$. We also define $\Omega := \Omega^- \cup \Sigma_0 \cup \Omega^+$ with $\Sigma_0 := \{0\} \times (-h, h)$. A point in $\Omega$ is denoted by $x = (x, y) \in \mathbb{R}^2$, and the PML function is given by

$$\alpha(x, y) := \begin{cases} 1 & |y| \leq h \\ \alpha_\infty & |y| > h, \end{cases}$$

with $-\frac{\pi}{2} < \arg(\alpha_\infty) < 0$. In order to write the forward problem, we introduce the modes of the left half-guide, which are the functions $\tilde{\varphi}_n^\pm(x, y) = e^{\pm h_{in} x} \tilde{\varphi}_n(y)$, with $(\lambda_n, \tilde{\varphi}_n)$ satisfying

$$\begin{cases} -\partial_y^2 \tilde{\varphi}_n - k_0^2 \tilde{\varphi}_n = \lambda_n^2 \tilde{\varphi}_n & \text{in } (-h, h) \\ d_y \tilde{\varphi}_n = 0 & \text{on } y = \pm h. \end{cases}$$

The scattering problem reads:

$$\text{find } \varphi \in H^1_\text{loc}(\Omega \setminus O) \text{ such that}$$

$$\begin{cases} -\Delta \varphi - k_0^2 \varphi = 0 & \text{in } \Omega^- \\ -\frac{2}{c^2} \partial_y (\alpha \partial_y \varphi) - \partial_y^2 \varphi - k^2 \varphi = 0 & \text{in } \Omega^+ \setminus \bar{O} \\ [\varphi_+] = 0 & \text{on } \Sigma_0 \\ \partial_\nu \varphi = 0 & \text{on } \partial \Sigma_0 \\ \varphi = 0 & \text{on } \partial O \\ \varphi - \tilde{w}_{n,0}^+ & \text{is outgoing}, \end{cases}$$

where $\tilde{w}_{n,0}^+$ is the extension of the mode $\tilde{w}_n^+$ of the left half-guide to the positive $x$ by 0 and $\nu$ is the unit normal to $\Omega$. In order to identify the obstacle $O$, we use the fact that our domain consists of the junction of two closed waveguides. In the following, we present first how the LSM can be adapted to the junction of two closed waveguides with real parameters. Then, we explain how this work has been extended to our configuration of interest, underlining the similarities but also differences arising with the PMLs.

2 The LSM for a junction of closed waveguides with real coefficients

We summarize here the main results obtained in [1] for a junction of an arbitrary number of waveguides, but limit the presentation to the simpler case of back-scattering identification in a junction of two branches with a constant wavenumber. To begin with, we define the reference fields $\tilde{r}_n$ which are the solution of the problems:

$$\text{find } \tilde{r}_n \in H^1_\text{loc}(\Omega) \text{ such that}$$

$$\begin{cases} -\Delta \tilde{r}_n - k^2 \tilde{r}_n = 0 & \text{in } \Omega \\ \partial_\nu \tilde{r}_n = 0 & \text{on } \partial \Omega \\ \tilde{r}_n - \tilde{w}_{n,0}^+ & \text{is outgoing}. \end{cases}$$
Then, we introduce for $x' \in \Omega$ the Green function solution of: find $G(\cdot, x') \in L^2_{\text{loc}}(\Omega)$ such that
\[
\begin{align*}
  -\Delta G(\cdot, x') - k^2 G(\cdot, x') &= \delta_{x'} & \text{in } \Omega \\
  \partial_n G(\cdot, x') &= 0 & \text{on } \partial \Omega \\
  G(\cdot, x') &= \text{is outgoing}.
\end{align*}
\] (3)

**Theorem 1** Problems (2) and (3) are well-posed, and we have for $x' < 0$ and $x \geq x'$ the decomposition:
\[
G(x, x') = -\sum_{n \geq 0} \frac{1}{2^n} \tilde{\tau}_n(x') \tilde{w}_n(x).
\] (4)

The decomposition (4) is obtained using the reciprocity property of the Green function. For $F \in H^\frac{1}{2}(\partial O)$, we also introduce the scattering problem: find $u^* \in H^1_{\text{loc}}(\Omega \setminus O)$ such that
\[
\begin{align*}
  -\Delta u^* - k^2 u^* &= 0 & \text{in } \Omega \setminus O \\
  \partial_n u^* &= 0 & \text{on } \partial O \\
  u^* &= F & \text{on } \partial O \setminus \partial O.
\end{align*}
\] (5)

The inverse problem consists in finding $O$ from the measurement of the $u_n^*$ on $\Sigma_{-R} := \{-R\} \times (-h, h)$, $R > 0$, for all $n \in \mathbb{N}$, where $u_n^*$ is the solution of (5) for $F = -\tilde{\tau}_n\delta_{\partial O}$. Let $z = (x_z, y_z)$, $x_z \geq -R$ be a sampling point. Let us introduce the so-called near-field equation: find $h \in L^2(\Sigma_{-R})$ such that
\[
\int_{\Sigma_{-R}} u^*(x, x') h(x') dx' = G(x, z), \quad \forall x \in \Sigma_{-R}.
\] (6)

where $u^*(\cdot, x')$ is the solution of problem (5) with $F = -\tilde{G}(\cdot, x')\delta_{\partial O}$. Using (4), we derive the following modal formulation of the LSM.

**Proposition 2** The near-field equation (6) reads: find $h(z) = \sum_{n \geq 0} h_n(z) \tilde{\tau}_n \in L^2(\Sigma_{-R})$ such that
\[
\sum_{n \geq 0} \frac{\lambda_n}{\bar{\lambda}_n} U_{mn} h_n(z) = \frac{c_n}{\bar{\lambda}_n} \tilde{\tau}_n(z), \quad \forall m \in \mathbb{N},
\] (7)

with $u_n^*|_{\Sigma_{-R}} = \sum_{m \geq 0} U_{mn} \tilde{\tau}_n$.

To image the defect, we plot the norm of the solution $h^{\text{reg}}(\cdot)$ of a Tikhonov-Morozov regularization of system (7) with the series truncated to the propagating modes, which are the modes satisfying $\lambda_n \in \mathbb{R}$. It is important to stress that the reference fields are computed once and for all during an offline phase, which leads to an efficient sampling procedure.

### 3 The LSM in a partially buried waveguide with a transverse PML

A partially buried waveguide truncated in its embedded part with transverse PMLs can be viewed as the junction of two closed waveguides, one of which involves a complex parameter. The LSM can be then derived like before by introducing the reference fields, the Green function and the near-field equation of the new structure. As for its mathematical justification, it presents two main difficulties: proving the well-posedness of problem (1) and obtaining a rigorous decomposition of the Green function on the reference fields. The first difficulty was addressed in [2], and the second one in a forthcoming article. These difficulties are consequences of the loss of the self-adjointness of the transverse operator appearing in the mathematical analysis, which is a consequence of the introduction of the complex-valued function $\alpha$ modelling the PML. The considered materials satisfy $c_0 > c_\infty$, which implies that there are no propagating modes in the right half-guide. Thus, all the waves leak in the surrounding medium, which results in a loss of information for the imaging. A numerical result is finally presented with Figure 1.

Figure 1: Level curves of the imaging function $z \mapsto -\log(\|h^{\text{reg}}(z)\|_{L^2(\Sigma_{-R})})$ for two Dirichlet obstacles in a steel plate partially buried in concrete, using 26 propagating modes. Parameters: $h = 5$, $h_{\text{in}} = 7.5$, $h_{\text{out}} = 12.5$, 10% of noise.

### References


High sensibility imaging of defects in elastic waveguides
using near resonance frequencies

Angèle Niclas\textsuperscript{1,*}, Éric Bonnetier\textsuperscript{2}, Laurent Seppecher\textsuperscript{1}, Grégory Vial\textsuperscript{1}

\textsuperscript{1}Institut Camille Jordan, Ecole Centrale de Lyon, Lyon, France
\textsuperscript{2}Institut Fourier, University Grenoble Alpes, Grenoble, France
*Email: angele.niclas@ec-lyon.fr

Abstract
This work presents a new multi-frequency inversion method to image shape defects in slowly varying elastic waveguides. Contrary to previous works in this field, we choose to take advantage of the near resonance frequencies of the waveguide, where the elastic problem is known to be ill-conditioned. A phenomenon close to the tunnel effect in quantum mechanics can be observed at these frequencies, and locally resonant modes propagate in the waveguide. These modes are very sensitive to width variations, and measuring their amplitude enables reconstructing the local variations of the waveguide shape with very high sensibility. Given surface wavefield measurements for a range of near resonance frequencies, we provide a stable numerical reconstruction of the width of a slowly varying waveguide and illustrate it on defects like dilation or compression of a waveguide.

Keywords: Waveguide, Inverse problems, Resonances

1 Scientific context
Reconstruction of defects in waveguides is of crucial interest in nondestructive evaluation of structures. This work is based on physical experiments done at Institut Langevin where one tries to reconstruct width defects in thin elastic plates using multi-frequency surface measurements (see [1]). Contrary to usual backscattering methods avoiding resonancies frequencies of the plate, they developed an experimental inversion method using these frequencies to obtain a high sensibility reconstruction of local defects in plates. We here try to provide a mathematical understanding of this inversion method and theoretical results on its stability.

2 Study of the forward problem
We consider an infinite 2D elastic plate with a slowly varying width $2h(x)$ (see and illustration in Figure 2). The wave field $u$ satisfies the elastic equation

$$\begin{cases}
-\omega^2 u - \text{div}(\sigma(u)) = f \quad \text{in } \Omega, \\
\sigma(u).\nu = 0 \quad \text{on } \partial \Omega, \\
\text{u is outgoing},
\end{cases}$$

where $\sigma(u) = \lambda \text{div}(u)I + 2\mu \nabla^\prime u$ and $(\lambda, \mu)$ are the Lamé coefficients of the plate $\Omega$. Using the formalism $X/Y$ developed in [2], vectors $X := (u_1, (\sigma(u)e_x)_2)$ and $Y := (-e_y, u_2)$ can be decomposed in Lamb modes $(X_n, Y_n)$:

$$\begin{pmatrix} X \\ Y \end{pmatrix}(x, y) = \sum_{n \in \mathbb{N}} \begin{pmatrix} a_n(x)X_n(x, y) \\ b_n(x)Y_n(x, y) \end{pmatrix}. \quad (1)$$

Each Lamb mode is associated to a wavenumber $k_n(x)$, represented in Figure 1.

Figure 1: Representation of $k_n(x)$ with respect to $\omega h(x)$. Purple branch: $k_n \in \mathbb{R}$, green branch: $k_n \in i\mathbb{R}$, yellow branch: $k_n \in \mathbb{C} \setminus (\mathbb{R} \cup i\mathbb{R})$.

We are interested in frequencies $\omega$, called resonant frequencies, such that $k_n(x)$ switches from a real number to a complex one when $x$ varies. We distinguish them in three cases, denoted (1), (2), (3) and represented in Figure 1. In each case, we prove that $a_n$ or $b_n$ are close to the solutions of

(2), (3) : $a_n^2 + k_n^2 a_n = F_1$, (1) : $b_n^2 + k_n^2 b_n = F_2$. 


where \( F_1 \) and \( F_2 \) depend explicitly on \( f \). These are Schrödinger equations, and we show that their solutions can be expressed using Airy functions of the first and second kind, denoted \( A \) and \( B \). It enables an explicit approximation of \( u \), denoted \( u^{\text{app}} \) (see an example in Figure 2). Adapting the proof of [3], we formally control the error of this approximation:

\[
\| u - u^{\text{app}} \|_{L^2(\Omega)} \leq \eta C_1 \| f \|_{H^1(\Omega)}. \tag{2}
\]

![Figure 2: Representation of \( |u_1^{\text{app}}| \) at a longitudinal resonance (1) in a slowly increasing waveguide.](image)

### 3 Imaging of the width of the waveguide

Using the study of the forward problem, we can now provide an approximation of the surface measurements for different frequencies \( \omega \). In case (1) (resp. (2), (3)), we see that \( d_\omega := u_1 \) (resp. \( d_\omega := u_2(x), d_\omega := |u_i(x)| \)) can be approached by

\[
d_\omega(x) \approx \alpha_\omega A(\beta_\omega(x - x_\omega^*)), \tag{3}
\]

where \( \alpha_\omega \in \mathbb{C}, \beta_\omega > 0 \), and \( x_\omega^* \) is a coordinate such that \( k_n(x_\omega^*) \) is at the junction of two different branches in Figure 1. Since the value of \( x_\omega^* \) is explicitly linked to the value of \( h(x_\omega^*) \) and varies when \( \omega \) varies, we plan on reconstructing \( h \) by finding the value of \( x_\omega^* \) for different frequencies \( \omega \) using data \( d_\omega \). To do so, we numerically minimize the function

\[
F : (x_\omega^*, \omega_\omega, x_\omega) \mapsto |d_\omega(x) - \alpha_\omega A(\beta_\omega(x - x_\omega^*))|_2.
\]

We prove the following result:

**Theorem 2** Under the same assumptions as in Theorem 1, there exists \( \eta_1 > 0 \) such that if \( \eta < \eta_1 \), the function \( F \) has a unique minimum. If we denote \( x_\omega^{\text{app}} \) the approximation of \( x_\omega^* \), there exists \( C_2 > 0 \) independent of \( \omega \) such that

\[
| x_\omega^* - x_\omega^{\text{app}} | \leq C_2 \eta. \tag{4}
\]

We represent in Figure 3 different points \( x_\omega^* \) and their approximations.

![Figure 3: Positions of \( x_\omega^* \) and \( x_\omega^{\text{app}} \) for different frequencies \( \omega \).](image)

![Figure 4: Two reconstructions of waveguide’s widths using a longitudinal resonance (1).](image)

Using the coordinates \( x_\omega^{\text{app}} \) and their associated width enables us to provide a stable reconstruction of the width in each case of resonance. We show in Figure 4 two reconstructions using a longitudinal resonance (1).

### References


On the construction of Shape Functions for Spacetime Trefftz-DG Formulations of Wave Problems with Perfectly Matched Layers

H. Barucq\(^1\), H. Calandra\(^1\), J. Diaz\(^1\), V. Vasanthan\(^1\)*

\(^1\)Project-Team Makutu, Inria, University of Pau, CNRS, TotalEnergies, France
\(^*\)Email: vinduja.vasanthan@inria.fr

Abstract

The Trefftz method is based on the construction of shape functions which are elementwise solutions of the equation to solve. We are interested here in the construction of shape functions that allow to solve Perfectly Matched Layers (PML) formulations of the acoustic wave equation in Trefftz-DG spaces. Different approximation spaces are considered and assessed with numerical experiments.

Keywords: Trefftz methods, Tent-Pitching, PML

1 Trefftz methods

Trefftz-DG approximations of wave equations in the frequency domain have shown clear potential in controlling numerical pollution (see e.g. [1–3]). They are based on spaces of shape functions which are local solutions of the equation to be solved. In this way, the associated variational problem is posed only on the edges or faces of the elements, and the computational load required for the inversion of the associated linear system is reduced. The extension of this approach to the time domain has been done by several authors (e.g. [4] and [5]) and its implementation involves integrating the equations in space and time using time and space dependent shape functions.

In our work, we consider Trefftz functions defined as elementwise solutions. They are Discontinuous Galerkin shape functions as the continuity at the interfaces of the elements is not strongly imposed. The resulting Trefftz-DG variational formulation involves integrals on the boundaries of each cell of the mesh of the domain of interest with appropriate transmission conditions between the cells.

In spacetime Trefftz-DG formulations, the solution is computed implicitly, which implies to invert a sparse but very large matrix. To overcome this difficulty, Tent-Pitching algorithms were first introduced for hyperbolic problems in space-time domain in [6]. They consist in building a causal mesh, which respects the wave propagation speed (see figure 1). This leads to solving the problem elementwise, which converts the original implicit scheme to a locally-implicit one. In practice, only small local matrices are inverted; either reference matrices that apply to all of the tents (structured meshes) or one matrix for each tent (unstructured meshes). These algorithms also have the major advantage of being conducive to parallel computing, which is mandatory when handling three dimensions and/or larger domains.

2 Acoustic wave equation with PML

Perfectly Matched Layers were first introduced by Bérenger in 1994 to absorb waves and avoid spurious reflections. For instance, the acoustic wave problem with PML in the y-direction in the domain \(\Omega\) can be written as:

\[
\begin{align*}
\rho \frac{\partial u_x}{\partial t} + \frac{\partial p}{\partial x} &= 0, \\
\rho \frac{\partial u_y}{\partial t} + (\frac{\partial}{\partial t} + \sigma)^{-1} \frac{\partial}{\partial t} \frac{\partial p}{\partial y} &= 0, \\
\frac{1}{c^2 \rho} \frac{\partial^2 p}{\partial t^2} + \frac{\partial u_x}{\partial x} + (\frac{\partial}{\partial t} + \sigma)^{-1} \frac{\partial}{\partial t} \frac{\partial u_y}{\partial y} &= 0,
\end{align*}
\]

with
$$\Omega = \mathcal{D} \times [0,T],$$

\(\mathcal{D}\), the space domain,

\(p(x,y,t)\), pressure,

\(u(x,y,t)\), velocity,

\(T\), the final time,

\(c\), wave speed,

\(\rho\), density,

\(u = (u_x, u_y)\)

and \(\sigma\) the absorption coefficient, depending only on \(y\).

In classical Trefftz-DG formulations, both shape and test functions are elementwise solutions to the problem under consideration. As a consequence, the resulting variational formulation only involves surface integrals which contributes to reduce the computational cost. In the PML, it turns out that shape and test functions have to be different to keep this property. This point will be discussed during the talk.

### 3 Shape functions

The implementation of Trefftz methods requires the construction of shape functions which are solutions in each element of the problem to solve. Ideally, we would like to have polynomial basis functions, but it turns out that their construction is not that obvious when considering PML.

However, according to [8], the Green’s function \(G_p\), associated with the pressure can be computed analytically and so does \(G^\text{pml}\_p\), the Green’s function inside of the absorbing layer.

With this in mind, exact solutions of the acoustic wave equation with PML can be computed as Green’s functions which are denoted \(G^\text{pml}\_p\), \(G^\text{pml}\_u_x\), \(G^\text{pml}\_u_y\), with \(u_x\) and \(u_y\) referring to the velocity in the \(x\) and \(y\) direction. They are null when \(t < \frac{r}{c}\), with \(r = \sqrt{x^2 + y^2}\) and when \(t > \frac{r}{c}\), they can be written as:

\[
G^\text{pml}\_p(x,y,t) = e^{-A(x,y,t)\cos[B(x,y,t)]}G_p
\]

\[
G^\text{pml}\_u_x(x,y,t) = \frac{tx}{\rho r^2}G^\text{pml}\_p - \frac{e^{-A(x,y,t)G_p}}{\rho r^2} \times \left( y \sqrt{t^2 - \frac{r^2}{c^2} \sin[B(x,y,t)]} \right)
\]

\[
G^\text{pml}\_u_y(x,y,t) = \frac{ty}{\rho r^2}G^\text{pml}\_p - \frac{e^{-A(x,y,t)G_p}}{\rho r^2} \times \left( x \sqrt{t^2 - \frac{r^2}{c^2} \sin[B(x,y,t)]} \right)
\]

With \(x = \{x - x_i\}_{i=1,n_x}\), \(x_i\) being the source points of the Green’s functions. We can achieve convergence by increasing \(n_x\).

---

**References**


Analysis and FDTD simulation of a perfectly matched layer for the Drude metamaterial

Jichun Li

1Department of Mathematical Sciences, University of Nevada, Las Vegas, USA
*Email: jichun.li@unlv.edu

Abstract

In this talk, I’ll present our recent work on analysis and application of a perfectly matched layer for the Drude metamaterial.

Keywords: Perfectly Matched Layer, metamaterial, FDTD scheme

1 Introduction

Since the Perfectly Matched Layer (PML) introduced for solving the three-dimensional (3D) time-dependent Maxwell’s equations by Bérenger in 1994, many PML models have been proposed and studied further for Maxwell’s equations (cf. [4, Ch.8] and references therein). The PML technique has also been extended to solve many other wave propagation problems, such as acoustics and elastodynamics (e.g. [1, 2]).

In late 1990s, the so-called negative index metamaterials (NIMs) was manufactured successfully and immediately became a very hot research topic as evidenced by numerous papers and books published on metamaterials (e.g., [4] and references therein). In the same time, many studies of PMLs in NIMs have been carried out and found that the classical PMLs fail in NIMs. Soon, some stable PMLs were developed for metamaterials. Here we will present our recent work on developing and analyzing a FDTD scheme for the metamaterial PML model proposed by Bécache et al. [2].

2 The 2-D metamaterial PML model and its stability

A general 2-D Transverse Electric (TEz) metamaterial PML model with 16 unknowns was developed in Bécache et al. Here we focus on the popular case whose governing equations can be written as follows (cf. [2, Eq.(48)]):

For any $(x, y, t) \in \Omega \times (0, T)$,

$$
\begin{align*}
\partial_t E_x + \omega^2_0 J_x + \epsilon_0^{-1} \sigma_y E_x - \epsilon_0^{-1} \partial_y (H^x + H^y),
\partial_t J_x - E_y = 0,
\partial_t E_y + \omega^2_0 J_y + \epsilon_0^{-1} \sigma_x E_y - \epsilon_0^{-1} \partial_x (H^x + H^y),
\partial_t J_y - E_x = 0,
\partial_t H^x + \mu_0^{-1} \sigma_y H^x - \mu_0^{-1} \partial_y E_x,
\partial_t K^x - H^y = 0,
\partial_t H^y + \omega_0^2 K^x + \mu_0^{-1} \sigma_y H^y - \mu_0^{-1} \partial_y E_y,
\partial_t K^y - H^x = 0.
\end{align*}
$$

where $\epsilon_0$ and $\mu_0$ are the permittivity and permeability in free space, $E = (E_x, E_y)$ and $H = H^x + H^y$ are the electric field and magnetic field (in split form) respectively, $J = (J_x, J_y)$ and $K = (K^x, K^y)$ are the auxiliary variables, $\sigma_x(x) \geq 0$ and $\sigma_y(y) \geq 0$ are the damping functions in the $x$ and $y$ directions, $\omega>0$ and $\omega_m>0$ are the electric and the magnetic plasma frequencies in the Drude model described by the following:

$$
\epsilon(\omega) = \epsilon_0 (1 - \frac{\omega^2}{\omega_0^2}), \quad \mu(\omega) = \mu_0 (1 - \frac{\omega^2}{\omega_m^2}).
$$

Here and in the rest of the paper, $\omega$ denotes the general wave frequency.

Since the PML is used in a rectangular domain outside the physical domain, we consider solving (1)-(8) in a rectangular domain $\Omega = [a, b] \times [c, d]$. To complete the model (1)-(8), we assume that the model problem is subject to the initial conditions

$$
\begin{align*}
E_x(x, 0) &= E_{x0}(x), \quad E_y(x, 0) = E_{y0}(x),
J_x(x, 0) &= J_{x0}(x), \quad J_y(x, 0) = J_{y0}(x),
H^x(x, 0) &= H_{x0}(x), \quad H^y(x, 0) = H_{y0}(x),
K^x(x, 0) &= K_{x0}(x), \quad K^y(x, 0) = K_{y0}(x),
\end{align*}
$$

and the perfect conduct (PEC) boundary condition

$$
E_x(x, y, t)|_{y = c, d} = 0, \quad E_y(x, y, t)|_{x = a, b} = 0,
$$

where $E_{x0}, E_{y0}, J_{x0}, J_{y0}, H_{x0}, H_{y0}, K_{x0}, K_{y0}$ are some properly given functions.

In the rest of the paper, we denote the $L^2$ norm over $\Omega$ as $\| \cdot \| := \| \cdot \|_{L^2(\Omega)}$.

Theorem 1 For the solution of (1)-(8), define the energy

$$
\begin{align*}
\mathcal{E}(t) &= \frac{1}{2} \left[ \epsilon_0 \| E_x \|^2 + \| E_y \|^2 + \epsilon_0 \omega_0^{-2} \| J_x \|^2 + \| J_y \|^2 \right] \\
&+ \mu_0 \| H^x \|^2 + \| H^y \|^2 + \mu_0 \omega_0^{-2} \| K^x \|^2 + \| K^y \|^2.
\end{align*}
$$
Then for any nonnegative functions \( \sigma_x(x) \) and \( \sigma_y(y) \), we have
\[
\frac{d}{dt} E_1(t) + \ldots \text{FDTD simulation of a perfectly matched layer for}
\]

Whenever \( \sigma_x = \sigma_y = \sigma \geq 0 \) (i.e., a positive constant), the energy is decreasing:
\[
\mathcal{E}_1(t) \leq \mathcal{E}_1(0), \quad \forall t \in [0,T].
\]

3 The FDTD scheme, stability analysis, and numerical simulation

To develop our difference scheme, we assume that the physical domain \( \Omega = [a,b] \times [c,d] \) is partitioned by a uniform rectangular grid
\[
a = x_0 < x_1 < \cdots < x_{N_x} = b,
\]
\[
c = y_0 < y_1 < \cdots < y_{N_y} = d,
\]
and the time interval \([0,T]\) is partitioned into \( N_T \) uniform intervals by points \( t_k = k\tau \), where \( \tau = \frac{T}{N_T}, k = 0, 1, \ldots, N_T \), grid points \( x_i = ih_x, h_x = \frac{b-a}{N_x}, i = 0, 1, \ldots, N_x \) in the \( x \)-direction, and grid points \( y_j = jh_y, h_y = \frac{d-c}{N_y}, j = 0, 1, \ldots, N_y \) in the \( y \)-direction. Our \( h_x \) and \( h_y \) can be different.

We introduce the following difference and averaging operators: For any discrete function \( u_{i,j}^n \),
\[
\delta_x u_{i,j}^{n+\frac{1}{2}} := \frac{u_{i+\frac{1}{2},j}^{n+1} - u_{i-\frac{1}{2},j}^{n+1}}{h_x}, \quad \nabla_{i,j}^n = \frac{u_{i+\frac{1}{2},j}^{n+1} - u_{i-\frac{1}{2},j}^{n+1}}{2h_x},
\]
\[
\delta_y u_{i,j}^{n+\frac{1}{2}} := \frac{u_{i,j+\frac{1}{2}}^{n+1} - u_{i,j-\frac{1}{2}}^{n+1}}{h_y}, \quad \delta_x u_{i,j}^n := \frac{u_{i+1,j}^n - u_{i,j}^n}{h_x}, \quad \delta_y u_{i,j}^n := \frac{u_{i,j+1}^n - u_{i,j}^n}{h_y}.
\]

We can develop the following FDTD scheme for solving the system of (1)-(8):
\[
\delta_x E_{x,i+\frac{1}{2},j}^{n+\frac{1}{2}} + \omega_2 J_{x,i+\frac{1}{2},j}^{n+\frac{1}{2}} + \epsilon_{x,j}^{n+\frac{1}{2}} \sigma_{y,j} E_{x,i+\frac{1}{2},j}^{n+\frac{1}{2}} = \epsilon_{x,j}^{n+\frac{1}{2}} \sigma_{y,j} E_{x,i+\frac{1}{2},j}^{n+\frac{1}{2}},
\]
\[
\delta_y J_{y,i,j+\frac{1}{2}}^{n+\frac{1}{2}} = -E_{x,i+\frac{1}{2},j+\frac{1}{2}}^{n},
\]
\[
\delta_x E_{y,i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} + \omega_2 J_{y,i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} + \epsilon_{x,i}^{n+\frac{1}{2}} \sigma_{x,i} E_{y,i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} = -\epsilon_{x,i}^{n+\frac{1}{2}} \sigma_{x,i} E_{y,i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}},
\]
\[
\delta_y J_{y,i,j+\frac{1}{2}}^{n+\frac{1}{2}} = -E_{y,i,j+\frac{1}{2}}^{n},
\]
\[
\delta_x H_{x,i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} + \omega_2 K_{x,i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} + \mu_{x,i}^{n+\frac{1}{2}} \sigma_{x,i} H_{x,i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} = \mu_{x,i}^{n+\frac{1}{2}} \sigma_{x,i} H_{x,i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}},
\]
\[
\delta_y K_{y,i,j+\frac{1}{2}}^{n+\frac{1}{2}} = -H_{x,i,j+\frac{1}{2}}^{n+\frac{1}{2}},
\]
\[
\delta_x H_{y,i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} + \omega_2 K_{y,i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} + \mu_{y,j}^{n+\frac{1}{2}} \sigma_{y,j} H_{y,i,j+\frac{1}{2}}^{n+\frac{1}{2}} = \mu_{y,j}^{n+\frac{1}{2}} \sigma_{y,j} H_{y,i,j+\frac{1}{2}}^{n+\frac{1}{2}},
\]
\[
\delta_y K_{y,i,j+\frac{1}{2}}^{n+\frac{1}{2}} = -H_{y,i,j+\frac{1}{2}}^{n+\frac{1}{2}},
\]
where we denote \( \sigma_{y,j} = \sigma_{y}(y_j) \), and \( E^v_{x,i+\frac{1}{2},j} \approx E_x(x_{i+\frac{1}{2}}, y_j, t_n), \) i.e., the approximate solution of \( E_x \) at point \((x_{i+\frac{1}{2}}, y_j, t_n)\). Similar notations are used for other variables. Many numerical tests are carried out, due to page limits, here we just present our simulation of a transmission problem between the vacuum and a Drude medium surrounded by Berenger's PML and the metamaterial PML respectively, originally proposed in [2].

Figure 1: Snapshots of \( H = H^x + H^y \) obtained by the scheme (18)-(25) with \( \tau = 0.01 \) at 800,2000,10000,12000 time steps.

References


Stability and convergence of time-domain perfectly matched layers in dispersive waveguides

Éliane Bécache\textsuperscript{1}, Maryna Kachanovska\textsuperscript{1}, Markus Wess\textsuperscript{1,\textasteriskcentered}
\textsuperscript{1}POEMS, CNRS, INRIA, ENSTA Paris, Institut Polytechnique de Paris, France
\textsuperscript{*}Email: markus.wess@disroot.org

Abstract
We consider the propagation of electromagnetic waves in dispersive waveguides in time domain. To treat the unbounded domains numerically we use so-called perfectly matched layers (PMLs). It is known (see [1]) that standard PMLs for such problems can lead to unstable solutions due to the possible occurrence of backward propagating waves. Here we adopt stabilized PMLs which have been designed to cope with the dispersive effects, following [1, 4]. Despite the fact that the use of PMLs is very popular, only very few and recent results (e.g., [2, 3]) on their convergence have been designed to cope with the dispersive effects, following [1, 4]. Despite the fact that the use of PMLs is very popular, only very few recent results (e.g., [2, 3]) on their convergence are available. Continuing the work done in [2] we consider general dispersive materials and study stability and convergence of the new PMLs.

Keywords: perfectly matched layers, time domain, dispersive media

1 Introduction and problem setting
We look for the solution $\mathbf{E}$, $\mathbf{H}$ of the TM system of Maxwell’s equations in a half-closed waveguide $\mathbb{R}^+ \times (0, l)$, $\ell > 0$,
\begin{align*}
\partial_t \mathbf{D} - \text{curl} \mathbf{H} &= 0, \\
\partial_t \mathbf{B} + \text{curl} \mathbf{E} &= 0.
\end{align*}
\text{(1)}

The above system is equipped with initial conditions, supported in $\Omega = (0, R) \times (0, l)$, and homogeneous (e.g. Neumann) boundary conditions. We consider materials given by the constitutive relations
\begin{align*}
\mathbf{D} &= \mathcal{L}^{-1}(\varepsilon(s) \hat{\mathbf{E}}), \\
\mathbf{B} &= \mathcal{L}^{-1}(\mu(s) \hat{\mathbf{H}}),
\end{align*}
\text{(2)}
where $\mathcal{L}$ is the Laplace transform and $\hat{\mathbf{H}} = \mathcal{L}(\mathbf{H})$, $\hat{\mathbf{E}} = \mathcal{L}(\mathbf{E})$. We assume that the dielectric permittivity and magnetic permeability of the medium $\varepsilon$, $\mu : \mathbb{C}^+ \to \mathbb{C}$ satisfy the following: $\eta \in \{\varepsilon, \mu\}$ is analytic for $s$ such that $\text{Res} > 0$, and
\begin{itemize}
\item $\text{Re}(s\eta(s)) > 0$ for $\text{Res} > 0$;
\item $\eta(s) = \eta(-s)$ (time-reality);
\item $\lim_{r \to +\infty} \eta(r) = 1$ (non-dispersivity for high frequencies).
\end{itemize}

Functions satisfying all these conditions will be called admissible. These assumptions cover the frequently considered cases of Drude and Lorentz materials (also with dissipation).

In the Laplace domain, problem (1) can be written as the dispersive Helmholtz equation
\begin{align*}
s^2 \hat{\varepsilon}(s)\mu(s)\hat{\mathbf{H}} - \Delta \hat{\mathbf{H}} &= 0.
\end{align*}
\text{(3)}

2 Waves in dispersive media
A decomposition into transversal modes $\phi_j$ corresponding to the eigenvalues $\lambda_j^2$ of the transversal Laplacian allows to represent $\hat{\mathbf{H}}$ as
\begin{align*}
\hat{\mathbf{H}}(x, y) &= \sum_{j=0}^{\infty} \hat{\mathbf{H}}_j(x)\phi_j(y),
\end{align*}
where $\hat{\mathbf{H}}_j$ for $x > R$ (i.e., outside of the support of the initial conditions) are given by
\begin{align*}
\hat{\mathbf{H}}_j(x) &= \hat{\mathbf{H}}_j(R) \exp(-\kappa_j(s)(x - R)),
\kappa_j(s) &= \sqrt{s^2 \mu(s)\varepsilon(s) + \lambda_j^2}.
\end{align*}
Let us for the moment assume that $\varepsilon$ and $\mu$ are meromorphic functions in $\mathbb{C}$, purely real on $i\mathbb{R}$. Then radiating waves with frequency $s = i\omega$, $\omega \in \mathbb{R}$, fall into one of the following classes: 1) forward propagating waves, where $\mu(i\omega) > 0$, $\varepsilon(i\omega) > 0$; 2) backward propagating waves, where $\mu(i\omega) < 0$ and $\varepsilon(i\omega) < 0$; note that in this case, the group velocity and the phase velocity have opposite signs; 3) evanescent waves, where $\mu(i\omega)\varepsilon(i\omega) < 0$.

3 PMLs for dispersive media
Because (1) is posed in an unbounded domain, its numerical simulation requires a truncation of the computational domain. Due to the presence of backward propagating waves, the classical, Bérenger’s PMLs are unstable. We thus employ the stabilized PML method of [1], adapted
to the dispersive nature of the problem. It is based on the change of variables
\[ \tilde{x} = x + \frac{1}{s\zeta(s)} \int_R^x \sigma(x') dx'. \]
Here \( \sigma > 0 \) is a damping parameter and \( \zeta : \mathbb{C}^+ \to \mathbb{C} \) is introduced to compensate for instabilities due to presence of backward propagating waves. Note that the classical PML corresponds to the choice \( \zeta \equiv 1 \). It was shown in [4] that if the function \( \zeta \) is such that \( \zeta \), as well as \( \mu \varepsilon / \zeta \) are admissible, then the respective PML system is stable for \( \sigma = \text{const} > 0 \). For Lorentz materials, this condition is equivalent to the necessary and sufficient stability conditions of [1]. Obvious simple choices include \( \zeta = \mu, \varepsilon \).

Subsequently, the unbounded part \( x > R \) of the waveguide is truncated to a finite computational domain of length \( L \) and equipped with a homogeneous boundary condition on the truncation boundary.

As a result, we obtain the following PML system, written in the Laplace domain:
\[
\left( 1 + \frac{a}{\zeta(s)} \right) s^2 \varepsilon(s) \mu(s) \dot{H} - \partial_x \left( 1 + \frac{a}{\zeta(s)} \right)^{-1} \partial_x \dot{H} \\
- \partial_x \left( 1 + \frac{a}{\zeta(s)} \right) \partial_x \ddot{H} = 0, \quad (5)
\]
posed in \((0, R+L) \times (0, \ell)\), equipped with initial and boundary conditions. This system has to be rewritten in the time domain by inverting the Laplace transform.

4 Main convergence result

Let \( H^0 \) solve the time-domain equivalent of (5), and \( H \) be the exact solution. Then the PML error \( E^\sigma(T) = \| H - H^\sigma \|_{L^2(0,T; L^2(0))} \) satisfies
\[
E^\sigma(T) \leq C \exp \left( -4\sigma L^2 T^{-1} \right) \mathcal{E}_d(T),
\]
where the constant \( C \) depends on \( \mu, \varepsilon, \zeta \) and polynomially on \( T \) and \( (L+R)^{-1} \). The quantity \( \mathcal{E}_d \) is the energy of the initial conditions and
\[
\sigma = L^{-1} \| \sigma \|_{L^1(R,R+L)} \text{ is the average damping.}
\]
Notably this bound is in accordance with the bounds for non-dispersive materials from [2, 3]. Let us remark that to prove this result we used similar techniques as in [2].

5 Numerical experiments

We conduct numerical experiments using a first order formulation of the time-domain version of (5) and high-order DG finite elements with explicit time-stepping. Figure 1a shows that the errors decay exponentially fast with respect to \( \sigma \). Figure 1b shows the expected deterioration of the convergence for larger times.

References


Perfectly Matched Layers for second order Maxwell’s equations in time domain

T.Cousin\textsuperscript{1,*}, A.Tonnoir\textsuperscript{2}, C.Fauchard\textsuperscript{3}, C.Gout\textsuperscript{2}

\textsuperscript{1}Routes de France, Paris, France
\textsuperscript{2}LMI, INSA Rouen, 76 000 Rouen, France
\textsuperscript{3}ENDSUM (Cerema), Rouen, France
*Email: theau.cousin@insa-rouen.fr

Abstract

In this work, we are interested in solving second order time-domain Maxwell’s equations in an unbounded domain. To restrict the computational domain, we propose a Perfectly Matched Layers (PMLs) formulation which implies only a reduced number of auxiliary functions (thus reducing the computational cost). This formulation has been validated numerically.

Keywords: Perfectly Matched Layers, Maxwell’s equations, time-domain.

An introduction

Maxwell’s equations appears in many contexts, especially in non-invasive procedures (in biomedical applications, geophysics, items detection, structures control...). In general, an unbounded domain is used to model the interaction between electromagnetic waves and the perturbations (such as tumor, rocks, buried item or water infiltration). One way to restrict the computational domain is to use PMLs, which consists in surrounding the bounded physical domain of interest by artificial non-reflecting absorbing layers. They have been initially developed for first order formulation of Maxwell’s equations (magnetic and electric field). More recently, the PMLs interpretation as a complex change for variables derived a new formulation for Maxwell’s equations in second order. Yet, although this approach has been well-developed for scalar wave equation (or TMz EM field [1]), it has not been reported to the best of our knowledge for the full electrical field.

In this work, we propose a PML formulation for second order time-domain Maxwell’s equations in dimension 2. Surprisingly, it leads to the introduction of "only" two auxiliary functions, as in TMz formulation.

1 In time-harmonic regime

The results are given for the two dimensional case, the three dimensional case will be discuss during the talk. Considering no magnetic source and constitutive law for linear materials, the Maxwell’s equations read

\[ \nabla \times \mu^{-1} \nabla \times \mathbf{E} + \partial_{\Gamma} \mathbf{E} = \mathbf{S} . \]

In time-harmonic domain, the equations become

\[ \nabla \times \mu^{-1} \nabla \times \mathbf{E} - \omega^2 \mathbf{E} = \mathbf{S} . \tag{1} \]

where \( \mathbf{E} \) (resp. \( \mathbf{S} \)) is the Fourier transform in time of \( \mathbf{E} \) (resp. \( \mathbf{S} \)). In time-harmonic regime, the PML formulation consists in applying a complex stretching \( x \rightarrow L_x(x) x \) and \( y \rightarrow L_y(y) y \), where here we take \( L_x(t) = 1 - i \frac{d(t)}{\omega} \), \( d(t) = \left( \frac{\epsilon(x,t-t_0)}{\epsilon_0} \right)^2 \), \( t_0 \) being the boundary in the \( t \) direction and \( l \) the PMLs width. This change of variables amounts in replacing in equation (1) the derivative with respect to \( x \) and \( y \) by \( \frac{1}{L_x} \partial_x \) and \( \frac{1}{L_y} \partial_y \). Applying PMLs, we get

\[ \nabla \times \mu^{-1} \nabla \times \tilde{\mathbf{E}} - \omega^2 \mathbf{E} L_x L_y \tilde{\mathbf{E}} = \mathbf{S} , \tag{2} \]

where:

- \( \tilde{\mathbf{E}} = \begin{bmatrix} L_x^{-1} & 0 \\ 0 & L_y^{-1} \end{bmatrix} \mathbf{E} \),
- \( \nabla_L = \begin{bmatrix} L_y L_x^{-1} \partial_x \\ L_x L_y^{-1} \partial_y \end{bmatrix} \),

and the 2D curl operators are defined by:

\[ \nabla \times f = \begin{pmatrix} \partial_y f \\ -\partial_x f \end{pmatrix} , \quad \nabla \times u = \partial_x u_2 - \partial_y u_1 . \]

Note that, we assume that the support of the source term is not in the PMLs, so it will not be impacted by the coefficients \( L_x \) and \( L_y \).

2 Back to time-domain regime

Very classically, coming back to time-domain involves time-convolution for the terms multiplied
by PMLs coefficients. To avoid these convolution, the idea is to introduce auxiliary functions. First, we have:

\[ \mathcal{F}^{-1} \left( -\omega^2 L_x L_y \tilde{E} \right), \]

which gives:

\[ \partial_t^2 \tilde{E} + (d(x) + d(y)) \partial_t \tilde{E} + d(x)d(y) \partial_x \tilde{E}_x. \quad (3) \]

Second, we set:

\[ \mathcal{F}^{-1} \left( [-L_x L_y^{-1} \partial_y - L_y L_x^{-1} \partial_x] \tilde{E} \right). \]

Let \( C_x = -L_x L_y^{-1} \partial_y \tilde{E}_x \) and \( C_y = L_y L_x^{-1} \partial_x \tilde{E}_y \), implying

\[
\begin{align*}
\partial_t (\tilde{E}_x - C_x) - d(x) \partial_y \tilde{E}_x + d(y) C_x &= 0, \\
\partial_t (\tilde{E}_y - C_y) + d(y) \partial_x \tilde{E}_y - d(x) C_y &= 0,
\end{align*}
\]

where \( C_x \) and \( C_y \) are the inverse Fourier transform of \( C_x \) and \( C_y \). Then, setting \( P_x = -\partial_y \tilde{E}_x - C_x \) and \( P_y = \partial_x \tilde{E}_y - C_y \), we get:

\[
\begin{align*}
\partial_t P_x - (d(x) - d(y)) \partial_y \tilde{E}_x + d(y) P_x &= 0, \\
\partial_t P_y - (d(y) - d(x)) \partial_x \tilde{E}_y + d(x) P_y &= 0,
\end{align*}
\]

which finally gives

\[ \mathcal{F}^{-1}(C_x + C_y) = \nabla \times \tilde{E} - (P_x + P_y). \quad (4) \]

To sum up, the new formulation in time-domain is:

\[
\begin{align*}
\partial_t^2 \tilde{E} &+ (d(x) + d(y)) \partial_t \tilde{E} + d(x)d(y) \tilde{E}_x \\
+ \nabla \times \mu^{-1} \nabla \times \tilde{E} - \nabla \times (P_x + P_y) &= \mathcal{S},
\end{align*}
\]

with the equation on \( \mathcal{P} \):

\[ \partial_t \mathcal{P} - (d(x) - d(y)) \left[ \frac{\partial_y \tilde{E}_x}{\partial_x \tilde{E}_y} \right] + \mathcal{D} \mathcal{P} = 0, \quad (6) \]

with \( \mathcal{D} = \begin{bmatrix} d(y) & 0 \\ 0 & d(x) \end{bmatrix} \).

3 Numerical results

The stable discretization of such system (5-6) is not obvious, see [2]. On Figure 1, the solution has been computed with a Finite Differences scheme that will be detailed during the talk. On Figure 3, we have represented the evolution in time of the energy. Further works are currently in progress to implement Finite Elements discretization in two and three dimensions.

References


Locally Implicit Preconditioning for Maxwell equations on a locally refined spatial grid

Marlis Hochbruck1,*, Jonas Köhler1, Pratik Kumbhar1

1Institute for Applied and Numerical Mathematics, Karlsruhe Institute of Technology, 76149 Karlsruhe, Germany

*Email: Marlis.Hochbruck@kit.edu

Abstract

In this talk, we discuss the construction and analysis of higher-order time integration schemes for the full discretization of linear Maxwell equations on locally refined spatial grids. The schemes are based on a higher-order implicit method, e.g., an algebraically stable Runge–Kutta method. Our main contribution is to propose a preconditioned Krylov subspace method for solving the linear systems arising in each time step, which is designed in such a way that its convergence only depends on the coarse mesh but not on the fine mesh. This is shown by approximation theory in the complex plane.

The advantage of this approach is that it is applicable to any implicit scheme and also works for exponential integrators. It is even applicable to nonlinear problems, where such linear systems arise within the Newton iterations.

Keywords: locally refined spatial grid, Maxwell equations, higher-order time integration, Krylov subspace methods, preconditioning.

1 Introduction

Let \( \Omega \subset \mathbb{R}^d, d = 1, 2, 3 \), be an open, bounded Lipschitz domain and \( T > 0 \) be the simulation time. The linear Maxwell equations in a medium with permeability \( \mu : \Omega \to \mathbb{R} \), permittivity \( \varepsilon : \Omega \to \mathbb{R} \), and a perfect conducting boundary are given by

\[
\begin{align*}
\mu \partial_t \mathbf{H} &= -\text{curl} \mathbf{E}, \quad (0, T) \times \Omega, \\
\varepsilon \partial_t \mathbf{E} &= \text{curl} \mathbf{H} - \mathbf{J}, \quad (0, T) \times \Omega, \\
\mathbf{H}(0) &= \mathbf{H}^0, \quad \mathbf{E}(0) = \mathbf{E}^0, \quad \Omega, \\
n \times \mathbf{E} &= 0, \quad (0, T) \times \partial \Omega.
\end{align*}
\]

Here, \( \mathbf{H}, \mathbf{E}, \mathbf{J} : (0, T) \times \Omega \to \mathbb{R}^d \) denote the unknown magnetic and electric field, and the given current density, respectively. The vector \( \mathbf{n} \) denotes the unit outward normal vector of the domain \( \Omega \). Discretization of (1) in space using a \( \text{dG} \) method with central flux [5, Section 2] leads to

\[
\partial_t \mathbf{u}_h(t) = \mathcal{C} \mathbf{u}_h(t) + \mathbf{j}_h(t), \quad \mathbf{u}_h^0 = \mathbf{u}_h(0),
\]

where

\[
\mathbf{u}_h = \begin{bmatrix} \mathbf{H}_h \\ \mathbf{E}_h \end{bmatrix}, \quad \mathcal{C} = \begin{pmatrix} 0 & -C_E \\ C_H & 0 \end{pmatrix}, \quad \mathbf{j}_h = \begin{bmatrix} 0 \\ -\mathbf{J}_h \end{bmatrix}.
\]

Here, \( \mathcal{C}_H \) and \( \mathcal{C}_E \) are spatially discretized curl-operators. The boundary condition for the electric field is weakly enforced in the definition of \( \mathcal{C}_E \).

We split the locally refined mesh \( T_h \) into a coarse mesh \( T_{h,c} \) and a fine mesh \( T_{h,f} \) with minimum mesh sizes \( h_c \) and \( h_f \), respectively.

The methods are attractive if \( h_f \ll h_c \) and card (\( T_{h,f} \)) \ll \text{card} (\( T_{h,c} \)). Based on this decomposition of the mesh, the split discrete curl operators \( \mathcal{C}_{H,c}, \mathcal{C}_{E,c}, \mathcal{C}_{E} \) defined in [5, Definition 2.7] satisfy

\[
\mathcal{C}_H = \mathcal{C}_H^c + \mathcal{C}_H^f, \quad \mathcal{C}_E = \mathcal{C}_E^c + \mathcal{C}_E^f \quad (3)
\]

and

\[
\mathcal{C}_{H,c} \mathcal{C}_E = \mathcal{C}_{H,c} \mathcal{C}_E, \quad \mathcal{C}_H^c \mathcal{C}_E^c = \mathcal{C}_H^c \mathcal{C}_E^c \quad (4)
\]

In fact, it was shown in [5], that not only the fine elements have to be treated implicitly but also their coarse neighbors. Then, the split operators \( \mathcal{C}_{H,c}^c, \mathcal{C}_{E,c}^c \) can be bounded independently of fine mesh sizes \( h_f \), i.e.,

\[
\| \mathcal{C}_{E,c} \| \leq c h_c^{-1}, \quad \text{and} \quad \| \mathcal{C}_{H,c} \| \leq c h_c^{-1},
\]

with a constant \( c \) that is independent of \( h_f \) and \( h_c \).

2 Higher-order time integration

The efficient implementation of an \( s \)-stage Gauss Runge-Kutta method [3, Section II.1] for the time integration of (2) with step size \( \tau > 0 \) requires solving linear systems of equations of the form

\[
\mathcal{A} \mathbf{x} = \mathbf{b}, \quad \text{where} \quad \mathcal{A} := \mathcal{I} + \tau^2 \alpha \mathcal{C}_H \mathcal{C}_E
\]

in each time step. The real or complex parameter \( \alpha := \alpha_R + i \alpha_I \) only depends on the coefficients of the Runge-Kutta method but neither on the problem nor on the mesh. Since \( \mathcal{C}_H \mathcal{C}_E \) is real and symmetric, \( \mathcal{A} \) is complex symmetric.
3 Krylov subspace methods

To exploit the structure of $A$, we suggest to use the quasi-minimal residual (QMR) algorithm for complex symmetric matrices [2, Section 3], which is based on the complex symmetric Lanczos process. For an initial guess $x_0$ and an initial residual $r_0$, QMR yields an approximation $x_m \in x_0 + \mathcal{K}_m(A, r_0)$, where $\mathcal{K}_m(A, r_0)$ is Krylov subspace generated by $A$ and $r_0$.

Analogously to [4, Theorem 2], one can prove that the error of the QMR iterates satisfies

$$
\|A^{-1}b - x_m\| \leq C \min_{p_m \in \mathcal{P}_m} \|p_m(A)\| \|r_0\|, \quad (7)
$$

with a constant $C$ independent of $\|A\|$. Here, $\mathcal{P}_m$ denotes the set of all polynomials of degree at most $m$. If the field of values $\mathcal{F}(A)$ is contained in a convex, bounded set $\mathcal{S}$, then, using Faber polynomials and complex approximation theory, cf. [1], we have

$$
\|p_m(A)\| \leq (1 + \sqrt{2}) \max_{z \in \mathcal{S}} |p_m(z)|. \quad (8)
$$

Note that the largest elements in $\mathcal{F}(A)$ are of the order $h_f^{-1}$.

4 Preconditioning

Obviously, a smaller set $\mathcal{S}$ in (8) leads to faster convergence. To speed up the convergence, we aim to construct a preconditioner such that the field of values of the preconditioned matrix can be bounded independently of $h_f$. Motivated by locally implicit methods for Maxwell equations in [5], we suggest to approximate $A$ by its dominant part,

$$
A \approx B := I + \tau^2 \rho C_H C_E, \quad \rho > 0, \quad (9)
$$

i.e., we replace the discrete curl operators $C_H, C_E$ in (6) defined on the full mesh by the split operators acting on the implicitly treated mesh elements and $\tau$ by a real parameter $\rho > 0$. Hence $B$ is a symmetric, positive definite matrix, which allows us to define the equivalent preconditioned linear system by

$$
\tilde{A}\tilde{x} = \tilde{b}, \quad \tilde{A} := B^{-1/2} A B^{-1/2}, \quad (10)
$$

where $\tilde{x} := B^{1/2}x$ and $\tilde{b} := B^{-1/2}b$. Since $A$ is complex symmetric and $B$ is real symmetric, the preconditioned matrix $\tilde{A}$ is again complex symmetric. We now apply the complex symmetric QMR method to the preconditioned linear system (10) and refer to this method as preconditioned QMR method (pQMR). For $\mathcal{F}(\tilde{A})$ we have proven the following theorem.

**Theorem 1** The field of values of $\tilde{A}$ defined in (10) satisfies $\mathcal{F}(\tilde{A}) \subset \tilde{\mathcal{S}}$, where $\tilde{\mathcal{S}}$ is bounded independently of the fine mesh.

By (7) and (8), this theorem shows that the convergence of the preconditioned QMR method is indeed independent of the fine mesh.

5 Acknowledgement

Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 258734477 – SFB 1173.

References


Efficient numerical method for time domain electromagnetic wave propagation in thin co-axial cables.

Akram BENI HAMAD1,∗, Sébastien IMPERIALE2, Patrick JOLY1

1POEMS (UMR CNRS-INRIA-ENSTA Paris) ENSTA Paris - Institut Polytechnique de Paris
2Inria-M3DISIM – LMS, École Polytechnique, CNRS – Institut Polytechnique de Paris

*Email: akram.beni-hamad@ensta-paris.fr

Abstract

In this work we construct an efficient numerical method to solve 3D Maxwell’s equations in coaxial cables. Our strategy is based upon an hybrid explicit-implicit time discretization combined with edge elements on prisms and numerical quadrature. One of our objectives is to validate numerically generalized Telegrapher’s models that are used to simplify the 3D Maxwell equations into a 1D problem.

Keywords: Coaxial cables, Maxwell’s equations, Telegrapher’s models, Numerical simulation.

1 Introduction

Coaxial cables have transverse dimensions that are small compared to the longitudinal one: we will consider mathematically that the transverse dimension is proportional to a small parameter δ ≪ 1, and, using an asymptotic analysis of the 3D Maxwell equations with δ → 0, establish several 1D simplified models. Such models were rigorously derived in [1]. To our knowledge, there is no existing quantitative numerical comparison between 1D model and 3D Maxwell’s theory. Doing so requires performing 3D simulations with 3D Maxwell’s equations. This is a computational challenge because the cable is thin.

2 The cylindrical case

Our space-time discretization strategy, will be developed for the second order formulation of the problem, obtained after elimination of the magnetic field,

$$\varepsilon \partial_2^2 E + \sigma \partial_3 E + \nabla \times \mu^{-1} \nabla \times E = 0.$$  (1)

Our approach is based on a particular rewriting of (1), that well separates the roles of the longitudinal and transverse space variables (resp, longitudinal and transverse electric fields).

In the considered applications, the wavelength λ is large compared to the diameter of the cross-section, but small compared to the size of the cable. This specificity has two impacts on the time discretization: first, an implicit scheme would be too costly given the size of the problem, second, an explicit scheme is to be avoided because the corresponding CFL condition would be too constraining. In this work we will present an efficient hybrid numerical method for solving our problem. The idea is to use an anisotropic prismatic mesh, with a transverse step size hT and a longitudinal step size h for the space discretization (with hT ≪ h), a trapezoidal quadrature rule in x3, and a hybrid implicit-explicit scheme for the time discretization [2].

To implement this method, the first step is to make a longitudinal discretization of the cable, then a transverse discretization of each section, and finally a discretization in time. The transverse field ET will then be approximated by Nedelec elements in each section Sj and by piecewise affine elements along the longitudinal direction. On the other hand, the longitudinal field E3 field will be approximated by P1 elements on each Sj+1/2 section and by P0 discontinuous elements along the longitudinal direction (See Figure 2).

In the end, the two unknown fields ET,j and E3,j+1/2 alternate from one cross section to the other (See Figure 3).
After writing a variational formulation and using trapezoidal quadrature for $x_3$ integration, the algebraic form of the semi-discrete problem is,

$$ M_h \frac{d^2 \mathbf{E}_h}{dt^2} + K_h \mathbf{E}_h = 0, \tag{2} $$

where $M_h$ and $K_h$ are the (infinite) mass and stiffness matrices.

$$ M_h = \begin{pmatrix} M_h & 0 \\ 0 & M_h \end{pmatrix}, \quad K_h = \begin{pmatrix} K_{T,h} & C_{3T,h} \\ C_{3T,h}^T & K_{T,h} \end{pmatrix}. $$

We used bold (normal) letters when they apply to differential operators in the longitudinal fields and mixes the $x_3$ and transverse derivatives. Finally thanks to double observation: $M_h$ is block diagonal by section.

Our method will be based on a tricky decomposition of the stiffness matrix $K_h = K_{h}^l + K_{h}^t$, where,

$$ K_{h}^l = \begin{pmatrix} K_{T,h} & 0 \\ 0 & K_{T,h} \end{pmatrix}, \quad K_{h}^t = \begin{pmatrix} K_{T,h} & C_{3T,h} \\ C_{3T,h}^T & 0 \end{pmatrix}. $$

The interest of the decomposition lies in the following double observation:

- $K_{h}^l$ is adapted to implicit time discretization because the matrix is positive and thanks to $x_3$ quadrature, block diagonal by section, thus easy to invert.
- $K_{h}^t$ is adapted to explicit time discretization because it corresponds to the discretization of the differential operators in the $x_3$ direction: this matrix couples all the interfaces and has no sign.

As a consequence, we propose the following scheme,

$$ \begin{align*}
M_h \frac{\mathbf{E}_h^{n+1} - 2 \mathbf{E}_h^n + \mathbf{E}_h^{n-1}}{\Delta t^2} + & K_h \mathbf{E}_h^n \\
+ K_{h}^l \{ \mathbf{E}_h^n \}_\theta = 0, \tag{3}
\end{align*} $$

$$ \{ \mathbf{E}_h^n \}_\theta := \theta \mathbf{E}_h^{n+1} + (1 - 2\theta) \mathbf{E}_h^n + \theta \mathbf{E}_h^{n-1}. $$

**Theorem 1** A sufficient stability condition for the fully discrete scheme (3) is that $\theta > \frac{1}{2}$ and, $c^t$ being the maximum velocity $c$, with $\varepsilon \mu c^2 = 1$.

$$ c^t \Delta t \frac{h}{\theta} < \sqrt{\frac{4 \theta - 1}{4 \theta}}. \tag{4} $$

3 The varying cross-section case

In the presence of deformations, the method needs to be modified. In order to preserve the longitudinal / transverse decoupling, we propose a hybrid method combining a conforming discretization in the longitudinal variable and a discontinuous Galerkin method in the transverse ones. This method is designed in order to coincide with the previous one in the cylindrical parts of the cable.

4 Numerical experiments

In Figure 4, we represent the norm $|E_{\delta}^x|$ on the boundary $\partial \Omega$ of the reference cable, and $|E_{\delta}^z|$ that is obtained by post-processing the solution of the limit model. We observe that the norm of 3D field cannot be distinguished from the one of the limit field when $\delta = 10^{-3}$.

In figure 5, we compare the evolution of the 1D (limit) voltage $V(x_3,t)$ issued from the numerical resolution of the 1D limit model, to the 1D voltage $V^\delta(x_3,t)$ for the 3D problem, and obtained by post-processing the 3D solution $E_{\delta}$. The limit solution $V$ is in red while $V^\delta$ is in blue. The numerics confirm that $V^\delta$ converge towards $V$.

**References**


The Hermite-Taylor Correction Function Method for Maxwell’s Equations

Yann-Meing Law\textsuperscript{1,\#}, Daniel Appelö
\textsuperscript{1}Michigan State University, East Lansing, USA
\textsuperscript{\#}Email: lawkamci@msu.edu

Abstract
A new approach, based on the Correction Function Method (CFM), to handle boundary conditions for Hermite-Taylor methods is proposed. In Hermite methods not only the solution but also its derivatives need to be determined on the boundary. Here we provide additional information to determine all degrees of freedom on the boundary by a pre-computation where a minimization problem is solved. The functional to be minimized is a square measure of the residual associated with the original problem, that is Maxwell’s equations in this work. Numerical examples are performed in 1-D and the expected convergence order is obtained.

Keywords: Hermite methods, Correction function method, Maxwell’s equations, High order, Boundary conditions

1 Introduction
Hermite methods achieve arbitrary order of accuracy while maintaining a stability condition only depending on the largest wave-speed, independent of the order of the method [1]. However, the imposition of general boundary conditions is cumbersome (and largely unexplored) since a \((2m+1)\)-order Hermite method requires the knowledge of all electromagnetic fields and their \(m\) first derivatives on the boundary. A possible solution to this is to use a hybrid DG-Hermite method as in [2] but this does require the use of local timestepping to maintain the large timesteps in the Hermite method. Here, we propose an alternative solution based on the CFM [3,4] to handle boundary conditions.

Let us assume a domain \(\Omega = [x_i, x_f]\) and a time interval \(I = [t_0, t_f]\), we focus on the following form of Maxwell’s equations in 1-D:

\begin{equation}
\begin{align*}
\mu \partial_t H + \partial_x E &= 0 \quad \text{in} \quad \Omega \times I, \\
\epsilon \partial_t E + \partial_x H &= 0 \quad \text{in} \quad \Omega \times I, \\
H(x, t_0) &= a(x), \quad \forall x \in \Omega, \\
E(x, t_0) &= b(x), \quad \forall x \in \Omega, \\
c_1 E(x_i, t) + c_2 H(x_i, t) &= g_1(t), \quad \forall t > t_0, \\
c_3 E(x_f, t) + c_4 H(x_f, t) &= g_4(t), \quad \forall t > t_0,
\end{align*}
\end{equation}

where \(H\) is the magnetic field, \(E\) is the electric field, \(\mu\) is the magnetic permeability, \(\epsilon\) is the electric permittivity, \(c_i\) for \(i = 1, \ldots, 4\) are known coefficients, and \(a(x), b(x), g_1(t)\) and \(g_4(t)\) are known functions.

2 Hermite-Taylor Methods
Hermite methods use a staggered grid in space and time defined by a primal grid \(x_i = x_f + i \Delta x, \ i = 0, \ldots, N\), and a dual grid \(x_i+1/2 = x_f + (i + 1/2) \Delta x, \ i = 0, \ldots, N-1\). Here \(\Delta x = \frac{x_f - x_i}{N}\) and \(N\) is the number of cells on the primal grid. The approximate solution on the primal grid is centered at times \(t_n = t_0 + n \Delta t\) while the approximation on the dual grid is centered at times \(t_{n+1/2} = t_0 + (n + 1/2) \Delta t\).

Assuming that the \(m\) first derivatives at the initial time are available, we construct Hermite interpolants of degree \(2m+1\). Afterward, we evolve the interpolant at the cell center through time using a recursive relation between time and space derivatives that comes from the system of PDEs. For linear hyperbolic problems, this evolution is exact. In other words, knowing all space derivatives of a given polynomial approximation at a given point \((x_i, t_{n+1/2})\) allows us to obtain the exact Taylor expansion in time for this polynomial and its derivatives, defining the update at \((x_i, t_{n+1})\).

3 Imposition of Boundary Conditions
Consider the problem of finding polynomials of degree \(m\) at \((x_N, t_{n+1})\) in Figure 1 that can be used together with the Hermite data at \(x_{N-1}\) to interpolate to \((x_{N-1/2}, t_{n+1})\) and subsequently
\[ J(H, E) = \frac{1}{2} \int_{I_h} \left[ \int_{\Omega_h} \left( (\mu \partial_t H + \partial_x E)^2 + (\epsilon \partial_t E + \partial_x H)^2 \right) dx + \left( c_3 E(x_r, t) + c_4 H(x_r, t) - g_r(t) \right)^2 \right] \] 
\[ + \int_{\Omega_h} \left( H(x_{N-1/2}, t) - H^*(x_{N-1/2}, t) \right)^2 + \left( E(x_{N-1/2}, t) - E^*(x_{N-1/2}, t) \right)^2 \right] dt \]

4 Numerical Examples

Consider a domain \( \Omega = \left[ \frac{1}{3}, \frac{8}{3} \right] \), a time interval \( I = [0, \frac{12}{\sqrt{3}}] \), \( \mu = 1 \) and \( \epsilon = 1 \). We set \( \Delta t = 0.5 h \), \( c_1 = c_3 = 0.5 \), \( c_2 = c_4 = 1 \), and set the initial and boundary data so find that the solution to the problem is \( H(x, t) = \sin(250x) \sin(250t) \), \( E = \cos(250x) \cos(250t) \). Figure 2 shows how the errors follow the expected \( 2m + 1 \) rates of convergence.

As a final numerical example, we solve the 2-D Maxwell’s equations in a \( 2 \times 2 \) PEC cavity with the Hermite-CFM of order of accuracy 3. As can be seeing in Figure 3, the errors are smooth and evenly distributed over the computational domain, indicating that the boundary treatment is stable and accurate.

Figure 3: Solution (left) and error (right) for a cavity problem in 2D.

References

A space–time quasi-Trefftz DG method for the wave equation with smooth coefficients

Lise-Marie Imbert-Gérard1, Andrea Moiola2,*, Paul Stocker3
1Department of Mathematics, University of Arizona, Tucson, USA
2Department of Mathematics, University of Pavia, Pavia, Italy
3Institute for Numerical and Applied Mathematics, University of Göttingen, Göttingen, Germany
*Email: andrea.moliola@unipv.it

Abstract
We propose a quasi-Trefftz method to approximate initial boundary value problems for the acoustic wave equation with piecewise-smooth material parameters. The key feature of the scheme is that all discrete trial and test functions are elementwise approximate solutions of the wave equation. The quasi-Trefftz scheme is framed in a space–time discontinuous Galerkin (DG) setting. We prove stability and high-order convergence, and show that the number of DOFs needed to obtain a given accuracy is considerably smaller than for schemes based on classical polynomial spaces. The quasi-Trefftz basis functions are polynomials in the space–time variable and can be computed with a simple algorithm. The inspiration comes from the generalised plane waves developed for time-harmonic problems with variable coefficients.

Keywords: quasi-Trefftz, space–time, discontinuous Galerkin, wave equation.

1 Trefftz and quasi-Trefftz methods
Trefftz schemes are Galerkin methods whose test and trial spaces are made of elementwise solutions of the PDE to be approximated. They are well-studied for homogeneous, linear PDEs with piecewise-constant coefficients, see [3] for the case of the wave equation. Other examples of Trefftz schemes use harmonic polynomials for the Laplace equation \( \Delta u = 0 \) and plane waves for the Helmholtz equation \( \Delta u + k^2 u = 0 \).

When the equation coefficients are not constant, it is usually very difficult to construct families of exact solutions with good approximation properties to use as basis functions, so Trefftz schemes are not viable in this case.

Quasi-Trefftz methods use discrete spaces of functions that are approximate solutions of the PDE. With this, we mean that the Taylor polynomial (of some given order \( m \)) of \( \mathcal{L}v_h \), \( \mathcal{L} \) being the PDE operator and \( v_h \) any discrete function, vanishes in a given point of each element of the computational mesh. In this way it is possible to construct low-dimensional discrete spaces with excellent approximation properties.

Existing quasi-Trefftz methods for time-harmonic problems use exponential basis functions called “generalized plane waves”, see [1]. Here, instead, we develop a quasi-Trefftz discretisation for the time-domain scalar wave equation with variable coefficients. Building on the Trefftz case studied in [3], we define space–time quasi-Trefftz polynomial bases, we show how to compute them and we use them in a DG scheme.

All details can be found in [2].

2 Variable-coefficient wave equation
We consider the following initial boundary value problem for the first-order system corresponding to the homogeneous acoustic wave equation:

\[
\begin{align*}
\nabla v + \rho \partial_t \sigma &= 0 & \text{in } Q = \Omega \times (0,T), \\
\nabla \cdot \sigma + G \partial_t v &= 0 & \text{in } Q, \\
\sigma(\cdot,0) &= \sigma_0 & \text{on } \Omega \subset \mathbb{R}^n, \\
v(\cdot,0) &= v_0 & \text{on } \partial Q \times (0,T).
\end{align*}
\]

Here \( \Omega \subset \mathbb{R}^n \) is an open, bounded, Lipschitz polytope, \( \rho, G > 0 \) are the material coefficients, independent of time and piecewise-smooth, and \( c := (\rho G)^{-1/2} \) is the wavespeed. Neumann (\( \sigma \cdot \mathbf{n} = g_N \)) and Robin (\( \partial v - \sigma \cdot \mathbf{n} = g_R \)) boundary conditions may also be included.

If \( \rho \sigma_0 \) is a gradient, then \( v = \partial_t u \) and \( \sigma = -\frac{1}{\rho} \nabla u \), where \( u \) is a solution of the second-order, scalar, homogeneous wave equation

\[
\Box_{\rho, G} u := -\nabla \cdot \left( \frac{1}{\rho} \nabla u \right) + G \partial_t^2 u = 0 \quad \text{in } Q.
\]

3 Local polynomial quasi-Trefftz spaces
Let \( K \subset Q \) be a space–time subdomain (a mesh element) that is star-shaped with respect to a centre point \( (x_K, t_K) \in K \). Assume that the material parameters \( \rho, G \) are sufficiently smooth
We define the local quasi-Trefftz spaces
\[ Q_U^p(K) := \{ f \in P^p(K) \mid \partial_i \square_{\rho,G} f(x_K,t_K) = 0, \forall i \in [n]^{p+1}, |i| \leq p - 2 \}, \quad p \in \mathbb{N}, \]
\[ Q_{PP}^p(K) := \left\{ \left( \partial_i f, -\frac{1}{\rho} \nabla f \right), \quad f \in Q_U^{p+1}(K) \right\}, \]
where \( P^p(K) \) is the space of polynomials of degree at most \( p \) on \( K \), and \( D^i \) with multi-index \( i = (i_1, \ldots, i_n, i_t) \), denotes the space-time partial derivative \( D^i = \partial_{x_1}^{i_1} \cdots \partial_{x_n}^{i_n} \partial_t^{i_t} \).

\( Q_U^p(K) \) is the space of polynomials \( f \) of degree at most \( p \) such that the degree-\((p-2)\) Taylor polynomial of \( \square_{\rho,G} f \) at \((x_K,t_K)\) is zero. Similarly, \( Q_{PP}^p(K) \) is the analogous space for the first-order system. It is possible to define a third kind of spaces \( Q_{U}^{p} \) for first-order systems not coming from second-order equations.

For all smooth solutions \( u \) of \( \square_{\rho,G} u = 0 \) in \( K \), the degree-\(p\) Taylor polynomial \( T[u](x,t) = \sum_{|i|\leq p} \frac{1}{i!} \partial_i^p u(x,t) \) belongs to the space \( Q_U^p(K) \). It follows that for all \( 0 \leq q \leq p \)
\[ \inf_{P \in Q_U^p(K)} |u - P|_{C^q(K)} \leq C_{p,q,r} r_K^{p+1-q} |u|_{C^{p+1}(K)}, \]
where \( r_K := \sup_{(x,t) \in K} |(x,t) - (x_K,t_K)| \). This means that the quasi-Trefftz space \( Q_{PP}^p(K) \) approximates all \( C^{p+1}(K) \) PDE solutions with the same \( h \)-convergence rates of the full polynomial space \( P^p(K) \). The advantage of the quasi-Trefftz space is that it is a much smaller space:
\[ \dim(Q_U^p(K)) = O_{p \to \infty}(p^n) \ll \dim(P^p(K)) = O_{p \to \infty}(p^{n+1}). \]

## 4 Basis function construction

We want to define a concrete basis of the quasi-Trefftz space. We note that the coefficients \( a_i \) of the monomial expansion \( v(x,t) = \sum_{i \leq p} a_i (x - x_K)^i (t - t_K)^n \) of any quasi-Trefftz polynomial \( v \in Q_U^p(K) \) satisfy the recurrence relations
\[ a_{i_1,i_2} = \sum_{j_1 < i_1} \frac{g_{j_1,i_1} - j_1}{g_0 a_{j_1,i_1 + 2}} + \sum_{l=1}^{n} \sum_{j_2 < i_2} \frac{(i_2 + 1)(i_2 + 1)}{(i_2 + 2)(i_2 + 1)g_0} a_{j_2 + i_2 + 1}, \]
where \( g_i \) and \( \zeta_i \) are the Taylor coefficients of \( G \) and \( \rho^{-1} \) at \((x_K,t_K)\). It is possible to order these relations in such a way that all coefficients of \( v \) can be computed from \( a_{i_1,0} \) and \( a_{i_1,1} \). It follows that \( v \) is determined by its value and the value of \( \partial_t v \) at time \( t = t_K \).

This implies that, given a basis \( \hat{B} \) of \( P^p(\mathbb{R}^n) \) and a basis \( B \) of \( P^{p-1}(\mathbb{R}^n) \) (these are polynomials in \( x \) only), we can construct a basis \( \tilde{B} \) of \( Q_{U}^{p} \) such that each \( b_j \in \tilde{B} \) satisfies either
\[ \begin{cases} b_j(\cdot, t_K) \in \hat{B}, \\ \partial b_j(\cdot, t_K) = 0, \end{cases} \quad \text{or} \quad \begin{cases} \partial b_j(\cdot, t_K) = 0, \\ \partial b_j(\cdot, t_K) \in \tilde{B}. \end{cases} \]

Then the relations above allow to explicitly compute the coefficients \( a_i \) of the monomial expansion of \( b_j \) with a simple iterative algorithm.

## 5 Quasi-Trefftz DG method

Let \( T_h \) be a polytopic mesh that partitions the space-time cylinder \( Q \). The global quasi-Trefftz space \( \coprod_{K \in T_h} Q_{PP}^p(K) \) is used as trial and test discrete space of a DG method that extends the one introduced in [3]. The formulation employs centred-in-space and upwind-in-time numerical fluxes on interior mesh faces.

In [2] we show that, under appropriate assumptions, the DG scheme is well-posed and we prove high-order \( h \)-convergence rates. These are optimal in a skeleton norm and half-order suboptimal at final time (i.e. in \( L^2(\Omega \times \{T\}) \) norm).

Numerical examples validate the theoretical results for both Cartesian-product and tent-pitched space-time meshes. These meshes give rise to a sort of implicit and explicit advancement in time, respectively. The main advantage compared to standard DG schemes is the faster convergence in terms of the number of degrees of freedom.

## References


Tuesday, July 26, First Afternoon Session
Numerical treatment of the vectorial equations of stellar oscillations

Martin Halla\textsuperscript{1}, Christoph Lehrenfeld\textsuperscript{2}, Paul Stocker\textsuperscript{2,*}
\textsuperscript{1}Max-Planck-Institut für Sonnensystemforschung, Göttingen, Germany
\textsuperscript{2}Georg-August-Universität Göttingen, Germany
\textsuperscript{*}Email: p.stocker@math.uni-goettingen.de

Abstract
We present a discretization for the vectorial equations of solar and stellar oscillations. Special attention is paid to preserving compatibility with the generalized Helmholtz decomposition used in the analysis of the continuous model to achieve stability.

Keywords: finite element method, Galbrun’s equation, helioseismology

1 Introduction
The Galbrun’s equation with additional rotational and gravitational terms model stellar oscillations. Recently, HDG numerical methods for the related scalar case, a convected Helmholtz equations, have been devised and analysed in [1]. Furthermore, in [2], it was shown that the vector valued problem is well-posed, when incorporating a simple damping term. A suitable generalized Helmholtz decomposition plays a crucial role in the analysis. In the discretization, we aim to preserve a discrete version of the generalized Helmholtz decomposition used in the analysis of the continuous model to achieve stability.

The variational problem states: Find $\mathbf{u} \in \mathcal{X}_b$ such that

$$a(\mathbf{u}, \mathbf{u}') = \sum_{i=1}^{3} a^i(\mathbf{u}, \mathbf{u}') = \langle \mathbf{f}, \mathbf{u}' \rangle, \forall \mathbf{u}' \in \mathcal{X}_b,$$

with

$$a^1(\mathbf{u}, \mathbf{u}') = \langle \rho \psi''' + (\mathbf{b} \cdot \nabla) \psi' + (\text{Hess}(\rho) - \rho \psi') \psi' + \rho \psi'' \psi = f \rangle (1)$$

$$-\frac{1}{4\pi G} \Delta \psi + \nabla (\rho \psi) = 0,$$

in the presence of density $\rho$, pressure $p$, sound speed $c_s$, background velocity $\mathbf{b}$, gravitational background potential $\phi$, damping coefficient $\gamma$, gravitational constant $G$, and source $f$. This problem was shown to be well-posed in [2]. For the discretization, we will focus on a common simplification of the problem, the Cowling approximation, given by setting $\psi = 0$ in (1).

We consider the resulting variational problem over the Hilbert space

$$\mathcal{X}_b = \{ \mathbf{u} \in L^2(\Omega, \mathbb{C}^3) : \nabla \cdot \mathbf{u} \in L^2(\Omega),$$
$$\mathbf{b} \cdot \nabla \mathbf{u} \in L^2(\Omega, \mathbb{C}^3), \mathbf{u} \cdot n_x = 0 \text{ on } \partial \Omega \}$$

over a bounded domain $\Omega$ and with inner product

$$\langle \mathbf{u}, \mathbf{u}' \rangle_{\mathcal{X}_b} = \langle \mathbf{u}, \mathbf{u}' \rangle + \langle \nabla \cdot \mathbf{u}, \nabla \cdot \mathbf{u}' \rangle + \langle \mathbf{b} \cdot \nabla \mathbf{u}, (\mathbf{b} \cdot \nabla) \mathbf{u}' \rangle.$$

2 Setting
Galbrun’s equation for time-harmonic acoustic waves for the unknowns $\mathbf{u}, \psi$ is given by the partial differential equation

$$\rho(-i\omega + (\mathbf{b} \cdot \nabla))^2 \mathbf{u} - \nabla (\rho \psi'' \nabla \cdot \mathbf{u})$$
$$+ (\nabla \cdot \mathbf{u}) \nabla p - \nabla (\nabla \cdot \mathbf{u}) - i\omega \gamma \rho \mathbf{u}$$
$$+ (\text{Hess}(p) - \rho \text{Hess}(\phi)) \mathbf{u} + \rho \nabla \psi = \mathbf{f}$$

in the presence of density $\rho$, pressure $p$, sound speed $c_s$, background velocity $\mathbf{b}$, gravitational background potential $\phi$, damping coefficient $\gamma$, gravitational constant $G$, and source $\mathbf{f}$. This
with $V \subset \{ v \in H^2(\Omega) | \nabla v \cdot n_\Omega = 0 \text{ on } \partial \Omega \}$, $W = \{ u \in X_b | (\nabla + q) \cdot u = 0 \}$ and $Z$ with size related to $\ker(B)$, with $B \in L(H^1)$. $\langle Bu, v \rangle := \langle \nabla u, \nabla v \rangle - \langle q \cdot \nabla u, v \rangle$. Second, the operator $A$, associated to the bilinear form $a(u, u') = \langle Au, u' \rangle_X$ is shown to be weak $T$-coercive, i.e.

$$AT = B^{\text{coerce}} + B^{\text{compact}}$$

for a coercive and a compact operator $B^{\text{coerce}}$, $B^{\text{compact}}$. Injectivity of $A$ is caused by the damping term. Well-posedness follows using Fredholm alternative. The choice of $T$, which we will also use in the discrete setting, is a sign switch operator. Let us denote by $P_V, P_W, P_Z$ the respective projections, then $T$ is chosen as

$$T := P_V - P_W + P_Z.$$  \tag{2}

3. Discretization

We follow [2], by considering two distinct cases for discretization, first focusing on the case with only background flow present without pressure and gravity and then the contrariwise case, which we later merge.

To approximate $u$ we consider discrete functions $u_h \in X_h$ on which we only impose normal continuity, i.e. $X_h$ is taken to be a $H_0(\nabla; \Omega)$-conforming finite element space, as we cannot expect functions in $X_h$ to be tangential continuous. Finding a generalized Helmholtz decomposition for the discretization space, similar to the one in the continuous setting, will be crucial for the stability analysis. We aim for an implicit decomposition of the form

$$X_h = V_h \oplus W_h,$$

here we will focus on the crucial spaces $V, W$, assuming that the finite dimensional space $Z$ only contains the zero function.

3.1 Background flow

We first consider the case of constant pressure and gravitational potential ($p = \text{const}$ and $\phi = \text{const}$). We obtain an orthogonal decomposition using the spaces $W_h = \{ u \in X_h | \nabla \cdot u = 0 \}$ and $V_h = \{ v_h \in X_h | \langle v_h, w_h \rangle_{1, h} = 0, \forall w_h \in W_h \}$. We introduce the discrete bilinear form

$$a_h(u_h, u'_h) = a^1(v_h, v'_h) + a^2(u_h, u'_h) + a^3(u_h, u'_h)$$

where $a^2(\cdot, \cdot)$ has additional DG penalization terms for the tangential jumps across interelement boundaries. Note that since $u_h = v_h + w_h$, with $w_h$ divergence free, the term $a^1(\cdot, \cdot)$ only depends on functions in $V_h$.

To show well-posedness we make use of a similar sign switch operator as in the continuous case $T_h := P_{V_h} - P_{W_h}$. Crucial for the numerical analysis is the observation that the divergence term can dominate the broken $H^1$-norm, which gives us control over the other $v_h$ terms in the bilinear form. Indeed, using tools from the numerical analysis of Stokes and linear elasticity problems for the space $X_h$, we obtain

$$\| \nabla \cdot v_h \|_{0, h} \geq c \| v_h \|_{1, h}, \forall v_h \in V_h.$$  \tag{3}

To prove convergence we derive a type of commutative property of the sign switching operators

$$\lim_{h \to 0} \| T_h p_h u - p_h T u \|_{X_h} = 0, \forall u \in X_b,$$

where $p_h$ is the projection onto $X_h$.

3.2 Pressure and gravity

Next we consider the case with no flow ($b = 0$), but with non-constant pressure and gravity. We must weaken the condition in $W_h$, else the discrete space may collapse to only containing the trivial solution. We consider $W_h = \{ u \in X_h | \langle (\nabla + q) \cdot u, r_h \rangle = 0, \forall r_h \in Q_h \}$ where $Q_h$ is a suitable scalar finite element space. Due to this relaxation we need to take extra care of the term $a^1(\cdot, \cdot)$, which now also depends on $w_h$. To obtain an estimate as in (3) we show an inf-sup stability result of the form

$$\inf_{r_h \in Q_h} \sup_{u_h \in X_h} \langle (\nabla + q) \cdot u_h, r_h \rangle \geq c \| u_h \|_{1, h} \| r_h \|_{Q_h}$$

for a constant $c$ independent of the discretization parameters.

References

[1] H. Barucq, N. Rouxelin and S. Tordeux,  

[2] M. Halla and T. Hohage,  
Capturing plasmonic behaviors in light scattering by spheres using finite element methods and asymptotic quadrature

Camille Carvalho2,1, Arnold Kim2, Benjamin Latham2,*
1Univ Lyon, INSA Lyon, UJM, UCBL, ECL, CNRS UMR 5208, ICJ, F-69621, France
2Department of Applied Mathematics, UC Merced, Merced, United States of America
*Email: blatham@ucmerced.edu

Abstract
We present a Finite Element Method (FEM) based approach to capture plasmonic behaviors light scattering by metallic spheres. Surface plasmons are highly oscillatory waves localized to the interface between a dielectric (air, vacuum) and a metal (gold, silver). As surface plasmons lead to large field enhancements, they are useful for high-resolution imaging and other applications. It is challenging to capture them merically, and standard methods do not succeed. In the context of spherical scatterers, we identify where plasmonic excitations can arise, propose an approach to extract the fast-oscillating plasmonic behavior from the formulation, owing FEM to approach the slow (smooth) part of the solution.

Keywords: Finite Element Methods, Surface plasmons, Resonances, Scattering

Problem setting
For simplicity we consider time-harmonic scattering of scalar waves in a homogeneous background medium. The plane wave \( u^a = e^{ikz} \) with wavenumber \( k > 0 \) is incident on the metal sphere corresponding to domain \( \Omega = \{ |x| < 1 \} \). The boundary \( \partial \Omega = \{ |x| = 1 \} \) and closure \( \bar{\Omega} = \Omega \cup \partial \Omega \). Let \( \varepsilon(x) = 1 \), \( x \in E := \mathbb{R}^3 \setminus \bar{\Omega} \) and \( \varepsilon(x) = \varepsilon_m < 1 \), \( x \in \bar{\Omega} \) denote the piece-wise constant permittivity characterizing this problem. The total field \( u \) satisfies the following undarly value problem:

\[
\mathbf{\nabla} \cdot (\varepsilon^{-1} \mathbf{\nabla} u) + k^2 u = 0, \text{ in } \mathbb{R}^3
\]

\[
[u]|_{\partial \Omega} = 0, \quad [\varepsilon^{-1} \mathbf{\nabla} u]|_{\partial \Omega} = 0
\]

\[
\text{lim}_{r \to \infty} r (\mathbf{n} \cdot -ik) u^\alpha = 0
\]

We can use \( \mathbf{T} \)-coercivity theory to establish that the problem is well-posed and FEM converges as long as the mesh is locally symmetric at the vicinity of the interface (e.g. [1]). We solve (1) using expansions in spherical harmonics, \( Y^m_l(\theta, \phi) \) with \( \phi \), denoting the azimuthal angle, polar angle, respectively. Using the Jacobi-Anger expansion for \( u^a \), we find that

\[
u^a(x) = \sum_{\ell=0}^{\infty} [A\ell u(k\ell r) - C\ell j(k\ell r)] Y^0_\ell(\theta, \phi),
\]

for \( x \in E \), with \( C\ell = i^{\ell}(\varepsilon - 1)2^{\ell+1}\pi \), and

\[
u^a(x) = \sum_{\ell=0}^{\infty} B\ell Y^0_\ell(\theta, \phi)
\]

for \( x \in \bar{\Omega} \). Here, \( B\ell = \sqrt{-\varepsilon_m} \), and \( h_\ell^l, j_\ell^l, i_\ell^l \) are the spherical Hankel functions, the spherical Bessel functions, and modified spherical Bessel functions of the first kind and of order \( \ell \), respectively. Using the transmission (jump) conditions in (1), the coefficients \( A\ell, B\ell \in \mathbb{C} \times \mathbb{C} \) satisfy

\[
M\ell(k) \begin{bmatrix} A\ell \\ B\ell \end{bmatrix} = C\ell \begin{bmatrix} j_\ell^l(k) \\ -Y^0_\ell(\theta, \phi) \end{bmatrix}
\]

The top left plot of Fig. 1 shows a plot of \( \|u^a\|_L^2(D) \) where \( D \) is a ball containing \( \Omega \) as a function of \( k \). We observe that the field peaks at some wavenumbers \( (k_\ell) \), where the corresponding FEM computations (see Fig. 1, top right) show plasmonic fields. Additionally, we plot larger errors occur at those peaks.

2 Plasmonic resonances
To identify the peaks seen in Fig. 1, we find the zeros of \( \text{det}(M\ell(k)) = 0 \) with \( M\ell(k) \) defined in (3), in particular those which correspond to surface plasmon resonances. We find surface plasmon resonances \( (k_\ell) \) close to the real axis (see Fig. 1, bottom). The large peaks of \( \|u^a\|_L^2(D) \) correspond to \( k = \Re(k_\ell) \). For fixed \( \ell \) the plasmonic resonance \( k_\ell \) corresponds to plasmonic resonant mode

\[
u^p(x) = \begin{cases}
j_l^{(1)}(k_\ell r) h_l^{(1)}(k_\ell r) Y^m_\ell(\theta, \phi), & x \in E \\
l_l^{(1)}(k_\ell r) Y^m_\ell(\theta, \phi), & x \in \bar{\Omega}
\end{cases}
\]
3 Extracting plasmonic behaviors from the formulation

In order to take into account the varying scale of the resonant mode, we assume a solution $u$ for the total field given as the sum:

$$u = u^u + u^{\text{reg}} + \alpha u^p, \quad \alpha \in \mathbb{C},$$

where $\alpha$ is related to the excitation source, and $u^{\text{reg}} \in H^1_\text{reg}(\mathbb{R}^3)$ is smooth. The goal is to compute $(u^{\text{reg}}, \alpha)$. Substituting (4) into (5), we derive a system for $(u^{\text{reg}}, \alpha)$ based on weak forms of (1). We compute discrete solution $(u^{\text{reg}}_N, \alpha_h) \in \mathbb{C}^N$ of:

$$\begin{bmatrix} \mathcal{K} + k^2 \mathcal{M} + \mathcal{S} & \mathcal{U} \mathcal{P} \\ \mathcal{T} \mathcal{Y} & C_2 \end{bmatrix} \begin{bmatrix} u^{\text{reg}}_N \\ \alpha_h \end{bmatrix} = \begin{bmatrix} f_N \\ C_1 \end{bmatrix}$$

(6)

for $N$ degrees of freedom (DOFs). Above, $\mathcal{K}$ is a weighted stiffness matrix, $\mathcal{M}$ is the mass matrix, $\mathcal{S}$ is the surface matrix (obtained using the Dirichlet-to-Neumann (DN) map on the truncated domain $D$), $f_N$ is the discrete right-hand side (related to $u^u$), and $C_1, C_2 \in \mathbb{C}$ are analytic constants. Finally, $\mathcal{T} \mathcal{Y}$, $\mathcal{U} \mathcal{P}$ contain the coupling terms (between $u^p$ and FEM basis function).

4 Asymptotic Quadrature

For the coupling terms in (6), one needs to accurately compute integrals such as

$$\int_D u^p \varphi_i dD, \quad i \in [1, N],$$

where $\varphi_i$ is a FEM basis function. Looking at (4), high frequency behavior from the spherical harmonics combined with relatively coarse mesh (in the case of limited computational resources to approximate three-dimensional problems), or low order FEM, leads to large errors. As an alternative to refining the mesh, we make use of the asymptotic expansion of the spherical harmonics for large $l$. For example when $m = 0$, we have the leading behavior (see [4, p. 140]):

$$Y_l^0(0, \phi) \sim \frac{\cos((l + 1/2)\phi - \pi/4)}{\sqrt{2\pi \sin(\phi)}},$$

(7)

when $l \to \infty$. Here, we have an explicit expression for the fast oscillations in (7) which we can use to develop a product quadrature method [2]. This product quadrature method uses exact integration of polynomials multiplied by those fast oscillations to derive weights. Those weights, in turn, analytically account for the fast oscillations in $u^p$ and relieve the FEM from having to compute them. By extending this analysis, we will develop a method for computing the coupling terms in (6) without having to resort to refining the mesh. Application to the scattering by multiple spheres (and other shapes starting with ellipsoids) and comparison with enriched elements methods will be considered in the future. Similar results could be observed for dispersive materials ($\varepsilon = \varepsilon(k)$).

Acknowledgements This work is partially funded by the National Science Foundation Grants: DMS-2009366 and DMS-1840265.

References

Revisiting the limiting amplitude principle for the wave equation with variable coefficients

Anton Arnold, Sjoerd Geevers, Ilaria Perugia, Dmitry Ponomarev

1 Institute of Analysis and Scientific Computing, Technical University of Vienna, Vienna, Austria
2 Faculty of Mathematics, University of Vienna, Vienna, Austria
3 St. Petersburg Department of V. A. Steklov Mathematical Institute, St. Petersburg, Russia

Abstract

The limiting amplitude principle is a well-known result connecting the solution of the Helmholtz equation with the large-time behavior of time-dependent wave equations with a source term which is periodic in time. Motivated by numerical analysis of time-domain methods for stationary scattering problems in heterogeneous media, we quantify the solution convergence of such time-dependent wave equations towards the stationary solution, under some assumptions on the coefficients and the source term. We also generalise the formulation of the limiting amplitude principle to the one-dimensional setting where the classical statement of the principle is known to be violated.

Keywords: limiting amplitude principle, time-domain wave equation, Helmholtz equation, large time behavior

1 An introduction

It is a common engineering wisdom that the wave equation with a periodic-in-time source term yields a solution that stabilises for large times to the solution of the corresponding Helmholtz equation modulated by a time-harmonic factor. This link between time- and frequency-domain wave problems is known as the limiting amplitude principle. This principle has been a subject of extensive research started nearly 70 years ago aiming at developing tools for the selection of a physically relevant unique solution of the Helmholtz equation in an unbounded domain. However, this viewpoint can be altered, and one can start with a problem governed by the Helmholtz equation (supplemented by classical Sommerfeld radiation conditions) which is known to admit a unique solution, and one can employ time-domain methods in order to efficiently find this solution. Despite a seemingly increased computational burden (due to the additional temporal dimension), some special time-domain methods such as [4,5] can be useful when wavenumber (frequency) is large and the original Helmholtz equation is difficult to solve numerically. In particular, in the time domain, one can take advantage of the presence of sharp wavefronts and resolve the problem on a suitably adapted mesh [1]. In the present communication, summarising [3], we focus on another aspect of evaluation of the efficiency of a time-domain approach to the Helmholtz equation. Namely, we are concerned with the speed of the convergence in time of the solution of the time-dependent wave equation to the solution of the underlying stationary problem.

2 Results

Given a frequency \( \omega > 0 \), a compactly supported source term \( F \in L^2 (\mathbb{R}^d) \) and non-trapping material parameters \( \alpha_{\min} < \alpha (x) \in C^\infty (\mathbb{R}^d), \beta_{\min} < \beta (x) \in C^\infty (\mathbb{R}^d) \) such that \( \alpha (x) = \alpha_0, \beta (x) = \beta_0 \) for \( x \in \mathbb{R}^d \setminus \Omega_0 \) with some bounded set \( \Omega_0 \subset \mathbb{R}^d \) and constants \( \alpha_{\min}, \beta_{\min} > 0 \), we consider the Helmholtz equation, for \( x \in \mathbb{R}^d \),

\[-\nabla \cdot (\alpha (x) \nabla U (x)) - \omega^2 \beta (x) U (x) = F (x), \]

supplemented by the Sommerfeld condition

\[ \lim_{|x| \to \infty} \left[ \frac{\partial}{|x|} U (x) - i \omega \sqrt{\beta_0/\alpha_0} U (x) \right] = 0. \]

The corresponding time-domain wave equation, for \( x \in \mathbb{R}^d, \ t > 0 \),

\[ \beta (x) \partial_t^2 u (x, t) - \nabla \cdot (\alpha (x) \nabla u (x, t)) = e^{-i \omega t} F (x) \]

is supplemented by the initial conditions

\[ u (x, 0) = 0, \quad \partial_t u (x, 0) = 0, \quad x \in \mathbb{R}^d. \]

Our main result pertaining the convergence in time of the solution \( u (x, t) \) and its derivatives can be formulated as the following theo-
rem which establishes and quantifies the limiting amplitude principle in the aforementioned setting.

**Theorem 1** Let $U$ and $u$ be the solutions to problems (1) and (2), respectively. Then, for any bounded domain $\Omega \subset \mathbb{R}^d$ and $t > 0$, the following estimates hold true.

For $d = 3$:
\[
\|u(\cdot, t) - e^{-i\omega t}U\|_{H^1(\Omega)} + \|\partial_t u(\cdot, t) + i\omega e^{-i\omega t}U\|_{L^2(\Omega)} \leq \frac{C_1}{(1 + t^2)^{1/2}}.
\]

For $d = 2$:
\[
\|u(\cdot, t) - e^{-i\omega t}U\|_{H^1(\Omega)} + \|\partial_t u(\cdot, t) + i\omega e^{-i\omega t}U\|_{L^2(\Omega)} \leq \frac{C_2 (1 + \log (1 + t^2))}{(1 + t^2)^{1/2}}.
\]

For $d = 1$:
\[
\|u(\cdot, t) - e^{-i\omega t}U - U_\infty\|_{H^1(\Omega)} + \|\partial_t u(\cdot, t) + i\omega e^{-i\omega t}U\|_{L^2(\Omega)} \leq C_3 e^{-\Lambda t}.
\]

Here, the constants $C_1$, $C_2$, $C_3 > 0$, $U_\infty := \frac{1}{2i\omega \sqrt{\alpha_0}} \int_{\mathbb{R}} F(x) \beta(x) \, dx$, and the decay rate $\Lambda > 0$ can be estimated explicitly.

Our proof of Theorem 1 is due to reduction towards several results concerning temporal decay for wave equations with sufficiently localised initial data or a source term. In particular, we build up on recent resolvent estimates from [6] and analysis of the one-dimensional wave equation [2].

Note that, in contrast to our setting, classical works (such as [7–10]) rarely quantify the limiting amplitude principle, and they deal with either constant-coefficient equations or variable-coefficient equations in the divergent form, with the main focus on the physical case $d = 3$. We also stress that our results show that, with a minor modification (by accounting for the additional constant term $U_\infty$), the validity of the limiting amplitude principle extends to the case $d = 1$.

During the talk, I will briefly describe some of the ingredients of the proof, touch on sharpness and non-sharpness aspects of the estimates in Theorem 1 and discuss further possible extensions of our results.

**References**


Gaussian wave packets for the magnetic Schrödinger equation

Selina Burkhard$^{1,*}$, Benjamin Dörich$^1$, Marlis Hochbruck$^1$

$^1$Institute for Applied and Numerical Mathematics, Karlsruhe Institute of Technology, 76149 Karlsruhe, Germany
$^*$Email: selina.burkhard@kit.edu

Abstract

In this talk, we consider the semiclassical magnetic Schrödinger equation, which describes the dynamics of particles under the influence of a magnetic field. Following [1], the solution of the Schrödinger equation is approximated by Gaussian wave packets via the time-dependent variational formulation by Dirac and Frenkel. For the numerical approximation we will derive ODEs for the parameters of the variational solution. Moreover, we obtain $L^2$-error bounds and observable error bounds for the approximating Gaussian wave packet.

Keywords: magnetic Schrödinger equation, semiclassical analysis, variational approximation, observables

1 Introduction

We consider the semiclassical magnetic Schrödinger equation

$$i\varepsilon \partial_t \psi(t) = H(t) \psi(t), \quad \psi(0) = \psi_0,$$ (1)

with Hamiltonian

$$H(t) = (i\varepsilon \nabla + A(t))^2 + V(t),$$

for $t \in [0, T]$ on $\mathbb{R}^d$ and the semiclassical parameter $0 < \varepsilon \ll 1$. The scalar, subquadratic potential $V$ and the vector valued, sublinear, magnetic potential $A$ are assumed to be smooth and might be time-dependent. We approximate the solution of (1) on the manifold $\mathcal{M}$ of Gaussian wave packets of the form

$$u(x, \cdot) = \exp \left( \frac{i}{\varepsilon} \left( \frac{1}{2} x_q^T C x_q + x_q^T p + \zeta \right) \right),$$ (2)

where $x_q = x - q$ with time-dependent parameters $q(t), p(t) \in \mathbb{R}^d$, $C(t) \in \mathbb{C}^{d \times d}$ symmetric with positive definite imaginary part, and phase $\zeta(t) \in \mathbb{C}$. To approximate in time we derive equations of motion (ODEs) for the parameters of the wave packet. Following the approach in [1], we derive $L^2$-error bounds and error bounds for observables.

Employing a perturbation result for relatively bounded operators, well-posedness of (1) is obtained via evolution families in the hyperbolic case, cf. [3–5].

2 Variational approximation

We consider the Dirac-Frenkel variational approximation introduced in [1, 2]: Seek $u \in \mathcal{M}$ such that $\partial_t u(t) \in T_{u(t)} \mathcal{M}$ and

$$\langle i\varepsilon \partial_t u(t) - H(t) u(t) | v \rangle = 0, \quad v \in T_{u(t)} \mathcal{M},$$ (3)

where we denote by $T_u \mathcal{M}$ the tangent space of the manifold $\mathcal{M}$ at $u$. Using the orthogonal projection $P_u : L^2(\mathbb{R}^d) \to T_u \mathcal{M}$ onto the tangent space, the variational approximation (3) can be reformulated as

$$i\varepsilon \partial_t u(t) = P_u(H(t) u(t)),$$ (4)

with initial value $u(0) = u_0 \in \mathcal{M}$.

The approximation by Gaussian wave packets seems appropriate due to the following exactness result shown in [1].

Proposition 1 ([1, Prop. 3.2]). Let $V(\cdot, t)$ be quadratic and $A(\cdot, t)$ be linear in space, $t \in [0, T]$. If the initial value $\psi_0$ is a Gaussian wave packet, then the solution of (1) is given by the variational approximation satisfying (4).

3 Equations of motion

The variational formulation (4) leads to ordinary differential equations for the parameters of the Gaussian wave packet. To see this we use the following projection formula from [1].

Proposition 2 ([1, Prop. 3.14]). For a Gaussian wave packet $u$ with $\|u\|_{L^2} = 1$ and a scalar smooth potential $W$ we have

$$P_u(W) = (\alpha + v^T x_q + \frac{1}{2} x_q^T B x_q) u,$$

where $\alpha, v, B$ are given by

$$\alpha = \langle W \rangle_u - \frac{\varepsilon}{4} \text{tr} \left( \text{Im} C^{-1} \langle \nabla^2 W \rangle_u \right),$$

$$v = \langle \nabla W \rangle_u, \quad B = \langle \nabla^2 W \rangle_u.$$

Here we used the notation $\langle W \rangle_u = \langle u | W u \rangle$. 
Comparing both sides of (4) and using Proposition 2 leads to ordinary differential equations for the parameters. The normalization is achieved by choosing an initial Gaussian wave packet of $L^2$-norm one and employing norm conservation. In order to apply Proposition 2 we make use of
\[\varepsilon A \cdot \nabla u = -A \cdot (C x q + p) u, \]
\[-\frac{\varepsilon^2}{2} \Delta u = \left( \frac{1}{2} x q^T C^2 x q + p^T C x q \right) u + \left( \frac{1}{2} |p|^2 - \frac{i\varepsilon}{2} \text{tr}(C) \right) u.\]

For the equations of motion we use the notation
\[\tilde{V} = \frac{1}{2}|A|^2 + V,\]
\[J_A = (\partial_j A_k)_{j,k=1}^d,\]
\[(D_A, C)_{k,l} = \sum_{j=1}^d \partial_l \partial_k A_j v_j, \quad v \in \mathbb{C}^d.\]

If the parameters of the Gaussian wave packet $u$ defined in (2) satisfy
\[\dot{q} = p - \langle A \rangle_u, \quad \dot{p} = (J_A^T \text{Re} C(x - q)) u + \langle J_A \rangle_u^T p - \langle \nabla \tilde{V} \rangle_u, \quad \dot{\zeta} = -C^2 + (D_A^2 \text{Re} C(x - q)) u + \langle D_A^2 p \rangle_u + (J_A \rangle_u^T C + C\langle J_A \rangle_u - \langle \nabla^2 \tilde{V} \rangle_u,\]
then $u$ is the variational solution (4). Moreover, $\zeta$ is defined by normalization of $u$.

4 $L^2$- and observable error bounds

If the potentials $A$ and $V$ can be approximated by linear or quadratic potentials, respectively, then by Proposition 1, the $L^2$-error is of order $\sqrt{\varepsilon}$, provided the following assumption holds.

**Assumption** The parameters $q, p \in \mathbb{R}^d$, $C \in \mathbb{C}^{d \times d}$, and $\zeta \in \mathbb{C}$ of the Gaussian wave packet $u$ satisfying (2) and (4) are bounded uniformly on $[0, T]$.

For our analysis in [6], we assume that the equations of motion for the parameters are solved exactly and therefore use (4). With this, we can state the following bound.

**Theorem 4.** Let $\psi$ be the solution of (1) and $u$ be the solution of (4). If the initial value $\psi_0$ is a Gaussian wave packet, then we have the error bound
\[\|\psi(t) - u(t)\|_{L^2} \leq c t \sqrt{\varepsilon},\]
where $c$ depends on the parameters and on the potentials, but is independent of $\varepsilon$ and $t$.

Next, we state the error of observables, i.e., selfadjoint operators on $L^2(\mathbb{R}^d)$, which are used to describe physical states. We consider operators $A = \text{opWeyl}(a)$ corresponding to a classical observable $a = a(q, p) \in C^\infty(\mathbb{R}^{2d})$ via the Weyl-quantization satisfying
\[\text{opWeyl}(\psi) = i\varepsilon \nabla \psi, \quad \text{opWeyl}(\psi) = x \psi.\]

**Theorem 5.** Let $\psi$ be the solution of (1) and $u$ be the solution of (4). If the initial value $\psi_0$ is a Gaussian wave packet, then we have the error bound
\[|\langle \psi(t) | A \psi(t) \rangle - \langle u(t) | A u(t) \rangle| \leq c t \varepsilon,\]
where $c$ depends on the parameters, on the potentials, and on $a$, but is independent of $\varepsilon$ and $t$.

5 Acknowledgement

Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 258734477 – SFB 1173.

**References**


Recent Advances in Elastodynamics
by Time-Domain Energetic Boundary Element Method

A. Aimi\textsuperscript{1}, L. Desiderio\textsuperscript{1}, G. Di Credico\textsuperscript{1}, C. Guardasoni\textsuperscript{1,*}

\textsuperscript{1}Department of Mathematical, Physical and Computer Sciences, University of Parma, Parma, Italy
\textsuperscript{*}Email: chiara.guardasoni@unipr.it

Abstract
This contribution aims at illustrating some recent advances in the application of the Energetic Boundary Element Method (EBEM) to the numerical resolution of Elastodynamic problems both in exterior and interior domains.

Keywords: Elastodynamics, Energetic Boundary Element Method

1 Introduction
From the initial work of [1] and [2], it has been clear that the energetic weak approach to boundary integral formulations gives a good theoretical setting for the investigation of elastodynamic wave propagation.

The method is based on a boundary integral representation formula for the differential problem solution, then a weak formulation linked to the energy of the system is applied in order to achieve, in the approximation phase, accurate and stable numerical results.

However, the extension of the EBEM implementation is not straightforward since the computation of linear system entries requires sophisticated numerical strategies depending on the problem at hand (2D or 3D, bounded or an unbounded domain equipped with Dirichlet and/or Neumann boundary conditions) and on the integral formulation used to represent the solution. In particular an accurate study of the numerical evaluation of double space integrals involved must be performed looking at the singularities of the integrand functions [3].

Further, the increasing complexity and dimensionality of test problems compels to perform a fast implementation by parallel computing on CPUs and GPUs and applying compression algorithms.

2 The model problem
Consider a domain $\Omega \subset \mathbb{R}^n$ with $n = 2, 3$, then the displacement $u = (u_1, \ldots, u_n)$ during the time interval $[0, T]$ in a linear, homogeneous, elastic and isotropic medium is described through the Navier equation by components:

\begin{equation}
\sum_{\substack{h,k,l=1 \atop i=1,\ldots,n}}^{n} \frac{\partial}{\partial x_h} \left( C_{ijkl} \frac{\partial u_l}{\partial x_i} (x,t) \right) - \rho \ddot{u}_i (x,t) = 0 \quad \forall (x,t) \in \Omega \times (0,T)
\end{equation}

with mass density $\rho$ and Hooke tensor $C_{ijkl}$ depending on the elastic material properties. The description of the problem is completed by initial and Dirichlet and/or Neumann boundary conditions

\begin{equation}
\begin{aligned}
u(x,0) &= 0; \quad \dot{u}(x,0) = 0 \quad x \in \Omega \\
u(x,t) &= g_D(x,t) \quad x \in \Sigma_D := \Gamma_D \times [0,T] \\
p(x,t) &= g_N(x,t) \quad x \in \Sigma_N := \Gamma_N \times [0,T]
\end{aligned}
\end{equation}

being $p_i(x,t) := \sum_{h,k,l=1}^{n} C_{ijkl} \left( \frac{\partial u_l}{\partial x_i} (x,t) \right) n_h(x)$ the $i$-th component of the traction $p$ defined with respect to a normal vector $n$ at a point $x$ of the boundary $\partial \Omega = \Gamma_D \cup \Gamma_N$.

3 The energetic boundary integral formulation
Starting from the Somigliana identity and applying the arguments related to energy as done in scalar wave propagation problems [4], the unknown traction $p$ on $\Gamma_D$ and displacement $u$ on $\Gamma_N$ appear to be solutions of the system

\begin{equation}
\left( \begin{array}{c}
\left( V_{ij} p_j \right)_{L_2(\Sigma_D)} - \left( K_{ij} u_j \right)_{L_2(\Sigma_D)} \\
\left( D_{ij} \psi_i \right)_{L_2(\Sigma_N)} - \left( K'_{ij} p_j \right)_{L_2(\Sigma_N)}
\end{array} \right) = \\
\left( \begin{array}{c}
\left( f_D, \psi_i \right)_{L_2(\Sigma_D)} \\
\left( f_N, \psi_i \right)_{L_2(\Sigma_N)}
\end{array} \right)
\end{equation}

involving the fundamental solution tensor through the classical integral operators $V, K, K'$. $\psi$ as defined in [5]. $\phi$ defined on $\Sigma_D$ and $\psi$ defined on $\Sigma_N$ are test functions belonging to the functional space of $p$ and $u$ respectively.

4 Numerical results
Preliminary numerical results have been published in [3] and in [6].

In the figure 1 there is the representation at
some time instants of the intensity (Euclidean norm) of the total displacement generated by an incident plane pressure wave that propagates in a 2D domain in the horizontal direction from left to right. The incoming plane pressure wave $u_{inc}$ propagates along the horizontal direction $k = (1, 0)^T$ with phase velocity equal to 2 and impacts on the left side of the disk at the time instant $t = 0.25$ with the following shape

$$u_{inc}(x, t) = -kg(cp_0(1/2) - k \cdot x)$$

defined by $g$ represented in Figure 2, setting the primary and the secondary waves velocities $cp = 2$ and $cs = 1$. The total displacement is obtained by summing to the incoming wave, the reflected wave that results solving the Dirichlet problem with datum $g_D(x, t) = -u_{inc}(x, t)$.

References


Experiences with the 3D-ACA in a CQM based Time Domain Boundary Element Method

Anita M. Haider\textsuperscript{1}, Martin Schanz\textsuperscript{2,}\textsuperscript{*}

\textsuperscript{1}Institute of Applied Mechanics, Graz University of Technology, Graz, Austria
\textsuperscript{2}Institute of Applied Mechanics, Graz University of Technology, Graz, Austria
\textsuperscript{*}Email: m.schanz@tugraz.at

Abstract

The proposed presentation is a continuation of the same topic presented at Waves 2019. The acoustic wave equation is solved in time domain with a boundary element formulation. The time discretisation is performed with the generalized convolution quadrature method and for the spatial approximation standard elements and a collocation scheme is applied. To increase the efficiency of the boundary element method the so-called 3D-ACA (three-dimensional Adaptive Cross Approximation) is applied. After introducing the model problem, a Dirichlet problem in acoustics, the 3D-ACA is discussed. The implementation is presented by several examples which serve, essentially, to show the properties of such an approach by numerical tests.

Keywords: BEM, 3D-ACA, CQM

1 Problem setting

As model problem, we consider the time domain boundary element method for the homogeneous wave equation with vanishing initial conditions and given Dirichlet boundary conditions. The generalized convolution quadrature method (gCQ) is used for the temporal discretization (see, e.g. \cite{2}) and collocation for the spatial discretization. Essentially, the gCQ requires to establish boundary element matrices of the corresponding elliptic problem in Laplace domain at several complex frequencies. Consequently, we get an array of system matrices. This array of system matrices can be interpreted as a three-dimensional array of data which we want to approximate by a data-sparse representation.

2 Generalization of the adaptive cross approximation

The idea of a generalization of adaptive cross approximation has been proposed in \cite{1} and is sketched in Algorithm 1. As discussed above, we generate a three-dimensional array of data $C_{ij,k}$.

\begin{algorithm}[H]
\caption{idea generalized ACA}
\begin{enumerate}
\item compute face $H_{ij}^\ell$ via low-rank approximation
\hspace{1cm} $h_{ij}^\ell = C_{ij,k}^\ell$
\item define pivot position
\hspace{1cm} $(i_\ell, j_\ell) := \arg \max_{i,j} |h_{ij}^\ell|$
\item compute fiber $F_f^\ell$
\hspace{1cm} $f_k^\ell = C_{i_\ell,j_\ell,k}$
\end{enumerate}
\end{algorithm}

The first two indices corresponds to the spatial discretization. One is related to the collocation point and the other to the basis function. The third index of the 3D array corresponds to the complex frequencies from the gCQ. The algorithm starts by assembling the system matrix at an arbitrary chosen but fixed frequency. Let the corresponding index be $k_\ell$. This system matrix, which we call face $H_i$, is compressed by the standard adaptive cross approximation. Therefore, we have to decompose the system matrix into a hierarchical scheme first. This hierarchical structure is based on the usual geometrical considerations and used for all further assembled faces. After the low-rank approximated face is determined, we have to define the position of the pivot element. In principle, the maximum entry of the matrix determines the pivot position, where $h_{ij}^\ell$ denotes the entries of the current face. Regarding to this position we compute the fiber $F$, an array with all frequencies where the indices related to the spatial discretization are fixed, i.e. one matrix entry at all frequencies for a distinct collocation point and shape function is assembled, $f_k^\ell$. In this way the first cross with an approximated face and a fiber is generated. For the next cross, the face or the fiber has to be updated. At further iterations the residual of the face and of the fiber has to be determined and based on this residual...
Figure 1: Approximation error in the Frobenius norm versus frequency

Figure 2: Convergence and compression of a Dirichlet problem computed at a cube

The position of the pivot element is computed. The algorithm terminates successfully if a suitable stopping criterion with a given accuracy $\varepsilon$ is satisfied. The current approximation is defined as $S^\ell = \sum_{d=1}^\ell \tilde{\mathbf{H}}^\ell \otimes \tilde{\mathbf{A}}^d$, where $\ell$ represents the used frequencies to obtain the preset accuracy.

3 Numerical results

How the introduced algorithm performs is shown by numerical experiments. In the first example, the three-dimensional array of data $\mathbf{C}$ is computed by assembling the single layer operator at 11 different frequencies given by the gCQ. The squared error of the approximation in the Frobenius norm is plotted in Fig. 1 against the iteration counter of the algorithm. Note, the iteration number corresponds to the number of necessary complex frequencies. The accuracy of the generalized ACA is chosen as $\varepsilon = 10^{-4}$. We perform the numerical experiment first without any low-rank approximation of the face, then with an approximation by a singular value decomposition and, last, by adaptive cross approximation. The accuracy of the low-rank approximated face is set as well to $\varepsilon = 10^{-4}$ for both approximation methods. For all three alternatives, the stopping criterion is satisfied after five iterations. At the fifth iteration, the ACA approximated face exhibits a slightly different approximation error. This indicates that the low-rank approximation error of the faces has already an effect. Nevertheless, it may be concluded that it is sufficient to evaluate the single layer operator only at a few instead of all frequencies and still a sufficiently quality of the data is maintained, resulting in a reduction of the computation time and the memory consumption.

The second example is the solution of a Dirichlet problem, where the given data represent an analytical solution of the wave equation. Again a cube is used as geometry and in Fig. 2 the $L_2$-error in space and time is plotted versus the mesh. It must be remarked that not only the spatial discretisation is uniformly refined but as well the time step size such that the relation between both is kept constant. In the same figure, the compression (see right axis) is plotted versus the refinement. The compression is the ratio of storage used by the dense BEM, i.e., all frequencies and dense matrices at each frequency, to the storage necessary for the 3D-ACA. Obviously, large savings are possible by keeping the convergence rate of the gCQ-BEM. The underlying time stepping was a 2-stage Radau IIA Runge-Kutta method. Above the SVD is used to compress the data within a face. In the presentation, as well results with ACA in the face will be shown and different geometries be used.

References


Enriched Space-Time Finite Element Methods for the Wave Equation

Kieran Quaine1,∗, Heiko Gimperlein2
1School of Mathematical & Computer Sciences, Heriot-Watt University, Edinburgh, UK
2Engineering Mathematics, University of Innsbruck, Innsbruck, Austria
∗Email: kq8@hw.ac.uk

Abstract
We propose a generalized finite element method based on plane-wave enrichments of the approximation space in space and time. It extends the established enriched methods for high-frequency wave propagation from the frequency to the time domain. The formulation studied is based on a discontinuous Galerkin method in time and continuous finite elements in space. Numerical results for example problems demonstrate the significant improvements in accuracy and computational effort compared with standard finite element methods.

Keywords: Generalized Finite Elements; Space-Time Methods; Plane-Wave Enrichment; Wave Equation.

1 Introduction

Generalized finite elements based on plane-wave enrichments have been shown since the late 1990s to significantly reduce the computational cost for the numerical approximation of wave emission and scattering problems in the frequency domain [4,6]. The enrichment of the approximation space allows good approximation of the oscillatory solutions at high frequencies even on coarse mesh grids, whereas standard finite elements are limited by fine meshes and proportionally small time-steps. Nonpolynomial enrichments of the approximation space have only recently been extended to time-dependent wave problems, e.g. in [5]. They combine spatial enrichments with standard time-stepping schemes and therefore remain limited by small time steps. In this work we initiate the study of space-time enriched methods, based on approximation spaces enriched by travelling plane waves.

2 Problem formulation

We consider a first-order formulation of the scalar wave equation in a domain \( \Omega \subset \mathbb{R}^2 \) for times \( t \in [0,T] \):

\[
\begin{align*}
\frac{\partial p}{\partial t} + \nabla \cdot \mathbf{u} &= f_1, \quad (1a) \\
\frac{\partial \mathbf{u}}{\partial t} + \nabla p &= f_2, \quad (1b) \\
p(\cdot,0) &= p_0, \quad \mathbf{u}(\cdot,0) = \mathbf{u}_0, \quad (1c)
\end{align*}
\]

with suitable initial conditions \( p_0, \mathbf{u}_0 \) and data \( f_1, f_2 \). Either homogeneous Neumann or periodic boundary conditions are imposed.

3 Numerical approximation

For the discretization we start from a standard discontinuous Galerkin formulation of (1a), (1b), see e.g. [1,3]. On each element we consider ansatz and test functions of the form

\[ \Pi_m(t) \Lambda_i(\mathbf{z}) G^m_{\mathbf{z}}(\mathbf{x},t), \]

defined from piecewise polynomials \( \Pi_m \) and \( \Lambda_i \) and enrichment functions \( G^m_{\mathbf{z}} \). To effectively enrich the approximation space we must choose basis functions which are appropriate for a given problem, here plane-waves \( G^m_{\mathbf{z}} \) are used [4,6]. To extend this we are considering the same spatial enrichments with the inclusion of temporal parameters which are scaled by the frequency of the given wave. These plane-wave enrichments corresponding to a lattice of frequencies,

\[
G^m_{\mathbf{z}}(\mathbf{x},t) = \exp(i(\mathbf{K} \cdot \mathbf{z} + \omega(t-t_m))),
\]

where \( L \) is of the order of the diameter of the domain and \( \mathbf{n} \in \mathbb{Z}^2 \) generates a lattice of wave vectors, \( \kappa \). The space-time \( \Omega \times [0,T] \) is discretised by a space-time mesh of product type with elements \( \mathbf{K} \times [t_m,t_{m+1}] \). This yields a time-stepping scheme with the same mass and stiffness matrices in each time step. Note the crucial shift by \( t_m \) in the definition of \( G^m_{\mathbf{z}} \) which assures that the matrices in different time-steps coincide. The resulting scheme for the numerical approximation of \( \mathbf{u} = (p, \mathbf{u}) \) takes the form

\[
(A + M_+ + S) \mathbf{u}_m = \mathcal{F} - M_- \mathbf{u}_{m-1},
\]
where $A$ is a convection matrix, $\mathcal{M}_\pm$ mass matrices and $S$ a stabilization matrix.

4 Numerical experiments

We consider a Gaussian Explosion [1] on a square $[0, 2\pi]^2$, corresponding to a circular source centred at $(x_0, y_0)$ which emits radial waves until a kill time. The right hand side is given by $f_1(x, y, t) = g_1(t)g_2(x, y)$ when $0 < t < 2\pi_0$ and $(x - x_0)^2 + (y - y_0)^2 < R^2$ and $g(x, y, t) = 0$ otherwise, where

\[
g_1(t) = 4 \exp \left(-\pi^2 f_0^2 (t - t_0)^2\right),
\]

\[
g_2(x, y) = \left(1 - \frac{(x - x_0)^2 + (y - y_0)^2}{R^2}\right) \theta \tag{4}
\]

Here $t_0 = \frac{1}{f_0}$, $f_0 = \frac{c_0}{N_L}$ is the central frequency, $N_L$ the number of points per wavelength and $c_0$ is the wave-speed. We choose $c_0 = N_L = 3$ and $R = \frac{1}{2}$. We must choose suitable enrichments corresponding to $K \in \{3, 4, 7\}$ following (2). Figure 1 shows the relative $L^2$ error in terms of the space-time degrees of freedom for both the proposed enriched method and for a standard finite element method (where $G^m_2 = 1$) on a fine mesh.

We see that the standard method achieves an error of the order $10^{-2}$ or $10^{-3}$ with a number of degrees of freedom which is several orders of magnitude smaller than for the standard method.

References


A space–time continuous and coercive variational formulation for the wave equation

Paolo Bignardi\textsuperscript{1,}\textsuperscript{*}, Andrea Moiola\textsuperscript{1}
\textsuperscript{1}Department of Mathematics, University of Pavia
\textsuperscript{*}Email: paolo.bignardi01@universitadipavia.it

Abstract

In recent years, several space–time formulations and discretizations for the wave equation have been proposed. With “space–time” we mean that they are posed in the space–time cylinder, as opposed to semi-discretizations in space combined with time stepping. To our knowledge, no continuous and coercive (i.e. sign-definite) variational formulation has been proposed yet. The aim of this paper is to fill this gap proposing a Lax–Milgram formulation on the space–time cylinder for the wave equation with impedance boundary conditions. In order to do this, we follow a strategy previously adopted for Helmholtz problems, which relies on Morawetz identities and multipliers. From this, a continuous and coercive bilinear form and a linear form on an appropriate space can be constructed. We also show the explicit coercivity constant.

Keywords: wave equation, variational problem, coercive, sign-definite, space–time

1 Introduction and notation

We consider an initial–boundary value problem (IBVP) for the wave equation with impedance boundary conditions:

\begin{equation}
\begin{cases}
  u_{tt} - c^2 \Delta u = f & \text{on } Q = (0, T) \times \Omega, \\
  \frac{\partial u}{\partial t} + \frac{1}{c} \nabla u = g & \text{on } \Sigma = (0, T) \times \partial \Omega, \\
  u = u_0 & \text{on } \Omega_0 = \{0\} \times \Omega, \\
  u_t = u_1 & \text{on } \Omega_0.
\end{cases}
\end{equation}

Here \( t \) denotes time differentiation, \( \Omega \subset \mathbb{R}^d \) is an open, bounded, Lipschitz domain, \( c > 0 \) and \( \theta > 0 \) are constants, and \( f, g, u_0 \) and \( u_1 \) are appropriate functions defined on \( Q, \Sigma \) and \( \Omega_0 \), respectively. Let also \( \Omega_T = \{T\} \times \Omega \).

Assume that exist \( L > 0 \) and \( \delta > 0 \) such that \( |x| \leq L \) for all \( x \in \Omega \) and \( x \cdot n(x) \geq \delta L \) for all \( x \in \partial \Omega \), where \( n(x) \) is the normal to \( \partial \Omega \) at \( x \). This implies that \( \Omega \) is star-shaped with respect to the ball \( B_{\delta L}(0) \).

We define the seminorm

\[ ||v||_V^2 := ||v_t||_Q^2 + c^2 ||\nabla v||^2_Q + T^2 ||u_t - c^2 \Delta u||^2_Q + L ||v_t||^2_\Sigma + c^2 L ||\nabla v||^2_\Sigma + c^2 T ||\nabla v||^2_{\Omega_0} + T ||v||^2_{\Omega_0} + c^2 T ||\nabla v||^2_{\partial \Omega_T} + T ||v||^2_{\partial \Omega_T}. \]

This is a norm on \( C^\infty(Q) := \{u \in C^\infty(\overline{Q}) : \int_{\Omega_0} u = 0\} \) and on \( V := C^\infty_0(\overline{Q}) \). We assume that the initial datum \( u_0 \) has zero average in \( \Omega_0 \). Problems with more general data can be treated by simply adding a constant to the solution.

2 Abstract framework

We introduce an abstract setting that includes coercive formulations for both the wave and the Helmholtz equations, generalising the approach in [2]. Consider a linear boundary value problem (BVP):

\begin{equation}
\begin{cases}
  Lu = f & \text{on } D \subset \mathbb{R}^n, \\
  Bu = g & \text{on } \partial D, \quad (2)
\end{cases}
\end{equation}

where the operators \( L \) and \( B \) act on the (either real or complex) Hilbert space \( H \subset L^2(D) \) with norm \( || \cdot ||_H \). We want to write the BVP (2) as a variational problem

\begin{equation}
\text{find } u \in H : b(u, v) = F(v) \quad \forall v \in H, \quad (3)
\end{equation}

whose sesquilinear form \( b \) is continuous and coercive (sign-definite) in \( H \), so that the problem is well-posed by Lax–Milgram theorem. To achieve this, we need an operator \( M : H \to L^2(D) \) (the “Morawetz multiplier”), and two sesquilinear forms \( X \) and \( G \) that are continuous on \( H \) and such that the following decomposition holds (the “integrated Morawetz identity”):

\begin{equation}
\int_D (LuMv + MuTv) = X(u, v) + G(u, v). \quad (4)
\end{equation}

We require that \( G(u, v) = G_g(v) \) for \( G_g \in H^* \) when \( B u = g \), so that \( G(\cdot, \cdot) \) collects the terms coming from the boundary conditions.
For $A > 0$, we define
\[ b(u, v) := -X(u, v) + \int_D [M u \nabla v + A L u \nabla v] , \]
\[ F(v) := G_\beta(v) + \int_D [-f M u v + A f L u v] . \]
It is immediate to check that, with these definitions, a solution of the BVP (2) solves (3).

The coercivity of $b$ is equivalent to the existence of $C > 0$ such that
\[ \frac{1}{2} [G(u, u) - X(u, u)] + A \| L u \|_{L^2(D)}^2 \geq C \| u \|_H^2 \]
for all $u \in H$. Indeed, from (4) it holds that
\[ \Re \int_D L u \nabla u = \frac{1}{2} [X(u, u) + G(u, u)] , \]
therefore $\Re b(u, u) \geq C \| u \|_H^2$ is (5).

By setting $L u = \Delta u + k^2 u$, $Bu = \frac{\partial u}{\partial n} - i k \beta u$, $M u = x \cdot \nabla u + \alpha u - i k \beta u$, $\mathcal{S}$ for suitable parameters $\alpha, \beta \in \mathbb{R}$, one recovers the coercive formulation for Helmholtz impedance BVPs described in [2].

3 A space–time formulation for the wave equation

Existing space–time formulations for second-order hyperbolic IBVPs, e.g. [3], do not satisfy Lax–Milgram assumptions. We formulate the IBVP (1) in the abstract framework described above. We let $H = V$, $D = Q$, $\mathcal{L} u := u_t - c^2 \Delta u$, $B$ be the operator collecting impedance conditions on $\Sigma$ and initial conditions on $\Omega_0$, and choose the Morawetz multiplier as
\[ (\mathcal{M} u)(t, x) := -\xi x \cdot \nabla u + \beta(t - T^*) u_t , \]
for all $(t, x) \in Q$, where $\beta, \xi > 0$ and $T^* = \nu T$, with $\nu > 1$ are fixed parameters.

We define $X$ and $G$ in (4) as
\[ X(u, v) := \int_{\partial \Omega} \beta T^*(u_t v_t + c^2 \nabla u \cdot \nabla v) \]
\[ + \int_{\Omega_0} \xi x \cdot (u_t \nabla v + \nabla u_t) \]
\[ + \int_Q (u_t v_t (\beta + \xi d) + c^2 \nabla u \cdot \nabla v (\beta + 2 \xi - \xi d)) \]
\[ - \int_{\Sigma} c^2 \left[ \mathcal{M} u \frac{\partial u}{\partial n} - \frac{1}{6c} u_t M v \right] \]
\[ - \int_{\Sigma} \xi x \cdot n \left[ c^2 \nabla u \cdot \nabla v - u_t v_t \right] , \]
\[ G(u, v) := \int_{\Omega_0} \beta T^* (u_t v_t + c^2 \nabla u \cdot \nabla v) \]
\[ + \int_{\Omega_0} \xi x \cdot (u_t \nabla v + \nabla u_t) \]
\[ - \int_Q c^2 \left[ \mathcal{M} u \frac{\partial u}{\partial n} - \frac{1}{6c} u_t M v \right] \]
\[ - \int_{\Sigma} \xi x \cdot n \left[ c^2 \nabla u \cdot \nabla v - u_t v_t \right] , \]

Then one can compute $G_\beta(\cdot)$ (by substituting $u_0, u_1$ and $g$ in $G(\cdot, V)$, $b(\cdot, V)$ and $F(\cdot)$ as defined above. Their continuity with respect to the seminorm $\| \cdot \|_V$ follows from repeated use of the Cauchy–Schwarz inequality, though it is not explicitly computed here.

4 Coercivity result

As observed in Section 2, to prove coercivity it is sufficient to prove (5). Indeed this is true, and the coercivity constant is reported explicitly. Only simple vector-calculus identities are used in the proof. Recall that $0 < \delta < 1$ measures the “star-shapedness” of $\Omega$.

Lemma. If
\[ \beta \geq \begin{cases} \xi (d - 1) \\ \xi \frac{1}{\nu^2} (\frac{\delta g^4}{T^2} + 1) \\ \xi \frac{1}{\nu^2} (\delta h + \frac{1}{\nu}) \end{cases} \]
and $\xi > 0$ and for any $\nu > 1$, then:
\[ b(v, v) \geq \min \left\{ \frac{\xi \delta}{4}, \frac{\xi}{\nu}, \frac{\xi}{\nu^2}, \frac{\xi}{\nu^3} \right\} \| v \|_V^2 \quad \forall v \in V. \]

Therefore the corresponding problem (3) is well-posed and any conforming Galerkin discretization is well-posed and quasi-optimal.

Standard $H^1(Q)$-conforming discretizations such as piecewise-(bi)linear finite elements are not acceptable for this formulation. Indeed they are not conforming in $V$, because of the $\| u_t - c^2 \Delta u \|_Q$ term in the norm, while $C^1(Q)$-conforming schemes can be used.

The complete proof of the lemma and more details will be available in [1].

References

Tuesday, July 26, Second Afternoon Session
An iterative hybrid numerical-asymptotic boundary element method for high-frequency scattering by multiple screens

Oliver Phillips\textsuperscript{1,*}, Stephen Langdon\textsuperscript{2}, Simon Chandler-Wilde\textsuperscript{1}

\textsuperscript{1}Department of Mathematics and Statistics, University of Reading, Reading, UK
\textsuperscript{2}Department of Mathematics, Brunel University London, London, UK

*Email: o.j.phillips@pgr.reading.ac.uk

Abstract
Standard Boundary Element Methods (BEM) for scattering problems, with piecewise polynomial approximation spaces, have a computational cost that grows with frequency. Recent Hybrid Numerical-Asymptotic (HNA) BEMs, with enriched approximation spaces consisting of the products of piecewise polynomials with carefully chosen oscillatory functions, have been shown to be effective in overcoming this limitation for a range of problems, focused on single convex scatterers or very specific non-convex or multiple scattering configurations. Here we present a novel HNA BEM approach to the problem of 2D scattering by a pair of screens in an arbitrary configuration, which we anticipate may serve as a building block towards algorithms for general multiple scattering problems with computational cost independent of frequency.

Keywords: High-frequency scattering, multiple scattering, BEM, hybrid numerical-asymptotic

1 Problem Statement
We consider the scattering of a plane wave \( u^i(x) := e^{i k d \cdot x} \), where \( d \) is a unit vector in the direction of the plane wave and \( k > 0 \) is the wavenumber, by the union of two disjoint 1D screens, \( \Gamma = \Gamma_1 \cup \Gamma_2 \), in \( D := \mathbb{R}^2 \setminus \overline{\Gamma} \), where \( \overline{\Gamma} \) denotes the closure of \( \Gamma \). The two screens can be in any orientation as long as they are not touching (e.g., Figure 1). The scattering problem we are looking to solve is to find \( u \in C^2(D) \cap W^1_{\text{loc}}(D) \) such that

\[
\Delta u + k^2 u = 0 \quad \text{in} \ D, \quad u = 0 \quad \text{on} \ \Gamma, \quad (1)
\]

and the scattered field \( u^s = u - u^i \) satisfies the Sommerfeld radiation condition. By Green’s 2nd identity (see, e.g., [2])

\[
u(x) = u^i(x) - \frac{i}{4} \int_{\Gamma} H_0^{(1)}(k|x - y|) \psi(y) \, ds(y), \quad x \in D, \quad (3)
\]

and the identity (see, e.g., [2])

\[
u(x) = u^i(x), \quad (6)
\]

\[
S_{11} \phi_1 + S_{12} \phi_2 = u^i|_{\Gamma_1}, \quad (6)
\]

\[
S_{21} \phi_1 + S_{22} \phi_2 = u^i|_{\Gamma_2}. \quad (7)
\]

Figure 1: \( \text{Re}(u) \) in \( D \), with \( \Gamma_1 \) on the left and \( \Gamma_2 \) on the right. The incident wave direction \( d \) is indicated by the arrow.

where \( \phi \in \tilde{H}^{-1/2}(\Gamma) \) is the jump in the normal derivative of \( u \) across \( \Gamma \), and \( H_0^{(1)} \) is the Hankel function of the first kind of order zero. Further, \( \phi \) satisfies the boundary integral equation

\[
\frac{1}{4} \int_{\Gamma} H_0^{(1)}(k|x - y|) \psi(y) \, ds(y) = u^i(x), \quad x \in \Gamma. \quad (4)
\]

2 Multiple scattering iterative method
For ease of notation, define \( \phi_j := \phi|_{\Gamma_j} \in \tilde{H}^{-1/2}(\Gamma_j) \), and let \( S_{ij} : \tilde{H}^{-1/2}(\Gamma_j) \rightarrow H^{1/2}(\Gamma_i) \) be defined by

\[
S_{ij} \psi(x) := \frac{1}{4} \int_{\Gamma_j} H_0^{(1)}(k|x - y|) \psi(y) \, ds(y), \quad (5)
\]

for \( x \in \Gamma_i, \ j, \ell \in \{1, 2\} \), and \( \psi \in \tilde{H}^{-1/2}(\Gamma_j) \). Equation (4) can then be written as

\[
S_{11} \phi_1 + S_{12} \phi_2 = u^i|_{\Gamma_1}, \quad (6)
\]

\[
S_{21} \phi_1 + S_{22} \phi_2 = u^i|_{\Gamma_2}. \quad (7)
\]
The first step in our iterative method is to ignore the effect of $\Gamma_2$ so (6) becomes

$$S_{11}\phi^{(0)} = u^1|_{\Gamma_1},$$

where the 0 in the superscript refers to the number of the iteration considered. We next solve (7) for $\phi^{(1)}_2$, replacing $\phi_1$ by $\phi^{(0)}_1$, thereby considering the first reflection from $\Gamma_1$ on $\Gamma_2$, solving

$$S_{22}\phi^{(1)}_2 = u^1|_{\Gamma_2} - S_{21}\phi^{(0)}_1.$$  

We then solve (6) with $\phi_2$ replaced by $\phi^{(1)}_2$; in order to find the $2r$th order reflection on $\Gamma_1$ and $(2r+1)$th order reflection on $\Gamma_2$ we solve, for $r = 0, 1, 2, \ldots$, with $\phi^{(r-1)}_2 := 0$,

$$S_{11}\phi^{(2r)} = u^1|_{\Gamma_1} - S_{12}\phi^{(2r-1)}_2,$$

$$S_{22}\phi^{(2r+1)}_2 = u^1|_{\Gamma_2} - S_{21}\phi^{(2r)}_1.$$  

### 3 High frequency approximation space

To solve (10) and (11) for a given $r$ we propose to use an HNA BEM approximation space adapting that in [2]. The solution $\phi^{(2r)}_1$ to (10) can be decomposed as

$$\phi^{(2r)}_1(s) = \Psi^{(2r)}_1(s) + v^1_{-2r}(s)e^{iks} + v^1_{-2r}(s)e^{-iks},$$

for $s \in [0, L_1]$, where $L_1$ is the length of $\Gamma_1$, and $s$ denotes the distance from one of the end points. $\Psi^{(2r)}_1$ is the leading order physical optics high-frequency approximation, defined as twice the normal derivative of the field incident on $\Gamma_1$. Precisely, at this iteration,

$$\Psi^{(2r)}_1 = 2\frac{\partial}{\partial n} \left( u^1 - S_{21}\phi^{(2r-1)}_1 \right)|_{\Gamma_1},$$

where, for $\psi \in \tilde{H}^{-1/2}(\Gamma_j)$, $S_j\psi \in C^2(D) \cap W^1_{loc}(D)$ is given, for $j = 1, 2$, by

$$S_j\psi(x) := \frac{1}{4}\int_{\Gamma_j} H_0^{(1)}(k|\mathbf{x} - \mathbf{y}|)\psi(y)ds(y), \ \mathbf{x} \in D,$$

and $\tilde{\psi}(x) := \psi(x)$ if a point source at $x$ is incident on the same side of $\Gamma_1$ as $u^1$, otherwise $\tilde{\psi}(x) := -\psi(x)$.

The term $\phi^{(2r)}_1(s) := v^1_{+2r}(s)e^{iks} + v^1_{-2r}(s)e^{-iks}$ captures the diffraction from the corners. As in [2], it can be shown that the functions $v^1_{+2r}$ in (12) are not oscillatory and hence can be approximated using standard piecewise polynomials with a number of degrees of freedom essentially independent of the wavenumber $k$. Therefore we can approximate $\phi^{(2r)}_1$ by a sum of products of piecewise polynomials and $e^{iks}$ (our HNA BEM approximation space). Substituting (12) into (10) means we are solving, for $r = 0, 1, 2, \ldots$,

$$S_{11}\phi^{(2r)}_1 = u^1|_{\Gamma_1} - S_{12}\phi^{(2r-1)}_2 - S_{11}\Psi^{(2r)}_1.$$  

These equations can each be solved by either the Galerkin method, as in [2], or the least squares collocation method of [1], using the above HNA BEM approximation space, whichever method we choose.

### 4 Results

In this section we test the iterative component of the algorithm for the geometry in Figure 1. Solutions for various $r$ can be seen in Figure 2, solving (10) and (11) by a conventional BEM. For this configuration we see convergence in very few iterations.

### References


A high-frequency approach for the acceleration of the Half-Space Matching method

Amond Allouko$^{1,2,*}$, Vahan Baronian$^1$, Anne-Sophie Bonnet-Ben Dhia$^2$, Sonia Fliss$^2$

$^1$Université Paris-Saclay, CEA, LIST, F-91120, Palaiseau, France
$^2$POEMS (CNRS-INRIA-ENSTA Paris), Institut Polytechnique de Paris, Palaiseau, France
$^*$Email: amond.allouko@ensta-paris.fr

Abstract
The Half-Space Matching (HSM) method has been recently developed as a numerical method for the solution of scattering problems with anisotropic backgrounds. After a finite element discretization, the HSM method couples a sparse matrix, corresponding to the vicinity of the scatterer, with dense matrices resulting from half-space representations of the solution. The computation of these dense matrices requires the evaluation of oscillating Fourier integral. We show here that a fast and accurate evaluation of these dense matrices results from half-space representations. For instance, knowledge of the normalized pulsation, and the traces $(\varphi_1, \varphi_2, \varphi_3, \varphi_4)$ of $u$ on the four infinite straight lines $x = \pm a$ and $y = \pm a$ delimiting four half planes, the derivation of the HSM system of equations is based on the so-called half-space representations. For instance, knowing $\varphi_1$, one can recover $u$ in the corresponding half-space $\Omega_1 = \{(x, y); x > a\}$ by the following integral formula:

$$u(M) = \int_{\partial \Omega_1} K(M, P)\varphi_1(P)d\gamma_P \quad (2)$$

where the kernel $K(M, P)$ is the normal derivative of the Dirichlet Green function in $\Omega_1$. Similar formulae hold for the three other half-spaces, and the HSM equations ensure the compatibility of the different representations of the solution, in the overlapping zones where they coexist [1].

In the problems we are interested in, there are generally no closed form for the kernel, and $K(M, P)$ has to be evaluated thanks to a Fourier integral, like the following one:

$$K(M, P) = \frac{1}{2\pi} \int_{\mathbb{R}} e^{i(\kappa(\xi)x+\xi y)}d\xi \quad (3)$$

where $x = xM - xp > 0$, $y = yM - yp$, and $\kappa(\xi) = \kappa_+(\xi)$ is one of the two solutions $\kappa_{\pm}(\xi)$ of the dispersion equation :

$$\mathbb{A}k(\xi) \cdot k(\xi) = \omega^2 \text{ with } k(\xi) = \left(\frac{\kappa(\xi)}{\xi}\right) \quad (4)$$

The choice of $\kappa_+$ is done as follows. If $\kappa_+ = \pi - \notin \mathbb{R}$, the evanescent wave is such that $\Im(\kappa_+ > 0)$, is selected. If $\kappa_+, \kappa_- \in \mathbb{R}$, $\kappa_+$ is chosen such that

$$\mathbb{A}k(\xi) \cdot e_0 > 0 \text{ with } e_0 = \left(\frac{\cos \theta}{\sin \theta}\right).$$

In the isotropic case ($\mathbb{A} = \mathbb{I}_2$), this leads to $\kappa_+ = \sqrt{\omega^2 - \xi^2}$ for $|\xi| < \omega$.

The difficulty comes from the function $\xi \mapsto e^{i(\kappa(\xi)x+\xi y)}$ which becomes highly oscillating when $x$ or $y$ increases, with oscillations that accumulate near the cutoff values $\xi = \pm \gamma$, where $\gamma$ is defined by $\mathbb{A}k(\gamma) \cdot e_0 = 0$ (see figure 1). This makes the numerical evaluation of the kernel very costly, and motivates the present work.

2 The far-field approximation
A first possibility to avoid an expensive naive quadrature to evaluate the Fourier integral is
to use a far-field approximation of the integral in (3) when \( r = d(M, P) = \sqrt{x^2 + y^2} \) is large. Setting \((x, y) = r(\cos \theta, r \sin \theta), \) the integral in (3) can be rewritten as

\[
\int_{\mathbb{R}} e^{ik(\xi) \cdot e_\theta} d\xi,
\]

so that the phase is stationary at \( \xi_0 \) given by

\[
k'(\xi_0) \cdot e_\theta = \kappa'(\xi_0) \cos \theta + \sin \theta = 0. \tag{5}
\]

On the other hand, (4) implies that for all \( \xi \)\( \kappa k(\xi) \cdot k'(\xi) = 0, \) which combined with (4) and (5), leads to

\[
k(\xi_0) = \left( \kappa(\xi_0) \frac{\omega}{\sqrt{\kappa^{-1} e_\theta \cdot e_\theta}} \kappa^{-1} e_\theta. \right.
\]

It means that the main contribution in the integral comes from the plane wave whose group velocity vector is aligned with the vector \( \overset{\rightarrow}{MP}. \)

Finally, the far-field approximation of the kernel \( K \) by the stationary phase theorem is:

\[
K(M, P) = \sqrt{2\pi \psi} \cos \theta e^{i\omega r \sqrt{\kappa^{-1} e_\theta \cdot e_\theta} / (1 + O(1/\tau))}
\]

where \( \psi = -\sqrt{\kappa^{-1} e_\theta \cdot e_\theta}^{-1/2} (\kappa e_\theta)_{\theta+\pi/2}^{-1} \) with \( e_\theta = e_{\theta+\pi/2}. \) For the isotropic case (\( \kappa = 1_2 \)), the formula can be directly obtained by using asymptotics of the Hankel function:

\[
K(M, P) = \sqrt{\frac{i\omega}{2\pi r}} \cos \theta e^{i\omega r (1 + O(1/\tau))}. 
\]

Let us mention that the above formulae are rigorously justified by splitting the integrals in two parts, one part containing the branch points \( \xi = \pm \gamma, \) which is proved to decay rapidly with the distance \( d(M, P), \) and another one around the stationary point to which the stationary phase theorem is applied.

3 The deformation of contour in the complex plane

Another approach, inspired by [2], is to move the path of Fourier integration in the complex plane. In practice in the HSM method, half integration paths (\( \xi > 0 \) or \( \xi < 0 \)) are considered separately. For instance, in the isotropic case, one can check by Cauchy theorem that

\[
\int_0^{+\infty} e^{i\omega(\xi)x + \xi y)} d\xi = \int_{D_0} e^{i\omega(\xi)x + \xi y)} d\xi
\]

where \( 0 < \alpha < \pi/2 \) and \( D_0 = \{ \eta e^{i\alpha}; \eta > 0 \}, \) as soon as \( |y| < x \cot \alpha. \) The advantage is that the function to integrate on this new path is much less oscillating (see 1). As a consequence, a same accuracy is obtained with much less points of discretization of the integral.

4 Numerical results

Both previous ideas are finally combined to optimize the evaluation of the kernel, using the far-field approximation when \( d(M, P) \) is larger than 7 wavelengths, and the deformation of the contour for intermediate values of \( d(M, P). \) This allows to get a cheap and accurate representation of the solution. One can see on Figure 2 the spurious effects which appear after 7 wavelengths when discretizing the oscillating integral, which disappear when using far-field formulae. In addition to this illustration of the benefits of our approach, quantitative speed-up results will be presented during the talk.

Figure 2: without/with far-field treatment

References


The inflection point problem - from modal to scattering behaviour

David P. Hewett\textsuperscript{1,*}, Valery P. Smyshlyaev\textsuperscript{1}

\textsuperscript{1}Department of Mathematics, University College London, London, UK
\textsuperscript{*}Email: d.hewett@ucl.ac.uk

Abstract

The “inflection point problem”, describing the local asymptotic behaviour of high frequency wave fields near an inflection point in the boundary of an obstacle, is a key unsolved canonical problem in wave scattering. In this talk we provide a historical perspective on the problem and describe recent work relating to it.

Keywords: Canonical problem, high frequency asymptotics, parabolic wave equation

In the high frequency/short wavelength regime, it is known that smooth concave boundaries can support so-called “whispering gallery” waves, which propagate along the boundary and are localised close to it. When such a whispering gallery wave encounters an inflection point in the boundary, one expects it to break up, generating exponentially decaying “creeping waves” on the subsequent convex portion of the boundary, along with a “searchlight beam” propagating away from the boundary (see Figure 1 for an illustration). However, determining the amplitude of the creeping waves and searchlight beam from the amplitude of the incoming whispering gallery wave remains an important open problem in scattering theory. One can argue that this should be considered a fundamental problem in PDE theory, since it connects asymptotically “modal” behaviour and “scattering” behaviour.

To describe the problem mathematically, consider the Helmholtz equation $\Delta u + k^2 u = 0$ near a Dirichlet boundary $\Gamma$ with an inflection point $O$. Let $(s, n)$ be local curvilinear coordinates representing arclength along and normal distance from $\Gamma$, with $s = n = 0$ at $O$, and suppose the curvature of $\Gamma$ satisfies $\kappa(s) = -s + O(s^2)$ as $s \to 0$. To investigate the high frequency behaviour near $O$ we introduce stretched coordinates $x = k^{3/5} s$ and $t = k^{1/5} n$ and seek a solution of the form

$$u \sim C(k)e^{ik^s} \psi(x, t), \quad k \to \infty,$$

for an appropriate $k$-dependent normalisation constant $C(k)$ (not discussed further here). Inserting this ansatz into the Helmholtz equation reveals that the function $\psi(x, t)$ satisfies

$$i \frac{\partial \psi}{\partial t} + \frac{1}{2} \frac{\partial^2 \psi}{\partial x^2} + xt \psi = 0, \quad x > 0, t \in \mathbb{R}, \quad \psi(0, t) = 0, \quad t \in \mathbb{R},$$

and to match with an incoming whispering gallery wave on the concave portion of $\Gamma$ we require

$$\|\psi(\cdot, t) - \psi_o^-(\cdot, t)\|_{L^2(0, +\infty)} \to 0, \quad t \to -\infty,$$

where, with $-\nu_j$ denoting a zero of $A_i$, $\psi^-(x, t) = (-2t)^{\frac{1}{2}} e^{i\nu_j \frac{1}{2} (-2t)^{\frac{1}{2}} A_i \left(x(-2t)^{\frac{1}{2}} - \nu_j\right)}$.

The problem can be equivalently formulated by introducing a new variable $\zeta = x - \frac{1}{2} t^3$, so that $(t, \zeta)$ represent approximate local Cartesian coordinates near $O$, and writing

$$\psi(x, t) = e^{\frac{i}{2} \zeta^2 + \frac{1}{12} t^3} \varphi(\zeta, t),$$

to find that $\varphi(\zeta, t)$ satisfies the parabolic wave equation (free Schrödinger equation)

$$i \frac{\partial \varphi}{\partial t} + \frac{1}{2} \frac{\partial^2 \varphi}{\partial \zeta^2} = 0, \quad \zeta > -\frac{1}{6} t^3, t \in \mathbb{R}, \quad \varphi(-\frac{1}{6} t^3, t) = 0, \quad t \in \mathbb{R},$$

with a homogeneous boundary condition on a cubic parabola $\zeta = -\frac{1}{2} t^3$, and an appropriate modification of (3) at $t = -\infty$.

The problem (1)-(3) was first formulated by Popov in [1], and has since been studied by a number of authors. Popov and Pahencik derived and analysed a finite difference method for
the numerical solution of the problem in [2], results generated from which are shown in Figure 1. In [3], Smyshlyaev and Babich proved well-posedness of the problem in an appropriate functional setting, along with certain regularity and decay properties of the solution.

In recent work [4], Smyshlyaev and Kamotski rigorously proved the existence of a unique “searchlight amplitude” \( G_0(\eta) \in H^1(\mathbb{R}) \) with \( \eta G_0(\eta) \in L^2(\mathbb{R}) \), such that

\[
\|\psi(\cdot, t) - \psi_0^+(\cdot, t)\|_{L^2(0, +\infty)}(t) \to 0, \quad \text{as} \quad t \to +\infty,
\]

where, with \( \eta := \frac{\zeta}{t} = \frac{\xi}{6} - \frac{1}{6} t^2 \) and \( t > 0 \),

\[
\psi_0^+(x, t) := t^{-\frac{3}{2}} e^{\frac{3\eta}{2t^3}} + \frac{i}{2} t^{-\frac{1}{2}} \eta^3 + \frac{i}{2} t^{-\frac{5}{2}} G_0(\eta).
\]

However, providing a closed-form expression for \( G_0(\eta) \) remains an open problem.

There have been numerous attempts to derive analytical solutions to (1)-(3), but so far all have proven unsuccessful. In particular, the Fourier transform approach used to derive the solution to the simpler Fock-Leontovich tangent ray diffraction problem (see e.g. [5]) fails here, because the problem (1)-(3) is non-separable.

In [6, 7] contour integral representations were considered for the solution of (5) in the form

\[
\varphi(\zeta, t) = \int_{\Gamma} F(z) e^{i\left(-\zeta z^2 + \frac{1}{2} \gamma z^3 + \frac{1}{6} \gamma^2 z^4\right)} dz,
\]

where \( \Gamma \) is a suitable contour in the complex \( z \)-plane, starting and ending at infinity, and \( F(z) \) is analytic in a neighbourhood of \( \gamma \). Such integrals are related to the classical catastrophe integrals described e.g. in [8], and to a recently-discovered representation for the solution of the Fock-Leontovich problem (see [5]).

In [7] it was shown using a steepest descent (saddle point) analysis that the function \( F(z) \) and contour \( \gamma \) can be chosen in such a way as to asymptotically recover either whispering gallery waves as \( t \to -\infty \), or creeping waves as \( t \to +\infty \). But as yet no choice of \( F(z) \) and \( \gamma \) has been found to produce both simultaneously.

Most recently [9], Naqvi and Smyshlyaev have investigated boundary integral equation reformulations of (1)-(3) that appear to shed new light on the problem both analytically and numerically. One exciting avenue of possible future research could be the development of accurate numerical methods for the solution of the boundary integral equations derived in [9], perhaps even using a hybrid numerical-asymptotic approach that incorporates the anticipated asymptotic structure of the solution.

References


Homogenisation of perforated plates

Shiza B. Naqvi1,∗, Lorna J. Ayton2

1DAMTP, University of Cambridge, Cambridgeshire, United Kingdom
2DAMTP, University of Cambridgeshire, Cambridge, United Kingdom

*Email: sn522@cam.ac.uk

Abstract
This paper considers the effects of periodic apertures perforating a thin plate and the appropriate homogenised boundary condition one should apply when such a plate is placed in flow. Specific attention is placed on a boundary condition applicable to acoustic scattering by an incident plane wave. The impact of homogenisation on the far-field scattered noise is investigated using the Wiener-Hopf technique. An explicit modelling of a perforated plate via Mathieu function collocation is also introduced.

Keywords: Rayleigh conductivity, impedance, homogenisation

1 Introduction
Aerofoil leading-edge noise may be attenuated by introducing permeability through apertures which perforate the entire thickness of the aerofoil. In particular, we consider the effect of periodically placed apertures, which have been seen experimentally to reduce noise.

The boundary condition upon such a plate is studied by replacing it with an effective impedance boundary condition, leading to a homogeneous model for the entire plate. We focus under the assumption that the size of each perforation is small compared to the distance between apertures, which is in turn much smaller than the wavelength of the incoming acoustic waves. The relevant parameter in the present model will be the Rayleigh conductivity: a measure of compliance, it characterises the fluctuating volume flow rate through the aperture [2]. In this paper, we shall investigate the far-field effects of different homogenised boundary condition models and how they compare against the computationally expensive route of modelling a perforated plate explicitly.

2 Body of the paper
Howe [2] originally assumes continuous displacement across the plate, so in the linearised approximation, the z-component of displacement of particles $\zeta(x, y) e^{i\omega t}$ lying just above and below $z = 0$ vanish outside the circular aperture and equal the displacement of the vortex sheet within the aperture. His method leads to an integro-differential equation for the non-dimensionalised displacement $Z$:

$$\int_S \frac{Z(\xi', \eta')d\eta'd\xi'}{\sqrt{(\xi - \xi')^2 + (\eta - \eta')^2}} = 1 + \alpha_1(\eta)e^{i\sigma_1 \xi} + \alpha_2(\eta)e^{i\sigma_2 \xi}, \quad (1)$$

where $S$ is the unit circle, $(\xi, \eta)$ are the non-dimensionalised physical coordinates, and $\sigma_i$ are the Kelvin-Helmholtz wavenumbers of instability waves on the vortex sheet. The amplitudes $\alpha_i(\eta)$ are set by the Kutta condition at the leading edge. The solution of (1) may then be used to determine the Rayleigh conductivity via

$$K_R = \pi R \int_S Z(\xi, \eta)d\xi d\eta. \quad (2)$$

Conversely to Howe’s assumption of continuous displacement, one can instead consider continuity of particle velocity [3, 7]. This route follows the same derivation, but merely includes an alternative jump condition between the two sides of the plate. The model considers a plate of thickness $T$ and an aperture with characteristic length $B$. The integro-differential equation to solve following this model is for the non-dimensional normal velocity $Z$:

$$\int_{S_0} \frac{Z(X', Y')dX'dY'}{\sqrt{(X - X')^2 + (Y - Y')^2}} - 2i\pi Sr \int_{LE}^X Z(X', Y) e^{i2Sr(X - X')}dX'$$

$$= 1 + \alpha(Y) e^{i2Sr X}. \quad (3)$$

$S_0$ is the non-dimensionalised version of the orifice with non-dimensional coordinates $(X, Y)$, $LE$ denotes the leading edge of the orifice, $Sr$ is
the Strouhal number. Again, $\alpha(Y)$ is set by imposing the Kutta condition at the leading edge.

We discuss the effectiveness of these homogenised models by comparing them with an explicit model. The Helmholtz equation in elliptic coordinates is separable, admitting a series solution expanded in terms Mathieu functions. Colbrook [4] developed a model for scattering by multiple plates. For our purposes, we construct a single perforated plate by aligning multiple, rigid, plates co-linearly to create a long perforated plate. The result is a scattered profile of a plane wave by a one-dimensional perforated plate. The following figures show the field for differing sizes of the perforations $\epsilon$, for the same incident wave.

![Scattered Field](image1)

(a) $\epsilon = 0.1$

![Scattered Field](image2)

(b) $\epsilon = 1$

These half-plane problems are then compared against the homogenised impedance parameters through solving the Wiener-Hopf problem for a general compliant plate, choosing the compliance parameter as dictated by each model. The resulting kernels from the problem without mean flow [1] and with mean flow [8] are factorised numerically. The inverse Fourier transforms are treated with the method of steepest descent to observe the far-field directivities.

3 Future work

Future work will take into the account boundary layers induced by the mean flow, which have been so far neglected by existing impedance models, or simplified to a vortex sheet. We follow the method of Brambley using the method of matched asymptotic expansions on the equations of motion for a perfect gas, in Cartesian coordinates. This will produce an effective impedance parameter from which we will be able to model the flow as uniform; the information pertaining to the boundary layer will be stored in the effective impedance.

4 References

References

Homogenization for transient waves in 1D periodic media: dispersion, interfaces and point sources

Rémi Cornaggia\(^{1,*}\), Bruno Lombard\(^2\)

\(^1\)Sorbonne Université, CNRS, UMR 7190, Institut Jean Le Rond d’Alembert, F-75005 Paris, France
\(^2\)LMA Aix Marseille Univ, CNRS, Centrale Marseille, LMA UMR 7031, Marseille, France

*Email: remi.cornaggia@sorbonne-universite.fr

Abstract

In the context of linear waves in 1D microstructured media, an homogenized model is proposed. It combines second-order asymptotic homogenization to account for dispersion, a reformulation into an hyperbolic system, and interface correctors to model transmission from or towards homogeneous media. The well posedness of this “total model” is proven and its efficiency is illustrated via numerical simulations. An extension to Dirac source terms is proposed.

Keywords: homogenization, dispersion, interfaces

1 Introduction

We first focus on waves propagating in unbounded one-dimensional media \((x \in \mathbb{R})\) characterized by density \(\rho(x) = \rho(x/\ell)\) and Young’s modulus \(E_\ell(x) = E(x/\ell)\), in terms of 1-periodic functions \((\rho, E)\) and the periodicity length \(\ell\). The material displacement is denoted \(u_\ell(x, t)\), and \(v_\ell = \partial_t u_\ell\), \(\sigma_\ell = E_\ell \partial_x u_\ell\) are the velocity field and stress field, satisfying the system:

\[
\begin{cases}
\partial_t v_\ell - \frac{1}{\rho_\ell} \partial_x \sigma_\ell = 0, \\
\partial_t \sigma_\ell - E_\ell \partial_x v_\ell = 0.
\end{cases}
\]

To avoid dealing with the oscillating coefficients \((\rho_\ell, E_\ell)\), an homogenization process is deployed. At leading-order, it leads to a similar system with constant coefficients \(\rho_0\) and \(E_0\), which are respectively the mean and harmonic mean of \(\rho\) and \(E\). The solutions of this system are reasonable approximations of \((v_\ell, \sigma_\ell)\) for very large wavelengths \(\lambda\), i.e. when the ratio \(\varepsilon = \ell/\lambda\) vanishes.

For larger wavelengths, however, the microstructural effects must be accounted for, notably dispersion and interface (or boundary) layers, see [1] and the references therein. This can be done by increasing the order of the homogenization process in \(\varepsilon\).

2 Stress-gradient system

Pushing the homogenization up to second order provides a family of enriched dispersive wave equations, featuring fourth-order space, time and “mixed” derivatives. In particular, the so-called \((mt)\) model studied in [1] can be reformulated into a system inspired by stress-gradient phenomenological models (see [2]):

\[
\begin{align*}
\partial_t w - \frac{a}{\rho_0} \partial_x \sigma &= -\frac{a - 1}{\rho_0} r, \\
\partial_t \sigma - E_0 \partial_x w &= 0, \\
\partial_t \varphi - \frac{a - 1}{\rho_0} \partial_x \sigma &= -\frac{a - 1}{\rho_0} r, \\
\partial_t r &= \frac{E_0}{\ell^2 \beta} \varphi.
\end{align*}
\]

where \((w, \sigma)\) are macroscopic fields gathering the slow variations of \((v_\ell, \sigma_\ell)\), and \((\varphi, r)\) are auxiliary fields. The second-order coefficient \(\beta > 0\) is imposed by the homogenization process, and the parameter \(a\) must satisfy:

\[a = -\beta_m/\beta_t\text{ with }\beta_m + \beta_t = -\beta.\quad (3)\]

The velocity \(v_\ell\) is finally approximated as:

\[v_\ell(x, t) \approx \sum_{j=0}^{2} P_j \left(\frac{x}{\ell}\right) \partial_x^2 w(x, t) - \varphi(x, t).\quad (4)\]

where \(P_0 = 1\) and the cell functions \(\{P_j\}_{j=1,2}\) solve auxiliary cell problems depending on \((\rho, E)\).

A similar expansion is found for \(\sigma_\ell\), with specific cell functions \(Q_j\). These cell functions are also used to define \(\beta\).

From hyperbolic systems properties [3], we prove the following proposition:

**Proposition 1** If the parameters \((\beta_m, \beta_t)\) satisfying (3) are chosen so that \(\beta_m < 0\) and \(\beta_t > 0\) (so that \(a > 1\)), then the system (2) is hyperbolic, the null solution is stable, and there is an associated positive conserved volume energy.
3 Interfaces: first-order correctors

We consider now an interface at $x = 0$ between a homogeneous medium ($x < 0$) characterized by $(\rho_-, E_-)$ and a microstructured medium ($x > 0$) characterized by $(\rho_1, E_1)$, see Figure 1. The interface is perfect, i.e. the velocity and stress continuity are imposed on $(v, \sigma)$. To use the homogenized system (2) in $\mathbb{R}^+$, interface correctors must then be found. Following [1], the continuity conditions above are applied to homogenized approximations such as (4). After some reformulations, and stopping the process at first order, the following "spring-mass" transmission conditions on the macroscopic fields $(w, \sigma)$ are obtained:

$$\begin{align*}
[w]_d &= \ell A_1 \partial_\ell (\sigma)_d , \\
[\sigma]_d &= \ell B_1 \partial_\ell (w)_d ,
\end{align*}$$

where $[f]_d$ and $(f)_d$ denote the jump and mean of a function $f$ across an enlarged interface $I^d = [-d\ell, d\ell]$ introduced to ensure stability, following earlier works on interface homogenization [4]. The coefficients $(A_1, B_1)$ above are then given by:

$$\begin{align*}
A_1 &= dE_-^{-1} + (d - P_1(0)) E_0^{-1} , \\
B_1 &= dp_- + (d - Q_1(0)) \rho_0 .
\end{align*}$$

(6)

To ensure the positivity of these coefficients, the interface parameter $d$ is chosen as:

$$d_{\text{opt}} := \max \left( \frac{E_- P_1(0)}{E_- + E_0}, \frac{\rho_0 Q_1(0)}{\rho_- + \rho_0}, 0 \right) .$$

(7)

We finally prove the proposition:

**Proposition 2** The "total model" made of the system (2) and the jump conditions (5) across an enlarged interface, where the interface parameter $d$ is given by (7), is stable: a positive total energy exists and is conserved.

As an example, Figure 1 presents a transmitted wave from a homogeneous to a laminated material for non-negligeable values of $\varepsilon$. The dispersive effects are clearly observed after a short propagation time, and also affect the reflected wave. All these features are well-captured by the homogenized model.

Finally, the same tools will be used to present extensions to the treatment of point-sources (modeled by Dirac source terms) in the microstructure.

**References**


The WaveHoltz Heterogeneous Multiscale Method for the Helmholtz Equation

Amit Rotem\textsuperscript{1,}\textsuperscript{*}, Daniel Appelö\textsuperscript{1}, Olof Runborg\textsuperscript{2}
\textsuperscript{1}Michigan State University, East Lansing, United States
\textsuperscript{2}Royal Institute of Technology, Stockholm, Sweden
\textsuperscript{*}Email: rotemami@msu.edu

Abstract
We are interested in finding solutions to wave equations posed in materials with rapidly varying coefficients, and time harmonic sources. For these problems, direct discretization is prohibitively costly, and instead multiscale methods are used. There are several multiscale methods, e.g. the popular heterogeneous multiscale methods (HMM) [4,5], that directly discretize in the frequency domain. In this work we instead start in the time-domain and combine a HMM method for the wave equation [2,3] with the newly introduced WaveHoltz method [1]. Each WaveHoltz iteration marches the wave equation towards the time-periodic Helmholtz solution. WaveHoltz has many advantages compared to traditional Helmholtz solvers: it is positive definite, has a bounded condition number, is memory lean, and can be parallelized, etc. All of these advantages will carry over to the multiscale method we present here. In addition our approach also eliminates the boundary errors present in other multiscale methods for the Helmholtz equation, where elliptic micro problems are used.

Keywords: HMM, Helmholtz, WaveHoltz

1 Introduction
Consider the Helmholtz equation on a smooth domain $\Omega$ and at frequency $\omega$,

$$
\nabla \cdot (A(x) \nabla u) + \omega^2 u = s(x), \quad x \in \Omega.
$$

The WaveHoltz method approximates the solution to this equation (for Dirichlet or Neumann boundary conditions) by iterating the equation,

$$
v^{n+1} = \Pi v^n, \quad v^0 \equiv 0,
$$

where $\Pi = \frac{2}{T} \int_0^T \left( \cos(\omega t) - \frac{1}{4} \right) w(x,t) \, dt, \quad T = \frac{2\pi}{\omega},

$$
where $T$ is the period, and $w$ solves

$$
w_{tt} = \nabla \cdot (A(x) \nabla w) - s(x) \cos(\omega t), \quad x \in \Omega,

w(x, 0) = v^n(x), \quad w_t(x, 0) \equiv 0.
$$

The WaveHoltz method thus finds the solution to the Helmholtz equation by repeatedly solving the wave equation [1].

The methods we propose work in multi-D but for brevity, we only consider the 1D case,

$$
(A^\varepsilon(x) u_x)_x + \omega^2 u = s(x), \quad x \in [a,b]. \quad (1)
$$

The source $s$ is independent of $\varepsilon$, but the coefficient $A^\varepsilon(x)$ is assumed to vary rapidly with smallest scale $\varepsilon \ll 1$, and has a scale separation property. We can for instance take locally periodic functions $A^\varepsilon(x) = A(x, x/\varepsilon)$, where $A$ is 1-periodic in the second argument. Then the solution $u$ can be expanded as

$$
u(t, x) = u_0(t, x) + \varepsilon u_1(t, x/\varepsilon) + \mathcal{O}(\varepsilon^2),
$$

where $u_0$ is independent of $\varepsilon$ and $u_1$ is locally periodic in $x$. Here we find $u_0$ by applying the WaveHoltz method to the HMM discretization of the problem

$$
w_{tt} = (A^\varepsilon(x) u_x)_x - s(x) \cos(\omega t), \quad x \in [a,b].
$$

We use the HMM method in [2], which solves the wave equation by discretizing the domain into $N + 2$ points with uniform spacing $H$. The solution is evolved using the second order centered differences in time and space:

$$
W_{j+1}^{n+1} = 2W_j^n - W_{j-1}^{n-1} + \frac{K^2}{H^2} \left( F_{j+1}^\frac{1}{2} - F_{j-1}^\frac{1}{2} \right)

- K^2 s(X_j) \cos(\omega t^n),
$$

with initial data $W_0^n = v(X_j)$. Here

$$
F_{j+1}^\frac{1}{2} = F \left( x_{j+1}^\frac{1}{2}, P_{j+1/2} \right), \quad P_{j+1}^\frac{1}{2} = \frac{1}{H} \left( W_{j+1}^n - W_j^n \right).
$$

The function $F$ represents the output from a microscale solver which evolves the wave-equation on a dense grid spanning $x \in [-\eta, \eta]$ for $\eta \ll H$, and $t \in [-\tau, \tau]$ for $\tau \ll K$. This microscale solver also uses a centered difference scheme with grid spacing $h$ and timestep $k$:

$$
w_{t+1}^\ell = 2w_{t}^\ell - w_{t-1}^{\ell-1} + \frac{k^2}{h^2} \left( f_{i+1/2}^{\ell} - f_{i-1/2}^{\ell} \right),

f_{i+1/2}^{\ell} = \frac{1}{h} \left( A(X_{j+1/2}^{\ell} + x_{i+1})w_{t+1}^{\ell} - A(X_{j+1/2}^{\ell} + x_{i})w_{t}^{\ell} \right).
$$
Figure 1: Convergence of the numerical flux produced by the micro-scale solver to the homogenized flux; for $p = 1, q = 5$ we see 7th order convergence (red line).

with initial data $w_0^i = x_i P_{j+1/2}^{-1}$. The computational domain of the micro-solver is $[-\eta', \eta']$ where $\eta' = \eta + \tau \sqrt{\max A'}$. The size of this patch follows from domain of dependence considerations, and guarantees that the microscale boundary conditions do not influence the solution in $[-\tau, \tau] \times [-\eta, \eta]$. Note that both $\eta$ and $\tau$ are chosen to be of size $O(\varepsilon)$ which makes the computational cost of the microscale solver virtually independent of $\varepsilon$.

Using the micro-scale solution, the quantity $F_{j+1/2}$ is the average:

$$F_{j+1/2} \leftarrow \frac{4}{\eta \tau} \int_{-\tau}^{\tau} \int_{-\eta}^{\eta} w(x, t) K(x/\eta) K(t/\tau) \, dx \, dt,$$

where $K = K^p_q$ is a high-order local averaging kernel derived in [2]. Here $p$ and $q$ control the approximation order of the kernel.

Note that, in the micro-solver, the forcing term $s(x) \cos(\omega t)$ can be excluded as it is approximately constant over $[-\tau, \tau] \times [-\eta, \eta]$, and any constant solution will result in a net-zero contribution to the integral. A detailed convergence analysis following [1,2] will be presented at the conference.

Numerical Results

We apply this method to problem (1) on $[-0.5, 0.5]$ with $A'(x) = 1.1 + \sin(2\pi x/\varepsilon)$, $s(x) = 170 \omega x e^{-144k^2}$, $\omega = 15$, and $\varepsilon = 10^{-5}$, and homogeneous boundary conditions. For this problem, we have a homogenized solution which represents the $O(1)$ terms of the expansion in $\varepsilon$; this solution is a solution to the same problem with $A \equiv \sqrt{21}/10$.

Figure 2: The red line represents the homogenized solution, and the black diamonds represent the solution found by WaveHoltz-HMM.

We first confirm the rate of convergence of the kernels in Fig. 1. Then we use the HMM solver with $N = 62$ interior points for the macro-solver, and 256 points for the micro-solver. We choose $\eta = \tau = 10 \varepsilon$, and the seventh order kernel, $K_{1.5}$. This solver drives the WaveHoltz method and the results are presented in Fig. 2.

References


Modeling and analysis of an inverse boundary value problem in a two dimensional viscoelastic medium

Frédérique Le Louër\textsuperscript{1,*}, Olha Ivanyshyn Yaman\textsuperscript{2,2}

\textsuperscript{1}Université de technologie de Compiègne, LMAC EA2222 - 60 203 Compiègne, France
\textsuperscript{2}Department of Mathematics, Izmir Institute of Technology, Urla, Izmir, 35430, Turkey

*Email: frederique.le-louer@utc.fr

Abstract
We consider the solution of a transmission problem at a thin layer interface of thickness $\varepsilon > 0$ in a two dimensional homogeneous viscoelastic medium. A multi-scale expansion for that solution as $\varepsilon$ tends to 0 enables to replace the thin layer with a generalized impedance boundary condition (GIBC) \cite{3,5}. This boundary condition involves a new second order surface symmetric operator with mixed regularity properties on tangential and normal components. Extending previous investigation for the Laplace equation case \cite{2}, the unique identification of the impedance parameters from measured data produced by the scattering of three linearly independent incident plane waves is established.

Keywords: linear viscoelasticity, thin layers, generalized impedance boundary conditions, inverse boundary value problem

1 Thin layer approximations
Let consider a simply connected bounded domain $\Omega$ in $\mathbb{R}^d$, $d = 2, 3$, with a closed orientable boundary $\Gamma$, as smooth as we need, representing a viscoelastic particle $\Omega^\varepsilon$ coated by a thin layer denoted $\Omega^\varepsilon_{int}$ with constant thickness $\varepsilon > 0$ and different material properties as below.

\begin{align*}
\text{In } \Omega^\varepsilon_{int}; & \quad u^{int}(x)e^{-i\omega t} \\
\text{div}(A^\varepsilon \nabla u^{int}) + \rho^\varepsilon \omega^2 u^{int} = 0 \\
A^\varepsilon & = \lambda^\varepsilon \text{Trace}[\xi]I + \mu^\varepsilon (\xi + T \xi)
\end{align*}

With a time-harmonic incident wave impinging upon $\Gamma$, the total wave is the solution of a transmission problem governed by the Navier equation in $\Omega_{ext}$ and $\Omega^\varepsilon_{int}$ with complex Lamé parameters characterized by $\text{Re}(\lambda, \mu) > 0$ and $\text{Im}(\omega \lambda, \omega \mu) \leq 0$. The continuity of the solution across the external boundary $\Gamma$ is described by the following boundary conditions on $\Gamma$

\begin{align*}
&u^\varepsilon_{ext} + u^{inc} = u^\varepsilon_{int} \\
&T(u^\varepsilon_{ext} + u^{inc}) = Tu^\varepsilon_{int}
\end{align*}

where $Tu = [A\nabla u]n$. This PDE system may be augmented by either a Dirichlet ($u^\varepsilon_{int} = 0$) or a Neumann ($Tu^\varepsilon_{int} = 0$) boundary condition on the internal boundary $\Gamma^\varepsilon$. In this context, the use of boundary and finite elements methods fails since some numerical instabilities arise due to different mesh scaling inside and outside the thin layer. To avoid the phenomena, we approximate the original model by a new exterior boundary value problem with GIBCs.

In the first part of the talk, we present the asymptotic analysis \cite{3,5} leading to an approximate solution with error estimates up to $O(\varepsilon^2)$. The GIBC involves a new nonnegative symmetric second order differential operator whose mapping properties enable the extension of previous investigation \cite{2} to linear viscoelasticity when $d = 2$. The regularity properties of the approximate solution are summarized in Section 2.

2 Regularity of the approximate solution
Let consider incident plane waves defined for a given unit direction $d$ and polarization $p$ by $u^{inc}(x) = e^{i\omega x \cdot d}d^{-1}(p \cdot d)$.

The approximate problem we consider may be formulated as follows: Given an incident plane wave $u^{inc}$ which is assumed to solve the Navier equations in the absence of any scatterer, find the scattered field $u$ satisfying

\begin{align*}
\mu \Delta u + (\lambda + \mu) \nabla \text{div } u + \rho \omega^2 u = 0 & \quad \text{in } \Omega^\varepsilon, \\
\text{where the positive constant } \rho & \text{ is the density, and} \\
\text{the impedance-like boundary condition on }\Gamma: & \\
Tu + i\omega \left\{ d_{\Gamma} - \text{div}_{\Gamma} (\beta \text{div}_{\Gamma} u_{\Gamma}) \right\} & = g,
\end{align*}

where $Tu = [A\nabla u]n$. This PDE system may be augmented by either a Dirichlet ($u^\varepsilon_{int} = 0$) or a Neumann ($Tu^\varepsilon_{int} = 0$) boundary condition on the internal boundary $\Gamma^\varepsilon$. In this context, the use of boundary and finite elements methods fails since some numerical instabilities arise due to different mesh scaling inside and outside the thin layer. To avoid the phenomena, we approximate the original model by a new exterior boundary value problem with GIBCs.

In the first part of the talk, we present the asymptotic analysis \cite{3,5} leading to an approximate solution with error estimates up to $O(\varepsilon^2)$. The GIBC involves a new nonnegative symmetric second order differential operator whose mapping properties enable the extension of previous investigation \cite{2} to linear viscoelasticity when $d = 2$. The regularity properties of the approximate solution are summarized in Section 2.

2 Regularity of the approximate solution
Let consider incident plane waves defined for a given unit direction $d$ and polarization $p$ by $u^{inc}(x) = e^{i\omega x \cdot d}d^{-1}(p \cdot d)$.

The approximate problem we consider may be formulated as follows: Given an incident plane wave $u^{inc}$ which is assumed to solve the Navier equations in the absence of any scatterer, find the scattered field $u$ satisfying

\begin{align*}
\mu \Delta u + (\lambda + \mu) \nabla \text{div } u + \rho \omega^2 u = 0 & \quad \text{in } \Omega^\varepsilon, \\
\text{where the positive constant } \rho & \text{ is the density, and} \\
\text{the impedance-like boundary condition on }\Gamma: & \\
Tu + i\omega \left\{ d_{\Gamma} - \text{div}_{\Gamma} (\beta \text{div}_{\Gamma} u_{\Gamma}) \right\} & = g,
\end{align*}

where $Tu = [A\nabla u]n$. This PDE system may be augmented by either a Dirichlet ($u^\varepsilon_{int} = 0$) or a Neumann ($Tu^\varepsilon_{int} = 0$) boundary condition on the internal boundary $\Gamma^\varepsilon$. In this context, the use of boundary and finite elements methods fails since some numerical instabilities arise due to different mesh scaling inside and outside the thin layer. To avoid the phenomena, we approximate the original model by a new exterior boundary value problem with GIBCs.
\[ g = -Tu^{inc} - \omega \left\{ \alpha u^{inc} - \operatorname{div}_\Gamma \left( \beta (\operatorname{div}_\Gamma u^{inc}) \right) \right\}, \]

where \( \tau = n^+ = T(-n_2, n_1), I_{\tau} = \tau \otimes \tau \) and \( \operatorname{div}_\Gamma u = \tau \cdot (\partial_n u) \) where \( \partial_n \) is the arc length derivative. The impedance parameters \( \alpha \in \mathcal{C}^1(\Gamma) \) and \( \beta \in \mathcal{C}^2(\Gamma) \) are complex functions with non-negative real parts. Moreover, the scattered field has to satisfy the Kupradze radiation condition rewritten in the form

\[ \lim_{|\hat{x}| \to +\infty} |\hat{x}|^{\frac{3}{2}} |\mathbf{T}(\partial_n \hat{x})u - i\mathcal{K}_\omega u| = 0, \]

which has to be satisfied uniformly for all unitary directions \( \hat{x} = \frac{x}{|x|} \) and where

\[ \mathcal{K}_\omega = \kappa_p(\lambda + 2\mu)I_2 + \kappa_s I_1, \]

\[ \kappa_p^2 = \omega^2 p(\lambda + 2\mu) \]

and \( \kappa_s^2 = \omega^2 p/\mu \) are the square \( P \) and \( S \)-wave numbers associated to longitudinal and transverse wave propagation, respectively, such that if \( \operatorname{Im}(\lambda, \mu) = 0 \) then \( \kappa_p = \omega \sqrt{\frac{\kappa_s^2}{\rho}} \) and \( \kappa_s = \omega \frac{\kappa_p}{p} \) or else \( \operatorname{Im}(\kappa_p, \kappa_s) > 0. \)

**Lemma 1** The surface differential operator \( \operatorname{div}_\Gamma \left( (\operatorname{div}_\Gamma \cdot) I_{\tau} \right) \) is bounded from \( H^{\frac{1}{2}}(\Gamma) \) to

\[ V^{-\frac{1}{2}}(\Gamma) := H^{-\frac{1}{2}}(\Gamma) \oplus H^{\frac{1}{2}}(\Gamma) \]

where \( H^{-\frac{1}{2}}(\Gamma) := \{ \varphi \in H^{-\frac{1}{2}}(\Gamma); n \cdot \varphi = 0 \} \)

and \( H^{\frac{1}{2}}(\Gamma) := \{ \varphi \in H^{\frac{1}{2}}(\Gamma); \tau \cdot \varphi = 0 \}. \)

**Theorem 2** (Existence) Assume that \( |\beta| > 0 \) and \( \omega^2 \tau^2 \) is not a Dirichlet eigenvalue of the Neumann operator \( -\Delta^s \). Then for each \( g \in V^{-\frac{1}{2}}(\Gamma) \), the generalized impedance scattering problem admits one and only one solution in \( H^{\frac{1}{2}}_{\text{inc}}(\Gamma; \overline{\Omega}) \).

3 An inverse boundary value problem

In the second part of this talk, we present uniqueness results for the inverse problem of identifying the impedance functions \( \alpha \) and \( \beta \), when the shape \( \Gamma \) is known, from a finite number of far field patterns defined by \( u^{\infty} = u^{\infty}_s + u^{\infty}_p \) where

\[ u(x) = |x|^{\frac{3}{2}} \left( e^{\kappa_s|x|}u^{\infty}_s(\hat{x}) - e^{\kappa_p|x|}u^{\infty}_p(\hat{x}) + O\left( \frac{1}{|x|} \right) \right), \]

uniformly in all directions \( \hat{x} = \frac{x}{|x|} \). The injectivity of the map \( \alpha \mapsto u^{\infty} \) obtained for the classical impedance acoustic problem in [2, Proposition 1] extends to linear (visco)elasticity as is. The case \( \beta \neq 0 \) is more involved.

For \( j = 1, 2, 3 \), we set \( u^{\text{tot}}_j = u_j + u^{\text{inc}}_j \). We introduce the Wronskian associated to the tangential components of the linear system

\[ \begin{cases} \chi_j u^{\text{tot}}_j + \chi_k u^{\text{tot}}_k = 0 \\
\chi_j\partial_n u^{\text{tot}}_j + \chi_k\partial_n u^{\text{tot}}_k = 0, \end{cases} \]

given by

\[ W_{j,k} = (u^{\text{tot}}_j \cdot \tau)(\operatorname{div}_\Gamma u^{\text{tot}}_k) - (u^{\text{tot}}_k \cdot \tau)(\operatorname{div}_\Gamma u^{\text{tot}}_j). \]

**Hypothesis H1.** The boundary curve \( \Gamma \) is such that given three linearly independent incident plane waves, the tangential components of the corresponding three total fields are linearly independent on \( \Gamma \) too, namely for \( j, k = 1, 2, 3 \) we have \( W_{j,k} \neq 0 \).

We prove the following results.

**Theorem 3** For a given shape \( \Gamma \), under Hypothesis H1, three far field patterns corresponding to the scattering of three incident plane waves, with linearly independent couples of directions and polarizations \( (d_j, p_j), j=1,2,3 \), uniquely determine the impedance functions \( \alpha \) and \( \beta \).

**References**


Domain Derivatives in Electromagnetism and Optimal Design of Chiral Objects

T. Arens1, F. Hagemann1, F. Hettlich1
1Department of Mathematics, Karlsruhe Institute of Technology, Karlsruhe, Germany
*Email: tilo.aren@kit.edu

Abstract

The concept of electromagnetic chirality allows the quantification of the difference in interaction of objects with electromagnetic fields of the two handednesses. Objects of high em-chirality are desirable in many technical applications. Domain derivatives are required to analyse the effect of variations of the shape of an obstacle on the scattered fields. They have been used both for inverse shape reconstruction problems as well as for optimal design. In the talk, their use in designing scatterers of (close to) maximal em-chirality is discussed.

Keywords: Electromagnetic scattering, chirality, inverse scattering, shape design.

1 Introduction

In nature, chirality is a phenomenon with important implications in physics, chemistry or biology. One field of interest is the interaction of chiral matter with electromagnetic fields. In applications, one is naturally interested in materials that interact very differently with fields of opposite helicity (e.g. circular polarization).

The traditional geometric definition of chirality does not allow for quantification. In Physics, this has lead to the concept of electromagnetic chirality (em-chirality) [3] and a corresponding scalar measure of this quantity. From a mathematical perspective, this was first discussed in [2]. Scatterers that have maximal measure of em-chirality, relative to all others with the same norm of the farfield operator, have special and desirable properties: at least in the case that reciprocity holds, they are invisible to incident fields of one helicity.

2 EM-Chirality

We consider a scattering problem for a penetrable object illuminated by a time-harmonic electromagnetic wave. The electromagnetic field $(E,H)$ is a solution to the Maxwell system

\[
\begin{align*}
\text{curl } E - i\omega\mu H &= 0 \quad \text{in } \mathbb{R}^3, \\
\text{curl } H + i\omega\varepsilon E &= 0
\end{align*}
\]

We assume that the material parameters $\varepsilon, \mu$ are equal to constant background parameters $\varepsilon_0, \mu_0 > 0$ outside of some bounded (Lipschitz) domain $D$. Inside of $D$ they are also assumed constant with $\mu > 0$ and $\arg(\varepsilon) \in [0, \pi)$. The incident field $(E^i, H^i)$ is assumed to be a solution of (1) for $\varepsilon_0, \mu_0$ in $\mathbb{R}^3$. The scattered field $(E^s, H^s) = (E, H) - (E^i, H^i)$ satisfies the Silver-Müller radiation condition at infinity. The standard asymptotics for scattered fields give rise to the far field operator $F : L^2(S^2) \to L^2(S^2)$, given by

\[
Fg(\hat{x}) = \int_{S^2} E^\infty(\hat{x}, \hat{y}, g(\hat{y})) d\sigma(\hat{y}), \quad g \in L^2(S^2).
\]

Here, $E^\infty(\hat{x}, \hat{y}, g(\hat{y}))$ is the farfield of $E^s$ for an incident plane wave propagating in direction $\hat{y}$ with amplitude $g(\hat{y})$, observed in direction $\hat{x}$. $L^2(S^2)$ denotes the space of square integrable tangential vector fields on the unit sphere.

A field is said to have helicity $\lambda$, if it is an eigenfunction with eigenvalue $\lambda$ of the operator $\frac{1}{\omega\sqrt{\mu}} \text{curl}$. For constant $\varepsilon$, $\mu$, a solution $(E, H)$ to the Maxwell system can always be represented as a linear combination of two such eigenfunctions for the eigenvalues $\pm 1$, the Beltrami fields $E \pm i \sqrt{\mu/\varepsilon} H$. For a plane wave, this is just the well known decomposition into left and right circularly polarized components. By approximation with Herglotz wave pairs in the case of an entire field, or through the far field in case of a radiating field, this decomposition extends to $L^2(S^2)$ and hence to $F$: the far field operator is split into

\[
F = F^+_q + F^+_q + F^+_q + F^-_q,
\]

with $F^q_{pq}$, $p, q \in \{+,-\}$ describing the scattering of fields of helicity $q$ onto fields of helicity $p$. Denote by $(\sigma^q_p)$ the sequences of singular values of $F^q_p$. The scatterer is called em-achiral if $(\sigma^+_-) = (\sigma^-_-)$ and $(\sigma^+_+) = (\sigma^-_+)$. Otherwise it is called em-chiral, and the relative measure of chirality

\[
\chi = \frac{||\sigma^+_- - (\sigma^-_-)||_2^2 + ||(\sigma^+_) - (\sigma^-_)||_2^2}{||F||_q^2}
\]
was proposed in [3]. Here, $\| \cdot \|_*$ denotes the Hilbert-Schmidt norm.

3 Domain Derivatives

Consider the map $F : \partial D \to E^\infty$ for a fixed incident field $(E^i, H^i)$. The Fréchet derivative of $F$ with respect to variations of $\partial D$ is called the domain derivative and may be computed by solving a transmission problem of the same type as the original scattering problem [6]. This derivative can be used in regularized Gauss-Newton schemes for solving the inverse scattering problem of reconstructing the shape of $\partial D$ from measurements of $E^\infty$ for one incident wave. The method was implemented for star-shaped obstacles and electromagnetic transmission problems in [5].

When only star-shaped scatterers are considered, the set of admissible parametrizations for $\partial D$ is a subset of a linear space. Obstacles for which high em-chirality can be expected are typically described by more complicated parameterizations with a non-linear dependence on the optimization variables. When discretizing the domain derivative in this case, a detailed derivation of corresponding expressions subject to the chosen class of parameterizations is required. A particular application, helical scatterers, and corresponding inverse problems, will be presented in the talk. Such scatterers are constructed as $C^1$-smooth surfaces from a center curve given as a B-spline and function specifying the diameter along the curve. Smooth caps close the surface at the two ends.

4 Optimal Design of EM-Chiral Objects

For problem of optimally designing a scatterer with respect to its em-chirality, one requires the Fréchet differentiability of an appropriately chosen measure of chirality with respect to variations of $\partial D$. It has been shown that $\chi$ as defined above does not have the required smoothness [4]. Hence the related measure

$$\tilde{\chi} = \frac{\left(\| F^+ \|_* - \| F^- \|_* \right)^2 + \left(\| F^+ \|_* - \| F^- \|_* \right)^2}{\| F \|_*^2}$$

has been proposed [4] and used in a related optimal design scheme based on an asymptotic representation formula of the scattered field [1]. Note that $\tilde{\chi} \leq \chi$ for all scatterers and that, in particular, $\tilde{\chi}$ attains the maximal value 1 if and only if $\chi$ does.

An expressions for the Fréchet derivative of $\| F \|_*^2$ and corresponding terms for the other operators are readily obtained from the definition of $F$ as a linear integral operator. One only requires variants of the estimates in [6] that make explicit the uniform bound on the $H(\text{curl})$-norm of the incident field. The implementation of the algorithm for the class of helical scatterers discussed in the previous section is subject to ongoing research.

References


Surface identification through back-scattering of an electromagnetic planar wave, by rational approximation

Paul Asensio\textsuperscript{1,*}, Laurent Baratchart\textsuperscript{1}, Juliette Leblond\textsuperscript{1}, Martine Olivi\textsuperscript{1}, Fabien Seybert\textsuperscript{1}
\textsuperscript{1}FACTAS, Inria Sophia Antipolis-Méditerranée, Valbonne, France
\textsuperscript{*}Email: paul.asensio@inria.fr

Abstract
By measuring the scattered electromagnetic field produced by a plane wave on a smooth object at various frequencies, we consider the inverse problem (nondestructive testing) of identifying the shape and certain physical characteristics of the object from the recovery of some singularities. When the object is smooth, these singularities coincide with the poles of some transfer function, that can be estimated by performing best quadratic rational or meromorphic approximation. We study the high-frequency behaviour of the scattered field and the separated contributions of its “optic” and “creeping waves” parts outside the measured frequency band and their respective influence in the reconstruction of the poles of the transfer function.

Keywords: Scattering, Inverse Problems, Shape Identification, High-frequency, Rational Approximation.

1 Introduction
We consider the scattering of a plane wave by an object \( \Omega \) as described in Figure 1. In this back-scattering configuration, we measure the total electric field \( E \) on a finite band of frequency at the point \( X_0 \in \mathbb{R}^3 \) (outside the object) of emission of the input plane wave. The goal of this study is to identify properties of the object from the poles of the transfer function:

\[ F(k) = \frac{E_{sc}(k, X_0) \cdot E_0}{E_{inc}(k, X_0) \cdot E_0}, \]

where \( k \) is the spatial pulsation (proportional to the frequency), and where the incident electric field \( E_{inc} \), which has a direction of propagation \( v \in \mathbb{R}^3 \), and the scattered electric field \( E_{sc} \) are given at \( X \in \mathbb{R}^3 \) (outside the object) by:

\[ E_{inc}(k, X) = E_0 e^{ikv \cdot X}, \quad E_{sc} = E - E_{inc}. \]

When the object is convex and smooth, the function \( F \) is meromorphic with poles lying in the upper half-plane. The scattered electric field is a solution to the Helmholtz equation outside \( \Omega \):

\[ \Delta E_{sc} + k^2 E_{sc} = 0, \]

\[ \nabla \cdot E_{sc} = 0, \]

\[ \lim_{r \to \infty} (r (X \cdot \nabla - ik) E_{sc}) = 0, \quad r = |X|, \]

\[ (E_{sc} + E_{inc}) \times \nu = 0 \text{ on } \partial \Omega, \]

for the outer normal vector \( \nu \) to \( \partial \Omega \).

In order to perform the rational approximation of \( F \), we need to describe its behaviour, hence that of the field \( E_{sc} \), at high frequency (outside the band of measured frequencies). We first consider the case in which the object \( \Omega \) is a spherical PEC (Perfectly Electric Conductor) of radius \( a \) in the back-scattering orientation \( (X = -r v \text{ with } r > a) \). In this case, the solution is given by its expansion (Mie series), [2]:

\[ E_{sc}(k, -rv) = \frac{E_0}{kr} \sum_{n=1}^{\infty} r^n \left( n + \frac{1}{2} \right) \times \]

\[ J_n(ka) H_n(kr) \left[ H_n'(ka) - i J_n'(ka) \right], \]

where the \( H_n \) are the spherical Hankel functions of the second kind and the \( J_n \) are the spherical Bessel functions of the first kind.

As the partial sums of these series converge slowly when \( k \) increases, it is not sufficient to model the high-frequency behaviour of \( E_{sc} \).

Figure 1: Setting of the scattering by a sphere.
2 Optical part

In order to study the high frequency behaviour of $F$, we consider a well-behaving ansatz under the form of a so-called Luneberg-Kline series, [1]. For $N > 0$:

$$E_{sc}(k, X) = \sum_{n=0}^{N} \frac{A_n(X)}{(ik)^n} e^{ikS(X)} + o \left( \frac{1}{k^N} \right). \quad (5)$$

By substituting this form into (1) to (4), we obtain the eikonal equation (6) and an infinite list of transport equations (7) that allow us to compute the ($\mathbb{R}$-valued) phase $S$ and the sequence of ($\mathbb{R}^3$-valued) coefficients $(A_n)_{n \in \mathbb{N}}$:

$$|\nabla S|^2 = 1, \quad (6)$$
$$\Delta S + 2\nabla S \cdot \nabla A_n = -\Delta A_{n-1}. \quad (7)$$

using the boundary conditions that for all $Y \in \partial \Omega$:

$$A_0(Y) \times Y = -E_0 \times Y, \quad \forall n \in \mathbb{N}^*, \quad A_n(Y) \times Y = 0, \quad \forall n \in \mathbb{N}, \quad \nabla S \cdot A_n(Y) = -\nabla \cdot A_{n-1}(Y), \quad S(Y) = v \cdot Y.$$

Using these equations, we can compute the successive terms of the Luneberg-Kline series for a PEC. In the back-scattering case, the first terms are given by:

$$S = (r - 2a),$$
$$A_0 = -\frac{a}{2r - a} E_0,$$
$$A_1 = -\frac{(r - a)^2}{(2r - a)^3} E_0,$$
$$A_2 = \frac{2(r - a)(2r^2 - 4ra + 3a^2)}{(2r - a)^5} E_0.$$

As we will show in section 4, this asymptotic expansion is not precise enough for our purpose and we thus consider, in the next section, terms that were neglected in the Luneberg-Kline series.

3 Creeping wave

In order to deeper understand the links between Luneberg-Kline expansions and Mie series, we apply Watson transformation [3,4] to the latter, as a way to transform the sum into an integral using the residue theorem. We show that, far from the spherical object $\Omega$ ($r$ large):

$$E_{sc}(k, -rv) = P(ka) \frac{\exp(ikr)}{kr} E_0,$$
$$P(ka) = P_c(ka) + P_o(ka),$$

where the optical part $P_o$ has the same high-frequency behaviour as the Luneberg-Kline series (5), and the creeping wave part $P_c$ has the following behaviour:

$$P_c(\rho) \sim \frac{\tau^4 e^{i\beta_1}}{\beta_1 \text{Ai}(-\beta_1)^2} \exp \left( i\rho - e^{-i\tau} \tau \pi \beta_1 \right),$$

where $\tau = \tau(\rho) = (\frac{\rho}{\beta_1})^{1/3}$ and $\beta_1$ is the first zero of the derivative $\text{Ai}'$ of the Airy function $\text{Ai}$.

4 Numerical comparison

As $P_c$ exponentially decreases when $k$ goes to infinity, it seems negligible with respect to $P_o$. Nevertheless, for a study of the compared importance of this terms when dealing with finite frequencies, we choose a frequency of 5 GHz for a sphere of radius $a = 0.15/2$ at a distance $r = 1$. Our computations show that the three optics terms represent respectively 86.11%, 4.87% and 0.01% of the field, while the creeping wave term represents 7.55% of the field. This confirms that in order to reconstruct the poles of the transfer function, we will need to use the creeping wave part of the scattered field, even if it is negligible w.r.t. the optic part at high-frequency.

References


Propagation of acoustic and gravity waves in the ocean: a new derivation for a general model

J. Dubois\textsuperscript{1}, S. Imperiale\textsuperscript{2}, J. Sainte-Marie\textsuperscript{1}

\textsuperscript{1}Inria Paris, 2 rue Simone Iff, 75589 Paris
\textsuperscript{2}Inria Saclay, 1 rue Honoré d’Estienne d’Orves 91120 Palaiseau

Abstract
In this work we are interested in the modeling of propagation of acoustic and gravity wave in the ocean. An original model is obtained by the linearization of the compressible Navier-Stokes equations with free surface written in Lagrangian coordinates. We present an asymptotic analysis for small Mach number allowing to compare the obtained model to existing linear models.

Keywords: Fluid mechanics, Free-surface flow, Modeling, Acoustic-gravity waves

1 Introduction
Several authors have proposed to use the propagation of acoustic-gravity waves in the ocean to detect tsunamis [2], as the sound travels much faster in water than the tsunami wave itself.

To model the acoustic-gravity waves, we consider the Navier-Stokes equations for an inviscid, weakly compressible and free-surface fluid and aim at a linear approximation of these nonlinear equations that retains the two types of waves.

The ocean is supposed to be close to an equilibrium, stratified, with a varying density $\rho$ and temperature $T$. The Navier-Stokes equations describing this state are written in Lagrangian coordinates for a rigorous treatment of the free surface. The system is then linearized around the state at rest, and a wave-like equation is obtained (it shares similarities with the Galbrun equation [4]). We compare our system with existing models in two ways: first we perform an asymptotic analysis for small Mach numbers and recover the equations governing an incompressible flow with free surface. Second we put the model back to eulerian coordinates and compare it with other well-known and widely used linear models [1, 3].

2 Lagrangian description
We start with the Navier-Stokes equations in Lagrangian coordinates. Let $\Omega$ be the domain of the ocean at rest, with boundary $\Gamma_b$ at the bottom and horizontal boundary $\Gamma_s$ at the surface. Let $d$ be the displacement from $\Omega$ to the deformed configuration. The gradient of $d$ is $F$, its Jacobian $J$ and the fluid velocity $U = \partial_t d$.

The Navier-Stokes equations are then

$$\partial_t \rho + \frac{\rho}{|J|} \nabla \xi \cdot (|J|F^{-1}U) = 0 \quad \text{in } \Omega, \quad (1)$$

$$\rho \partial_t U + F^{-T} \nabla \xi \rho \rho g = \rho g \quad \text{in } \Omega, \quad (2)$$

with the boundary conditions, $p^a$ being the atmospheric pressure and $f$ a source term,

$$p = p^a \text{ on } \Gamma_s \text{ and } U \cdot n_b = f \text{ on } \Gamma_b. \quad (3)$$

The pressure and the density must satisfy the state law

$$p = f_0(\rho, T) \text{ with the temperature assumed given. With this law and energy conservation, an equation for the pressure is obtained}$$

$$\partial_t p + \frac{\rho c^2}{|J|} \nabla \xi \cdot (|J|F^{-1}U) = 0. \quad (4)$$

Where $c$ is the speed of sound in the fluid.

3 Linearization and the limit state
The equations (1)-(4) are linearized around a steady state for the ocean at rest: there is no mean current and the pressure, density and temperature have only vertical variations. This corresponds to an asymptotic expansion with $\epsilon \ll 1$:

$$d = \epsilon d_1 + \mathcal{O}(\epsilon^2), \quad \rho = \rho_0 + \epsilon \rho_1 + \mathcal{O}(\epsilon^2),$$

$$p = \rho_0 + \epsilon p_1 + \mathcal{O}(\epsilon^2). \quad (5)$$

Using these expressions in Eq.(1)-(4) and separating powers of $\epsilon$ yields a limit system and a system for the first order corrections.

For limit terms, one finds that the pressure $p_0$ and density $\rho_0$ depend only on the vertical coordinate $\xi^3$, with

$$\rho_0(\xi^3) = -\rho_0 \beta, \quad p_0 = p^a \text{ on } \Gamma_s. \quad (6)$$

They must also satisfy $p_0 = f_0(\rho_0, T_0)$ where $T_0$ is the initial temperature. These equations are compatibility conditions between the choice of a state at rest and the hypothesis that this is a stable equilibrium.
4 A wave equation for the velocity

The system for the correction terms is written in $\Omega$ and reads

$$\frac{\rho_0}{\partial t} \frac{\partial U_1}{\partial t} + \nabla \xi p_1 - (\nabla \xi d)^T \nabla \xi \rho_0 = \rho g,$$  

(7)

$$\frac{\partial \rho_1}{\partial t} + \rho_0 \nabla \xi \cdot U_1 = 0,$$  

(8)

$$\frac{\partial \rho_1}{\partial t} + \rho_0 c_0^2 \nabla \xi \cdot U_1 = 0,$$  

(9)

with boundary conditions

$$p_1 = 0 \text{ on } \Gamma_s \text{ and } U_1 \cdot n_b = f \text{ on } \Gamma_b.$$  

(10)

Differentiating in time (7) and replacing $\rho$ and $\rho_1$ with (8), (9) we obtain a second order equation for $U_1$,

$$\rho_0 \frac{\partial^2 U_1}{\partial t^2} - \nabla \xi (\rho_0 c_0^2 \nabla \xi \cdot U_1)$$

$$- (\nabla \xi U_1)^T \rho g + \rho_0 \nabla \xi \cdot U_1 g = 0.$$  

(11)

We introduce for the weak formulation the space

$$V = \{ U_1 \in H(\text{div}, \Omega) \mid U_1 \cdot n \in L^2(\partial \Omega) \text{ and } U_1 \cdot n_b = 0 \text{ on } \Gamma_b \}.$$  

(12)

The variational formulation of (11) is not straightforward to obtain but reads:

Find $U_1 \in C^1([0, T]; L^2(\Omega)^3) \cap C^0([0, T]; V)$ solution to

$$\frac{d^2}{dt^2} (U_1, V)_H + a(U_1, V) = L(V) \quad \forall V \in V,$$  

(13)

where $a$ is a symmetric bilinear form

$$a(U_1, V) = \int_{\Gamma_s} \rho_0 g U_1 \cdot e_3 V \cdot e_3 \, ds$$

$$+ \int_{\Omega} \rho_0 \left( c_0 \nabla \xi \cdot \psi - \frac{g}{c_0} (U_1 \cdot e_3) \right)$$

$$\times \left( c_0 \nabla \xi \cdot \psi - \frac{g}{c_0} (V \cdot e_3) \right) \, d\xi$$

$$+ \int_{\Omega} N^2 \rho_0 U_1 \cdot e_3 V \cdot e_3 \, d\xi,$$  

(14)

with the Brunt-Väisälä frequency $N^2$ defined by

$$N^2(\xi) = - \left( \frac{g^2}{c_0(\xi)^2} + \frac{\rho_1(\xi)}{\rho_0(\xi)} \right),$$

and $L$ is a linear form

$$L(V) = \int_{\Omega} \rho_0 V \cdot f \, d\xi.$$  

For values of $\rho$, $\rho_0$ and $c_0$ in the literature, $N^2$ is positive and so is the bilinear form $a$.

5 Asymptotic analysis for small Mach number

All the quantities are put in non-dimensional form. Introducing the non-dimensional number $\delta = Ma/Fr$, we obtain the equation

$$\rho_0 \frac{\partial^2 U_1}{\partial t^2} - \frac{1}{\delta^2} \nabla \xi \left( \rho_0 c_0 \nabla \xi \cdot U_1 \right)$$

$$- (\nabla \xi U_1)^T \rho g + \rho_0 \nabla \xi \cdot U_1 g = 0.$$  

(15)

An asymptotic expansion for $\delta \ll 1$ is carried out. The limit solution is divergence free. In the limit equation the divergence term is replaced by a Lagrange multiplier. When $f = 0$ and the density is constant, the Lagrange multiplier $\varphi$ is solution to

$$\Delta \varphi = 0 \text{ on } \Omega, \quad \partial_n \varphi - \partial_3 \varphi = 0 \text{ on } \Gamma_s.$$  

(16)

In other cases (density not constant) the obtained limit equation can be seen as a generalization of the classical Cauchy-Poisson equation for incompressible flow.

6 Comparison with linear models in Eulerian coordinates

The first order system is written in Eulerian coordinates. The set of equations of [1] is obtained. Compared to [3], our model retains more terms because of two modelling choices: the fluid is not assumed irrotational, and the density depends not only on the pressure but also on the temperature. The interest of our model is demonstrated by numerical simulations.

References


Symmetric-hyperbolic conservation laws
modelling viscoelastic flows

Sébastien BOYAVAL\textsuperscript{1,}\textsuperscript{*}

\textsuperscript{1}Laboratoire d’hydraulique Saint-Venant (Ecole des Ponts ParisTech – EDF R&D), EDF’lab Chatou & MATHERIALS, Inria Paris ; France. (sebastien.boyaval@enpc.fr)

\textsuperscript{*}Email: me@my.domain

Abstract

Keywords: viscoelastic flows, symmetric-hyperbolic systems, balance laws

1 Problem setting

Many equations have been proposed to model flows with a viscoelastic behaviour, for various applications (polymer suspensions, turbulent fluids averaged in time/space...). Seminal equations have been proposed by Maxwell in 1867 for viscoelastic fluids, with stress relaxation \textsuperscript{3}. In particular, the Upper-Convected Maxwell (UCM) equations are useful for one-dimensional flows. But for multi-dimensional flows, the usability of such viscoelastic fluid systems as the UCM equations remains limited.

For many configurations useful e.g. in materials engineering, where the viscoelastic fluid rheology is often invoked, numerous numerical simulations have shown that reasonable multi-dimensional extensions of the UCM equations do not converge when the discretization parameters are refined beyond a critical value for the relaxation-time of the stress \textsuperscript{4}.

2 A new model

As a remedy to the computations with existing equations, we propose to consider a new system of conservation laws with algebraic source terms (balance laws) to model viscoelastic flows:

\begin{equation}
\begin{aligned}
\partial_t (\rho u^i) + \partial_j (\rho u^i u^j) &- \partial_j \left( -p \delta_{ij} + 2\rho (K F^i_\alpha A^{\alpha\beta} F^j_\beta - \theta \delta_{ij}) \right) = \rho f^i \\
\partial_t (\rho F^i_\alpha) + \partial_j (\rho u^j F^i_\alpha - \rho u^i F^j_\alpha) &= 0 \\
\partial_t \rho + \partial_j (u^j \rho) &= 0 \\
\partial_t (\rho A^{\alpha\beta}) + \partial_j \left( \rho u^j A^{\alpha\beta} \right) &= \frac{4\rho}{\xi} \left( \theta \left( [F^{-1}]^{\alpha\beta}_i [F^{-1}]^{i\beta}_i \right) - K A^{\alpha\beta} \right)
\end{aligned}
\end{equation}

(1)

The system (1) is an extension of the elastodynamics with an additional material variable, the anelasticity tensor $A^{\alpha\beta}$, that is symmetric definite positive and relaxes at a time rate $\xi$ to the inverse Cauchy-Green deformation tensor. Note that in (1), we used classical notations:

- $u^i$ are the components of the velocity field in the Euclidean ambient space,
- $F^i_\alpha$ are the components of the deformation gradient relative to the material manifold,
- $\rho = |F|^{-1} \rho_0$ is the mass density, and
- $p(\rho)$ is a pressure term.

We have denoted $K$ and $\theta$ two constants, to be fixed in an isothermal setting.

Then, it is noteworthy that the Eulerian system (1) has a Lagrangian that is equivalent for smooth flows, and symmetric-hyperbolic \textsuperscript{1}. Classically, the proof in \textsuperscript{1} consists in exhibiting a mathematical entropy for (1) that is strictly convex in the conservative variable.

Moreover, the extended elastodynamics system (1) unifies hardly-elastic fluid models with hardly-compressible solid models, similarly to the famous K-BKZ integral viscoelastic models \textsuperscript{4}, but in a more versatile (purely differential) way based on an evolution equation for the anelasticity metric tensor.

3 Perspectives

Contrary to the Navier-Stokes equations (i.e. momentum equations with velocity diffusion), our equations can model the viscous friction using shear waves of finite-speed.

The new system can be manipulated for various applications of the viscoelastic flow concept in environmental hydraulics (shallow-water flows) \textsuperscript{1} or materials engineering (non-isothermal flows) \textsuperscript{2}.

Acknowledgements

This research has been supported by ANR project 15-CE01-0013 SEDIFLO: “Modelling and simulation of solid transport in rivers”.
4 References

References


Stability analysis of the JCAPL equivalent fluid model equations for porous media

Ilyes Moufid\textsuperscript{1,2,*}, Denis Matignon\textsuperscript{1}, Rémi Roncen\textsuperscript{2}, Estelle Piot\textsuperscript{2}
\textsuperscript{1}ISAE-SUPAERO - Université de Toulouse, 31055 Toulouse, France
\textsuperscript{2}ONERA, The French Aerospace Laboratory - Université de Toulouse, 31055 Toulouse, France
\textsuperscript{*}Email: ilyes.moufid@onera.fr

Abstract
The equivalent fluid model (EFM) describes the acoustic properties of rigid porous media by defining it as a fluid with an effective density and an effective compressibility. Their definition are based on the dynamic tortuosity $\alpha$ and the dynamic compressibility $\beta$, known to be complex-valued functions depending on frequency. Among the different models describing $\alpha$ and $\beta$, this paper focuses on the Johnson-Champoux-Allard-Pride-Lafarge (JCAPL) model \cite{1} where these parameters are defined as irrational functions, behaving like fractional derivatives in the time domain. Here, we present the proof of stability of the time-domain EFM using the JCAPL model thanks to their oscillatory-diffusive (OD) representations.

Keywords: porous media, equivalent fluid model, JCAPL model, OD representation, stability.

1 Introduction
The EFM equations for rigid porous materials are recalled below in the Laplace domain:
\begin{align*}
\begin{cases}
\rho_0 \alpha(s) \bar{\mathbf{v}} + \mathbf{\nabla} \bar{\rho} &= 0, \\
\chi_0 \beta(s) \bar{\mathbf{v}} + \mathbf{\nabla} \cdot \bar{\mathbf{v}} &= 0,
\end{cases}
\end{align*}
(1)
where $\rho_0$ is the ambient fluid density, $\chi_0$ the ambient adiabatic compressibility; velocity $\mathbf{v}$ and pressure $p$ are defined on $(0, \infty) \times \Omega$, with $\Omega \subset \mathbb{R}^n$. $\hat{f}$ denotes the Laplace transform of $f$ and $s$ is the complex variable.

The JCAPL model defines $\alpha$ and $\beta$ as
\begin{align*}
\alpha(s) := \alpha_\infty \left[ 1 + \frac{M}{s} + N \sqrt{1 + \frac{M}{s} - 1} \right],
\end{align*}
(2)
\begin{align*}
\beta(s) := \gamma^{-1} \left[ 1 + \frac{M'}{s} + N' \sqrt{1 + \frac{M'}{s} - 1} \right],
\end{align*}
(3)
with parameters detailed in \cite{2}. These expressions are based on the exact description of $\alpha$ and $\beta$ at the high and low frequency limits, connected by a function whose singularities lie on the negative real axis of the complex plane \cite{3}.

In order to study the stability of the whole JCAPL - EFM system, a methodology based on $a$ poles and cuts technique \cite{4} is used. It enables to recast a complex function $f$ in a formulation built from an OD representation \cite{4}, containing an infinite number of real or complex weights and poles, but no $\sqrt{s}$-type terms.

\begin{align*}
\hat{f}(s) = \sum_{k \in \mathbb{Z}} \frac{r_k}{s - s_k} + \int_0^{\infty} \frac{\mu(\xi)}{s + \xi} d\xi,
\end{align*}
(4)
with the well-posedness condition $\int_0^{\infty} |\mu(\xi)| d\xi < \infty$ for $\hat{f}$ to admit an OD representation \cite{2}.

2 Oscillatory-diffusive representation
The irrational parts of $\alpha$ and $\beta$ are first studied in order to find their OD representation. The focus is therefore on the two following transfer functions:
\begin{align*}
\hat{g}(s) := \frac{1}{N} \left[ \alpha(s) - \alpha_\infty \right] = \frac{\sqrt{1 + \frac{M}{s} - 1}}{s},
\end{align*}
\begin{align*}
\hat{h}(s) := \frac{\beta(s) - 1}{\gamma - 1} = \frac{N' \sqrt{1 + \frac{M'}{s} + M' - N'}}{s + N' \sqrt{1 + \frac{M'}{s} + M' - N'}}.
\end{align*}
Function $\hat{g}$ admits a diffusive representation with $\mu(\xi) \propto \xi^{-1/2}$, a positive diffusive weight defined for $\xi \in (L, \infty)$ and verifying the well-posedness condition.

Function $\hat{h}$ has an oscillatory-diffusive representation containing a diffusive part and an additional isolated term, which is null for certain values of the parameters $M'$, $N'$ and $L'$ \cite{2}.

\begin{align*}
\hat{h}(s) = \frac{r_0}{s - s_0} + \int_{L'}^{\infty} \frac{\nu(\xi)}{s + \xi} d\xi,
\end{align*}
(5)
with $s_0 < 0$, $r_0 \geq 0$ and $\nu(\xi) \propto \xi^{-1/2}$ $\left( (\xi - M' - N')^2 + N'^2(\xi - L')^{-1} \right)\frac{1}{1 - (\xi - L')^{-1}}$, which is positive and verifies the well-posedness condition.

3 Extended diffusive realization
Based on the OD representations of $\hat{g}$ and $\hat{h}$, system (1) in the time domain reads:
\begin{align*}
\partial_t \mathbf{u} + M \mathbf{u} + N (g * \partial_t \mathbf{u}) + \frac{1}{\rho_0 \alpha_\infty} \mathbf{\nabla} p &= 0, \\
\partial_t p + (\gamma - 1) (h * \partial_t p) + \frac{1}{\chi_0} \mathbf{\nabla} \cdot \mathbf{u} &= 0.
\end{align*}
(6)
The interest of the OD representation is in the associated diffusive realization, which gives a time-local formulation of the convolution products present in (6). In this work, extended diffusive realizations, as

\[
\begin{align*}
\mathbf{z}_u(t, x) &= \int_{L} \mu(\xi) \partial_t \phi(\xi; t, x) \, d\xi, \\
\partial_t \phi(\xi; t, x) &= -\xi \phi(\xi; t, x) + \mathbf{u}(t, x), \\
\phi(\xi; 0, x) &= \mathbf{u}(0, x)/\xi, \\
\end{align*}
\]

for \( \mathbf{z}_u = (g \ast \partial_t \mathbf{u}) \) with \( \phi \) the diffusive variable, are used and differ from usual diffusive realizations by the presence of a time derivative in the convolution product. Non-null initial conditions are set for the diffusive variable to have a finite value for \( \mathbf{z}_u \) at \( t = 0 \) [5]. The energy functional

\[ E_{\phi}(t) := \frac{1}{2} \int_{\Omega} \int_{L} \mu(\xi) \xi \| \phi(\xi; t, x) \|^2 \, d\xi \, dx, \quad \] (8)

defined for the extended diffusive realization (7). A realization analogous to (7) is used for \( z_p := (h \ast \partial_t p) \) with \( \psi \) denoting its associated diffusive variable and \( E_{\psi} \) its associated energy. The additional first-order system \( r_0/(s - s_0) \) in (5) is handled by the same diffusive variable \( \psi \) and its associated energy, included in \( E_{\psi} \), is

\[ E_{\psi}(t) := \frac{1}{2} \int_{\Omega} r_0 (-s_0) \| \psi(-s_0; t, x) \|^2 \, dx, \]

Using the realization of the convolution products in (6) leads to the augmented system:

\[
\begin{align*}
\partial_t \mathbf{u} + M \mathbf{u} + N \mathbf{z}_u + \frac{1}{\rho_0} \alpha_\infty \nabla p &= 0, \\
\partial_t p + (\gamma - 1) z_p + \frac{1}{\rho_0} \nabla \cdot \mathbf{u} &= 0, \\
\partial_t \phi(\xi; t, x) &= -\xi \phi(\xi; t, x) + \mathbf{u}(t, x), \\
\partial_t \psi(\xi; t, x) &= -\xi \psi(\xi; t, x) + p(t, x), \\
\phi(\xi; 0, x) &= \mathbf{u}(0, x)/\xi, \\
\psi(\xi; 0, x) &= p(0, x)/\xi. \\
\end{align*}
\]

4 Stability analysis

The stability analysis of system (9) is performed thanks to the augmented energy functional

\[ \mathcal{E}(t) := E_{\text{int}}(t) + E_{\text{diff}}(t), \]

where the classical mechanical energy is

\[ E_{\text{int}}(t) := \frac{\rho_0 \alpha_\infty}{2} \int_{\Omega} \| \mathbf{u} \|^2 \, dx + \frac{\chi_0}{2} \int_{\Omega} |p|^2 \, dx, \]

and a diffusive energy is defined as

\[ E_{\text{diff}} := \rho_0 \alpha_\infty N \mathbf{E}_{\phi}(t) + \chi_0 (\gamma - 1) \mathbf{E}_{\psi}(t). \]

The positivity of the JCAPL diffusive weights, and the known sign of \( r_0 \) and \( s_0 \), enables to prove the following proposition.

**Theorem 4.1** In a bounded domain \( \Omega \) with no contribution at the boundary (either \( p = 0 \), or \( \mathbf{u} \cdot \mathbf{n} = 0 \) on \( \partial \Omega \)), the augmented energy \( \mathcal{E} \) of the JCAPL-EFM satisfies \( \frac{d}{dt} \mathcal{E}(t) \leq 0 \).

The key point of the proof lies in noticing that certain terms in

\[ \frac{d}{dt} E_{\text{int}}(t) = -\rho_0 \alpha_\infty \left( M \int_{\Omega} \| \mathbf{u} \|^2 \, dx + N \int_{\Omega} \mathbf{u} \cdot \mathbf{z}_u \, dx \right) - \rho_0 \alpha_\infty + \chi_0 \int_{\Omega} p \, d\Omega p \, dx, \]

have an opposite sign of those in the time derivative of the diffusive energy (see the first term of (8)) and can compensate exactly with \( \frac{d}{dt} E_{\text{diff}} \). Moreover, following [6], Prop. 4.1 can be proved.

**Proposition 4.1** The dynamical system (9) is asymptotically stable, i.e. \( (\mathbf{u}, p, \phi, \psi) \rightarrow (0, 0, 0, 0) \) as \( t \rightarrow \infty \) in the appropriate energy space.

Hence, \( \mathcal{E} \) describes an energy functional for (9), which enables to ensure the stability of the system without external inputs.

**Acknowledgment** This research has been financially supported by ONERA and by ISAE-SUPAERO, through the EUR TSAS under grant ANR-17-EURE-0005.

**References**

Wednesday, July 27, Morning Session
Scattering by a Body in a Pipe

P. A. Martin$^{1,*}$, A. T. Skvortsov$^2$

$^1$Department of Applied Mathematics and Statistics, Colorado School of Mines, Golden, USA
$^2$Maritime Division, Defence Science and Technology Group, Fishermans Bend, Australia

Email: pamartin@mines.edu

Abstract

The scattering of long waves by an obstacle in a rigid pipe is considered. Various approximations are obtained. These involve the blockage coefficient, which is a far-field quantity associated with potential flow along the pipe.

Keywords: acoustics, matched asymptotics

1 Introduction

Many years ago, the first author co-authored a paper [4] in which matched asymptotics were used for a two-dimensional waveguide problem. The waveguide occupies the strip $|x| < a$, $-\infty < z < \infty$ in the $xz$-plane. It contains a bounded obstacle $B$ (with boundary $S$) which is assumed to be symmetric about the line $z = 0$. A low-frequency plane wave is incident on $B$, and is partly reflected and partly transmitted. Thus, with $e^{-ika}$ suppressed, the solution $u$ satisfies

$$u \sim \begin{cases} e^{ikz} + R e^{-ikz}, & z \to -\infty, \\ T e^{ikz}, & z \to \infty, \end{cases}$$

(1)

together with $(\nabla^2 + k^2)u = 0$ in the waveguide, $\partial u/\partial x = 0$ at $x = \pm a$ (the boundary is sound-hard (rigid)) and a boundary condition on $S$. The problem is to estimate the reflection coefficient $R$ and the transmission coefficient $T$, assuming that $ka \ll 1$.

Intuitively, we might expect Laplace’s equation $\nabla^2 u = 0$ to be appropriate near $B$. Indeed, this is part of the story, but not the whole story. Historically, Lamb followed the intuitive path for a hard circular $S$, and he obtained a wrong estimate for $R$, whereas Twersky obtained the correct result some years later; see [4] for details and references.

In [4], two inner problems are identified, one for $\nabla^2 u = 0$, and one for Poisson’s equation, $\nabla^2 u = 1$. The first of these requires the determination of a certain constant, known as the blockage coefficient. This constant is needed in the matching between the outer expansion of the inner solution, and the inner expansion of the outer (wave-like) solution.

More recently, the authors have generalized the basic methods from [4] (which apply to two-dimensional problems with sound-hard obstacles) to three-dimensional problems in which long waves along a rigid cylindrical waveguide interact with an obstacle $B$; the boundary of $B$, $S$, can be hard (rigid, Neumann condition) or soft (Dirichlet condition) [5]. Here, we describe our recent work on rigid obstacles, with some remarks on soft obstacles in section 4.

2 A rigid body in a rigid pipe

Consider a cylindrical pipe of infinite length containing an obstacle $B$. Both the pipe’s wall and the boundary of $B$ are rigid. Assume that $B$ is symmetric about the plane $z = 0$, where the $z$-axis is along the pipe. The solution $u$ satisfies (1). In [5], estimates for $R$ and $T$ are obtained:

$$R = D_a - D_n, \quad T = 1 + D_s + D_n$$

where

$$D_s = \frac{i\kappa M}{1 - i\kappa M}, \quad D_n = \frac{i\kappa L}{1 - i\kappa L},$$

$\kappa = ka$, $a$ is defined by equating the pipe’s cross-sectional area to $\pi a^2$, $M = -|B|/(2\pi a^3)$ and $|B|$ is the volume of the body $B$. The quantity $L$ is the blockage coefficient; see section 3.

The approximations found for $R$ and $T$ satisfy known constraints, $|R|^2 + |T|^2 = 1$ and $RT^\ast + RT = 0$, exactly, where the $\ast$ denotes complex conjugation. They also agree with rigorous long-wave asymptotic approximations for a sphere in a pipe of circular cross-section [2].

3 The blockage coefficient

The blockage coefficient $L$ is a dimensionless constant defined uniquely by solving a boundary-value problem for a potential $\Phi$: $\nabla^2 \Phi = 0$ in the pipe, the normal derivative $\partial \Phi/\partial n = 0$ on the pipe’s wall and on $S$, and $\Phi$ satisfies

$$\Phi = (z/a) \pm L + o(1) \quad \text{as} \quad z \to \pm \infty; \quad (2)$$

for a hard circular obstacle $B$ of sectional area $\pi a^2$ in a hard cylindrical waveguide $S$ of axial length $L = 2\pi a/\kappa$.

Suggested members of the Scientific Committee:

Bojan Guzina, David Hewett, Vincent Pagneux
the far-field conditions (2) eliminate an arbitrary additive constant. We see that \( \Phi \) is the velocity potential for uniform flow along the pipe; \( L \) can be regarded as giving a measure of the obstruction, or blockage, to the flow caused by the presence of the body in the pipe.

In order to use our simple approximations for \( R \) and \( T \), we need \( L \), but we do not want to solve the full boundary-value problem for \( \Phi \): it is complicated! If the pipe is a circular cylinder (a tube) we could contemplate solving a boundary integral equation over \( S \) using Green’s function for the tube [3].

We do have Hurley’s useful exact formula [1]

\[
L = \frac{1}{2\pi a^2} \int_S \Phi \frac{\partial z}{\partial n} \, dS, \tag{3}
\]

where the normal vector on \( S \) points outwards. This formula relates the far-field quantity \( L \) to \( \Phi \) evaluated on \( S \), a near-field quantity.

If \( B \) is small (with diameter small compared to the diameter of the pipe’s cross-section), we could replace \( \Phi \) in (3) by the corresponding potential for flow past \( B \) in an infinite fluid. Doing this works well; see [5] for examples.

For thin objects in a tube, such as a rigid disc in the plane \( z = 0 \), approximations can be developed using dual integral equations when the centre of the disc is on the axis of the tube. Of interest are situations where the disc almost blocks the tube, leaving a small gap between the edge of the disc and the tube wall; see [6].

Suppose now that \( B \) is slender and aligned with the flow; for example, \( B \) could be a prolate spheroid with its axis along the \( z \)-axis. Such geometries recall Webster’s horn equation: for waves along a rigid pipe of slowly-varying cross-section (the horn), the three-dimensional wave equation may be approximated by

\[
\frac{1}{A(z)} \frac{\partial}{\partial z} \left( A(z) \frac{\partial u}{\partial z} \right) = \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2}, \tag{4}
\]

where \( A(z) \) is the cross-sectional area at station \( z \); the derivation of (4) assumes that the horn is rigid, with \( \partial u/\partial n = 0 \) on the boundary. We can use (4) for wave propagation along the pipe containing a slender body \( B \); in this context, \( A(z) \) is the area of the annular fluid cross-section. When applied to the estimation of \( L \) (no dependence on \( t \)), we obtain an ordinary differential equation; solving it gives

\[
L = \frac{1}{2a} \int \frac{\pi a^2 - A(z)}{A(z)} \, dz, \tag{5}
\]

note that \( A(z) = \pi a^2 \) outside \( B \). It turns out that this simple formula works remarkably well, and it also gives good approximations when \( B \) almost fills the waveguide; for details and comparisons, see [6].

4 Discussion

We have considered the reflection and transmission of long waves by an obstacle \( B \) in a rigid cylindrical waveguide. For a rigid obstacle, this led us to study the blockage coefficient \( L \). This far-field quantity appears in other related applications of matched asymptotic approximations. Further applications are noted in [6].

The situation for sound-soft obstacles is more complicated: one is required to calculate two additional coefficients, denoted by \( P \) and \( Q \) in [5]; \( P \) is related to the electrostatic capacity of \( B \) in the pipe.

References

Waveguide acoustic black holes: non-helpful and helpful damping mechanisms

Martin Berggren1,∗, Abbas Mousavi 1, Eddie Wadbro2
1Department of Computing Science, Umeå University, Umeå, Sweden
2Department of Mathematics and Computer Science, Karlstad University, Karlstad, Sweden
∗Email: martin.berggren@cs.umu.se

Abstract
Motivated by puzzling experimental results for a waveguide acoustic black hole, we investigate through computations which sources of damping that are significant for a successful function of the device. As opposed to analogous structural devices, the addition of damping material towards the end of the device has essentially no effect. Our results suggest instead that damping at the outer tube in combination with visco-thermal boundary-layer losses are the most critical sources of damping.

Keywords: waveguide, acoustic black hole

1 Introduction
Mironov [3] introduced a broad-band damping device for a beam or plate, usually referred to as an acoustic black hole, which very efficiently damps vibrations above a given critical frequency. A gradual tapering of the structural thickness causes a decrease in wave velocity and an increase in amplitude, which means that a small amount of damping material at the thin side can effectively dampen the vibrations.

An analogous device for guided wave propagation in air has been suggested and analyzed by Mironov and Pislyakov [4]. The experimental investigations by El Ouahabi et al. [5] of this type of device gave quite surprising results. The performance, in terms of the reflection coefficient at the inlet, agrees reasonably well with predictions [4] even without explicitly added damping material. However, unlike the structural counterpart, the addition of damping material at the device’s peripheral end does not significantly improve performance (figure 1).

Here we systematically investigate, through numerical simulations, the relative importance of possible sources of damping in this device, and we suggest likely candidates for the most important damping mechanisms. All numerical investigations are carried out by solving the Helmholtz equation for the acoustic pressure in

\[ \nabla^2 p_c - \frac{\omega^2}{c^2} p_c = 0 \]

where \( \omega \) is the angular frequency of the incident wave and \( c \) is the speed of sound.

2 Non-helpful damping
The idea behind the design of figure 2 is to slow the propagation speed and increase the wave amplitude as the wave progresses towards the right end. Theory predicts an operational range for frequencies \( f \geq f_{\text{crit}} = \frac{c}{L} \sim 425 \text{ Hz} \) [2], where \( c \) is the speed of sound. In analogy to structural black holes, it seems reasonable to focus on damping effects at the end of the device. We therefore consider a surface-impedance boundary condition at \( \Gamma^R \), a wooden wall in the experiments, and simulate damping materials in the last cavity through a Rayleigh-damping model. As can be seen in figure 3, we note a complete failure of this setup to provide any damping.

Suggested members of the Scientific Committee:
Vincent Pagneux, Manfred Kaltenbacher

Figure 1: Measured reflection coefficients (data from El Ouahabi et al. [5], used with permission)

Figure 2: The axisymmetric acoustic black hole

2D axial symmetry for the geometry illustrated in figure 2. A simple radiation condition at \( \Gamma^L \) imposes a right-traveling planar wave and absorbs reflected planar waves. We restrict the analysis to the frequency range below the first higher (circumferential) mode at 866 Hz.
in the predicted operational range. Even very aggressive damping in this region has no helpful effect above $f_{\text{crit}}$.

3 A somewhat helpful damping effect

Due to the radial rings, the device contains a quite large area of sound-hard material. It is therefore reasonable to expect losses due to visco-thermal boundary-layer effects. To account for these, we use the model devised by Berggren et al. [1], which, in cylindrical symmetry, models these effects through the boundary condition

$$-\delta V \frac{i}{2} \nabla T \cdot (r \nabla T p) + \delta T k^2 (i - 1)(\gamma - 1) \frac{1}{2} r p + r \frac{\partial p}{\partial n} = 0,$$

where $\gamma$ is the heat capacity ratio, $k$ the wavenumber, $\delta V$ and $\delta T$ the wave-number-dependent viscous and thermal boundary-layer thicknesses, and $\nabla T$ the tangential gradient operator. Including also these losses, in addition to the previous, we indeed obtain a discernible effect on the reflections, as is clear from figure 4.

4 A crucially helpful damping effect

As designed by Mironov and Pislyakov [4], the purpose of the concentric rings in figure 2 is to provide an increasingly compliant wall admittance. Indeed, this property holds reasonably well for low frequencies. However, the cavities are deep enough to cause a more complicated wall-admittance load at higher frequencies. A combined compliant/inertial effect creates local resonances in the cavities, located progressively further from the far end the higher the frequency, explaining why damping material towards the end has no effect. The high localized sound pressures in the ring cavities likely generate losses at the outer (plastic) tube, a conjecture supported by the reflection spectrum in figure 5, where a small amount of surface damping also has been added to the outer tube. Although we lack data to make a quantitatively accurate prediction, our results supports the hypothesis that the main sources of damping that makes the waveguide acoustic black hole work is a combination of losses at the outer tube and visco-thermal boundary-layer losses. A natural next step would be to apply numerical optimization to the geometry and the location of supplemental damping to further improve performance.

References

Thermoviscous acoustic propagation in thin rough tubes

Henri Boutin$^1$, Juliette Chabassier$^2$, Thomas Hélie$^1$, Alexis THIBAULT$^2,*$

$^1$3SAM team, STMS, 1 place Igor Stravinsky, 75004 Paris – France
$^2$MAKUTU team, Inria Bordeaux Sud–Ouest, 200 avenue de la Vieille Tour, Talence – France

*Email: alexis.thibault@inria.fr

Abstract

Thermoviscous acoustic propagation in a tube with corrugated isothermal rigid walls is considered. At long wavelengths, it amounts to a 1D transmission line equation, in which the coefficients depend on the solution to a 2D diffusion problem. These coefficients are shown to display predictable behaviors at low, high, and intermediate frequencies. These results are demonstrated on a numerical example.

Keywords: roughness, thermoviscous acoustics, scale separation, losses

1 Introduction

Wind instruments made out of wood often exhibit small-scale detail (roughness) on the inner wall. It has been shown experimentally to modify the effective dissipation and dispersion of acoustic waves in the air inside the instrument [2]. However, this phenomenon is usually neglected in musical acoustics models.

This work proposes a computation method for thermoviscous acoustics in a thin tube with a rough (here, grooved) wall. It consists in separating the acoustic propagation, which occurs mostly in the longitudinal direction $z$ (1D), from the viscous and thermal diffusion, which occurs mostly in the transverse directions (2D).

2 Long wavelength approximation

We consider a simplified rough tube, represented by a domain $\Omega = \Sigma \times \mathbb{R}$, where the cross-section $\Sigma \subset \mathbb{R}^2$ is the union of a disk of radius $R = 7.45$ mm, with smaller disks of radius $R_{\text{rough}} = 0.16$ mm intersecting its boundary, spaced by $w = 0.3$ mm (see Figure 1).

We assume that the acoustic velocity $\hat{u}$, pressure $\hat{p}$, density and temperature are solutions to the time-harmonic linearized Navier-Stokes equations in $\Omega$, with no-slip and isothermal boundary conditions. Assuming that the acoustic wavenumber $\lambda = 2\pi c_0/\omega$ (where $c_0$ is the isentropic sound velocity, and parameter $\omega > 0$ is the angular frequency) is much larger than both the tube radius $R$ and the viscous and thermal characteristic lengths, then the pressure $\hat{p}(z)$ and total flow $\hat{U}(z) = \int_{\Sigma} \hat{u}(x, y, z) \cdot e_z \, dx \, dy$ are solution to a 1D transmission line equation [3]

\[
\begin{cases}
\frac{d}{dz} \hat{p}(z) + |\Sigma| \hat{U}(z) = 0, \\
\frac{d}{dz} \hat{U}(z) + Y_t \hat{p}(z) = 0.
\end{cases}
\]

(1)

with $Z_v = \frac{1}{\kappa} \frac{\omega \rho_0}{\mu C_p}$, $Y_t = (1 + (\gamma - 1) K_t) \frac{\omega |\Sigma|}{\rho_0 c_0^2}$, where $\rho_0$ is the static density, $|\Sigma|$ is the cross-section area, and the coefficients $K_v = 1 - (\psi_{\beta_v})$, $K_t = 1 - (\psi_{\beta_t})$, quantify the influence of the viscous and thermal effects respectively, and would be zero in the lossless case. Constants $\beta_v = \mu / \rho_0$ and $\beta_t = \kappa / \rho_0 C_p$ are related to the viscous and thermal diffusion rates, and $(\psi_{\beta})$ is the mean over $\Sigma$ of the solution $\psi_{\beta}$ to a heat equation on the cross-section

\[
\begin{cases}
i\omega \psi_{\beta}(x, y) - \beta \Delta \psi_{\beta}(x, y) = -\beta |\Sigma| & \text{on } \Sigma \\
\psi_{\beta}(x, y) = 0 & \text{on } \partial \Sigma.
\end{cases}
\]

(2)

We propose to solve the equations sequentially, by first calculating the solutions $\psi_{\beta_v}$ and $\psi_{\beta_t}$ of the transverse problem (§3-4), and then by using the resulting values of $K_v$ and $K_t$ to solve the transmission line equation (§5).

3 Analysis in the harmonic domain at low, high and medium frequency

Since the solution $\psi_{\beta}$ of the transverse problem depends on the frequency, so do $K_v$ and $K_t$. Since $K_v$ and $K_t$ are equal up to a frequency scaling factor of $\beta_v / \beta_t = \mu C_p / \kappa = 0.71$ for air, only $K_v$ is considered hereafter.

In the low frequency limit, $\psi_{\beta}$ tends to zero and therefore $\lim_{\omega \to 0} K_v = 1$. In the high frequency limit, boundary layers form in the vicinity of the walls, with thickness $\delta = \sqrt{\beta / \omega}$, and $\psi_{\beta}$ quickly approaches 1 away from the boundaries [1]. One can show that the influence of the boundary layers is asymptotically

\[
K_v(\omega) = (1 - i) \frac{|\Sigma|}{2\omega} \sqrt{\frac{\beta_v}{2\omega}} + o(\omega^{-1/2}).
\]

(HF rough)
This suggests that increasing the perimeter-to-area ratio $|\partial \Sigma|/|\Sigma|$ should increase the amount of losses. Moreover, in the high-frequency limit, thermal and viscous effects contribute equally to dispersion (real part) and dissipation (imaginary part).

As the frequency decreases, the boundary layer thickness may exceed the characteristic size $R_{\text{rough}}$ of the asperities. We would thus expect $K_v$ to follow approximately equation (HF rough), but with a frequency-dependent effective perimeter length. If $R_{\text{rough}} \ll R$, a regime should appear where $\Sigma$ can be approximated as a disk:

$$K_v(\omega) \approx (1 - i) \frac{2}{R} \sqrt{\frac{\beta_v}{2\omega}}.$$  

(HF smooth)

4 Numerical calculations: 2D problem

Equation (2) is solved on a 2D mesh representing a small triangular portion of domain $\Sigma$. The domain is virtually symmetrized by using Neumann conditions on the cutting lines. Calculations are performed using high-order finite element library Montjoie. Elements of order 8 are used, leading to a relative $L^2$ error lower than $2 \times 10^{-4}$ at all frequencies.

The solution $\psi_{\beta_v}$ is computed at 30 frequencies with geometric progression spanning $6 \times 10^{-4}$ Hz to 20 kHz. The dependency of $K_v$ with respect to frequency is plotted in figure 2, together with the asymptotes predicted by equation (HF rough) for a smooth tube and for the considered rough tube.

The three regimes predicted in the previous section are visible: the low-frequency asymptote below $10^{-2}$ Hz (below human hearing, 20 Hz-20 kHz), the high-frequency asymptote (HF rough) above 1 kHz, and a region from $10^{-1}$ Hz to $10^1$ Hz where $K_v$ is close to the "smooth tube of same radius" approximation (HF smooth).

5 Solving the transmission line equations

System (1) is solved for the values of $K_v(\omega)$ and $K_t(\omega)$ computed in §4, using high-order 1D finite elements [4]. Assuming that the tube is closed with condition $\hat{U}(L) = 0$ at $L = 238.5$ mm, and driven with unit flow $\hat{U}(0) = 1$, we compute the acoustic impedance $Z = \hat{p}(0)/\hat{U}(0)$. The result is plotted in figure 3 for the rough tube and for a smooth circular tube of same radius.

We observe a resonance around 1430 Hz, which remain of finite amplitude because of the dissipation. The roughness appears to lower the quality factor of the resonance, and to shift the resonance frequency down by about 3Hz.

6 Perspectives

A first perspective is to extend the results from the time-harmonic domain to the Laplace and the time domain, in view of using the theory of diffusive representations to provide time-domain simulations of rough tubes. A second perspective is to consider the case of tapered tubes, which encompass more musical instruments.

References

Multipole-model approximation of the equivalent fluid model equations for porous media in the time domain

Ilyes Moufid\textsuperscript{1,2,*}, Denis Matignon\textsuperscript{1}, Rémi Roncen\textsuperscript{2}, Estelle Piot\textsuperscript{2}

\textsuperscript{1}ISAE-SUPAERO - Université de Toulouse, 31055 Toulouse, France
\textsuperscript{2}ONERA, The French Aerospace Laboratory - Université de Toulouse, 31055 Toulouse, France
\textsuperscript{*}Email: ilyes.moufid@onera.fr

Abstract

The equivalent fluid model (EFM) describes the acoustic properties of rigid porous media by defining it as a fluid with an effective density \( \rho_{eq} \) and an effective compressibility \( C_{eq} \). These physical quantities are complex-valued functions depending on frequency, and are irrational due to their behaviour at the high and low frequency limits. Hence, the system of equations derived from the EFM is first expressed in the Fourier domain, and can involve fractional derivatives in the time domain. Here, an approach is presented to formulate the EFM equations in the time domain, leading to a system with additional differential equations, on which an energy method is used to prove its stability under certain conditions.

Keywords: porous media, equivalent fluid model, multipole model, stability conditions.

1 Introduction

This work focuses on the equations of the EFM:

\[
\begin{align*}
\rho_{eq}(s) s \hat{u} + \nabla \cdot \hat{p} &= 0, \\
C_{eq}(s) s \hat{p} + \nabla \cdot \hat{u} &= 0,
\end{align*}
\]

where \( u \) and \( p \) are defined on \( (0, \infty) \times \Omega \), with \( \Omega \subseteq \mathbb{R}^n \), \( f \) denotes the Laplace transform of \( f \) and \( s \) is the complex variable. In order to reformulate these equations in the time domain, recent studies have used the additional differential equations (ADE) method \cite{1}, approximating \( \rho_{eq} \) and \( C_{eq} \) by rational functions of \( s \) or using the oscillatory-diffusive (OD) representation method \cite{2}, based on a pole and cut technique \cite{3}.

Choosing to approximate \( \rho_{eq} \) and \( C_{eq} \) by rational functions or by using the OD representation approach leads, in both cases, to write their discrete expressions using multipole models.

\[
\rho_{eq}(s) = \rho_{\infty} \left(1 + \sum_{k=1}^{N} \frac{r_k}{s - s_k}\right),
\]

\[
C_{eq}(s) = C_{\infty} \left(1 + \sum_{k=1}^{M} \frac{l_k}{s - q_k}\right).
\]

On that account, the following work is based on \( \rho_{eq} \) and \( C_{eq} \) approximated as above.

2 Time-domain representation of the EFM

It is assumed here that the studied porous media have a purely dissipative behaviour, hence all parameters \( r_k, l_k, s_k \) and \( q_k \) of \( \rho_{eq} \) and \( C_{eq} \) are real. Then, using expressions (2) and (3), system (1) becomes:

\[
\begin{align*}
\rho_{\infty} \hat{u} + \nabla \cdot \hat{p} &= 0, \\
C_{\infty} \hat{p} + \nabla \cdot \hat{u} &= 0.
\end{align*}
\]

However, as suggested by Xie et al. for a Biot model \cite{4}, it can also be rewritten as follows, which can ease the numerical computation.

\[
\begin{align*}
\rho_{\infty} \hat{u} + \nabla \cdot \hat{p} &= 0, \\
C_{\infty} \hat{p} + \nabla \cdot \hat{u} &= 0.
\end{align*}
\]

In order to compare these two equivalent systems in the time domain, the inverse Laplace transform is applied. This leads to a new set of equations containing causal convolution. To compute them, additional variables, \( \varphi_k \) and \( \psi_k \) for system (4), \( \varphi_k^* \) and \( \psi_k^* \) for system (5), are introduced. Therefore, the global systems for (4) and (5) read:

\[
\begin{align*}
\partial_t \hat{u} + \frac{1}{\rho_{\infty}} \nabla \cdot \hat{p} &= -\sum_{k=1}^{N} r_k \varphi_k, \\
\partial_t \hat{p} + \frac{1}{C_{\infty}} \nabla \cdot \hat{u} &= \sum_{k=1}^{M} l_k \psi_k, \\
\partial_t \varphi_k + \frac{1}{\rho_{\infty}} \nabla \cdot \hat{u} &= s_k \varphi_k - \sum_{k=1}^{N} r_k \varphi_k, \\
\partial_t \psi_k + \frac{1}{C_{\infty}} \nabla \cdot \hat{u} &= q_k \psi_k - \sum_{k=1}^{M} l_k \psi_k.
\end{align*}
\]
\[
\begin{align*}
\partial_t \mathbf{u} + \frac{1}{\rho_\infty} \nabla p &= -\sum_{k=1}^{N} r_k \mathbf{u} - \sum_{k=1}^{N} r_k s_k \phi_k^* , \\
\partial_t p + \frac{1}{C_\infty} \nabla \cdot \mathbf{u} &= -\sum_{k=1}^{M} l_k p - \sum_{k=1}^{M} l_k q_k \psi_k^* , \\
\delta \phi_k^* &= s_k \phi_k^* + \mathbf{u} , \\
\delta \psi_k^* &= q_k \psi_k^* + \rho_\infty .
\end{align*}
\]

In (7), there are no spatial derivatives in the ADE, compared to (6). Hence, when the system is discretized with a numerical scheme based on fluxes, these fluxes depend on the velocity and pressure variables, but not on the additional variables. Consequently, the problem to solve at each mesh interface does not grow with the number of additional variables. Moreover, for problems with multiple subdomains (porous media and air domain), there are no additional fluxes to manage for the interface between them.

3 Stability analysis

Hereafter, a stability analysis of system (7) is performed thanks to an energy functional defined below:

\[ E(t) = \rho_\infty E_u(t) + C_\infty E_p(t) , \]

where \[ E_u = \frac{1}{2} \int_{\Omega} \| \mathbf{u} \|^2 \, dx - \frac{1}{2} \sum_{k=1}^{N} r_k s_k \int_{\Omega} \| \phi_k^* \|^2 \, dx , \]

and \[ E_p = \frac{1}{2} \int_{\Omega} \rho_\infty \rho_\infty \| \mathbf{u} \|^2 \, dx - \frac{1}{2} \sum_{k=1}^{M} l_k q_k \int_{\Omega} (\delta \psi_k^*)^2 \, dx . \]

It is straightforward to take its derivative:

\[
\frac{dE}{dt} = -\rho_\infty \sum_{k=1}^{N} r_k \int_{\Omega} (\partial_t \phi_k^*)^2 \, dx \\
- C_\infty \sum_{k=1}^{M} l_k \int_{\Omega} (\partial_t \psi_k^*)^2 \, dx \\
- \int_{\partial \Omega} (p \mathbf{u}) \cdot \mathbf{n} \, ds .
\]

From these equations, combined with the fact that \(\rho_\infty\) and \(C_\infty\) are necessarily positive, we impose the following sufficient conditions on the parameters:

\((C_1)\) the weights \((r_k, l_k)_k\) are positive,
\((C_2)\) the poles \((s_k, q_k)_k\) are negative.

Hence, \(E\) is positive-definite and decreasing without external contributions at the boundary of the domain \(\Omega\). Thus, under these conditions, \(E\) describes an energy functional for (7), that enables to ensure the stability of the system without external inputs.

A numerical application with a Discontinuous Galerkin (DG) scheme was carried out to apply previous results.

Figure 1: Normalized energy over time in a 2D domain for different multipole-model parameters approximating a toy model and an initial Gaussian field for \(\mathbf{u}\) and \(p\). Increasing parts of the energy are marked in red.

Furthermore, these 2 conditions are met by several approximated models describing \(p_{\text{eq}}\) and \(C_{\text{eq}}\) for a realistic range of physical parameters. Indeed, the OD representation of the JCAPL model or the Horoshenkov model can be discretized in the form of (2) and (3) with parameters verifying the conditions \((C_1)\) and \((C_2)\).

4 Conclusion

This work formulates the EFM equations for porous media in the time domain, with the functions \(p_{\text{eq}}\) and \(C_{\text{eq}}\) described by a set of weights and poles. In addition, a proof of stability is given under certain conditions on the sign of these weights and poles. In order to apply the theoretical results obtained, a DG scheme was implemented in 2D [5].

Acknowledgment

This research has been financially supported by ONERA and by ISAE-SUPAERO, through the EUR TSASE under grant ANR-17-EURE-0005.

References

Efficient numerical solvers for frequency- and time-domain electromagnetic simulation, optimization and design

Oscar P. Bruno\textsuperscript{1,*}

\textsuperscript{1}Computing and Mathematical Sciences, Caltech, Pasadena, USA
\textsuperscript{*}Email: obruno@caltech.edu

Abstract

We present a family of numerical methods for the solution of the acoustic and electromagnetic wave equations, with application to simulation, optimization, and design. In particular, a novel rectangular-polar integral equation solver will be described which can produce solutions to the time harmonic Helmholtz and Maxwell’s equations, with high order accuracy, for general 2D and 3D structures, with an extension to time domain problems on the basis of a time re-centering synthesis technique. An effective integral equation acceleration method, the IFGF method (Interpolated Factored Green Function) will be presented which, without recourse to the FFT, and, thus, lending itself to effective distributed memory parallelization, evaluates the action of Green function-based integral operators for an N-point surface discretization at a computational cost of $O(N \log N)$ operations. A number of computational illustrations, including applications to photonic optimization and design problems, will be presented.

Keywords: Fast Integral Equation Solvers, Frequency and Time Computational Electromagnetics, Photonic Device Simulation and Optimization

1 Scattering solvers and applications

We present a range of methodologies developed recently for the solution of the frequency domain and time domain Maxwell and acoustic wave equations, with application to the simulation of wave propagation and scattering by a variety of structures and media, as well as analysis, optimization, and design of photonic structures. In particular, a novel rectangular-polar high-order integral-equation solver will be discussed which can produce accurate solutions to the Helmholtz and Maxwell’s equations, with high order accuracy, for general two- and three-dimensional structures in the frequency domain\cite{4,8} and, by additionally exploiting a time windowing-and-recentering Fourier-time synthesis technique\cite{1}, in the time domain as well. Associated optimization and design methods\cite{7,9} will be demonstrated, including mention of the fabricated and tested grating demultiplexer device introduced in\cite{10}. An enabling technique underlying these design applications, the Windowed Green Function method (WGF)\cite{5–7}, will be mentioned.

An effective integral acceleration technique, the IFGF (Interpolated Factored Green Function)\cite{2} will be presented which, without recourse to the Fast Fourier Transform (FFT), evaluates the action of Green function-based integral operators for surface discretization containing N points at an $O(N \log N)$ computing cost, instead of the $O(N^2)$ cost associated with unaccelerated methods. The IFGF algorithm, which is well suited for treatment of extremely large scattering problems, exploits the slow variations of certain “factored Green functions” and thus enables the fast evaluation of fields generated by groups of sources on the basis of a recursive interpolation scheme. Owing in part to its independence from the FFT, the IFGF is amenable to efficient parallelization on massively parallel computers. But the parallel IFGF approach is effective on small computers as well: a recent IFGF-accelerated parallel implementation\cite{8} of the combined IFGF and rectangular-polar method\cite{4} will be presented, which, based on the OpenMP programming interface can be used to tackle problems of scattering by large engineering structures on small parallel computer nodes. For example, on the basis of a 28-core computing node, full scattering solutions with several digits of accuracy can be obtained for realistic engineering structures of the order of one hundred wavelengths in size in computing times of the order of a few minutes per iteration and a few tens of iterations of the GMRES iterative solver; see e.g. Figure 1.

A massively parallel implementation of the IFGF algorithm\cite{3}, in turn, will also be presented which relies on both the Message Passing Interface (MPI) and OpenMP. This hybrid
parallel IFGF implementation, which is suitable for implementation in modern high-performance computing (HPC) systems, provides excellent parallel efficiency without limitations in the size of the computer system used. In recent test cases, for example, an ellipsoid 4,096 wavelengths in diameter (resp. a sphere 1,389 wavelengths in diameter) containing approximately 400 million discretization points (resp. 1.610 billion points) was considered, for which the discrete forward operator was evaluated with an error of $1.5 \cdot 10^{-2}$ (resp. $4.0 \cdot 10^{-3}$), requiring, in both cases, a computing time of under one hour in a 30-node, 1,680-core parallel cluster, with a memory requirement of 30 GB per node (resp. 125 GB per node).

In all, the Green function methods presented, which are based on a small set of basic underlying ideas, span a wide range of applications, problem complexity, computer architectures and varied capabilities.

![Figure 1: Upper left image group: High-order rectangular-polar integral solver [4] on a patch geometry (upper left), IFGF acceleration box- and-cone octree [2] (upper right), nacelle geometry (lower left) and nacelle patch description (Lower right). Lower left, center and right images: Total field magnitude $|u(x)| = |u_i(x) + u_s(x)|$ under point source incidence (lower left and center) and 82-wavelength plane-wave incidence (right) [8]. Details can be appreciated by enlarged pdf viewing.](image)

References


Optical cloaking refers to making an object invisible by preventing the light scattering in some directions as it hits the object. There is interest in developing devices in radar and other applications. Developing a model to accurately capture cloaking comes with numerical challenges, however. We must determine how light propagates through a medium composed by multiple, in layers of materials with different electromagnetic properties. In this paper, we consider a \textit{ulti}-layered scalar transmission problem in 2D and use boundary integral equation methods to compute the field. The Kress product quadrature rule [2] is used to approximate singular integrals evaluated on boundaries, the Boundary Integral Equation Formulation \textit{(RIE)} method [1] with Periodic Trapezoid Rule \textit{(PTR)} is employed to treat nearly singular \textit{(BRIE)} method [2] with the PTR, we also treat singular members of the Scientific Committee.

\section*{Abstract}

\textbf{Problem Setting}

\textbf{Boundary Integral Equation System}

\textbf{Keywords:} boundary integral methods, close evaluation, multi-layered media

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{Sketch and notations for the problem.}
\end{figure}

\begin{equation}
\begin{aligned}
\vartheta_m(x) &= - D_{j-1,1} u_j + \frac{\varepsilon_j}{\varepsilon_{j-1}} S_{j-1,1} \partial_n u_{j-1} \\
&+ D_{j,j} u_j - S_{j,j} \partial_n u_j \quad \text{in } \tilde{\mathcal{L}}_j,
\end{aligned}
\end{equation}

Above, \( D_{i,j} \) and \( S_{i,j} \) represent the double-layer potential and single-layer potential, respectively, defined on \( \Gamma_i \) for \( i = j - 1, j \), evaluated in \( L_j \):

\begin{align*}
D_{i,j}[u_j](x) &= \int_{\Gamma_i} \frac{\partial \Phi_i}{\partial n}(x,y) u_j(y) d\sigma_y, \quad x \in \tilde{\mathcal{L}}_j \\
S_{i,j}[\partial_n u_j](x) &= \int_{\Gamma_i} \Phi_i(x,y) \partial_n u_j(y) d\sigma_y, \quad x \in \tilde{\mathcal{L}}_j
\end{align*}

with the fundamental solution to the Helmholtz equation \( \Phi_i(x,y) := \frac{i}{4} H_0^{(1)}(k_i|x-y|) \) with \( H_0^{(1)} \) denoting the Hankel function of first kind. We also write \( u_0 = u^{in} + D_{00}[u_0] - S_{00}[\partial_n u_0] \) and \( u_N = -D_{N-1,N}[u_{N-1}] + \frac{\varepsilon_{N-1}}{\varepsilon_N} S_{N-1,N}[\partial_n u_{N-1}] \).

As long as one knows the traces and normal traces \( (u_j(y), \partial_n u_j(y)) \) for \( y \in \Gamma_j \), then one can evaluate the solution of the problem everywhere. To that aim, we solve the boundary integral equation (BIE) system shown below (obtained by evaluating the above representations on the boundaries and using known layer potential properties) [2].

\section{Near-Boundary Evaluation with BRIE}

To treat singularities in the BIE system, we use the Kress product quadrature rule [2]. Using the BRIE method with the PTR, we also treat
the nearly singular integrals in (1) close to the boundaries. To use BRIEF [1], we consider auxiliary functions \( \psi_j \), \( j \in [0, N - 1] \):

\[
\psi_j(x) = u_j(x_j^b)g_j(x) + \partial_n u_j(x_j^b)f_j(x), \quad x \in L_j,
\]

with \( g_j \) and \( f_j \) satisfying the associated Helmholtz equation in \( L_j \) with the boundary conditions \( g_j(x_j^b) = 1 \), \( \partial_n g_j(x_j^b) = 0 \), \( f_j(x_j^b) = 0 \), \( \partial_n f_j(x_j^b) = 1 \), with \( x_j^b \in \Gamma_j \), the point on the boundary closest to \( x = (x_1^b + n\ell, \ell \neq 0) \). Using Green’s identities, we subtract the nearly singular behaviors using \( \psi_j \) as follows:

\[
\begin{align*}
\psi_j(x) &= \psi_j - D_{j-1,j} [u_{j-1} - \psi_{j-1}] \\
&\quad + \frac{\varepsilon_j}{\varepsilon_{j-1}} S_{j-1,j} [\partial_n u_{j-1} - \partial_n \psi_{j-1}] \\
&\quad + D_{j,j} [u_j - \psi_j] - S_{j,j} [\partial_n u_j - \partial_n \psi_j].
\end{align*}
\]

As illustrated in Figures 2-3 the error (or the field’s amplitude) is reduced at the vicinity of the boundaries with BRIEF. The incident field is a plane wave with angle \( \alpha = \frac{\pi}{4} \) and for the discretization a body-fitted grid with 100 points on each boundary and 100 points along the radial direction was used.

Figure 2: Absolute log error for standard solution (left) and BRIEF solution (right) for homogeneous case, where boundaries are circles of radii 2 and 1.

5 Ongoing Work

Future goals include reducing the time needed to generate multi-layered models, which will be done with parallel computing; investigating relevant applications with effects on the solvability of the BIE system. In particular, in order to efficiently simulate optical cloaking, we will consider different electromagnetic properties [3] and different (non convex) boundary shapes. One can also create lossy cloaking devices. In that case, one choose some \( k_j \in \mathbb{C} \) with \( \Im(k_j) > 0 \), and other quadratures than Kress will be needed to preserve accuracy. Extensions to 3D will also be considered.

Acknowledgements. E.C. is supported by the UC Merced Eugene Cota-Robles Fellowship. C.C. acknowledges support from the National Science Foundation Grant DMS-1819052.

References


Coupled Single-Trace Formulations with Volume Integral Operators for Acoustic Transmission Problems

Ignacio Labarca\textsuperscript{1,}\textsuperscript{*}, Ralf Hiptmair\textsuperscript{1}
\textsuperscript{1}Seminar for Applied Mathematics, ETH Zürich, Zürich, Switzerland
\textsuperscript{*}Email: ignacio.labarca@sam.math.ethz.ch

Abstract

We study acoustic transmission problems in two dimensions with a bounded inhomogeneity. By means of defining reference constant coefficients, a representation formula for the exterior and interior domains is derived. The latter contains a volume integral operator, related to the one in the Lippmann-Schwinger equation. Following the approach of first and second-kind single-trace formulations (STF), a block operator is obtained and discretized. Numerical experiments confirm the convergence of the method and show its potential for high-contrast problems and scatterers with small inhomogeneities.

Keywords: integral equations, volume integral operators, boundary integral operators, single-trace formulations, acoustic transmission problems.

1 Introduction

We are interested in solving the acoustic wave transmission problem in presence of an inhomogeneous medium of compact support $\Omega \subset \mathbb{R}^2$ with Lipschitz boundary $\Gamma := \partial \Omega$. Material properties are given by functions $a : \mathbb{R}^2 \to \mathbb{R}$ and $\kappa : \mathbb{R}^2 \to \mathbb{C}$ where

$$a(x) \equiv 1, \kappa(x) \equiv \kappa_0 \in \mathbb{C}$$

for $x \in \mathbb{R}^2 \setminus \Omega$. The equation governing the problem of finding the total wave $u_{\text{tot}} := u + u_{\text{inc}}$ in the whole space is

$$\text{div}(a(x) \nabla u_{\text{tot}}(x)) - \kappa(x)^2 u_{\text{tot}}(x) = 0,$$

for $x \in \mathbb{R}^2$, where $u$ is the scattered field that satisfies radiation conditions

$$\lim_{r \to \infty} r \left( \frac{\partial u}{\partial r} - i \kappa_0 u \right) = 0,$$

and $u_{\text{inc}}$ corresponds to an incident field that satisfies

$$-\Delta u_{\text{inc}}(x) - \kappa_0^2 u_{\text{inc}}(x) = 0,$$

for $x \in \mathbb{R}^2$.

2 Volume Integral Equations

We can rewrite (2) as

$$-\Delta u_{\text{tot}} - \kappa_0^2 u_{\text{tot}} = \text{div}(\alpha \nabla u_{\text{tot}}) + \beta u_{\text{tot}},$$

where $\alpha(x) := a(x) - 1, \beta(x) := \kappa(x)^2 - \kappa_0^2$. The right-hand side of (5) is now a compactly supported function. Let $N_0$ denote the Newton potential for the Helmholtz equation with wavenumber $\kappa_0 \in \mathbb{C}$. It is possible to obtain from (5) the following integral equation, typically known as the Lippmann-Schwinger equation

$$u_{\text{tot}} - \text{div}N_0(\alpha \nabla u_{\text{tot}}) - N_0(\beta u_{\text{tot}}) = u_{\text{inc}},$$

where $u_{\text{tot}} \in H^1(\Omega)$. Fredholmness of equation (6) has been studied in [2, 4], with remarkable limitations for the case $\alpha \in C^1(\Omega)$ instead of $C^1(\mathbb{R}^2)$.

3 Single-Trace Formulations

If we focus on the constant coefficients case, a useful approach to solve transmission problems requires boundary integral equations. Based on a representation formula for the interior and exterior domains

$$u = S_I(\partial_n^- u) - D_I(\gamma^- u), \quad \text{in } \Omega,$$

$$u = -S_0(\partial_n^+ u) + D_0(\gamma^+ u), \quad \text{in } \mathbb{R}^2 \setminus \Omega,$$

where $\gamma^\pm, \partial_n^\pm$ denote exterior/interior Dirichlet and Neumann trace operators, $S_I$ and $D_I$ are the layer potentials for the Helmholtz equation with wavenumber $\kappa_j, j = 0, 1$. By taking traces on the representation formula, we obtain the following identities

$$\left( \frac{1}{2} I - A_I \right) \left( \frac{\gamma^- u}{\partial_n^- u} \right) = 0,$$

$$\left( \frac{1}{2} I + A_0 \right) \left( \frac{\gamma^+ u}{\partial_n^+ u} \right) = 0,$$

with $A_j$ the Calderón operator with $\kappa_j, j = 0, 1$. By enforcing transmission conditions in (7), we
obtain
\[
\left( \frac{1}{2} I - A_1 \right) \left( \gamma^- \frac{\partial}{\partial_n} u \right) = 0, \tag{8}
\]
\[
\left( \frac{1}{2} I + A_0 \right) \left( \gamma^- \frac{\partial}{\partial_n} u \right) = \left( \frac{\gamma u_{\text{inc}}}{\partial_n u_{\text{inc}}} \right).
\]
First-kind STF is obtained by subtracting the expressions in (8):
\[
(A_0 + A_1) \left( \gamma^- \frac{\partial}{\partial_n} u \right) = \left( \gamma u_{\text{inc}} \right). \tag{9}
\]
Second-kind STF is obtained by adding them:
\[
(I + A_0 - A_1) \left( \gamma^- \frac{\partial}{\partial_n} u \right) = \left( \frac{\gamma u_{\text{inc}}}{\partial_n u_{\text{inc}}} \right). \tag{10}
\]

The appropriate functional setting for both equations has been previously studied in [1,3].

4 Coupled STF-VIE

In the presence of a compactly supported source \( f \) in the right-hand side of the Helmholtz equation, the representation formula reads
\[
u = S_1(\partial^-_n u) - D_1(\gamma^- u) + N_1(f), \tag{11}
\]
for \( \mathbf{x} \in \Omega \). We define reference coefficients
\[
a_1 := \frac{1}{|\Gamma|} \int a(\mathbf{x}) d\mathbf{x}, \quad \kappa_1 := \frac{1}{|\Gamma|} \int \kappa(\mathbf{x}) d\mathbf{x}.
\tag{12}
\]
This definition reduces the problem to the constant coefficient case of Section 3 when \( a \) and \( \kappa \) are constant functions. Following the approach from the STF and denoting
\[A := N_1(\text{div}(\alpha_1 \nabla u) + \beta_1 u),\]
where \( \alpha_1(\mathbf{x}) := a(\mathbf{x}) - a_1, \beta_1(\mathbf{x}) := \kappa(\mathbf{x})^2 - \kappa_1^2 \),
we can derive an extended version of the first-kind STF
\[
\begin{pmatrix}
M^{-1} A_0 M + A_1 \\
-D_1
\end{pmatrix}
\begin{pmatrix}
\gamma A \\
I - A
\end{pmatrix}
\begin{pmatrix}
\gamma^- u \\
\frac{\partial}{\partial_n u}
\end{pmatrix}
= \begin{pmatrix}
\gamma u_{\text{inc}} \\
\partial_n u_{\text{inc}}
\end{pmatrix},
\tag{13}
\]
in \( H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma) \times H^1(\Omega) \), where
\[
M = \begin{pmatrix}
1 & 0 \\
0 & a
\end{pmatrix}.
\]
Similarly, an extended version of the second-kind STF can be derived.

These new formulations have some properties that make them desirable to be studied and compared with existing alternatives. We discuss:

- (a) Well-posedness of the continuous and discrete formulations.
- (b) Robustness of the formulation.
- (c) Limit cases: boundary integral equations.
- (d) Conditioning of the resulting matrix.

5 Numerical Experiments

Several numerical experiments illustrate the capabilities of our proposed formulations. We discretize with low-order finite elements on the boundary and in the domain. We study errors in the \( L^2(\Omega) \) and \( H^1(\Omega) \) norms.

Figure 1: Scattering by a disk.

References


Volume integral equations on fractal domains and the Koch snowflake transmission problem

Joshua Bannister\textsuperscript{1,*}, Andrew Gibbs\textsuperscript{1}, David P. Hewett\textsuperscript{1}
\textsuperscript{1}Department of Mathematics, University College London, London, UK
\textsuperscript{*}Email: joshua.smith.14@ucl.ac.uk

Abstract
We study volume integral equation (VIE) reformulations of the inhomogeneous Helmholtz equation with piecewise constant refractive index on inhomogeneities with rough, possibly fractal, interface. We focus in particular on the case of scattering by the Koch snowflake. To obtain a numerical approximation we replace the inhomogeneity by a smoother “prefractal” approximation, and solve the VIE on the prefractal using piecewise constants on a suitable triangulation. Using the concept of Mosco convergence we prove the convergence of the corresponding Galerkin approximations on the prefractals to the true solution of the VIE on the fractal in the joint limit as the pre-fractal level \( j \to \infty \) and mesh width \( h \to 0 \). We discuss the relationship between the convergence rate of the method and the Hausdorff dimension of the fractal boundary and present supporting numerical results.

Keywords: Helmholtz transmission problem, Volume integral equation, Mosco convergence

1 Motivation
We recall the classical Helmholtz transmission problem in \( \mathbb{R}^d, d = 2, 3 \): given wavenumbers \( k_i, k_e > 0 \), an incident plane wave \( u^{inc} = e^{ik_e x} \), \( |d| = 1 \), and a bounded Lipschitz open set \( D \subset \mathbb{R}^d \), find an interior field \( u_i \in H^1(D) \) and an exterior field \( u_e \in H^{1,loc}(\mathbb{R}^d \setminus \overline{D}) \) such that
\[
\begin{align*}
\Delta u_i + k_i^2 u &= 0 \quad \text{in } D, \\
\Delta u_e + k_e^2 u &= 0 \quad \text{in } \mathbb{R}^d \setminus \overline{D},
\end{align*}
\]
\[
\begin{align*}
u_e &= u_i \quad \text{on } \partial D, \\
\partial_n u_e &= a \partial_n u_i \quad \text{on } \partial D,
\end{align*}
\]
where \( a > 0 \) is a coupling constant, and the scattered field \( u_s = u - u^{inc} \) satisfies the Sommerfeld radiation condition (SRC) at infinity. For bounded Lipschitz \( D \), the problem (1)-(4) is well-posed, and can be recast as a system of boundary integral equations (BIEs) on \( \partial D \) \cite{1}, which, when \( \partial D \) is piecewise smooth, can be solved numerically using the boundary element method.

![Figure 1: Scattering of a plane wave by the Koch snowflake, with \( k_e = 30 \) and \( k_i = 45 \).](image)

However, for general non-Lipschitz \( D \), such as the Koch snowflake, which has fractal boundary, the transmission problem (1)-(4) and its BIE reformulation no longer make sense, because one does not in general have well-defined Dirichlet and Neumann trace operators on \( \partial D \).

The question we investigate in this work is: how can we pose “transmission problems” on such sets, and how can we efficiently approximate their solutions numerically?

2 Inhomogeneous Helmholtz equation and VIE reformulation
For general bounded open \( D \subset \mathbb{R}^d \) with \( |\partial D| = 0 \), in place of the transmission problem (1)-(4) we seek a solution \( u \in H^{1,loc}(\mathbb{R}^d) \) of the inhomogeneous Helmholtz equation
\[
\Delta u + k_e^2 n(x) u = 0,
\]
with refractive index
\[
n(x) = \begin{cases} 
  k_i^2 / k_e^2, & x \in D, \\
  1, & x \in \mathbb{R}^d \setminus \overline{D},
\end{cases}
\]
such that the scattered wave \( u^{sca} = u - u^{inc} \), which should satisfy the equation
\[
\Delta u^{sca} + k_e^2 n(x) u^{sca} = k_e^2 f,
\]
where $f = (1-n)u^{inc}$, satisfies the SRC at infinity. The problem is well-posed (by a standard Riesz-Fredholm theory argument), and can be reformulated equivalently as a VIE on $D$ via the Lippmann-Schwinger equation (LSE) (cf. [3–6]):

$$ (I + k^2 V (1-n)) u^{eca} = F, \quad \text{on } D, \quad (7) $$

where $V$ is the Newton potential, defined by

$$ V\phi(x) = \int_D \Phi(x,y) \phi(y) \, dy, \quad \phi \in L^2(D), $$

with $\Phi$ denoting the fundamental solution of $(\Delta + k^2)u = 0$, and $F = -k^2 V f$. It is well known that $V : L^2(D) \to H^2(G)$ is bounded, and hence $V : L^2(D) \to L^2(G)$ is compact, for any bounded open $D, G \subset \mathbb{R}^n$. Hence the LSE operator is a compact perturbation of the identity operator on the space $L^2(D)$, and by the well-posedness of (5) and the equivalence of the latter with (7), equation (7) is well-posed.

3 Discretization and numerical analysis

To discretize (7) we replace $D$ by a polygonal or polyhedral “prefractal” approximation $D_j$, and then compute an approximate solution $u^{eca}_j$ of (7), with $D$ replaced by $D_j$, using a Galerkin piecewise constant approximation on a convex mesh of $D_j$. To prove convergence of $u^{eca}_j$ to $u^{eca}$ we use the notion of Mosco convergence, which implies convergence of Galerkin solutions for operators that are compact perturbations of coercive operators [2].

**Definition 1** Let $W$ and $W_j$, for $j \in \mathbb{N}$, be closed subspaces of a Hilbert space $H$. We say $W_j$ Mosco converges to $W$ if

(i) $\forall w \in W, \exists w_j \in W_j, j \in \mathbb{N}, s.t\:
\|w - w_j\|_H \to 0 \text{ as } j \to \infty$;

(ii) if $\{W_{ja}\}$ is a subsequence of $\{W_j\}$ and $w_{ja} \in W_{ja}$ with $w_{ja} \to w$, then $w \in W$.

Applying this definition with $H = L^2(B)$ for some ball $B$ containing $D$ and $D_j$, we can prove Mosco convergence of $L^2(D_j)$ to $L^2(D)$, and hence of $u^{eca}_j$ to $u^{eca}$, under quite general conditions on the prefraactal approximations $D_j$.

When $D_j \subset D$ for each $j$ we also have asymptotic quasi-optimality, so that for sufficiently large $j$ the Galerkin error can be controlled in terms of the best approximation error of $u \in L^2(D)$ by elements $v_h$, for which we have

$$ \|u - v_h\|_{L^2(D)} \leq \|u\|_{L^2(D \setminus \overline{D_j})} + \|u - v_h\|_{L^2(D)}. $$

Hence the best approximation error comprises two parts - the first due to the approximation of $D$ by $D_j$, and the second due to the approximation of $u$ on $D_j$ by a piecewise constant function. Since $u \in H^1(D)$, we have the standard bound

$$ \|u - v_h\|_{L^2(D_j)} \leq \frac{h_j}{\pi} \|u\|_{H^1(D)}, $$

where $h_j$ is the maximum mesh width on $D_j$, and since $u \in H^2(D) \subset C(\overline{D})$ we have

$$ \|u\|_{L^2(D \setminus \overline{D_j})} \leq \|D \setminus \overline{D_j}\|^{1/2} \|u\|_{C(\overline{D})}. $$

The magnitude of $|D \setminus \overline{D_j}|$ depends on the fractal dimension of the boundary $\partial D$, which affects how well it can be approximated by polygons/polyhedra. For the particular case of the Koch snowflake we investigate the corresponding errors for different choices of $D_j$ and $h_j$, including the standard prefractional approximations (unions of triangles), and the “pixelizations” commonly used in VIE solvers e.g. VINES [6].

References


Homogenization of a thin layer of randomly distributed nano-particles: effective model and error estimates

Amandine Boucart\textsuperscript{1}, Sonia Fliss\textsuperscript{1}, Laure Giovangigli\textsuperscript{1,*}

\textsuperscript{1}Department of Applied Mathematics, Poems, ENSTA, IP Paris, Palaiseau, France.
*Email: laure.giovangigli@ensta-paris.fr

Abstract
We study the time-harmonic scattering by a heterogeneous object covered with a thin layer of randomly distributed nanoparticles. We propose, via a multi-scale asymptotic expansion of the solution, an effective model where the layer of particles is replaced by an equivalent boundary condition. Under the assumption that the particles are distributed given a stationary and ergodic random point process, we prove that the so-called corrector problems are well-posed and establish quantitative error estimates between the original and effective solutions.

Keywords: Stochastic homogenization

1 Introduction
Let us consider an infinite plane, denoted $\Sigma_0 := \{x_d = 0\}$, covered by a thin layer of width $\varepsilon h_L$ of randomly distributed particles $\mathcal{P}_\varepsilon^\omega$ of size $\varepsilon$.

Let $D_\varepsilon^\omega := \mathbb{R}^{d-1} \times \mathbb{R}^+ \setminus \mathcal{P}_\varepsilon^\omega$ be the half space above $\Sigma_0$ outside the particles $\mathcal{P}_\varepsilon^\omega$ for a given distribution.

For a given source function $f \in L^2(D_\varepsilon^\omega)$ whose support lies far away from the layer, we look for the solution $u_\varepsilon^\omega$ of the Helmholtz equation

$$-\Delta u_\varepsilon^\omega - k^2 u_\varepsilon^\omega = f \quad \text{in } D_\varepsilon^\omega,$$

where $k$ is the wavenumber. The infinite plane models a multilayer object through a Robin boundary condition

$$\nabla u_\varepsilon^\omega \cdot e_d = \gamma u_\varepsilon^\omega \quad \text{on } \Sigma_0,$$

where $\gamma \in \mathbb{C}$ is such that $\text{Im} [\gamma] > 0$. At the boundary of the particles $\partial \mathcal{P}_\varepsilon^\omega$, we impose to the field either a homogeneous Dirichlet condition

$$u_\varepsilon^\omega = 0 \quad \text{on } \partial \mathcal{P}_\varepsilon^\omega,$$

or a homogeneous Neumann boundary condition

$$\nabla u_\varepsilon^\omega \cdot n = 0 \quad \text{on } \partial \mathcal{P}_\varepsilon^\omega.$$

Finally, the problem formulation has to be completed by a radiation condition.

Let $L$ denote the infinite strip $L := \mathbb{R}^{d-1} \times [\delta, h_L + \delta]$ where $\delta > 0$. Let $\{x_n\}_n^\omega$ denote the point process corresponding to the centers of the particles. Let $B(x_n^\omega)$ be the particle with radius 1 centered at $x_n^\omega$. We suppose that $\{x_n\}_n^\omega$ is stationary and ergodic and that the particles lie in $L$ at least at a distance of $\delta$ from one another. We introduce $\mathcal{P}_\varepsilon^\omega := \bigcup_n B(x_n^\omega)$ the set of particles in $L$ and $\mathcal{P}_\varepsilon^\omega := \bigcup_n B(x_n^\omega)$ the set of particles of size $\varepsilon$ in the rescaled strip $L^\varepsilon := \varepsilon L$.

2 A formal asymptotic expansion
Let $D_\varepsilon^\omega := \mathbb{R}^{d-1} \times (0, \varepsilon H) \setminus \mathcal{P}_\varepsilon^\omega$ and $D_{\varepsilon H, \infty} := \mathbb{R}^{d-1} \times [\varepsilon H, +\infty)$ for a given $H > 0$.

We propose the following Ansatz for $u_\varepsilon^\omega$:

$$u_\varepsilon^\omega(x) = \sum_{n \in \mathbb{N}} \varepsilon^n \left[ U_n^\omega, NF \left( x_\varepsilon, x_d \right) + U_n^\omega, FF \left( x_\varepsilon \right) \right] \text{ in } D_{\varepsilon H, \infty}$$

$$= \sum_{n \in \mathbb{N}} \varepsilon^n U_n^\omega, NF \left( x_\varepsilon, x_d \right) \text{ in } D_{\varepsilon H, \infty}.$$

The so-called far-field terms $U_n^\omega, FF$ depend only on the macroscopic variable $x := (x_\varepsilon, x_d)$ and the so-called near-field terms $U_n^\omega, NF$ depend on the tangential components $x_n$ of $x$ and on the microscopic variable $y := x/\varepsilon$.

We impose that, $\forall n \in \mathbb{N}$, $U_n^\omega, NF$ verifies for all $x_n \in \mathbb{R}^{d-1}$

- $\forall y_\omega \in \mathbb{R}^{d-1}$, $\lim_{\|y_\omega\| \to +\infty} U_n^\omega, NF (x_n; y_\omega, y_d) = 0$ a.s.,
- $\forall y_d \in \mathbb{R}^+$, $(\omega, y_d) \mapsto U_n^\omega, NF (x_n; y_\omega, y_d)$ stationary.

After injecting the development into the equations verified by $u_\varepsilon^\omega$, we obtain for all $n \in \mathbb{N}$

- $U_n^\omega, FF$ verifies:

$$\forall x \in D_{\\varepsilon, H} := \Omega - \Delta U_n^\omega, FF (x) - k^2 U_n^\omega, FF (x) = \varepsilon f, \quad (1)$$

and the radiation condition.

- $U_n^\omega, NF$ satisfies a Laplace-type problem parametrized by $x_\varepsilon$ and set in an infinite half-space.
with a Robin bc on $\Sigma_0$ and either a Dirichlet or Neumann bc on $\partial P_\omega$. This problem depends on $U_{n-1,\omega}^{\gamma,\alpha,FF}$ and the far-field terms $u_n^{\omega,FF}$ and $u_n^{\omega,FF}$.

We still need to determine a boundary condition for $u_n^{\omega,FF}$ on $\Sigma_\epsilon H$. This condition will arise as a necessary condition for the existence and uniqueness of the near-field terms.

3 Dirichlet boundary condition on $\partial P_\omega$

Let $D_\omega := \mathbb{R}^{d-1} \times (0, H) \setminus \mathbb{R}^{d-1} \times (H, +\infty)$. In order to study the well-posedness of the problem verified by $U_{n,\omega}^{\gamma,\alpha,FF}$ for $n = 0, 1, 2$ we consider the following problem: we look for a $y_\omega$-stationary solution $U^{\omega}$ to

$$
\begin{cases}
\Delta U^{\omega} = \nabla \cdot G_1^{\omega} & \text{in } D^{\omega} \\
\nabla U^{\omega} \cdot n = G_2^{\omega} & \text{on } \Sigma_0 \\
U^{\omega} = 0 & \text{on } \partial D^{\omega} \\
\left[\nabla U^{\omega} \cdot n\right]_H = G_3^{\omega}
\end{cases}
$$

(2)

We suppose here that $G_1, G_2$ and $G_3$ are $y_\omega$-stationary processes $\mathcal{S}$. $G_1^{\omega} \in L^2(\Omega, L^2(D^{\omega}))$, $G_2^{\omega} \in L^2(\Omega \times \Sigma_0)$, $G_3^{\omega} \in L^2(\Omega \times \Sigma_H)$, $\omega \in (2, +\infty)$. We introduce the following space: $H_0 := \{a.s. \ U^{\omega} = H_1(\Omega, D^{\omega})\} \\
\forall y_\omega \in \mathbb{R}^+, (\omega, y_\omega) \mapsto 1_D - U^{\omega}(y_\omega, y_\omega)$ stationary, $U^{\omega} = 0$ on $\partial D^{\omega}$.

Under additional assumptions on $\{x_n\}_{n \in \mathbb{N}}$, $H_0$ can be proven to be a Hilbert space. [2]

Theorem 1 In this setting, there exists a unique solution $U$ in $H_0$ to (2). Moreover, there exists $c \in \mathbb{R}$ s.t. a.s. $\lim_{y_\omega \to +\infty} U^{\omega} = c$.

By imposing that a.s. $\lim_{y_\omega \to +\infty} U_{n,\omega}^{\gamma,\alpha,FF} = 0$, we get $u_0^{\omega,FF} |_{\Sigma_\epsilon H} = 0$ and $u_1^{\omega,FF} |_{\Sigma_\epsilon H} = c_0^{(1)} \partial_{\alpha} u_0^{\omega,FF} |_{\Sigma_\epsilon H}$ where $c_0^{(1)}$ is the limit at $+\infty$ of a profile function solution of (2).

4 Neumann boundary condition on $\partial P_\omega$

We study the existence and uniqueness of $U_{n,\omega}^{\gamma,\alpha,FF}$ for $n \leq 2$. First $U_{1,\omega}^{\gamma,\alpha,FF} := U_{1,\omega}^{\gamma,\alpha,FF} - u_1^{\omega,FF}$ verifies

$$
\begin{cases}
-\Delta U_{1,\omega}^{\gamma,\alpha,FF} = 0 & \text{in } D^{\omega} \\
\nabla U_{1,\omega}^{\gamma,\alpha,FF} \cdot n = -\gamma u_0^{\omega,FF} |_{\Sigma_\epsilon H} & \text{on } \Sigma_0 \\
\nabla U_{1,\omega}^{\gamma,\alpha,FF} \cdot \tilde{\gamma} = - \nabla u_0^{\omega,FF} |_{\Sigma_\epsilon H} \cdot n_\epsilon & \text{on } \partial D^{\omega} \\
\left[\nabla U_{1,\omega}^{\gamma,\alpha,FF} \cdot n\right]_H = \partial_{\alpha} u_0^{\omega,FF} |_{\Sigma_\epsilon H}
\end{cases}
$$

(3)

Theorem 2 If the compatibility condition $-\gamma u_0^{\omega,FF} + \partial_{\alpha} u_0^{\omega,FF}$ on $\Sigma_\epsilon H = 0$ holds, then there exists a unique solution $U_{1,\omega}^{\gamma,\alpha,FF}$ to (3) defined up to a constant in $H := \{\tilde{U} \in L^2(\Omega, H^1_\epsilon(D^{\omega})|)$.

$$
\forall y_\omega \in \mathbb{R}^+, 1_D - \nabla U^{\omega}(y_\omega, y_\omega) \text{ stationary, } \\
E \left[\int_0^{+\infty} 1_D |\nabla U^{\omega}|^2 d\gamma_\omega\right] < +\infty
$$

Given a quantitative mixing assumption on $\{x_n\}_{n}$, for $d = 3$, this solution can be constructed to be $y_\omega$ stationary. It then verifies $\lim_{y_\omega \to +\infty} U_{1,\omega}^{\gamma,\alpha,FF} = 0$.

The proof via regularity relies on classical arguments in stochastic homogenization. [3]

Applying a similar method to $U_{2,\omega}^{\gamma,\alpha,FF}$, the compatibility condition gives us the boundary condition for $u_1^{\omega,FF}$ on $\Sigma_\epsilon H$.

$$
\begin{cases}
\nabla u_1^{\omega,FF} \cdot \tilde{\gamma} + \gamma u_1^{\omega,FF} = a^{(2)}_{\alpha_1} u_1^{\omega,FF} + \sum_{i=1}^2 a^{(2)}_{\alpha_i} \partial_{\alpha} u_1^{\omega,FF}. 
\end{cases}
$$

The constants $a^{(2)}$ are computed via profile functions solution of type (3) problems.

5 Effective model and error estimates

$\nu_2(x) := \tilde{u}_0^{\omega,FF} + \varepsilon \tilde{u}_1^{\omega,FF}$ verifies (1), the radiation condition on and $\Sigma_\epsilon H$.

$$(D) - \varepsilon u^{(1)}_\omega \nabla v_2, \tilde{\gamma} + \nu_2 = 0,$$

$$(N) \nabla v_2, \tilde{\gamma} + (\gamma - \varepsilon a^{(2)}_{\alpha_1}) v_2 \cdot \varepsilon \sum_{i=1}^2 a^{(2)}_{\alpha_i} \partial_{\alpha} v_2 = 0.$$

Theorem 3 (Error estimates for Dirichlet) For all $M, R > 0$,

$$
\sup_{R > 0} \mathbb{E} \left[\int_{D_R \setminus M} |v_2 - v_2| d\gamma\right] \leq o(\varepsilon).
$$

Error estimates in the Neumann case are still in progress.

References


Modelling acoustic metasurfaces using homogenization of fluid-structure interaction on strongly heterogeneous perforated plates in thin layers

Eduard Rohan\textsuperscript{1,*}, Vladimír Luke\textsuperscript{2}
\textsuperscript{1}Department of Mechanics, NTIS, Faculty of Applied Sciences, University of West Bohemia, Pilsen, Czech Republic
\textsuperscript{*}Email: rohan@kme.zcu.cz

Abstract
We consider acoustic waves propagating in a so-called transmission layer containing a perforated plate and inviscid fluid. The plate behavior is influenced by a strong heterogeneity of the elasticity in the form of periodically distributed holes and soft inclusions which may induce antiresonance effects well known in acoustic metamaterials. As a particular novelty, we study acoustic perturbations of the permanent flow interacting with the plate modeled using the Reissner-Mindlin theory. The modelling based on the homogenization leads to a 3D-to-2D model reduction of the layer which, in the limit, is represented by an acoustic metasurface. An efficient method is proposed to compute frequency-dependent homogenized coefficients involved in the limit model which are responsible for a strong wave dispersion.

Keywords: acoustic transmission, periodic homogenization, fluid-structure interaction, acoustic metasurface

1 Introduction
We consider a transmission layer $\Omega_3 \subset \mathbb{R}^3$ of the thickness $\delta = \varepsilon \kappa$ with a given fixed $\kappa > 0$, being introduced via its midsurface $\Gamma_0$, see Fig. 1. The solid structure (an elastic perforated plate) $\Sigma'$ is embedded in the layer, such that the acoustic fluid occupies domain $\Omega^e = \Omega_3 \setminus \Sigma'$. The scale parameter $\varepsilon \sim \delta$ characterizes the microstructure sizes (holes and soft elastic inclusions, the resonators), whereby $\varepsilon = \delta / \kappa$, with a given fixed $\kappa > 0$.

The acoustic harmonic wave with the frequency $\omega$ propagating in the layer is described by the acoustic potential $p^e$ in the fluid $\Omega^e$, the corresponding wave in the elastic body is described by the displacement field $u^e$ defined in $\Sigma'$. These fields satisfy the following equations and transmission conditions on the solid-fluid interface $\partial_e \Sigma'$, where $\sigma(u^e)$ is the stress,

$$
c^2 \nabla^2 p^e + \omega^2 p^e - (\theta \omega \partial_w p^e + \tau \partial_w^2 p^e) = 0 \quad \text{in } \Omega^e, \\
\nabla \cdot \sigma(u^e) + \omega^2 \rho u^e = 0 \quad \text{in } \Sigma',
$$

where $\theta = (\tau + 1)/2$, with $\tau = 3$ in 3D, and the derivatives $\partial_w p = w \cdot \nabla p$ and $\partial_w^2 = \partial_w (\partial_w p)$ depend on the steady advection field $w$.

The elastic structure is represented by the Reissner-Mindlin (RM) plate featured heterogeneity, such that it is generated by the representative cell $\Xi = [0,1]^2 \subset \mathbb{R}^2$ as a periodic lattice, where $\Xi = \Xi_S \cup \Xi^* \cup \partial \Xi$. The solid part involves the matrix and the soft inclusions, as treated in [1]. This latter aspect extends the work published in [2], such that vibroacoustic problem is featured by the large contrast in the differential operator associated with the RM plate equation. The weak formulation is constituted by the following variational equalities governing $p^e \in H^1(\Omega^e)$ and $\{u^e, \theta^e\} \in (H^1_0(\Omega))^5$,

$$
c^2 \int_{\Omega^e} \nabla p^e \cdot \nabla q^e - \omega^2 \int_{\Omega^e} p^e q^e + \theta \omega \int_{\Omega^e} \partial_w p^e \partial_w q^e - \tau \int_{\Omega^e} \partial_w^2 p^e \partial_w q^e = 0, \\
- \omega \int_{\Omega^e} \partial_w p^e \partial_w q^e - \tau \int_{\Omega^e} \partial_w^2 p^e \partial_w q^e = 0,
$$

for all $q \in H^1(\Omega^e)$, where $U^e = \overline{u^e} - \varepsilon \kappa \theta^e$, $\zeta \in [-1/2, +1/2]$ determines the displacement within the plate for the transversal position $\varepsilon \kappa \zeta$, being given by the plate kinematics defined in terms of the midsurface displacements $u = (\overline{u}, u_3)$.
and rotations $\theta$, satisfying
\[
\omega^2 \left( \int_{\Gamma^0} \rho u^0 \cdot v^0 + \frac{h^2}{12} \int_{\Gamma^0} \rho \theta^0 \cdot \psi^0 \right) \\
+ \frac{h^2}{12} \int_{\Gamma^0} \left[ E^H \nabla^S \psi^0 + \int_{\Gamma^0} \left[ E^H \nabla^S \mathbf{u}^0 \right] : \nabla^S \vartheta \right] \\
- \frac{1}{\varepsilon h} \int_{\partial_0 \Gamma^0} \left( f^\varepsilon(p^0) \cdot v^0 + \bar{m}^\varepsilon(p^0) \cdot \psi^0 \right) \\
= \frac{1}{\varepsilon h} \int_{\partial_0 \Gamma^0} \left( f^\varepsilon(p^0) \cdot v^0 + \int_{\partial_0 \Gamma^0} \bar{m}^\varepsilon(p^0) \cdot \psi^0 \right),
\]
for all $(v^0, \psi^0) \in (H^1(\Gamma_0))^5$. The r.h.s. terms represent plate loading by $p^0$ on its surface.

2 Homogenized transmission layer

Pursuing analogical upscaling procedure based on the unfolding homogenization, as reported in [2], autonomous cell problems defined in $Y^+$ and $\Xi$, see Fig. 2, are solved for characteristic responses. These are needed to establish the macroscopic problem involving homogenized coefficients. In the context of a global acoustic problem, the homogenized layer model presents a Dirichlet-to-Neumann operator which links the acoustic fluxes $g^0 = \partial_n \tilde{P}$ to the pressure jump $\Delta \tilde{P}$, thus representing transmission conditions on $\Gamma_0$, which involve internal variables $(p^0, u^0, \theta^0)$ satisfying the fluid equation,
\[
\int_{\Gamma_0} \left[ (A \nabla x p^0 + i \omega y^0 B \omega) \cdot \nabla x q^0 - \omega^2 (\zeta^* + M_w) p^0 q^0 \right] \\
+ i \omega \int_{\Gamma_0} q^0 (i \omega T_w q^0 + W \cdot \nabla x p^0) + i \omega \int_{\Gamma_0} q^0 \Delta G^1 \\
+ i \omega \int_{\Gamma_0} q^0 (h H : \nabla^S u^0 + \nabla x q^0 \cdot D a^0) = 0,
\]
for $q^0 \in H^1(\Gamma_0)$, the plate equation
\[
\int_{\Gamma_0} \left( (H^H \nabla x u^0 - \theta^0) \cdot (\nabla x v^0 - \vartheta) \right) \\
+ \frac{h^2}{12} \int_{\Gamma_0} \left( E^H \nabla^S \psi^0 \right) : \nabla^S \vartheta + \int_{\Gamma_0} \left[ E^H \nabla^S \mathbf{u}^0 \right] : \nabla^S \vartheta \\
- i \omega \rho \int_{\Gamma_0} \left[ p^0 H : \nabla^S \psi^0 + \frac{1}{h} v \cdot (D \nabla p^0 + i \omega C g^0) \right] \\
- \omega^2 \int_{\Gamma_0} \left( (\mathbf{M} u^0) \cdot v + \frac{h^2}{12} (\Delta \theta^0) \cdot \vartheta \right) = 0,
\]
satisfied $\forall (v, \theta) \in (H^1(\Gamma_0))^5$ and a coupling condition (for a given scale $\varepsilon_0 > 0$)
\[
\int_{\Gamma_0} \psi (i \omega C \cdot u^0 - i \omega F y^0) = \frac{1}{\varepsilon_0} \int_{\Gamma_0} \psi \Delta \tilde{P}.
\]

References


Effective dynamics for low-amplitude transient elastic waves in a 1D periodic array of non-linear interfaces

Cédric Bellis$^{1,*}$, Bruno Lombard$^1$, Marie Touboul$^1$, Raphaël Assier$^{2,2}$

$^1$Aix Marseille Univ, CNRS, Centrale Marseille, LMA, Marseille, France
$^2$Department of Mathematics, The University of Manchester, Oxford Road, Manchester, UK
$^*$Email: bellis@lma.cnrs-mrs.fr

Abstract
This presentation focuses on the time-domain propagation of elastic waves through a 1D periodic medium that contains non-linear imperfect interfaces, i.e. interfaces exhibiting a discontinuity in displacement and stress governed by a non-linear constitutive relation. In this context, we investigate transient waves with both low-amplitude and long-wavelength, and aim at deriving homogenized models that describe their effective motion.

Keywords: Homogenization – Correctors – Imperfect interfaces – Non-linear waves – Time-domain numerical simulations

1 Objectives
The array of interfaces considered is generated by a, possibly heterogeneous, cell repeated periodically and bonded by interfaces that are associated with transmission conditions of non-linear “spring-mass” type. More precisely, the imperfect interfaces are characterized by a linear dynamics but a non-linear elasticity law. The latter is not specified at first and only key theoretical assumptions are required. To establish an effective model, the two-scale asymptotic homogenization method is deployed, up to the first-order. To begin, an effective model is obtained for the leading zeroth-order contribution to the microstructured wavefield. It amounts to a wave equation with a non-linear constitutive stress-strain relation that is inherited from the behavior of the imperfect interfaces at the microscale. The next first-order corrector term is then shown to be expressed in terms of a cell function and the solution of a linear elastic wave equation. Without further hypothesis, the constitutive relation and the source term of the latter depend non-linearly on the zeroth-order field, as does the cell function. Combining these zeroth- and first-order models leads to an approximation of both the macroscopic behavior of the microstructured wavefield and its small-scale fluctuations within the periodic array.

2 Setting: microstructured configuration
We consider the propagation of transient waves in a 1D periodic elastic medium containing imperfect interfaces. The latter have spacing $h$ and, for simplicity but with no loss of generality, we consider that they are located at $X_n = nh$ with $n \in \mathbb{Z}$. The elastic medium is supposed to be $h$-periodic and linear elastic with mass density $\rho_h(X)$ and Young’s modulus $E_h(X)$. Given a source term $F$, the displacement field $U_h$ is governed by the time-domain wave equation

$$\rho_h(X)\frac{\partial^2 U_h}{\partial t^2}(X,t) = \frac{\partial \Sigma_h}{\partial X}(X,t) + F(X,t)$$

where

$$\Sigma_h(X,t) = E_h(X) \frac{\partial U_h}{\partial X}(X,t),$$

with $\Sigma_h$ being the stress field. Moreover, the interfaces are assumed to be characterized by the interface mass and rigidity parameters $M$ and $K$, respectively, together with the, possibly non-linear, constitutive relation $\mathcal{R}$, so that the following transmission conditions apply at any interface point $X_n$, see [1–4]:

$$M \left\langle \frac{\partial U_h}{\partial t^2}(\cdot, t) \right\rangle_{X_n} = [\Sigma_h(\cdot, t)]_{X_n}, \quad K \mathcal{R} \left\langle [U_h(\cdot, t)]_{X_n} \right\rangle$$

where, for any function $g(X)$, we define the jump and mean operators $\llbracket g \rrbracket_{X_n}$ and $\langle g \rangle_{X_n}$ as

$$\llbracket g \rrbracket_{X_n} = g(X_n^+) - g(X_n^-),$$

$$\langle g \rangle_{X_n} = \frac{1}{2} \left( g(X_n^+) + g(X_n^-) \right).$$

In addition, both the displacement $U_h$ and the stress field $\Sigma_h$ are continuous on the open intervals $(X_n, X_{n+1})$. 
3 Main homogenization results

We now consider a reference wavelength λ∗ and introduce the following parameters

\[ k^* = \frac{2\pi}{\lambda^*} \quad \text{and} \quad \eta = hk^*, \]  

where \( k^* \) being the reference wavenumber. In this study it is assumed that \( \eta \ll 1 \) and that the source term \( F \) is of relatively low-amplitude (an issue that will be discussed). The objective is to derive an effective dynamical model, up to the first-order, for the waves propagating in the periodic interface array considered. More precisely, we seek an approximation \( U^{(1)} \) of the solution \( U_h \) to (1–2) of the form:

\[ U_h(X, t) = U^{(1)}(X, t) + o(h). \]

The main results of this study is that the sought-after approximation is given by

\[ U^{(1)}(X, t) = U_0(X, t) + hU_1(X, t), \]  

where the zeroth-order field \( U_0 \) in (5) is continuous and is solution of the problem

\[ \rho_0 \frac{\partial^2 U_0}{\partial t^2}(X, t) = \frac{\partial \Sigma_0}{\partial X}(X, t) + F(X, t) \]

with

\[ \Sigma_0(X, t) = \mathcal{G}_0(X, t)). \]

Here, \( \mathcal{E}_0 = \partial U_0/\partial X \) and \( \mathcal{G}_0 \) is an effective strain-stress relation that is local and, generally speaking, non-linear, while \( \rho_0 \) is an effective mass density. Moreover, the first-order corrector field \( U_1 \) in (5) can be written as

\[ U_1(X, t) = \mathcal{U}_1(X, t) + \mathcal{P}(y, \mathcal{E}_0(X, t)) \mathcal{E}_0(X, t) \]

with \( y = (X - nh)/h \) for \( X \in (nh, (n+1)h) \) and where the cell function \( \mathcal{P} \) is, generally speaking, a non-linear function of \( \mathcal{E}_0 \). The mean field \( \overline{U}_1 \) is solution to the linear problem:

\[ \rho_0 \frac{\partial^2 \overline{U}_1}{\partial t^2}(X, t) = \frac{\partial \overline{\Sigma}_1}{\partial X}(X, t) + \mathcal{S}(U_0(X, t)) \]

with

\[ \overline{\Sigma}_1(X, t) = \mathcal{G}_0(X, t)) \overline{\Sigma}_1(X, t), \]

where \( \overline{\Sigma}_1 = \partial \overline{U}_1/\partial X \), while both the parameter \( \mathcal{G}_0(X, t)) \), which is the derivative of \( \mathcal{G}_0 \), and the source term \( \mathcal{S}(U_0(X, t)) \) depend explicitly on the zeroth-order field, locally in space and time, and in a non-linear fashion.

Particularizing for a prototypical non-linear interface law and in the cases of a homogeneous periodic cell and a bilaminated one, the behavior of the obtained models will then be illustrated on a set of numerical examples and compared with full-field simulations. Both the influence of the dominant wavelength and of the wavefield amplitude will be investigated numerically, as well as the characteristic features related to non-linear phenomena.

References


High-frequency homogenisation in periodic media with imperfect interfaces and elastodynamic co-dipole metachusters

Marie Touboul\textsuperscript{1,*}, Raphael Assier\textsuperscript{1}, Bruno Lombard\textsuperscript{2}, Cédric Bellis\textsuperscript{2}, Philip Cotterill\textsuperscript{1}, David Nigro\textsuperscript{3}, William Parnell\textsuperscript{1}

\textsuperscript{1}Department of Mathematics, The University of Manchester, Oxford Road, Manchester, M13 9PL, UK
\textsuperscript{2}Aix Marseille Univ, CNRS, Centrale Marseille, LMA, Marseille, France
\textsuperscript{3}Thales UK, 350 Longwater Avenue, Reading, Berkshire RG2 6GF

Abstract

This work will tackle two independent issues that are of interest in the framework of metamaterials which take advantage of a specific structure of the material in order to control the propagation of waves at a macroscopic scale. Metamaterials are usually divided into two categories: periodic media at high frequency usually named phononic crystals and locally resonant metamaterials that allow the occurrence of bandgaps at lower frequencies and with no need of periodicity.

(i) In a first part, the concept of high-frequency homogenisation, which is relevant in the framework of phononic crystals, is extended to the case of one-dimensional periodic media with imperfect interfaces of the spring-mass type.

(ii) The framework of the second part is local resonances for non-periodic configurations in full elasticity. We study the manner by which the dipole resonance arising from a soft-in-rigid configuration is affected by coupling and geometry when several scatterers are in close proximity.

Keywords: (i) High-frequency homogenisation, Periodic media, Imperfect interfaces
(ii) Elastodynamic metamaterials, Dipole resonance, Metachusters

1 High-frequency homogenisation in periodic media with imperfect interfaces

Phononic crystals are exactly described by the Floquet-Bloch theory that provides the exact relation of dispersion that can be solved numerically. This allows to describe the occurrence of bandgaps that are intervals of frequency in which wave propagation is forbidden.

However, the wave fields associated with these short wavelengths can also present large evolution lengths and this information is not directly accessible by the Floquet-Bloch approach. The concept of high-frequency homogenisation \cite{1-3} allows to study this question of large scale modulation of wave fields with short wavelengths. This concept is extended to the case of one-dimensional periodic media with imperfect interfaces of the spring-mass type. In other words, when considering the propagation of elastic waves in such media, discontinuities are allowed across the borders \( X_n \) of the periodic cell for the displacement \( U_h \) and the stress \( E_h \) as follows:

\[
[U_h]_{X_n} = \frac{1}{K} \left( E_h \frac{dU_h}{dX} \right)_{X_n}, \tag{1}
\]

\[
[E_h \frac{dU_h}{dX}]_{X_n} = -M \omega^2 \left( U_h \right)_{X_n}, \tag{2}
\]

with \( \omega \) the frequency, \( [\cdot] \) and \( \langle \cdot \rangle \) the jump and the mean value across the interface, and \( M \) and \( K \) the mass and stiffness characterizing the imperfect interface.

The homogenisation is carried out about the periodic and antiperiodic solutions corresponding to the edges of the Brillouin zone. Due to the discontinuities at the interfaces, the zeroth-order eigenvalue problem obtained is unusual since the eigenvalue also appears in the boundary conditions. This requires to introduce a tailored inner product to prove the symmetry and non-negativity of the associated operator.

Asymptotic approximations are provided for both the branches of the dispersion diagram (second order) and the resulting wave field (leading order, see Figure 1). Compared to the usual homogenisation, the main difference is that the macroscopic variable is the amplitude of the eigen-mode associated to the edges of the Brillouin zone instead of the displacement field itself.

The case of two branches of the dispersion diagram intersecting with a non-zero slope at an edge of the Brillouin zone (occurrence of a so-called Dirac point) is also considered, result-
ing in an approximation of the dispersion diagram (first-order) and the wave field (zeroth-order) near these points. Finally, a uniform approximation valid for both Dirac and non-Dirac points is provided. Numerical comparisons are made with the exact solutions obtained by the Bloch-Floquet theory. Convergence measurements are carried out on the wave fields to validate the approach. For both the wave field and the dispersion relation (see Figure 2), we show that the uniform approximation remains a very good approximation even far from the edges of the Brillouin zone.

Figure 2: Exact dispersion diagram (plain lines) and homogenized approximations (dotted lines). (left): single approximation. (right): uniform approximation

2 Elastodynamic co-dipole metaclusters

In the framework of metamaterials, resonances are of great interest since they allow to reach a subwavelength response and do not require periodicity compared to phononic crystals. In elasticity, a dipole resonance was first studied in [4] in which a rigid core inclusion is placed in a softer layer of silicone rubber itself placed in a hard epoxy matrix. The concept of metacluster introduced in [5] takes advantage of a collection of scatterers in order to tune the far-field response due to some incident field. In [6], a metacluster of voids leading to a monopole resonance, i.e. voids in an elastic matrix which has a bulk modulus much greater that its shear modulus, is studied and it is shown that the configuration of circular cylin-
drical voids can have a significant effect on the resonant frequency and the far-field response. In the present work, we extend the latter study for coated cylinders of circular cross-section that present the physical contrasts of [4], and consequently give rise to a dipole resonance. More precisely, we study the manner by which the resonance arising from this soft-in-rigid configuration in close proximity is affected by coupling, i.e. multiple scattering. In particular, we show that by modifying the configuration of the metacluster, e.g. reducing the distance between them, the resonance can be enhanced. Therefore, the scattering amplitude and the directionality can be tailored and tuned playing on the geometry of the configuration. Such metaclusters could then be used in the design of elastodynamic metamaterials in order to control both wave propagation and effective properties.

References

Design of a mode converter using thin resonant ligaments

Lucas Chesnel1,∗, Jérémy Heleine1, Sergei A. Nazarov2
1Inria, UMA/Ensta Paris, Institut Polytechnique de Paris, Palaiseau, France
2Saint-Petersburg State University, St. Petersburg, Russia
∗Email: lucas.chesnel@inria.fr

Abstract
The goal of this work is to design an acoustic mode converter. The wave number is fixed so that two modes can propagate. We explain how to construct geometries such that the energy of the modes is completely transmitted and additionally the mode 1 is converted into the mode 2 and conversely.

Keywords: acoustic waveguide, mode converter, asymptotic analysis, thin resonators, scattering coefficients, complex resonance

1 Setting of the problem
To create our mode converter, we work in a specific geometry that we start by describing.

![Figure 1: Geometry of the waveguide $\Omega^\varepsilon$.](image)

Define the domains $\Pi_{\pm} := \{(x, y) \in \mathbb{R}^2 \mid (\pm x, y) \in (1/2; +\infty) \times (0; 1)\}$, connect them by two thin non intersecting ligaments $L_{\pm}^\varepsilon$ of constant width $\varepsilon > 0$ and finally set (see Figure 1)

$$\Omega^\varepsilon := \Pi_- \cup L_-^\varepsilon \cup L_+^\varepsilon \cup \Pi_+.$$

Considering the propagation of acoustic waves in $\Omega^\varepsilon$ leads us to study the problem

$$\begin{align*}
\Delta u^\varepsilon + k^2 u^\varepsilon &= 0 & \text{in } \Omega^\varepsilon \\
\partial_{\nu} u^\varepsilon &= 0 & \text{on } \partial \Omega^\varepsilon.
\end{align*}$$

We fix $k \in (\pi; 2\pi)$ so that only the modes

$$w_1^\pm(x, y) = e^{\pm ik_1 y} \varphi_1(y), \quad w_2^\pm(x, y) = e^{\pm ik_2 y} \varphi_2(y)$$

with $\varphi_1(y) = 1/\varepsilon$, $\varphi_2(y) = \sqrt{2} \cos(\pi y)$ and $k_1 = k$, $k_2 = \sqrt{k^2 - \pi^2}$, can propagate. We are interested in the solutions to the diffraction problem (1) generated by the incoming waves $w_1^+, w_2^+$ in the channel $\Pi_-$. They admit the decompositions

$$u_1^\varepsilon = w_1^+ \circ s^+ + \sum_{j=1}^{2} r_{1j}^\varepsilon w_j^- \circ s^+ + \ldots \text{ in } \Pi_-$$

$$u_2^\varepsilon = w_2^+ \circ s^+ + \sum_{j=1}^{2} r_{2j}^\varepsilon w_j^- \circ s^+ + \ldots \text{ in } \Pi_-.$$

Here the shifts $s^+(x, y) = (x \pm 1/2, y)$ are introduced only to simplify notation below and $r_{ij}^\varepsilon, t_{ij}^\varepsilon \in \mathbb{C}$ are reflection and transmission coefficients. Moreover ellipsis stand for remainders which decay exponentially at infinity. We define the reflection and transmission matrices

$$R^\varepsilon := \begin{pmatrix} r_{11}^\varepsilon & r_{12}^\varepsilon \\ r_{21}^\varepsilon & r_{22}^\varepsilon \end{pmatrix}, \quad T^\varepsilon := \begin{pmatrix} t_{11}^\varepsilon & t_{12}^\varepsilon \\ t_{21}^\varepsilon & t_{22}^\varepsilon \end{pmatrix}.$$

In general, due to the geometrical features of $\Omega^\varepsilon$, almost no energy of the incident waves passes through the thin ligaments $L_{\pm}^\varepsilon$ and one observes almost complete reflection (see Figure 2). More precisely, as $\varepsilon$ tends to zero, one gets

$$R^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + o(1), \quad T^0 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} + o(1).$$

Our goal is to show that by choosing carefully the parameters defining the thin ligaments, we can get almost complete transmission of energy of the incident waves $w_1^+, w_2^+$ and additionally, we can ensure that all the energy carried by the incident mode 1 is transferred on the mode 2 only and vice versa. More precisely, we establish that as $\varepsilon$ tends to zero, we can have

$$R^\varepsilon = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + o(1), \quad T^\varepsilon = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + o(1).$$

2 Exploiting symmetry
To diminish the number of parameters to play with, we assume that $\Omega^\varepsilon$ is symmetric with respect to $(Oy)$. Then we set $\omega^\varepsilon := \{(x, y) \in \Omega^\varepsilon \mid x < 0\}$. Introduce the two problems

$$\begin{align*}
\Delta u_N^\varepsilon + k^2 u_N^\varepsilon &= 0 & \text{in } \omega^\varepsilon \\
\partial_{\nu} u_N^\varepsilon &= 0 & \text{on } \partial \omega^\varepsilon.
\end{align*}$$
\[
\begin{align*}
\Delta u_\epsilon + k^2 u_\epsilon & = 0 \quad \text{in } \omega^\epsilon \\
\partial_\nu u_\epsilon & = 0 \quad \text{on } \partial \omega^\epsilon \cap \partial \Omega^\epsilon \\
u_\epsilon & = 0 \quad \text{on } \partial \omega^\epsilon \setminus \partial \Omega^\epsilon.
\end{align*}
\] (3)

For \(i = 1, 2\), they admit the solutions
\[\begin{align*}
u^{\epsilon}_{N_i} & = w^+ + \sum_{j=1}^2 r_{ij} \nu^{\epsilon}_j \quad \text{in } \omega^\epsilon \\
u^{\epsilon}_{D_i} & = w^+ + \sum_{j=1}^2 r_{ij} \nu^{\epsilon}_j \quad \text{in } \omega^\epsilon.
\end{align*}\]

We define the reflection matrices
\[\begin{align*}
R^\epsilon_N & := \begin{pmatrix} r_{11}^N & r_{12}^N \\ r_{21}^N & r_{22}^N \end{pmatrix}, \\
R^\epsilon_D & := \begin{pmatrix} r_{11}^D & r_{12}^D \\ r_{21}^D & r_{22}^D \end{pmatrix}.
\end{align*}\]

Playing with symmetries, one shows that
\[R^\epsilon = \frac{R^\epsilon_N + R^\epsilon_D}{2}, \quad T^\epsilon = \frac{R^\epsilon_N - R^\epsilon_D}{2}.
\]

Therefore our goal is to find geometries \(\omega^\epsilon\) where, as \(\epsilon\) tends to zero,
\[\begin{align*}
R^\epsilon_N & = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + o(1), \\
R^\epsilon_D & = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} + o(1).
\end{align*}\] (4)

3 Asymptotic analysis

Denote by \(L^\epsilon_\pm\) the half ligaments \(L^\epsilon_\pm|_{\omega^\epsilon}\). Pick two different \(y_\pm \in (0; 1)\) and set \(A_\pm := (-1/2, y_\pm)\).

We assume that \(L^\epsilon_\pm\) are connected to \(\Pi_-\) at the points \(A_\pm\). Moreover we assume that \(L^\epsilon_\pm\) is of length \(\ell^\epsilon_\pm := \ell_\pm + \epsilon \ell'_\pm\) where the values \(\ell_\pm > 0\), \(\ell'_\pm > 0\) will be fixed below.

Next we derive asymptotic expansions of the \(u^{\epsilon}_{N_i}, u^{\epsilon}_{D_i}\) as \(\epsilon \to 0\). We employ the technique of matched asymptotic expansions. In the process, the properties of the 1D problems
\[\begin{align*}
(\mathcal{P}^\epsilon_N) & \quad \frac{\partial^2 \nu^\epsilon}{\partial x^2} + k^2 \nu^\epsilon = 0 \quad \text{in } (0; \ell_\pm) \\
(\mathcal{P}^\epsilon_D) & \quad \frac{\partial^2 \nu^\epsilon}{\partial x^2} + k^2 \nu^\epsilon = 0 \quad \text{in } (0; \ell_\pm)
\end{align*}\]

obtained by considering the restriction of (2) and (3) to \(L^\epsilon_\pm\) play a central role. Let us fix \(\ell_+\) (resp. \(\ell_-\)) coinciding with a resonant length of (\(\mathcal{P}^\epsilon_D\)) (resp. \(\mathcal{P}^\epsilon_N\)). In other words, we take
\[k\ell_+ = m\pi \quad \text{and} \quad k\ell_- = (m + 1/2)\pi\] (5)

for some \(m \in \mathbb{N}\). Then we can prove that \(L^\epsilon_\pm\) (resp. \(L^\epsilon_\pm\)) has no influence at order \(\epsilon^0\) on the \(u^{\epsilon}_{N_i}\) (resp. \(u^{\epsilon}_{D_i}\)). This key remark allows us to decouple the action of the ligaments. At the end of the asymptotic procedure, we obtain expansions where the features of the geometry appear explicitly. For example for \(u^{\epsilon}_{D_1}\), we get the following statement:

**Proposition** There is \(\ell'_\epsilon(\epsilon)\) such that as \(\epsilon \to 0\),
\[\begin{align*}
u^{\epsilon}_{D_1} & = w^+ \pm w^- + ak\gamma + o(1) \quad \text{in } \Pi_- \\
u^{\epsilon}_{D_1} & = O(1) \quad \text{in } L^\epsilon_+ \\
u^{\epsilon}_{D_1} & = \epsilon^{-1} a \sin(ks) + O(1) \quad \text{in } L^\epsilon_+
\end{align*}\]

where \(a \in \mathbb{R}\), \(\gamma\) is a certain Green function centered at \(A_+\), and \(s\) is the curvilinear abscissa.

Finally, thanks to similar formulas for \(u^{\epsilon}_{D_2}, u^{\epsilon}_{N_i}\), we can find values of \(\ell'_\epsilon(\epsilon)\) and \(\ell'_\pm\) such that as \(\epsilon \to 0\), the expansions (4) for \(R^\epsilon_N, R^\epsilon_D\) are valid. This leads to the numerics of Figure 3. We emphasize that in the method, it is crucial to work around the resonance lengths to get effect of order \(\epsilon^0\) with ligaments of width \(\epsilon\).

4 Numerics

---

Figure 2: \(\Re \ u^{\epsilon}_{1}(\epsilon)\) (top) and \(\Re \ u^{\epsilon}_{2}(\epsilon)\) (bottom) for \(\epsilon = 0.01\). Here the lengths of the ligaments are close to the critical values (5) but not particularly selected to get mode conversion.

Figure 3: \(\Re \ u^{\epsilon}_{1}(\epsilon)\) (top) and \(\Re \ u^{\epsilon}_{2}(\epsilon)\) (bottom) for \(\epsilon = 0.1\). The features of the ligaments have been tuned to get mode conversion.

---

References

Spectral analysis of generalized normal modes

Anne-Sophie Bonnet-Ben Dhia
POEMS, ENSTA, Palaiseau, France

Christophe Hazard
1POEMS, ENSTA, Palaiseau, France
2School of Mathematics, The University of Edinburgh, Edinburgh, UK

Matias Ruiz
Poems, ENSTA, Palaiseau, France

Abstract
We study a spectral problem defined by an unforced Helmholtz equation when using the permittivity as the eigenvalue. The eigensolutions of such problems, so-called generalised normal modes (GNM), have been recently applied by different authors for modal expanding electromagnetic scattering fields by resonant nanocavities in nanophotonic systems. In this work we make progress in the theoretical underpinnings of GNM by proving their completeness in a pertinent energy functional space. We further prove that they form a Riesz basis in some particular configurations.

Keywords: Electromagnetic resonances, modal expansion, spectral theory, non-selfadjoint operators.

1 Introduction
An efficient approach to the analysis of the electromagnetic field scattered by a nanoresonator subject to radiation losses (i.e., in an open system), is to proceed by a modal expansion approach wherein the resonant response can be described as an infinite sum using as basis functions the eigenfunctions of a spectral problem defined by the unforced Maxwell’s equations. One of these spectral problems stems from considering the permittivity as the eigenvalue, yielding the so-called generalized normal modes (GNM) [1, 2]. This approach entails several advantages over the alternative quasi-normal modes where the frequency is considered as the eigenvalue: GNM correspond to real stationary states (for a given real frequency), they don’t suffer from an exponential growth at infinity, and are underpinned by a linear eigenvalue problem. However, to date, this approach is restricted to numerical experimentation only and lacks theoretical grounds. For instance, an important open question is whether the (generalized) eigenfunctions define a Riesz basis and therefore one can rigorously justify the modal expansion.

Owing to radiation conditions, the linear spectral problem underpinning GNM is non-self-adjoint, which is at the source of numerical and theoretical difficulties. Furthermore, the problem is non-standard in that its eigenvalues both diverge and accumulate at finite points. We are accordingly motivated to study the spectral properties of the GNM spectral problem. We focus, in particular, in GNM modes in 2D which are governed by the Helmholtz equation. We consider different scenarios, which are detailed in section 2. Our main results are the proof of the completeness of these modes in \( H^1(D) \), where \( D \) is the domain occupied by the resonant cavity. We also show that they define a Riesz basis in the particular cases of the domains depicted in Fig. 1.

2 Problem formulation
Consider a domain \( \Omega \subset \mathbb{R}^2 \), which extends (at least in one coordinate) to infinity. In particular we consider \( \Omega \) to be a 2D waveguide or \( \Omega = \mathbb{R}^2 \). Consider also a compact and simply-connected domain \( D \subset \Omega \) which we assume to be smooth over the transmission boundary with \( \Omega \). Fig. 1 shows two examples. We are interested in the following PDE spectral problem defined in \( \Omega \):

Find \( \mathcal{E} \in \mathbb{C} \) and \( u \in H^1_{\text{loc}}(\Omega) \) such that, for \( \varepsilon = \chi(D) \mathcal{E} + \chi(\Omega \setminus D) \),

\[
\nabla \left( \frac{1}{\varepsilon} \nabla u \right) + \omega^2 u = 0, \\
\lim_{x \to \infty} |x| \left( \frac{\partial}{\partial x} - i\omega \right) u(x) = 0
\]

(1)

Here \( \chi(\cdot) \) denotes the indicator function. If \( \Omega \) is a waveguide, we further consider Neumann boundary conditions on the waveguide boundary.

3 Spectral analysis
We proceed by a variational approach and use a Dirichlet-to-Neumann mapping (which accounts for the radiation conditions) to reduce problem (1) to the study of a linear operator \( \mathcal{A}_\omega : H^1(D) \to H^1(D) \) with eigenvalues \( 1/\mathcal{E} \). The spectral properties of \( \mathcal{A}_0 \) are well understood.
D \Omega
(a) \( D = \{(x, y); x^2 + y^2 < R\}; \Omega = \mathbb{R}^2 \).

(b) \( D = \{(x, y); -a < x < 0, 0 < y < 1\}; \Omega = \{(x, y); -a < x, 0 < y < 1\}. \) In this case, we also consider Neumann boundary conditions on the upper walls and a Dirichlet boundary condition at \( x = -a \).

Figure 1: Examples of domains \( D \) and \( \Omega \).

[3]. Furthermore, it can be shown that \( A_\omega - A_0 \) is compact. This yields the following result.

**Lemma 1** The spectrum of \( A(\omega) \) is discrete with two accumulation points at \( \mathcal{E} = \infty \) and \( \mathcal{E} = -1 \). Plus, all eigenvalues have a non-negative imaginary part.

Each of this accumulation points is associated with a different family of modes. \( \mathcal{E} = \infty \) is associated with bulk modes which can be used to describe resonances in high-index cavities; \( \mathcal{E} = -1 \) is associated with boundary modes which can be used to describe resonances in plasmonic resonators. This is illustrated in Fig. 2 and Fig. 3, which show some of the eigenfunctions for \( D \) of Fig. 1.(b). The numerical computation of these modes was carried out using the finite element software XLIFFE++.

Using the above lemma along with the Riesz decomposition (or splitting) theorem we can show the existence of two subspaces \( \mathcal{H}_\infty \) and \( \mathcal{H}_{-1} \) such that \( H^1(D) = \mathcal{H}_\infty \oplus \mathcal{H}_{-1} \), where \( A_\omega \) restricted to \( \mathcal{H}_i \) is invariant, with only one accumulation point (\( \mathcal{E} = \infty \) or \( \mathcal{E} = -1 \)), and of type Hilbert-Schmidt. Thus, using the theory of Hilbert-Schmidt operators yields the following result.

**Theorem 2** The generalized eigenfunctions of \( A_\omega \) are complete in \( H^1(D) \).

To further show that the generalized eigenfunctions of \( A_\omega \) form a Riesz basis of \( H^1(D) \) it is sufficient to show that the application \( T(\alpha) := \sum_k \alpha_k u_k \), where \( \{u_k\} \) is the sequence of generalized eigenfunctions of \( A_\omega \), defines an isomorphism of \( l^2 \) into \( H^1(D) \). One can show that this property is directly linked to the asymptotic behaviour of the eigenvalues of \( A_\omega \). In the particular case of the configurations depicted in Fig. 1 such asymptotic behaviour can be estimated using separation of variables techniques, which yields the following result.

**Theorem 3** The eigenvalues of the operator \( A_\omega \) stemming from the domains depicted in Fig. 1 are not defective. Moreover, their eigenfunctions form a Riesz basis of \( H^1(D) \).

Figure 2: First four "bulk" eigenfunctions for \( D \) of Fig. 1.(b).

Figure 3: First four "plasmonic" eigenfunctions for \( D \) of Fig. 1.(b).

**Acknowledgements**

Matias Ruiz acknowledges support from the RSE Saltire Research Award.

**References**


Sheared nanoribbons

Philippe Briet\textsuperscript{1,∗}, D. Krejčiřík\textsuperscript{2}, Hamza Abdou Soimadou\textsuperscript{1}

\textsuperscript{1}Centre de Physique Théorique, Université de Toulon, Toulon, France
\textsuperscript{2}Department of Mathematics, Czech Technical University in Prague, Prague, Czechia
∗Email: briet@univ-tln.fr

Abstract

The purpose of this note is to study some spectral properties of the Dirichlet Laplacian defined on a two-dimensional infinite band subjected to a "shear". We give geometric conditions leading to a Hardy inequality and the absence of a discrete eigenvalue. The second part is devoted to the discussion of the presence of discrete spectrum. Apart from a few details, the bulk of proof can be found in [1].

Keywords: Quantum waveguide, sheared band, Hardy inequality.

1 Introduction

Recent work has shown that certain deformations of a straight waveguide have a repulsive effect, i.e. the absence of a discrete spectrum of the corresponding Dirichlet Laplacian; see for example BHK, BH, Kre. We want to study this fact for a two-dimensional quantum waveguide subjected to shear. To this end we introduce the following model. Let \( f : \mathbb{R} \to \mathbb{R} \) such that \((h) the derivative \( f' \in L^\infty(\mathbb{R}) \) and \( f'(s) \to \beta \) as \( |s| \to +\infty, \beta \in \mathbb{R} \cup \{ \pm \infty \} \).

If \( \beta \in \mathbb{R} \) the deviation is denoted by \( \varepsilon := f'(s) - \beta \). Let \( d > 0 \). Consider the domain in \( \mathbb{R}^2 \) (see Figure 1):

\[ \Omega = \Omega_f = \{(x, y) \in \mathbb{R}^2; f(x) < y < f(x) + d \} \]

We are focusing on the spectral analysis of the "Dirichlet Laplacian" denoted by \(-\Delta_D\) in \( L^2(\Omega) \) i.e. the self-adjoint operator in \( L^2(\Omega) \) defined from the quadratic form:

\[ \mathbb{Q}_D[\psi] = \int_{\Omega} |\nabla \psi(x, y)|^2 dx dy, \quad \psi \in H^1_0(\Omega). \]

For finite \( \beta \) it is convenient to use an appropriate change of variables:

\[ (s, t) \in \Omega_0 \to L(s, t) = (s, f(s) + t) \in \Omega \]

Denote by \( H_f \) the operator obtained in the curvilinear coordinates \((s, t)\), it is associated to the following quadratic form:

\[ q[\varphi] = \| (\partial_s - f' \partial_t ) \varphi \|^2 + \| \partial_t \varphi \|^2; \varphi \in D(q) \]

By direct calculation we see that \( q \) is closed on \( D(q) = H^1_0(\Omega_0) \). Let us give the location of the essential spectrum of the operator \( H_f \) which is a necessary step for our purpose. Let \( E_1(\beta) = (1 + \beta^2)^{-1} E_1 \), where \( E_1 = \left( \frac{x^2}{X} \right)^2 \) is the first transverse mode: \( -\partial^2_\beta \chi(t) = E_1 \chi(t) \).

Theorem 1 Suppose \((h) holds. Then,

\( i) if \beta \in \mathbb{R} \). Then, \( \sigma_{ess}(H_f) = [E_1(\beta), +\infty) \)

\( ii) if f' \to \pm \infty. \) Then \( \sigma_{ess}(H) = \emptyset. \)

The proof of the Theorem 1 can be found in [1]. Note that for \( \beta = \pm \infty \) the spectrum of the operator \( H_f \) is purely discrete so from now we only consider the finite \( \beta \) case.

2 Hardy inequalities

Theorem 2 (repulsive shearing) Suppose \((h) holds, \varepsilon \) a nonzero function, \( \beta \in \mathbb{R} \), and \( \beta \varepsilon \geq 0 \).

Then there exists \( c > 0 \) s.t.

\[ -\Delta_D - E_1(\beta) \geq \frac{c}{1 + s^2} \]

holds in the quadratic form sense in \( L^2(\Omega) \).

Let us give few remarks. The last theorem implies the non existence of discrete eigenvalue for \( H_f \). If \( \varepsilon = 0 \), a limiting argument show that (2) cannot be true see [2]. Finally, note also that the presence of positive term in the r.h.s of (2) shows that the result is stable by adding a small perturbation to \( H_f \) of order 0.

The proof of the Theorem is given in [1]. The key point comes from the so called "the ground state decomposition", it is the following identity which is valid for every finite \( \beta \) and \( \varepsilon \in L^\infty_{loc}(\mathbb{R}) \).

Let \( \psi \in C^\infty_0(\Omega_0) \), then

\[ q[\varphi] - E_1(\beta) \| \psi \|_2^2 = \| (\partial_s \psi - \varepsilon \partial_t \psi - \beta \partial_t (\chi^{-1} \psi) \|_2^2 + \| \chi \partial_t (\chi^{-1} \psi) \|_2^2 + \int_{\Omega_0} \beta \varepsilon \left( E_1(\beta) + \left( \frac{x^2}{X} \right)^2 \right) |\psi|^2 \]

Then by (3), since the r.h.s. is positive if \( \beta \varepsilon \geq 0 \) then the associated operator \( H_f \) has no spectrum below \( E_1(\beta) \) even for \( \varepsilon = 0 \).
3 Discrete spectrum

Theorem 3 (Attractive shearing) Suppose that \( \varepsilon \) is a nonzero function, \( \varepsilon^2 + 2\beta \varepsilon \in L^1(\mathbb{R}) \) and either one of the following conditions is satisfied,

\[
\int_{\mathbb{R}} (\varepsilon^2 + 2\beta \varepsilon) < 0 \quad (4)
\]

\[
\varepsilon \in W^1_{\text{loc}}(\mathbb{R}), \varepsilon \neq -2\beta \text{ and } \int_{\mathbb{R}} (\varepsilon^2 + 2\beta \varepsilon) = 0 \quad (5)
\]

Then \( \sigma_d(H_f) \neq \emptyset \).

The criterion (4) of existence of discrete eigenvalues has been used in [5] for a different model. In fact here we prove more i.e. the discrete eigenvalues persist even when (4) is saturated (see (5)). This last result is more delicate to obtain and we need here an additional condition on the regularity of the deviation. Of course this result is consistent with Theorem 2 since for repulsive shearing assumptions (4) and (5) are clearly not satisfied.

4 Large coupling

We close this work, by considering a particular case namely \( f \) is s.t. \( f'(x) = \beta + \alpha \varepsilon(x) \), \( \beta > 0 \), \( \alpha < 0 \), \( \varepsilon \) is a bounded positive function with support \([0,1]\). Then we get:

Theorem 4 Suppose that there exist \( 0 < c_1 \leq \varepsilon(x) \leq c_2 \), \( x \in [0,1] \). Then for \( \alpha < 0 \) and large \( \sigma_d(H_f) = \emptyset \).

References


Figure 1: sheared nanoribbon
A trace theorem on an infinite $b$-adic tree

Kiyan Naderi$^{1,*}$, Konstantin Pankrashkin$^1$

$^1$Institute of Mathematics, Carl von Ossietzky University, Oldenburg, Germany

*Email: kiyan.naderi1@uol.de

Abstract

We discuss the construction of the trace operator defined on Sobolev spaces over a class of infinite radial trees based on an identification of the abstract boundary with an Euclidean domain. The case of dyadic trees was covered by Maury, Salort, Vannier in [2], and we adapt their constructions and results in order to include to the case of $b$-adic trees with arbitrary $b \geq 2$. While the overall approach is very similar, one has to introduce several new steps related to the discrete Fourier transform and to a more careful analysis of various characterizations of Besov and Sobolev spaces.

Keywords: Trace theorems, Sobolev spaces, Fractal graph, Boundary values

1 Motivation

A wave propagation or diffusion process inside an object occupying some region in the space is typically described by a suitable differential or finite-difference equation, while the interaction with the surrounding is taken into account using a boundary or transmission condition. In many cases, one looks for solutions of boundary value problems in suitable Sobolev spaces, and the regularity of boundary data (−traces) implies important conclusions on the existence and the regularity of the solutions. While there is an established trace theory for Sobolev spaces over smooth domains, many important questions remain open for more involved geometric objects (in particular, for the objects that become “degenerate” near the boundary, even the rigorous definition and the existence of boundary traces represent a difficult problem). In the present work, we address the related questions for a class of fractal objects represented by Laplace-type operators on special self-similar trees, which is a natural extension of the mathematical model of respiratory systems introduced in [2] and can be viewed as a discrete approximation to the study of wave propagation in thin networks proposed in [1].

2 Resistive trees

The infinite $b$-adic tree $T$ with root $o$ is shown in Figure 1. Its internal properties will be taken into account using an additional parameter $\alpha \in (0, b)$ as follows: the resistance $r(x, y)$ of an edge $xy$ in the $n$th generation is $\alpha^n$. Denote by $V(T)$ the set of all vertices of $T$, then the first Sobolev space is defined as

$$H^1(T) = \left\{ p : V(T) \to \mathbb{C} : \|p\|^2 := \sum_{x \sim y} \frac{|p(x) - p(y)|^2}{r(x, y)} < \infty \right\}$$

equipped with the norm $\|p\|^2 := |p|^2 + |p(0)|^2$.

The $H^1$-closure of the set of $p$ with finite supports will be denoted as $H^1_0(T)$. It is straightforward to show the decomposition

$$H^1(T) = H^1_0(T) \oplus H^1_\Delta(T),$$

where $H^1_\Delta(T)$ is the null space of a linear operator (a kind of discrete Laplacian) $\Delta$ associated with $T$.

It is natural to interpret $H^1_\Delta(T)$ as the set of functions vanishing at the boundary and the quotient $H^1/H^1_0$ as the space of functions at the boundary, which then reduces to the study of boundary values of the “harmonic functions”, i.e. of the elements of $H^1_\Delta$.

![Figure 1: Structure of a $b$-adic tree](image)

3 Abstract trace operator

The abstract trace operator is constructed using a suitable basis in $H^1_\Delta$. For that, the tree is
decomposed in a special way.

Each point of the boundary can be naturally identified with an infinite sequence \((c_n)\) with 
\[c_n \in \{0, 1, \ldots, b - 1\},\]
which corresponds to an infinite path from the root through the vertices 
\[X_{n,k}, \quad k_n = \sum_{i=1}^{n} c_i b^{n-i}.\]
The set of such paths passing through \(X_{n,k}\) will be denoted by 
\(C_{n,k}\). If one identifies the whole boundary with a set \(\Omega\) (having a finite volume \(|\Omega|\)), then one can naturally expects that the portion \(\Omega_{n,k}\) identified 
with \(C_{n,k}\) has the volume \(b^{-n}|\Omega|\).

Denote by \(T_{n,k}\) the infinite subtree composed of \(X_{n,k}\) and all its children. Using an adapted discrete Fourier transform one is able to show that there exists a basis \(\{\phi_{n,k}\}\) in \(H^2(\Omega)\) such that 
\[\phi_0 = 1\] and \(\phi_{n,k}^{(s)}\) vanish outside \(T_{n,k}\) and are radial along \(T_{n,k}\). The main idea for the construction of the trace operator is that the trace of \(\phi_{n,k}\) is identified with the (suitably normalized) indicator function of \(\Omega_{n,k}\).

## 4 Embedding

In order to implement rigorously the above idea, one needs additional assumptions on the subsets \(\Omega_{n,k}\). Namely, assume that \(\Omega \subset \mathbb{R}^d\) is a bounded connected Lipschitz domain and \(\Omega_{n,k} \subset \Omega\) with 
\(n \in \mathbb{N}\) and \(k = 0, \ldots, b^n - 1\) be its measurable subsets building a kind of multiscale decomposition in the following sense:

\[
\bigcup_{k} \Omega_{n,k} = \overline{\Omega} \quad \text{for all } n,
\]
\[
\bigcup_{n,k} \Omega_{n+1,k,k+j} = \overline{\Omega_{n,k}} \quad \text{for all } n, k,
\]
\[
|\Omega_{n,k}| = b^{-n}|\Omega|,
\]
\[
(\Omega_{n,k})_{k=0}^{b^n-1} \quad \text{are disjoint for all } n;
\]
and satisfying some additional (explicitly formulated) assumptions ensuring that \(\Omega_{n,k}\) do not “degenerate” (i.e. \(\Omega_{n,k}\) should become “small” in all directions as \(n\) becomes large). We give explicit examples of suitable decompositions in every dimension.

If one accepts the above approach and hypotheses (which then reduces to the identification of \(C_{n,k}\) with \(\Omega_{n,k}\)), then the “reasonable” trace operator \(\gamma\) is uniquely defined by the identifications

\[
\gamma^\Omega(\phi_{n,k}^{(s)})^2(x) = \begin{cases} 
\frac{b^{2n} - \alpha}{b - \alpha} & \text{if } x \in \Omega_{n+1,k,k+j}, \\
0 & \text{otherwise},
\end{cases}
\]

\[
\gamma^\Omega(\phi_0)^2(x) = \mathbb{I}_\Omega, \quad \gamma^\Omega(H^1_0(T)) = 0.
\]

Specifically, the Sobolev regularity of these trace functions can then be studied and we obtain our main result:

**Theorem 1** Denote

\[
s = \frac{d}{2}(1 - \frac{\ln \alpha}{\ln b}),
\]
then

\[
\gamma^\Omega(H^1(T)) = H^s(\Omega) \text{ if } s < \frac{1}{2},
\]
\[
\gamma^\Omega(H^1(T)) \hookrightarrow H^{s'}(\Omega) \text{ if } s \geq \frac{1}{2} \text{ and } s' < \frac{1}{2}.
\]

If time permits, we will discuss an ongoing work dealing with an extension of the above approach to the trace theory of some self-similar metric graphs recently discussed in [1, 3].

**References**


Valentin Ritzenthaler\textsuperscript{1,}\textsuperscript{*}, Pierre Cantin\textsuperscript{2}, Xavier Ferrières\textsuperscript{1}, Sébastien Pernet\textsuperscript{3}, Guillaume Puigt\textsuperscript{4}

\textsuperscript{1}ONERA/DEMR, Université de Toulouse, F-31055 Toulouse, France
\textsuperscript{2}Institut de Mathématiques de Toulouse - UMR CNRS 5219, Université Paul Sabatier, France
\textsuperscript{3}ONERA/DTIS, Université de Toulouse, F-31055 Toulouse, France
\textsuperscript{4}ONERA/DMPE, Université de Toulouse, F-31055 Toulouse, France
*Email: valentin.ritzenthaler@onera.fr

Abstract

This article introduces a new way to discretize Maxwell’s equations. It is a discontinuous high-order method based on local polynomial interpolations, named the Spectral Difference method. This approach mainly differs from the standard Discontinuous Galerkin method by solving the strong form of the equation, instead of the weak form. This article gives the main lines of the Spectral Difference method for a 1D conservation law and explains how it applies to transient Maxwell’s equations. The method is then evaluated on a test-case with well-known analytical solution.

Keywords: High-order method, Spectral Difference, Maxwell’s equations, Time domain.

1 Introduction

The Spectral Difference (SD) method is a discontinuous high-order method based on local polynomial interpolations. This method was introduced in [1] as a scheme that is conservative, high-order, geometrically flexible, computationally efficient and simply formulated. It solves the strong form of the equation, as in Finite Difference. This method has been widely explored in Computational Fluid Dynamic (CFD) as an alternative to the Discontinuous Galerkin method (DG) [2]. The present article starts from the formulation in [1] for Maxwell’s equations but accounts for specific location of the degrees of freedom associated with stable SD schemes [3]. This paper is organized as follows. Section 1 explains how the SD method works for a 1D conservation law and how it generalizes to Maxwell’s equations. Section 2 shows a test-case, on a non-Cartesian grid, with well-known analytical solution.

2 Spectral Difference method

In 1D, the main idea of the SD method, for a conservative system \((\partial_t u = -\partial_x F(u))\), is to compute the conserved variables \(u\) as a polynomial of degree \(p\) \((p \in \mathbb{N}^*)\) and to compute the flux as a polynomial of degree \(p+1\) so that solution and flux divergence are both polynomials of degree \(p\). Solution and flux polynomials are defined by Lagrange interpolation using two sets of points, \(p+1\) solution points and \(p+2\) flux points (Figure 1).

![Figure 1: Example of point positions over a segment, for \(p = 2\): solution points (\(\circ\)) and flux points (\(\blacktriangle\)).](image)

Figure 1: Example of point positions over a segment, for \(p = 2\): solution points (\(\circ\)) and flux points (\(\blacktriangle\)).

The stability of the method only depends on the location of the latter [3]. In 1D, two of the flux points must be taken as the segment end points, the \(p\) remaining are taken inside the element. The formulation is shown linearly stable for any degree \(p\) [4]. The SD algorithm consists of four steps:

1. The solution is extrapolated to the flux points.
2. For the two boundary points, the flux is the solution of a Riemann problem. On the internal points, the flux is a linear combination of the unknowns.
3. The flux polynomial is interpolated from the flux points.
4. The flux is differentiated at the solution points in order to update the solutions.

For 2D/3D configurations, problems are considered using tensorized 1D formulation. An efficient implementation can easily be obtained using matrix/vector products.
The SD formulation is applied to Maxwell’s equations written in conservative form; they consist of two coupled linear advection equations (in 1D, \( u = (E, H) \) and \( F(u) = (H, E) \)). From there, everything described above applies: each component of the fields \( E \) and \( H \) is approximated by a polynomial of degree \( p \), and the interpolations are taken in every directions using a tensorial rule.

3 Numerical results

As a primary validation, the method is tested by considering a propagating mode (here the \((1,1,0)\) mode) inside the unit cube of \( \mathbb{R}^3 \). For computation, \( p = 3 \). The mesh is a structured non-Cartesian grid (Figure 2), with 32,768 degrees of freedom and 512 cells.

Figure 2: Structured non-Cartesian mesh used for the simulation. 32,768 degrees of freedom, 512 cells.

Figure 3 shows the good agreement between the SD numerical solution and the analytical solution. Other configurations will be presented during the conference.

4 Conclusion

In this article, a new way (the SD method) to discretize Maxwell’s equations is introduced and validated for a cavity mode by using a non-Cartesian grid. For the presentation further details will be given on the formulation of the SD method, in particular stability results and comparisons with both FDTD [5] and DG schemes [6].

References


Stabilization of the high-order discretized wave equation for data assimilation problems

Tiphaine Delaunay¹, Sébastien Imperiale¹*, Philippe Moireau¹

¹Inria — LMS, Ecole Polytechnique, CNRS — Institut Polytechnique de Paris, Palaiseau, France
*Email: sebastien.imperiale@inria.fr

Abstract

The objective of this work is to propose and analyze numerical schemes to solve data assimilation problems by observers for wave-like hyperbolic systems. The efficiency of the considered data assimilation strategy relies on the exponentially stable character of the underlying system. The aim of our work is therefore to propose a discretization process that enables to preserve the exponential stability at the discrete level when using high-order finite element approximation. The main idea is to add to the wave equation a stabilizing term which damps the oscillating components of the solutions (such as spurious waves). This term is built from a discrete multiplier analysis that gives us the exponential stability of the semi-discrete problem at any order without affecting the order of convergence.

Keywords: Data assimilation, Control, Numerical discretisation

1 Statement of the problem

We aim at studying data assimilation strategies for wave equation problems compatible with their high-order discretization. In sequential approaches, also called observer approaches [2], we aim at stabilizing exponentially fast – using the available measurements – the error between the observed trajectory initialized from an unknown initial condition and the simulated trajectory starting from a vanishing initial state.

Obtaining the exponential stabilization properties at the continuous level is widely studied – see for example [2]. However, discretizing the observer so that the stabilization property is preserved at the discrete level is an additional difficulty due to spurious high frequencies [1]. We propose, in the context of high order spectral finite elements schemes in space [3] and leap-frog discretisation in time, new remedies and associated analysis with a discretization - then - control strategy.

Let $\Omega = (0,1)$ be the domain of propagation, we consider a scalar wave equation with damping at the boundary $x = 1$,

$$\begin{align*}
\partial_t u + \partial_x v &= 0 \quad \text{in } \Omega \\
\partial_t v + \partial_x u &= 0 \quad \text{in } \Omega
\end{align*}$$

with $\gamma > 0$. The initial data corresponds to the unknown discrepancy between the observed trajectory (that is assumed observed at $x = 1$) and the reconstructed trajectory. By linearity, the system above corresponds to the system of the error between observed and reconstructed trajectory, and the question is to prove that such system – that is known to be exponentially stable – preserves its exponential stability property after discretization.

2 Eigenvalues behavior investigations

As a key indicator of the behavior of the discrete system we investigate the eigenvalues of the generator of the corresponding semi-group: we introduce

$$z = \begin{pmatrix} u \\ v \end{pmatrix}, \quad A = \begin{pmatrix} 0 & -\partial_x \\ \partial_x & 0 \end{pmatrix},$$

where $A : L^2(0,1) \times L^2(0,1) \to L^2(0,1) \times L^2(0,1)$ is an unbounded operator with domain $D(A) \subset H^1(0,1) \times H^1(0,1)$ that takes into account the boundary conditions. The consider dynamics read

$$\dot{z} = Az, \quad \dot{z}_h = A_h z,$$

where $A_h \in \mathcal{L}(V_h)$ is an approximation of the operator $A$ in a finite-dimensional space $V_h$ that is a subspace of $D(A)$ obtained using spectral-finite elements. Since we look for exponential stability we aim at constructing approximations for which the eigenvalues of $A_h$ lies in the complex plane not close to the imaginary axis.

In Figure 1 is represented the spectrum of $A_h$ obtained with a standard $P_1$ approximation (on both components $u$ and $v$). We also represents the spectrum obtained when vanishing (with $h$) viscosity is added – as a classical stabilization strategy, see [1]. Only in the latter
case eigenvalues are well separated uniformly in $h$ from the imaginary axis. The problem persists when using higher order finite elements and is in fact stronger since the classical stabilization strategy is less efficient, see Figure 2 and Figure 3 (left) in terms of quality of approximation.

3 A high-order stabilizing term

We use the following variational formulation of our problem: find $z_h(t) = (u_h(t), v_h(t)) \in V_h$ solution to, for every $(\tilde{u}_h, \tilde{v}_h) \in V_h$,

$$
\begin{align*}
\int_0^1 (\tilde{u}_h u_h + \tilde{v}_h v_h) dx + \int_0^1 (\tilde{u}_h u_h + \tilde{v}_h v_h) dx \\
+ \tilde{v}_h(1) (\gamma v_h(1) - u_h(1)) \\
+ d_h(u_h, \tilde{u}_h) + d_h(v_h, \tilde{v}_h) = 0,
\end{align*}
$$

where $\int_0^1$ denotes the use of the Gauss-Lobatto quadrature formulae and $d_h$ the correcting bilinear form used to obtain the desired stabilization property. Denoting $\{x_i\}$ the set of vertices of a partition of $[0, 1]$, it is defined by

$$
d_h(u_h, \tilde{u}_h) = C_r h^{2r} \sum_i \int_{x_i}^{x_{i+1}} \tilde{u}_h^{(r)}(x) \tilde{u}_h^{(r)}(x) dx,
$$

where $C_r$ is a positive scalar depending only on the order $r$ of the finite-element method.

Denoting $I_h$ the interpolation operator of continuous function into the finite element space, we use an original discrete multiplier strategy: choosing $\tilde{u}_h = I_h(x \varphi_h)$ and $\tilde{v}_h = I_h(x \psi_h)$ in the formulation above we show that

$$
\|z_h(t)\|_{L^2(\Omega) \times L^2(\Omega)} \leq C e^{\sigma t} \|z_h(0)\|_{L^2(\Omega) \times L^2(\Omega)},
$$

where $C$ and $\sigma$ are positive scalars independent of $h$. This exponential stability property is confirmed by an eigenvalue analysis (see Figure 3). Note that our method extends the standard stabilization strategy recovered here when $r = 1$.

We complete our analysis by proposing and studying first an implicit then an explicit time discretization that are shown to preserve – under a time step condition – the efficiency, accuracy and exponential stability properties of the semi-discrete problem.

Extension to 2d problems and other choices of discretisation spaces will be discussed and numerical results will be presented.

References

Stability of space–time isogeometric methods for wave propagation problems

Sara Fraschini\textsuperscript{1,*}, Andrea Moiola\textsuperscript{2}, Giancarlo Sangalli\textsuperscript{2}

\textsuperscript{1}Faculty of Mathematics, University of Vienna, Vienna, Austria
\textsuperscript{2}Department of Mathematics, University of Pavia, Pavia, Italy
\textsuperscript{*}Email: sara.fraschini@univie.ac.at

Abstract

We investigate the first steps towards an unconditionally stable space–time isogeometric (IGA) discretization for the second-order wave equation. Inspired by a finite element formulation proposed by Steinbach and Zank, we propose a stabilization of the isogeometric method for an ordinary differential equation that is closely related to the wave equation. This suggests an extension to wave propagation problems.

Keywords: Isogeometric Analysis, wave equation, space–time Galerkin formulation, stability.

1 Introduction

The space–time discretization of evolution equations is a fairly recent tool that offers approximate solutions that are available at all times in the interval of interest, in contrast to semi-discretization and time-stepping techniques.

We focus on the following scalar, second-order wave-propagation problem with homogeneous conditions

\[
\begin{cases}
\partial_t u - \Delta u = g & \text{on } \Omega \times (0, T), \\
u = 0 & \text{on } \partial \Omega \times (0, T), \\
u = \partial_t \nu = 0 & \text{on } \Omega \times \{0\},
\end{cases}
\]

where $\Omega \subset \mathbb{R}^d$ is an open, bounded, Lipschitz domain. A variational formulation of (1) with integration by parts in both space and time is considered in \cite{2}. A CFL condition $h_t \leq C h_x$ is required for the stability of conforming tensor-product space–time discretizations with piecewise-linear polynomials. Different approaches have been proposed in order to overcome the CFL condition. In \cite{1} the stability of the conforming piecewise-linear FEM is addressed by first studying the same discretization applied to the Helmholtz ODE initial value problem

\[
\begin{cases}
\partial_t u(t) + \mu u(t) = f(t) & t \in (0, T), \\
u(0) = (\partial_t u)(0) = 0
\end{cases}
\]

with $\mu > 0$. Linear-FEM unconditional stability and optimal convergence rates in space–time norms are proved for both (1) and (2) using a perturbed variational formulation.

Motivated by the excellent numerical properties of the IGA method, we aim at extending the techniques of \cite{1} to high-order space–time isogeometric discretizations.

2 Abstract variational problem

As in \cite{1}, our model problem is the ODE (2).

Define the following subspaces of $H^1(0, T)$:

\[
H^1_{0,*}(0, T) = \{ w \in H^1(0, T) : w(0) = 0 \},
\]

\[
H^1_{1,0}(0, T) = \{ v \in H^1(0, T) : v(T) = 0 \},
\]

endowed with the Sobolev seminorm $| \cdot |_{H^1(0, T)}$.

The variational formulation of (2) reads

\[
\begin{cases}
\text{Find } u \in H^1_{0,*}(0, T) & \text{such that} \\
(a(u, v) = \langle f, v \rangle_{(0, T)} & \forall v \in H^1_{1,0}(0, T),
\end{cases}
\]

where $T > 0$ and $f \in [H^1_{1,0}(0, T)]'$ are given, and where the bilinear form is

\[
a(\cdot, \cdot) : H^1_{0,*}(0, T) \times H^1_{1,0}(0, T) \rightarrow \mathbb{R}
\]

\[
a(w, v) := -\langle \partial_t w, \partial_t v \rangle_{L^2(0,T)} + \mu \langle w, v \rangle_{L^2(0,T)}.
\]

As proven in \cite{3}, problem (3) is well-posed.

3 Isogeometric discretization

As discrete trial and test spaces for a conforming Galerkin discretization of (3) we consider

\[
V^h_{0,*} := S^p_h(0, T) \cap H^1_{0,*}(0, T),
\]

\[
V^h_{1,0} := S^p_h(0, T) \cap H^1_{1,0}(0, T),
\]

where $S^p_h(0, T)$ is the space of degree-$p$ piecewise-polynomials in $C^{p-1}(0, T)$ (i.e. maximal-regularity splines), and $h$ is the mesh size. The conforming Petrov–Galerkin isogeometric discretization of (3) is

\[
\begin{cases}
\text{Find } u_h \in V^h_{0,*} \text{ such that} \\
a(u_h, v_h) = \langle f, v_h \rangle_{(0, T)} & \forall v_h \in V^h_{1,0}.
\end{cases}
\]

By extending Theorem 4.7 of \cite{2} (in the case $p = 2$) and by the use of compact perturbations
techniques (for any $p$), we get two results of conditional (w.r.t. $h$) stability for (4). However, numerical results show that these two constraints are not sharp; their improvement is currently ongoing. Our numerical experiments also suggest that, if the mesh size satisfies

$$h < \sqrt{\frac{9}{\mu}},$$

then the quadratic isogeometric discretization (4) is inf-sup stable; see Figures 1–2.

The stabilized bilinear form in [1, (17.13)] can easily be written as

$$a_h(w_h, v_h) = -\langle \partial_t w_h, \partial_t v_h \rangle_{L^2(0,T)} + \mu \langle w_h, v_h \rangle_{L^2(0,T)} - \frac{\mu}{12} \sum_{l=1}^{N_F} h_l^2 \langle \partial_l w_h, \partial_l v_h \rangle_{L^2(\tau_l)},$$

where $\{\tau_l\}_{l=1,...,N_F}$ are the elements of the FEM mesh. We thus propose to substitute in place of $a(\cdot, \cdot)$ in (4) the discrete bilinear form

$$a_h(w_h, v_h) := -\langle \partial_t w_h, \partial_t v_h \rangle_{L^2(0,T)} + \mu \langle w_h, v_h \rangle_{L^2(0,T)} - \delta_p \mu \sum_{l=1}^{N_F} h_l^2 \langle \partial_l w_h, \partial_l v_h \rangle_{L^2(\tau_l)},$$

where $\delta_p > 0$ is a penalty parameter. The effect of this stabilization for $p = 2$ and $\delta_p = \frac{1}{100}$ is visible in Figures 3–4, where we can observe the enlargement of the stable region that corresponds to inf-sup values larger than $\approx e^{-5}$.

In particular, the inf-sup constant is stable for $h \to 0$ and fixed $\mu$.

4 Wave equation

Numerical tests show that a conforming isogeometric discretization of the space–time variational formulation of (1), as introduced in [2], requires a CFL condition. Following Section 3, we propose to replace the bilinear form of the space–time IGA scheme with

$$-\langle \partial_t w_h, \partial_t v_h \rangle_{L^2(Q)} + \langle \nabla_x w_h, \nabla_x v_h \rangle_{L^2(Q)}$$

$$- \delta_p^W \sum_{m=1}^{d} \sum_{l=1}^{N_F} h_l^2 \langle \partial_l^m w_h, \partial_l^m v_h \rangle_{L^2(\Omega \times \tau_l)}$$

for $\delta_p^W > 0$. Numerical tests are ongoing.

References


A comparison of Hermite and Lagrange finite element methods for the wave equation

Ivy Weber\textsuperscript{1,*}, Gunilla Kreiss\textsuperscript{1}

\textsuperscript{1}IT Department (Scientific computing division), Uppsala University, Sweden
*Email: ivy.weber@it.uu.se

Abstract
We use finite element methods with Hermite and Lagrange interpolation polynomials to solve the wave equation and compare the performance of these methods. When the same time-step is used for both we see comparable accuracy and computation time. When the time-step is chosen according to the stability properties of the methods we see that Hermite finite elements can produce a numerical solution up to twice as fast.

Keywords: Hermite interpolation, Lagrange interpolation, finite element method, wave equation

1 Hermite finite elements
We use rectangular elements in 2D with Lagrange and Hermite tensor product interpolation polynomials. In particular, we use the existing implementation in deal.II\textsuperscript{1} for Lagrange interpolation polynomials, and define a basis of Hermite interpolation polynomials\textsuperscript{2} $f_i, g_i$ for $i = 0, 1, \ldots, r$ of degree $2r + 1$ on the 1D reference interval $[0, 1]$ as follows:

$$\frac{d^j}{dx} [f_i(x)]_{x=0} = 4^j i! \delta_{i,j}, \quad \frac{d^j}{dx} [g_i(x)]_{x=0} = 0,$$

$$\frac{d^j}{dx} [f_i(x)]_{x=1} = 0, \quad \frac{d^j}{dx} [g_i(x)]_{x=1} = 4^j i! \delta_{i,j}.$$

In the above the polynomials $f_i$ correspond to derivative degrees of freedom at $x = 0$, and $g_i$ correspond to degrees of freedom at $x = 1$. For Hermite polynomials we enforce continuity of all derivatives up to order $r$ across element boundaries, which leads to fewer degrees of freedom in total for the same polynomial order. These elements are implemented in the deal.II framework to allow a quick comparison with Lagrange elements.

One drawback of Hermite finite elements is the difficulty in enforcing derivative continuity on unstructured meshes. However the intention is to use these elements in an immersed boundary framework where a regular Cartesian grid can be used with a more general domain shape. Another drawback that occurs with the higher order elements is the basis functions do not approximate orthogonality, so the mass matrix is not diagonally dominated and mass-lumping cannot be applied.

For all numerical experiments we consider the wave equation on the spatial domain $\Omega = [0, 3]^2$ and time period $[0, 2)$:

$$\begin{align*}
    u_{tt} &= u_{xx} + u_{yy}, \quad (x, y, t) \in \Omega \times (0, 2), \\
    u(x, y, 0) &= \sin (\pi x) \sin (\pi y), \quad (x, y) \in \Omega, \\
    u_t(x, y, 0) &= 0, \quad (x, y) \in \Omega, \\
    u(x, y, t) &= 0, \quad (x, y, t) \in \partial \Omega \times (0, 2),
\end{align*}$$

where $\partial \Omega$ denotes the boundary of $\Omega$ and the exact solution is

$$u(x, y, t) = \sin (\pi x) \sin (\pi y) \cos (\sqrt{2} \pi t).$$

We use the second order leapfrog method to discretise $u_{tt}$ directly, and initialise the system with the exact solution at times $t = 0$ and $t = \delta t$.

2 Initial conditions
The first row of the tables gives the dimensions of the spatial grid (16 denotes a $16 \times 16$ grid), and the first column gives the polynomial degree of the finite element basis.

### Lagrange FEM:

Initial $L^2$-errors over $\Omega$:

<table>
<thead>
<tr>
<th>$p$</th>
<th>$N = 16$</th>
<th>$N = 32$</th>
<th>$N = 64$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1$</td>
<td>2.8588e-02</td>
<td>6.9298e-03</td>
<td>1.7189e-03</td>
</tr>
<tr>
<td>$3$</td>
<td>5.2059e-05</td>
<td>3.1889e-06</td>
<td>1.9828e-07</td>
</tr>
<tr>
<td>$5$</td>
<td>3.7683e-08</td>
<td>5.8017e-10</td>
<td>9.0409e-12</td>
</tr>
</tbody>
</table>

### Hermite FEM:

Initial $L^2$-errors over $\Omega$:

<table>
<thead>
<tr>
<th>$p$</th>
<th>$N = 16$</th>
<th>$N = 32$</th>
<th>$N = 64$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1$</td>
<td>2.8588e-02</td>
<td>6.9298e-03</td>
<td>1.7189e-03</td>
</tr>
<tr>
<td>$3$</td>
<td>2.0817e-04</td>
<td>1.4095e-05</td>
<td>9.0036e-07</td>
</tr>
<tr>
<td>$5$</td>
<td>1.0568e-07</td>
<td>1.5650e-09</td>
<td>2.4098e-11</td>
</tr>
</tbody>
</table>

Calculating order of accuracy from these results indicates that both methods are $(p + 1)^{th}$ order accurate in projecting initial conditions.

3 Fixed CFL number
We first consider the results when a CFL number of 0.05 is used for all simulation set-ups. This value was found to be numerically stable
for both methods up to polynomial degree \( p = 5 \). The \( L^2 \)-errors after the final time-step and CPU time in seconds are shown below:

### Lagrange FEM:

**Final \( L^2 \)-errors over \( \Omega \):**

<table>
<thead>
<tr>
<th>( p )</th>
<th>( N = 16 )</th>
<th>( N = 32 )</th>
<th>( N = 64 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8.7399e-02</td>
<td>2.4609e-02</td>
<td>6.2750e-03</td>
</tr>
<tr>
<td>3</td>
<td>4.7439e-04</td>
<td>1.2220e-04</td>
<td>3.0537e-05</td>
</tr>
<tr>
<td>5</td>
<td>4.7049e-04</td>
<td>1.2200e-04</td>
<td>3.0537e-05</td>
</tr>
</tbody>
</table>

Simulation times (CPU seconds):

<table>
<thead>
<tr>
<th>( p )</th>
<th>( N = 16 )</th>
<th>( N = 32 )</th>
<th>( N = 64 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.7134e+00</td>
<td>1.1035e+01</td>
<td>7.9023e+01</td>
</tr>
<tr>
<td>3</td>
<td>3.0569e+00</td>
<td>1.8632e+01</td>
<td>1.3382e+02</td>
</tr>
<tr>
<td>5</td>
<td>6.2698e+00</td>
<td>3.8880e+01</td>
<td>2.7534e+02</td>
</tr>
</tbody>
</table>

### Hermite FEM:

**Final \( L^2 \)-errors over \( \Omega \):**

<table>
<thead>
<tr>
<th>( p )</th>
<th>( N = 16 )</th>
<th>( N = 32 )</th>
<th>( N = 64 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8.7399e-02</td>
<td>2.4609e-02</td>
<td>6.2750e-03</td>
</tr>
<tr>
<td>3</td>
<td>5.0804e-04</td>
<td>1.2268e-04</td>
<td>3.0548e-05</td>
</tr>
<tr>
<td>5</td>
<td>4.7049e-04</td>
<td>1.2200e-04</td>
<td>3.0537e-05</td>
</tr>
</tbody>
</table>

Simulation times (CPU seconds):

<table>
<thead>
<tr>
<th>( p )</th>
<th>( N = 16 )</th>
<th>( N = 32 )</th>
<th>( N = 64 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.1218e+00</td>
<td>1.2389e+01</td>
<td>8.7286e+01</td>
</tr>
<tr>
<td>3</td>
<td>3.4353e-00</td>
<td>2.0078e+01</td>
<td>1.4209e+02</td>
</tr>
<tr>
<td>5</td>
<td>6.4353e-00</td>
<td>4.0642e+01</td>
<td>2.9798e+02</td>
</tr>
</tbody>
</table>

We see that the error at the final time is dominated by the time-stepping error, which is second order. We also note that the errors at the final time and the computation time are very similar for Lagrange and Hermite methods. Interestingly this is despite Hermite having fewer degrees of freedom, indicating more work is needed to find a good preconditioner for the mass matrix.

### 4 Relaxed CFL numbers

As found in [3], it is possible to take significantly larger time-steps for higher order Hermite finite elements than Lagrange while maintaining numerical stability over time. The CFL numbers used for the different methods and polynomial degrees are chosen to be below but not at the stability limit, and are listed below to three significant figures:

<table>
<thead>
<tr>
<th>( p )</th>
<th>Lagrange</th>
<th>Hermite</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.406</td>
<td>0.367</td>
</tr>
<tr>
<td>3</td>
<td>0.0979</td>
<td>0.184</td>
</tr>
<tr>
<td>5</td>
<td>0.0460</td>
<td>0.122</td>
</tr>
</tbody>
</table>

All methods remained stable with these CFL numbers. The Lagrange polynomials were tested with a CFL of 0.12 and became unstable for \( p = 3, 5 \). The difference in CFL for \( p = 1 \) was purely due to using an approximate formula to generate CFL numbers, and in practice a Hermite method would not be used with \( p = 1 \).

The final errors for these experiments were again dominated by the time-step errors, which led to worse accuracy for Hermite than Lagrange due to larger time-steps. Methods to improve the accuracy of the Hermite system over time exist but are beyond the scope of this short paper.

### Lagrange FEM:

Simulation times (CPU seconds):

<table>
<thead>
<tr>
<th>( p )</th>
<th>( N = 16 )</th>
<th>( N = 32 )</th>
<th>( N = 64 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.4382e-01</td>
<td>1.4153e+00</td>
<td>1.0287e+01</td>
</tr>
<tr>
<td>3</td>
<td>1.7566e+00</td>
<td>9.8094e+00</td>
<td>6.8715e+01</td>
</tr>
<tr>
<td>5</td>
<td>6.7261e+00</td>
<td>4.1602e+01</td>
<td>2.9929e+02</td>
</tr>
</tbody>
</table>

### Hermite FEM:

Simulation times (CPU seconds):

<table>
<thead>
<tr>
<th>( p )</th>
<th>( N = 16 )</th>
<th>( N = 32 )</th>
<th>( N = 64 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5.6322e-01</td>
<td>1.7037e+00</td>
<td>1.2634e+01</td>
</tr>
<tr>
<td>3</td>
<td>1.4320e+00</td>
<td>6.7186e+00</td>
<td>4.2364e+01</td>
</tr>
<tr>
<td>5</td>
<td>3.3575e+00</td>
<td>1.9046e+01</td>
<td>1.3433e+02</td>
</tr>
</tbody>
</table>

The larger time-steps that Hermite elements allow produce a significant improvement in computation time compared to Lagrange. This indicates that Hermite elements can offer a significant performance benefit over Lagrange for simulations over long time periods due to the larger maximum stable time-step.

### References


Thursday, July 28, Morning Session
Wave propagation in unbounded quasiperiodic media, Part 1: the absorbing case

Pierre Amenoagbadji1, Sonia Fliss1, Patrick Joly1

1POEMS (UMA-ENSTA Paris-IPP), Palaiseau, France
*Email: pierre.amenoagbadji@ensta-paris.fr

Abstract
This work is devoted to the numerical resolution of the Helmholtz equation in a 1D unbounded quasiperiodic absorbing medium. Using the definition of quasiperiodicity, this problem is lifted onto a 2D non-elliptic problem with periodic coefficients. The periodicity of the new problem allows to adapt some tools developed for the elliptic case [2]. However, the non-elliptic nature of Dirichlet-to-Neumann (DtN) type: solve (1) by constructing transparent conditions as explained in Figure 3.

Keywords: quasiperiodic media, waveguides

1 Introduction

We are interested in the Helmholtz equation

\[ -\left(\mu u\right)'' - \mu \omega^2 u = f \quad \text{in} \quad \mathbb{R}, \tag{1} \]

where \(\mu_0\) and \(\rho_0\) have positive upper and lower bounds. The source term \(f \in L^2(\mathbb{R})\) has a compact support denoted by \((-a,a)\), where \(a > 0\). We additionally assume that \(\Im \omega > 0\).

Under these assumptions, (1) admits a unique solution in \(H^1(\mathbb{R})\). Our objective is to solve (1) numerically when \(\mu_0\) and \(\rho_0\) are quasiperiodic, that is, when there exists \(\theta \in (0,\pi/2)\) and \(\theta\)-periodic coefficients \(\mu_p, \rho_p \in \mathcal{C}^0(\mathbb{R}^2)\) such that

\[ \mu_0(x) = \mu_p(e_\theta x) \quad \text{and} \quad \rho_0(x) = \rho_p(e_\theta x), \tag{2} \]

where \(e_\theta = (\cos \theta, \sin \theta)\) – see Figure 1. Note that without loss of generality, \(\mu_0\) and \(\rho_0\) could also be locally perturbed quasiperiodic functions, where the local perturbation can be supposed to be compactly supported in \((-a,a)\).

Using the properties of \(\mu_0, \rho_0\) and \(f\), we want to solve (1) by constructing transparent conditions of Dirichlet-to-Neumann (DtN) type:

\[ \pm\left(\mu_0 u\right)'(\pm a) + \lambda^\pm_0 u(\pm a) = 0, \tag{3} \]

where the DtN coefficients \(\lambda^\pm_0\) are computed by solving problems of the following generic form: Find \(u_0 \in H^1(\mathbb{R}^+_)\) such that

\[ -\left(\mu_0 u\right)' - \mu_0 \omega^2 u = 0, \quad \text{in} \quad \mathbb{R}^+_, \tag{4} \]

The quasiperiodicity of \(\mu_0\) and \(\rho_0\) can be exploited to solve (4). The idea to do so is to use as in [1] that the study of an elliptic quasiperiodic PDE comes down to the study of a 2D non-elliptic periodic PDE.

2 Lifting in a periodic 2D PDE

As the coefficients \(\mu_0\) and \(\rho_0\) in (4) are defined as traces of 2D functions along the half-line \(\mathbb{R}^+\), the main idea is to seek \(u_0\) as the trace along the same line of a 2D function \(U_0\). Using the chain rule [\(U_0(\mathbb{R}^+)\) = \(D_\theta U(\mathbb{R}^+)\) with \(D_\theta := e_\theta \nabla\), and exploiting the periodicity of \(\mu_p\) and \(\rho_p\) in their first variable, it is natural to introduce the half-guide problem: \((y_1,y_2) \in \Omega := (0,1) \times \mathbb{R}^+_\),

\[ -D_\theta \left(\mu_p D_\theta U_0\right) - \rho_p \omega^2 U_0 = 0 \quad (\Omega), \]

\[ U_0 = \varphi \quad (y_2 = 0), \tag{5} \]

\[ U_0 \text{ is periodic wrt. } y_1, \]

where \(\varphi \in \mathcal{C}^0(\mathbb{R})\) is an arbitrary \(1\)-periodic function that must satisfy \(\varphi(0) = 0\) for the sake of consistency with \(u_\theta(0) = 1\).

By Lax-Milgram’s theorem, (5) admits a unique solution \(U_0\) which belongs to

\[ H^1_0(\Omega) := \{ U \in L^2(\Omega), \ D_\theta U \in L^2(\Omega) \}. \]

Furthermore, \(u_0\) is given by \(u_0(x) = U_0(e_\theta x)\).

3 Resolution of the half-guide problem

The periodicity of \(\mu_p, \rho_p\) and the well-posedness of (5) allow one to show that for \(\varphi \in L^2(0,1)\) and \(\ell \in \mathbb{N}\), \(U_0(\varphi)\) has the structure:

\[ U_0(\varphi)(\cdot + \ell \mathbf{e}_2) = U_0(\mathcal{P}^\ell \varphi)(\cdot) \tag{6} \]

where \(\mathcal{P} : \varphi \mapsto U_0(\varphi)|_{y_2=1} \in L^2(0,1)\) is the so-called propagation operator. Provided that \(\mathcal{P}\) is known, \(U_0(\varphi)\) can be obtained using the solutions of local cell problems \((C := (0,1)^2)\)

\[ U_0(\varphi)(\cdot + \ell \mathbf{e}_2)|_{\mathcal{L}} = E^0(\mathcal{P}^\ell \varphi) + E^1(\mathcal{P}^{\ell+1} \varphi), \tag{7} \]

where \(E^0\) and \(E^1\) satisfy the PDE in (5) in \(C\), with periodic conditions in the \(y_2\) direction and Dirichlet conditions as explained in Figure 3.
Figure 1: $\mu_p(y_1, y_2) = 1.5 + \cos(2\pi y_1) \cos(2\pi y_2)$ (left), its quasiperiodic trace along $\vec{e}_\theta$, $\theta = \pi/3$ (right)

Figure 2: Solution of (1) for $\omega = 10 + 0.1i$

Figure 3: Local cell problems

By imposing that $U_\theta$ defined by (7) has a directional derivative which is continuous across the interface $\{y_2 = 1\}$, one deduces that $P$ satisfies the stationary Riccati equation

$$T^{10} p^2 + (T^{00} + T^{11}) P + T^{01} = 0, \quad (\mathcal{A})$$

where $T^{jk}$ are local cell DtN operators defined from the $E^j$'s. One shows that $P$ is the unique solution of (\mathcal{A}) with a spectral radius $\rho(P) < 1$.

Our method is very similar to [2], but its justification is more delicate due to the non-elliptic principal part of the operator in (5). In particular, this non elliptic nature induces a lack of compactness, and the spectral properties of the propagation operator $P$ differ than the ones for the elliptic case (cf [2]).

4 Discretization and numerical results

Along the justification of the method, we also focus on the Finite Elements discretization of the 2D local cell problems solved by $E^0$ and $E^1$.

One natural idea to approximate $E^0$ and $E^1$ is to solve the local cell problems on arbitrary unstructured 2D meshes. Although this approach always gives efficient results, it seemed more judicious to introduce a quasi-1D approach. As for the method of characteristics, the main idea is to exploit the fibered structure of the operator in (5) to solve 1D bounded cell problems, and to “concatenate” the solutions to get $E^0$ and $E^1$. This allows to approximate the local DtN operators $T^{jk}$ and solve the Riccati equation.

The solution $U_\theta$ can then be computed cell by cell (see Figure 4), and the DtN coefficients $\lambda^\pm_\theta$ in (3) can be deduced. Finally, one can reconstruct $u$ in the whole line (see Figure 2).

References


Wave propagation in unbounded quasiperiodic media, Part 2: the non-absorbing case

Pierre Amenoagbadji, Sonia Fliss, Patrick Joly
1POEMS (UMA-ENSTA Paris-IPP), Palaiseau, France
*Email: patrick.joly@inria.fr

Abstract
We are interested in the Helmholtz equation in a 1D unbounded quasiperiodic medium (see Part 1 for the absorbing case). We propose a numerical procedure to compute the outgoing solution assuming that a limiting absorption principle holds. The problem is lifted onto a 2D non-elliptic problem with periodic coefficients. However, the method has to be adapted: the Dirichlet-to-Neumann (DtN) coefficients are replaced by Robin-to-Robin (RtR) ones, and with respect to the non-absorbing case, a condition has to be added to characterize the propagation operator.

Keywords: quasiperiodicity, waveguides

1 Problem setting
We are interested in the Helmholtz equation with frequency $\omega \in \mathbb{R}$:

$$-(\mu_\theta u')' - \rho_\theta \omega^2 u = f \quad \text{in} \quad \mathbb{R}, \quad (1)$$

where $f \in L^2(\mathbb{R})$ has a compact support $(-a,a)$, $a > 0$, and where $\mu_\theta$ and $\rho_\theta$ are quasiperiodic, that is, there exists $\theta \in (0, \pi/2)$ and $1$-periodic functions $\mu_p, \rho_p \in C^0(\mathbb{R}^2)$ such that

$$\mu_\theta(x) = \mu_p(x \bar{\theta}), \quad \text{and} \quad \rho_\theta(x) = \rho_p(x \bar{\theta}). \quad (2)$$

The well-posedness of (1) is unclear. One expects that the physical solution $u$, if it exists, may not belong to $H^1(\mathbb{R})$ due to a lack of decay at infinity. In this case, one needs a so-called radiation condition that imposes the behaviour at infinity. Such a condition can be obtained in practice using the limiting absorption principle, which consists in (i) adding some absorption to the problem, and (ii) studying the limit of the solution $u$ as $\Im \omega^2 \to 0$.

2 Mathematical issues
Understanding the limit process described above is closely related to the spectral analysis of the self-adjoint differential operator in $L^2(\mathbb{R}; \rho_\theta \, dx)$:

$$H_\theta u = -\frac{1}{\rho_\theta} (\mu_\theta u'),$$

$$D(H_\theta) = \{u \in H^1(\mathbb{R}), \ (\mu_\theta u')' \in L^2(\mathbb{R})\}.$$
Robin half-line problem instead of (3):
\[
\begin{align*}
-(\mu_\theta \hat{u}_\theta)' - \rho_\theta \omega^2 \hat{u}_\theta &= 0, \quad \text{in } \mathbb{R}^*_+, \\
[\mu_\theta \hat{u}_\theta](0) + i \omega \hat{u}_\theta(0) &= 1,
\end{align*}
\]
with $\Re \omega > 0$, so that the associated operator has no discrete spectrum. We look for solutions $\hat{u}_\theta$ as $\tilde{u}_\theta(x) = \tilde{U}_\theta(x \hat{e}_\theta)$, where $\tilde{U}_\theta$ satisfies for $(y_1, y_2) \in \Omega := (0, 1) \times \mathbb{R}^*_+$, the problem
\[
\begin{align*}
-D\theta (\mu_p D\theta \tilde{U}_\theta) - \rho_p \omega^2 \tilde{U}_\theta &= 0 \quad (\Omega), \\
\sin \theta \mu_p D\theta \tilde{U}_\theta + i \omega z \tilde{U}_\theta &= \varphi, \quad (y_2 = 0),
\end{align*}
\]
with $\varphi \in \mathcal{C}^0(\mathbb{R})$, an arbitrary 1-periodic function that must satisfy $\varphi(0) = 0$ for the sake of consistency with the condition satisfied by $\tilde{u}_\theta$.

(1) If $\omega^2$ is not in $\sigma_{\text{ess}}(H_\theta)$, the essential spectrum of $H_\theta$, then (5) is well-posed in $H^1_\theta(\Omega) := \{U; D\theta U \in L^2(\Omega)\}$, and the procedure is similar to the absorbing case. More precisely,
\[
\tilde{U}_\theta(\varphi)(y_1, y_2 + \ell) = \tilde{U}_\theta(\overline{P}(\varphi))(y_1, y_2)
\]
where the propagation operator $\overline{P}$ is defined by
\[
\overline{P}\varphi = [\sin \theta \mu_p D\theta \tilde{U}_\theta(\varphi) + i \omega z \tilde{U}_\theta(\varphi)]|_{y_2=1}.
\]

In this case, $\tilde{U}_\theta$ can be computed cell by cell in terms of the solutions $E^0, E^1$ of Robin local cell problems, i.e. the PDE in (5) completed with periodic conditions in the $y_1$ direction and Robin conditions (cf Figure 3). For any $\omega^2 \in \mathbb{R}$, these local cell problems are well-posed, contrary to the Dirichlet ones. One can show that $\overline{P}$ is the unique solution of a Riccati system with a spectral radius $\rho(\overline{P}) < 1$.

(2) If $\omega^2 \in \sigma_{\text{ess}}(H_\theta)$, then (5) is no longer well-posed in $H^1_\theta(\Omega)$. In other terms, the outgoing solution can oscillate without vanishing until infinity. In order to construct the outgoing solution, we use the same procedure as in the previous case by computing $\tilde{E}^0, \tilde{E}^1$, and by solving the Riccati system. To allow oscillations at infinity for the outgoing solution, one has to look for a solution of the Riccati system of spectral radius equal to 1 (see (6)). However, the Riccati system may admit an infinity of such solutions. To recover uniqueness and characterize the outgoing propagation operator, we adapt the spectral condition proposed in [1]. This condition, obtained by limiting absorption for the classical Helmholtz equation, is linked to the energy flux of the outgoing solution.

Once $\overline{P}$ is obtained, using the solutions of the local cell problems, one can deduce $\tilde{U}_\theta$ cell by cell and then, provided that $\omega^2$ is not in the discrete spectrum of $H_\theta$, compute coefficients $\lambda^\pm_\theta \in \mathbb{C}$ so that
\[
\pm (\mu_\theta u')(\pm \alpha) + \lambda^\pm_\theta u(\pm \alpha) = 0
\]
are transparent conditions for (1).

References
Asymptotic analysis of Berry phase governed by the scalar wave equation

Bojan Guzina\textsuperscript{1,∗}, Othman Oudghiri-Idrissi\textsuperscript{1}, Shixu Meng\textsuperscript{2}

\textsuperscript{1}Dept. of Civil, Environmental, & Geo-Engineering, University of Minnesota, Twin Cities, U.S.
\textsuperscript{2}Institute of Applied Mathematics, Chinese Academy of Sciences, Beijing, China

∗Email: guzin001@umn.edu

Abstract
We deploy an asymptotic model for the interaction between nearby dispersion surfaces and respective eigenstates toward explicit evaluation of the Berry phase governed by the scalar wave equation in 2D periodic continua. The model, featuring a pair of coupled Dirac equations, endows the interacting Bloch eigenstates with an explicit gauge that caters for analytical integration in the wavenumber domain. Among the featured parameters, the one (\(s \in [0, \frac{1}{2}]\)) that synthesizes the phase information on the coupling term is shown to decide whether the Berry connection round the loop is singular (\(s = 0\)) or analytic (\(s > 0\)). We show that the Berry phase is \(\pi\)-quantal and topological when \(s = 0\), equalling \(\pi\) when the contour encloses the apex of a Dirac cone and zero otherwise. The analogous result is obtained when \(s \simeq 0\) and similarly for \(s \simeq \frac{1}{2}\). In the interior of the \(s\)-domain, we find that the Berry phase either equals \(\pi\) or is not quantal.

Keywords: Berry phase, scalar wave equation, periodic continua

1 Introduction
In 1984, Michael Berry discovered [1] that when an eigenstate of quantum system is cycled “slowly” (i.e. adiabatically) in the parametric space, it acquires a geometrical phase factor, the so-called Berry phase \(\Upsilon\), that is not removable under a gauge transformation. This finding has permeated all branches of physics and bears analogues in gauge theory and differential geometry [2]. In the original paper [1] it is shown, under a particular restriction on the parametric space, that \(\Upsilon = \pi\) (modulo \(2\pi\)) when the closed contour encloses the apex of a Dirac cone and \(\Upsilon = 0\) otherwise. Even though originally derived within the framework of quantum mechanics, this concept is readily applicable throughout wave physics, see e.g. [3] in the context of classical electromagnetism and Bloch waves – which allow for system cycling in the physical, i.e. wavenumber (as opposed to parametric) space [4]. In principle, evaluation of the Berry phase is inherently numerical and entails quadrature of the phase increment, the co-called Berry connection, over a loop in the wavenumber space enclosing the suspect degeneracy. For 2D systems, \(\Upsilon\) is known to be “generally” 0/\(\pi\) quantal and possibly topological [3,4]. In the absence of analytical results, however, it is difficult to draw definitive conclusions.

2 Berry phase
Consider the wave equation in an unbounded periodic medium \(S \subseteq \mathbb{R}^2\) at frequency \(\omega\), namely

\[
\nabla \cdot (G(x) \nabla u) + \omega^2 \rho(x) u = 0 \quad \text{in} \ S, \quad (1)
\]

where \(0 < G < \infty\) and \(0 < \rho < \infty\) are \(Y\)-periodic and bounded away from zero. We next seek the Bloch-wave solutions of (1) as

\[
\n(x) = \tilde{u}(x)e^{ik \cdot x}, \quad \tilde{u} : Y\text{-periodic} \quad (2)
\]

where \(\tilde{u}\) depends implicitly on \(k \in \mathcal{B}\) and \(\omega \in \mathbb{R}^+\) (\(\mathcal{B}\) denotes the first Brillouin zone). With such premise, (1) reduces to

\[
\nabla_k \cdot (G(x) \nabla_k \tilde{u}) + \omega^2 \rho(x) \tilde{u} = 0 \quad \text{in} \ Y \quad (3)
\]

subject to the usual quasi-periodic boundary conditions, where \(\nabla_k = \nabla + ik\).

As demonstrated in [5], for given \(k \in \mathcal{B}\) the field equation (3) (with relevant boundary conditions) is affiliated with the eigensystem \(\{\lambda_n(k) \in \mathbb{R}, \phi_n(k) \in H^1_{\text{pp}}(Y), \|\phi_n\| = 1\}\) that satisfies

\[
\rho(x)^{-1} \nabla_k \cdot (G(x) \nabla_k \tilde{\phi}_n) + \lambda_n \tilde{\phi}_n = 0 \quad \text{in} \ Y, \quad (4)
\]

where \(H^1_{\text{pp}}(Y) = \{\tilde{g} \in L^2_{\text{pp}}(Y) : \nabla \tilde{g} |_{\partial Y} \in (L^2_{\text{pp}}(Y))^2\}\), and \(L^2_{\text{pp}}(Y) = \{\tilde{g} : Y\text{-periodic, } \int_Y \rho g \tilde{g} dx < \infty\}\).

On denoting by \(C \subseteq \mathbb{R}^2\) be a closed path enclosing some \(k_s \in \mathcal{B}\), we consider the Berry phase characterizing the \(n\)th dispersion branch at \(k = k_s\) as a closed line integral

\[
\Upsilon_n(k_s) = \oint_C d\Upsilon_n(k), \quad (5)
\]
where $\mathrm{d}\Upsilon_n$ is an infinitesimal phase difference between neighboring eigenstates [6] given by

$$\mathrm{d}\Upsilon_n(k) = -i \, \mathrm{d}k \cdot (\rho \tilde{\phi}_{n,k}(k), \tilde{\phi}_n(k)); \quad (6)$$

$\tilde{\phi}_{n,k} = \partial \phi_n / \partial k$; $(\cdot, \cdot)$ is the usual inner product over $Y$, and the quantity contracted with $\mathrm{d}k$ is referred to as the Berry connection. We aim to evaluate (5) in instances where branches $n$ and $n+1$ are close to each other at $k_s$.

3 Asymptotic model

Let the eigenvalue problem due to (4) yield a pair of nearby eigenvalues $\lambda_n := \omega_n^2$ and $\lambda_{n+1} := \omega_{n+1}^2$ for some $k_s \in B$, and consider the affiliated dispersion map over a small neighborhood

$$k = k_s + \epsilon k, \quad \epsilon = o(1). \quad (7)$$

Writing $\omega_{nj}^2(k) := \omega_{n+1,j}^2(k) \ (j = 1, 2)$, we assume “tight” eigenvalue separation in that

$$\omega_{nj}^2(k_s) = \omega_{n+1,j}^2(k_s) + \epsilon \gamma, \quad \gamma = o(1).$$

As shown in [5], eigenfunctions $\tilde{\phi}_n$ within spectral neighborhood (7) can be expanded as

$$\tilde{\phi}_n(k_s + \epsilon k) = u^{\dagger}(\epsilon) \cdot \tilde{\phi}_n(k_s) + O(\epsilon), \quad (8)$$

where $u^{\dagger} \in \mathbb{C}^2$ solve the eigenvalue problem

$$\begin{pmatrix} \mathbb{A}^\dagger + \lambda_j \mathbb{I} \end{pmatrix} u^{\dagger} = 0, \quad (9)$$

$$\mathbb{A}^\dagger = \begin{pmatrix} \theta_{11} \cdot i k & \theta_{12} \cdot i k \\ -\theta_{12} \cdot i k & \theta_{22} \cdot i k - \gamma \end{pmatrix}. \quad (10)$$

Here $\mathbb{I}$ is the $2 \times 2$ identity matrix, and $\theta_{pq} = (G \nabla_k \tilde{\phi}_p, \tilde{\phi}_q) - (G \nabla_k \tilde{\phi}_p, \tilde{\phi}_q)$ are evaluated at $k_s$. Note that the coefficient matrix $\mathbb{A}^\dagger$ is Hermitian [5]; specifically, we have $\theta_{pq} \in i \mathbb{R}^2$ thanks to the fact that $\theta_{pq} = -\theta_{qp}$. In the sequel, we write $\theta_{12} := (t_1, t_2)$. Note that (8) resembles the tight binding model in the condensed matter physics literature.

4 Results

Assuming the circular path of integration in (5) by letting $k = e \theta$ where $e \in \mathbb{R}^2$ is a unit vector and $\theta = O(1)$, from (5)–(6) and (8)–(11) one finds that the Berry phase can be recast in a 4-dimensional parametric space as

$$\Upsilon_n(k_s) = F(s, |\Delta \theta|, \gamma, \theta, \beta),$$

where

$$s = |\theta_{12}|^{-2} |2 \Re (\Delta \theta)| \in [0, \frac{1}{2}];$$

$$|\Delta \theta| = |\Delta \theta / |\theta_{12}||; \quad \Delta \theta = \Upsilon(\theta_{11} - \theta_{22})/|\theta_{12}|; \quad \gamma_0 = \gamma/|\theta_{12}|; \quad \beta_2 = \beta_1 + \pi, \quad \text{and } \beta_1 \quad \text{is the angle between the directions where } |\Upsilon_{12} \cdot e| \quad \text{and } |\Delta \theta \cdot e|$$

are respectively minimized. In this setting, $s$ is shown to decide whether the Berry connection round the loop is singular ($s = 0$) or analytic ($s > 0$). The analysis demonstrates that the Berry phase for 2D lattices is $\pi$-quantal and topological when $s = 0$, equalling $\pi$ (modulo $2\pi$) when the contour encloses a Dirac i.e. diabolical point and zero in all other situations (avoided crossings or line crossings). The analogous result is obtained, up to an $O(s)$ residual, when $s \simeq 0$ and similarly for $s \simeq \frac{1}{2}$. In the interior of the $s$-domain, on the other hand, we find that the Berry phase either approximately equals $\pi$ (for sufficiently small $\gamma_0$) or is not quantal. Beyond shedding light on the anatomy of the Berry phase for 2D periodic continua, the featured analysis carries a practical benefit for it permits single-wavenumber evaluation of this geometrical phase quantity.

References


Numerical solution for non-periodic scattering problems in the 3D periodic structure

Nasim Shafieeabaneh\textsuperscript{1,*}, Ruming Zhang\textsuperscript{1}

\textsuperscript{1}Department of Mathematics, KIT, Karlsruhe, Germany

\textsuperscript{*}Email: nasim.shafieeabaneh@kit.edu

Abstract

This paper is devoted to solving non-periodic acoustic scattering problems from periodic structure in three-dimensional (3D) space. These problems, which have a substantial role in mathematical physics, are modeled by the Helmholtz equation on an unbounded domain. The main step is to use the Floquet-Bloch transform, which has been known as a powerful tool for 2D scattering problems. However, the straightforward extension of the method used in the 2D problems is not suitable for the 3D case because singularities of the Bloch transformed field are no longer in a finite number of points; in fact, they lie on the union of circles. Then, a new high-order numerical method needs to be proposed for the 3D problem. Hence, we apply a high-order method based on a nonuniform mesh by generating the fine mesh near the singular circles. Eventually, the exponential convergence of the proposed method is proved.

Keywords: Non-periodic scattering problems, 3D periodic surface, Floquet-Bloch transform, finite element method.

1 Introduction

In this article, we propose a high-order method for solving non-periodic scattering problems with an unbounded periodic structure. The classical methods used for quasi-periodic scattering problems no longer work for non-periodic problems. Then, it is necessary to find a way out of the mentioned difficulty. In this case, the Floquet-Bloch transform can establish a link between a non-periodic problem in an unbounded domain and a family of quasi-periodic problems in a bounded domain. In [1], the Floquet-Bloch transform has been applied for this kind of problem, but the reported convergence rate is low.

Assume that $\Gamma$ is a $\Lambda$-periodic Lipschitz surface lying in the 3D space and $\Omega$ is the unbounded domain above $\Gamma$. Moreover, let $\Gamma_H$ be a flat surface parallel to $\Gamma$, i.e., $\Gamma_H = \mathbb{R}^2 \times \{H\}$ and $\Omega_H$ denotes the domain between $\Gamma$ and $\Gamma_H$ as depicted in Fig. 1.

The main objective of this paper is to find the total field $u$ that satisfies the following Helmholtz problem

$$\Delta u + k^2 u = 0, \quad \text{in } \Omega \subset \mathbb{R}^3, \quad (1)$$

$$u = 0 \quad \text{on } \Gamma. \quad (2)$$

For a non-periodic incident field $u^i$, the total field is related to the scattered field $u^s$ as $u := u^i + u^s$. The upward propagating radiation condition of $u^s$ yields another boundary condition

$$\frac{\partial u}{\partial x_3} - T^+ u = \frac{\partial u^i}{\partial x_3} - T^+ u^i, \quad \text{on } \Gamma_H, \quad (3)$$

in which the Dirichlet-to-Neumann (DtN) map $T^+$ introduced in [1]. In [3], it has been indicated that the DtN map is continuous from $H^\frac{3}{2}(\Gamma_H)$ into $H_{r^{-\frac{3}{2}}(\Gamma_H)}$ for $|r| < 1$.

2 Floquet-Bloch transform

The Floquet-Bloch transform is a generalization of Fourier transform, which is defined as follows

$$v = (\mathcal{F}_H u)(\boldsymbol{\alpha}, \boldsymbol{x}) := \frac{1}{2\pi} \sum_{j \in \mathbb{Z}^2} u(\hat{\boldsymbol{x}} + \Lambda j, x_3)e^{-i\boldsymbol{\alpha} \cdot \Lambda j},$$

where $\boldsymbol{x} = (\hat{\boldsymbol{x}}, x_3) \in \Omega^\Lambda_H$ ($\Omega^\Lambda_H$ has been illustrated in Fig. 1) and $\boldsymbol{\alpha} \in W^* := [0, 1]^2$. It is straightforward to check that the Floquet-Bloch transform of $u$ is $\alpha$-quasi-periodic in $\boldsymbol{x}$ and 1-periodic in $\boldsymbol{\alpha}$.

Taking the Floquet-Bloch transform from Eqs. (1)-(3) and using the periodized versions of transformed field $v$ and $\mathcal{F}_H u^i$, i.e.,

$$v_\alpha := e^{-i\alpha \cdot \hat{\boldsymbol{x}}} v(\boldsymbol{\alpha}, \boldsymbol{x}), \quad \psi_\alpha(x) := e^{-i\alpha \cdot \hat{\boldsymbol{x}}} \mathcal{F}_H u^i(\boldsymbol{\alpha}, \boldsymbol{x}),$$

indicate that $v_\alpha$ satisfies in the following variational problem

$$a_\alpha(v_\alpha, \varphi) = \int_{\Gamma_H^1} F(\boldsymbol{\alpha}, \cdot) \varphi dS, \quad \forall \varphi \in V_{\text{per}}, \quad (4)$$

Figure 1: Illustration of domain (left image) and periodic structure (right image)
4 High-order numerical method

The next step is to evaluate the original total field $u$ by the inverse Bloch transform as follows:

$$u = \mathcal{F}^{-1}v = \frac{|\det \Lambda|^{1/2}}{2\pi} \int_0^1 \int_0^1 v(\alpha, x)e^{i\alpha \cdot \cdot} \, d\alpha, \quad x \in \Omega_2^N.$$ 

In comparison with the 2D case in [2] where singularities only lie on at most three points in a bounded interval, the 3D case is much more difficult. Our idea for computing the above double integral is based on the nonuniform mesh so that we generate fine mesh in the neighborhood of the singular circles (see Fig. 3). On the coarse elements, the Gaussian quadrature rule is applied. Moreover, we use the midpoint rule on fine elements near singularities.

**Theorem 1** Suppose that $u_{N,M,\varepsilon}$ is the numerical solution of the mentioned problem which is obtained by the finite element method with mesh size $\varepsilon$. Then, the error between $u_{N,M,\varepsilon}$ and the exact solution $u$ is bounded by

$$\|u_{N,M,\varepsilon} - u\|_{L^2(\Omega)} \leq C \left[ \varepsilon^2 + \delta^{-C_1M} + 2^{-C_2N} \right],$$

where $\delta$ is the number of divisions for nonuniform mesh in $\alpha$ space, $M$ denotes order of Gaussian quadrature rule and $\delta > 1$.

**References**


A data compact representation for frequency dependent BEM matrices

Dirckx S.1,∗, Huybrechs D.2, Meerbergen K.3
1Department of Computer Science, KULeuven, Leuven, Belgium
2Department of Computer Science, KULeuven, Leuven, Belgium
3Department of Computer Science, KULeuven, Leuven, Belgium
*Email: simon.dirckx@kuleuven.be

Abstract

Boundary integral equation discretizations for the scalar Helmholtz equation lead to large dense linear systems. Efficient boundary element methods (BEM) solvers, such as the fast multipole method (FMM) and H-matrix based methods, focus on structured low-rank approximations of subblocks in these systems. The ranks of these subblocks increase linearly with the wavenumber. We explore a data-sparse representation of BEM-matrices valid for a range of frequencies, based on extracting the known phase of the Green’s function. We show that the resulting H-matrix can be constructed efficiently using a small number of frequency samples, even for geometrically complex three-dimensional scattering obstacles.

Keywords: boundary element method, low-rank approximation, rational approximation

1 Introduction

The scalar Helmholtz equation

$$\nabla^2 \psi + \kappa^2 \psi = 0 \quad \text{on } \Omega \subset \mathbb{R}^3, \kappa \in \mathbb{R} \quad (1)$$

models time-harmonic wave-propagation. Boundary element methods (BEM) rely on re-writing (1) into a boundary integral equation (BIE) and then discretizing the resulting equation.

For moderate frequencies, the dense BEM matrices can be approximated by data-sparse matrices, either explicitly or implicitly. This results in, amongst others, the Hierarchical Matrix (H-matrix) framework, fast multipole methods (FMM), and wavelet methods. These methods reduce assembly and solution cost of BEM-systems to near-linear. Their complexity increases linearly with the wave number though, and the precise wavenumber dependence of these solvers is an open problem.

In this paper, we propose writing the Galerkin discretisation matrix of BEM operators as the Hadamard product of a frequency matrix with an H-matrix, i.e.,

$$B(\kappa) = H(\kappa) \circ \hat{B}(\kappa)$$

with $H(\kappa)_{ij} := \exp(\im \kappa ||\xi_i - \eta_j||)$, and in which $||\xi_i - \eta_j||$ is the distance between the centers of the ith test DOF and the jth ansatz DOF. We show that the matrix $\hat{B}$ has a significantly reduced assembly time compared to $B$ and allows for a convenient compact representation of the wavenumber dependence $\kappa \mapsto \hat{B}(\kappa)$, based on the (set-valued) AAA algorithm [1].

Our research has two aims. The most important one is to introduce a compact representation for the wavenumber dependence of these BEM matrices that can be constructed in near-linear time as a function of the grid size. Secondly, we provide a method for the fast construction of BEM matrices whose data-spariness is preserved at high frequencies.

The problem of increasing complexity for oscillatory kernels has been tackled in a number of ways, focused mainly on directional approximations (e.g. [2]). However, the admissibility criteria involved in these methods include an aperture requirement of $O(1/\kappa)$ leading (algebraically) to many small subblocks needing to be compressed and managed, resulting in high overhead and a large fixed constant in the asymptotic complexity.

2 Description of the methods used

For bounded $\Omega \subset \mathbb{R}^3$ with orientable (weakly) Lipschitz boundary $\partial \Omega$, let $\Gamma := \{\tau_n\}_{n=1}^N$ be some triangular mesh of $\partial \Omega$. Let $I$ and $J$ denote sets of test and ansatz DOFs respectively, with test and ansatz functions $\{\phi_i\}_{i \in I}$ and $\{\psi_j\}_{j \in J}$, each supported on a small cluster of mesh triangles. Of interest here are discrete oscillatory kernel operators $B \in \mathbb{C}^{I \times J}$, i.e.,

$$B_{ij} = \int_I \int_I \mathcal{E}^{\im \kappa ||x-y||} \hat{k}(x,y) \phi_i(x) \psi_j(y) dx dy$$

with $\hat{k}$ asymptotically smooth and non-oscillatory. A typical example is the 3D Helmholtz Green’s
kernel
\[ G(x, y; \kappa) = \frac{e^{i\kappa \|x-y\|}}{\|x - y\|}. \]
A well-known consequence of asymptotic smoothness is that at low wavenumber, whenever two blocks are well-separated in the sense of
\[ \eta \text{dist}(t, s) > \max\{\text{diam}(t), \text{diam}(s)\} \] (2)
for some separation parameter \( \eta \), the corresponding \( B_{t \times s} \) is low-rank. However, this rank increases linearly with \( \kappa \). In contrast, we were able to show that the extracted matrix \( \hat{B} \), defined by
\[ \hat{B}_{ij} := e^{-i\kappa \|x_i-y_j\|} \cdot B_{ij}, \]
does retain its low rank in the mid-to-high frequency regime. This operation allows us to write for all \( \kappa \in [\kappa_{\min}, \kappa_{\max}] \) the linearization
\[ \hat{B}_{t \times s}(\kappa) \approx \hat{B}_{t \times s}^{B_T}(\kappa) = \sum_{k=1}^{R_T} M_k f_k(\kappa) \] (3)
with \( R_T \) modest, \( M_k \in \mathbb{C}^{s \times s} \), and \( f_k \) in some function set for which an approximate projection exists. We use fixed-degree rational functions \( p_n(x)/q_n(x) \) computed by the AAA algorithm (see [1]) as approximate projection. We built a custom tensorial adaptive cross approximation scheme. The details can be found in [3]. In the end our scheme returns a block-wise representation with a further factorization of \( M_k \) above in the form \( M_k = \sum_{\nu=1}^{R} C_{\nu,k} X_k Y_k^T \). The cost of the scheme scales with the ranks involved and with the integral quadrature order, but it is nearly linear in the total number of degrees of freedom. Furthermore, the ranks are only weakly dependent on the wavenumber. The cost of reconstruction of the BEM matrix at any frequency is equally efficient, and no longer depends on the order of quadrature – which is a significant saving in practice.

3 Numerical results

Construction time and memory usage are shown in Figs. 1–2, for a spherical domain and the Stanford bunny. Both are almost constant as a function of the wavenumber after the proposed frequency extraction. Table 1 reports the timing, memory use and errors of the compact representation over the frequency range. Table 2 shows the reconstruction times at a fixed wave number.

Table 1: Memory use and timing of the compact representation, compared to original timings of \( B(\kappa) \) (time\(_F\)) and \( B(\kappa) \) (time\(_O\)).

<table>
<thead>
<tr>
<th>Shape</th>
<th>time(_F)</th>
<th>time(_O)</th>
<th>Err(_F)</th>
<th>Err(_O)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sphere</td>
<td>10.50</td>
<td>147.36</td>
<td>1.01e-5</td>
<td>1.01e-4</td>
</tr>
<tr>
<td>Bunny</td>
<td>17.88</td>
<td>262.32</td>
<td>8.51e-5</td>
<td>8.51e-5</td>
</tr>
</tbody>
</table>

Table 2: High-frequency reconstruction time from compact representation, compared to original timings of \( \hat{B}(\kappa) \) (time\(_F\)) and \( B(\kappa) \) (time\(_O\)).

<table>
<thead>
<tr>
<th>Shape</th>
<th>time(_F)</th>
<th>time(_O)</th>
<th>time(_O)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sphere</td>
<td>10.50</td>
<td>147.36</td>
<td>374.28</td>
</tr>
<tr>
<td>Bunny</td>
<td>17.88</td>
<td>262.32</td>
<td>430.86</td>
</tr>
</tbody>
</table>

References
Numerical Modelisation of Interaction between Plasma Thruster Plume and Antennas on Small Satellites

Toufic Abboud¹, Benoît Chaigne¹,*, Marek Fleščí¹, Alexandre Piche³, Guillaume Sylvand⁴

¹IMACS, Palaiseau, France
²Inria Bordeaux Sud-Ouest, Talence, France
³Airbus Defence&Space, Toulouse, France
⁴Airbus Central R&T, Issy-Les-Moulineaux, France

*Email: chaigne@imacs.polytechnique.fr

Abstract

Electric propulsion is now widely used on satellites, due to its efficiency with respect to its reduced weight. When ignited, the thruster creates a plasma plume, that interferes with the electromagnetic fields propagation in the area. Consequently, it can alter the work in transmission or reception of the antennas situated on the satellite. In this study, we are interested in the numerical modeling of this phenomenon using different finite element methods, and to its high performance solution using fast solvers.

Keywords: plasma plume, BEM, FEM-BEM, HPC, FMM, H-matrix.

1 Introduction

The plasma plume created by ion thrusters is considered as an axisymmetric domain with varying permittivity. In this paper we investigate the use of either a coupled method between volume Finite Element Method (FEM) and Boundary Element Method (BEM), or a pure BEM approach (where the heterogeneous plasma plume is simplified into piecewise constant domains), presented in section 2. We use the symmetric FEM-BEM coupling formulation introduced in [5]. For the fast solution of the linear systems produced by these schemes, in section 3 we use acceleration techniques such as the Fast Multipole Method [1] or H-matrix representations [2] (BEM part), as well as the open source sparse direct solver MUMPS [4] (FEM part) and specific coupled scheme [3] for the FEM-BEM coupling. Finally, we present in section 4 results of radiation diagrams and performance measurements illustrating the interests of the different choices studied.

2 Modelisation and Meshing

The model is made of: a perfectly conducting (PEC) satellite BEM model on which a simple λ/4-long monopole antenna at 400MHz is connected and excited by a 1V voltage generator; a volumic plasma plume.

The plasma plume is a discrete axisymmetric Drud model with \(\mu_r = 1\) and \(\varepsilon_r\) given on isosurfaces generatrices: from inner to outer isolines we have \(\varepsilon_r \in (0.7, 0.8, 0.9, 0.95, 0.97, 0.99)\) yielding 6 bounded volumes. We note \(\varepsilon_i\) the relative permittivity in each volume with \(\varepsilon_1\) in the innermost and \(\varepsilon_7 = 1.0\) in the exterior domain.

Figure 1: Plasma plume model: linear interpolation of the permittivity (left); volumes id for piecewise constant model (right).

We consider 3 numerical models: (1) Full BEM model: constant \(\varepsilon_i\) (mean value of boundary values and \(\varepsilon_1 = 0.7\)); (2) FEM/BEM model with constant permittivity as with the BEM model; (3) FEM/BEM model with linear interpolation between isosurfaces using a convex-hull algorithm.

The satellite mesh is a uniform triangular mesh with \(h_{\text{mean}} = \lambda/30\). The plume BEM (triangular) or FEM (tetrahedral) mesh is such that \(h_{\text{mean}} = \lambda/15\) in each domain. The mesh is locally refined where isosurfaces are close. The plume mesh is obtained by revolution of a 2-dimensional mesh. The full BEM model has...
These results have been obtained in 324s for the full BEM model using the H-matrix solver while the best FEM-BEM solver runs in about 2295s using the multi-facto algorithm. All computations are performed on one node of two Intel®R Xeon® Gold 6142 CPU at 2.60GHz, for a total of 32 cores and 384 GiB of RAM available.

Figure 2: Comparison of the gain diagrams

Conclusion

In this study, we have demonstrated our capacity to model and solve numerically the impact of a plasma thruster plume on the radiation pattern of nearby antennas using coupled FEM-BEM approach and homegrown dense-sparse solvers. We have shown that the plume has indeed a significant impact on the gain diagrams. Moreover, on this specific case, a piecewise constant plume is a good approximation, allowing us to use BEM and H-matrix to solve accurately the whole problem in extremely fast times.

References

**Abstract**

Hierarchical methods for $N$-body problems have important applications in the fast solving of integral equations. When dealing with wave scattering problems in the high frequency regime, the design of efficient hierarchical methods is still a hard problem. In this talk, we aim at presenting our work on \textit{defmm}, the C++ library which implements our new and efficient approach exploiting Fast Fourier Transforms (FFTs) for this class of problem. Both the mathematical and high performance computing aspects are studied and comparison results with a state-of-the-art library are provided.

**Keywords:** Fast Fourier Transforms, directional Fast Multipole Methods, integral equations, oscillatory kernels, symmetries, High performance computing

**Introduction**

We are concerned by the fast evaluation of $N$-body problems of the form

$$p(x) = \sum_{y \in Y} G(x, y)q(y), \ x \in X$$

where $X, Y \subset \mathbb{R}^3$ are two large point clouds and $G$ is an asymptotically smooth function, possibly oscillatory. Typically, $G$ can refer to the Helmholtz Green’s kernel $e^{i|\mathbf{x} - \mathbf{y}|/(4\pi|\mathbf{x} - \mathbf{y}|)}$ involved in integral equations in wave scattering problems. Fast Multipole Methods (FMMs) [1] allow this problem to be solved in a linear or linearithmic time (depending on the frequency regime), at the cost of a controllable approximation error. Kernel-independent approaches (i.e. requiring only the user to provide routines for evaluating $G$ but no explicit expansion of it) exploit directional approximations of $G$ in the high frequency regime [2, 3], leading to complex algorithmic and strongly increasing the precomputation cost compared to the low-frequency or non-oscillatory cases.

**A FFT-based directional FMM**

Interpolation-based FMMs using equispaced interpolation [4] are kernel-independent methods lowering the precomputation cost while keeping fast evaluation timings for non-oscillatory kernels, compared to low-rank compression-based techniques. This existing approach uses the Fourier expression of the far-field matrix blocks $M = [G(x_k, y_l)]_{k,l}$ obtained after a coarse interpolation on equispaced grids $\{x_k\}_k, \{y_l\}_l$:

$$M = \mathbb{F}^* D \mathbb{F}$$

where $\mathbb{F}$ refers to the Fourier matrix (that can be evaluated in linearithmic time through Fast Fourier Transforms) and $D$ is a diagonal matrix (evaluated in linear time). However, this interpolation process is known to suffer from the Runge’s phenomenon. We thus introduced the first FFT-accelerated wideband directional FMM based on exploiting equispaced interpolation, for which we demonstrated the convergence. Because we target possibly highly non-uniform particle distributions (such as appearing in Boundary Element Method, especially with mesh refinement), we considered a slightly modified Dual Tree Traversal method [5] to traverse the trees obtained thanks to the hierarchical space decomposition in the FMM algorithm, allowing to flexibly switch between high- and low-frequency regimes depending on the local particle distribution (and exploiting directional or non-directional approximations accordingly). This led us to the design, implementation and optimization of the \textit{defmm} (for directional equispaced
interpolation-based fast multipole method) library, which is the synthesis of our work.

**Symmetries**

`dfmm` mathematically-based optimizations are widely built on the invariances of both the kernel $G$ and the underlying octree structure in the method: both are invariant under the action of $\mathcal{D}_3$, the set of rotations preserving the cube

$$G(g \cdot x, g \cdot y) = G(x, y), \forall g \in \mathcal{D}_3.$$  

This allows to strongly reduce the number of far-field matrices $M$ to be precomputed at the cost of application of permutation matrices $P_g$ associated to each $g \in \mathcal{D}_3$ (i.e. computations of $P_g^{-1}MP_g$). Because the far-field matrices are evaluated in the Fourier domain, we extended these symmetries to this domain, leading to a new formulation of the diagonalized far-field matrices:

$$P_{g}^{-1}MP_g = \mathbb{F}^* \cdot \mathcal{D}_g \cdot \mathbb{F}$$

where $\mathcal{D}_g$ is a diagonal matrix whose diagonal terms are permutations of the $D$ ones. We then derived fast evaluations of the far-field matrices under rotations, thanks to vectorized Hadamard products for the application of $\mathcal{D}_g$ to a vector.

**High Performance Computing**

Our FMM is optimized for one CPU core and we provided efficient approaches for the fast evaluation of the different FMM operators. Among them, the deinterleaving of complex data plays an important role, for which we described different applications leading to important gains. By comparing our work to a state-of-the-art library (namely `dfmm` [3]), we validated the efficiency of our new approach, as illustrated in Fig. 1. We shall discuss in details how the algorithmic design of `dfmm` combined with our handling of symmetries, as well as low-level optimizations allow us to obtain these performance results, especially on realistic test cases with space decomposition tree nodes in the high-frequency regime near the root as well as leaves at very low-frequency regimes.

**References**


Massively Parallelized Interpolated Factored Green Function Method

Christoph Bauinger¹*, Oscar P. Bruno¹

¹Department of Computing and Mathematical Sciences, California Institute of Technology, Pasadena, USA

*Email: cbauinge@caltech.edu

Abstract

We present the first parallel implementation of the novel “Interpolated Factored Green Function” (IFGF) method introduced recently for the accelerated evaluation of discrete integral operators arising in wave scattering and other areas (Bauinger and Bruno, Jour. Computat. Phys., 2021). On the basis of the hierarchical IFGF interpolation strategy, the proposed (hybrid MPI-OpenMP) parallel implementation results in a highly efficient data communication, and it exhibits in practice excellent parallel scaling up to large numbers of cores, which is demonstrated on the basis of numerical results for problems of up to 4,096 wavelengths in electrical size, and scaling tests spanning from 1 compute core to all 1,680 cores available in the HPC cluster used.

Keywords: Wave Scattering, Integral Equations, High Performance Computing

1 Parallel IFGF Method

We present a hybrid MPI-OpenMP parallel implementation of the novel “Interpolated Factored Green Function” (IFGF) method for the accelerated evaluation of discrete integral operators arising in wave scattering and other areas [1]. The proposed implementation demonstrates in practice excellent parallel scaling up to large numbers of cores essentially without any hard limitations on the number of cores concurrently employed in an efficient manner — even for small problems — while preserving the linearithmic complexity (O(N log N) computing cost) inherent in the sequential IFGF algorithm. The IFGF method accelerates the evaluation of discrete integral operators by relying on a certain factorization of the Green function into two factors, a “centered factor” that is incorporated easily as a common factor in the calculation, and an “analytic factor” which enjoys a property of analyticity up to and including infinity — and which thus motivates the IFGF strategy, namely, evaluation of a given discrete integral operator by means of a hierarchical interpolation approach which relies on use of a large number of small and independent interpolation procedures. In particular, the IFGF approach does not utilize acceleration elements commonly used by other acceleration methods [2–7] such as the FFT (Fast Fourier Transform), spherical harmonics expansions, high-dimensional linear algebra factorizations, translation operators, equivalent sources, or parabolic scaling.

The parallelization of other accelerated Green function methods has been the subject of a significant literature [8–12]. In contrast to these approaches, the IFGF method admits an elegant and highly efficient parallelization strategy due to its algorithmic simplicity. This parallel strategy is based on adequately partitioning the interpolations performed on each level of the underlying octree structure, which facilitates the spatial decomposition of the surface discretization points. As shown in [1], the number of interpolations performed on each level is large and approximately constant (as a function of the octree level), thus admitting a large number of independent tasks suitable for parallelization. The decomposition and distribution of the interpolation data is based on a total order in the set of spherical cone segments representing the interpolation domains, which is an extension of a domain decomposition based on a Morton curve to the box-cone data structure inherent in the IFGF approach. While the usage of space-filling curves for the representation of octree structures underlying the various acceleration methods is not a novel concept [13–15], it requires some adjustments to be applicable to the present box-cone data structure inherent in the IFGF approach. In view of its strong reliance on the IFGF’s box-cone structure, the proposed parallelization strategy is not applicable to other acceleration methods such as the Fast Multipole Method.

In addition to the IFGF method itself and the proposed parallelization strategy, this talk will include a variety of numerical results, which
illustrate the character of the proposed parallel method, are presented in this talk. They include results showing excellent weak and strong parallel scaling properties in all cases considered—for problems of up to 4,096 wavelengths in electrical size, and scaling tests spanning from 1 compute core to all 1,680 cores on 30 nodes available in the HPC cluster used.

2 Numerical Results

![Figure 1: Measured speedup $S_{1,N_c}$ (vertical axis) versus number of cores $N_c$ (horizontal axis) in a strong scaling test transitioning from 1 core to 1,680 cores ($= 30$ compute nodes) for three geometries: a sphere of size 128 wavelengths (blue), an oblate spheroid of size 128 wavelengths (red), and prolate spheroid of size 256 wavelengths (yellow). The dash-dotted purple line indicates the theoretical perfect speedup.](image)

References


Adaptive Spectral Decomposition for Time-Dependent Inverse Problems

Daniel H. Baffet, Yannik G. Gleichmann, Marcus J. Grote

1Department of Mathematics and Computer Science, University of Basel, Basel, Switzerland

*Email: yannik.gleichmann@unibas.ch

Abstract

Inverse medium problems involve the reconstruction of a spatially varying medium, $u(x)$, from available observations. Typically, they are formulated as PDE-constrained optimization problems and solved by an inexact Newton-like iteration. Clearly, standard grid-based representations of $u$ are very general but often too expensive due to the resulting high-dimensional search space. Adaptive spectral inversion (ASI) instead expands the unknown medium in a basis of eigenfunctions of a judicious elliptic operator, which depends itself on the current iterate. Rigorous $L^2$-error estimates of the adaptive spectral (AS) approximation are proved for an arbitrary piecewise constant medium.

Keywords: wave equation, inverse scattering, regularization

1 Inverse scattering problem

Consider the time-dependent wave equation

$$\frac{\partial^2 y}{\partial t^2} - \nabla \cdot (u(x)\nabla y) = f \quad \text{in } \Omega \times (0, T),$$

in a bounded domain $\Omega \subset \mathbb{R}^d$ and time interval $0 < t < T$, together with appropriate initial and boundary conditions on the boundary $\Gamma$ of $\Omega$. Here $u(x)$ denotes the (unknown) squared wave speed inside $\Omega$ and $f(t, x)$ is a known source.

Given (noisy) observations $y_{\ell}^{\text{obs}}$ on $\Gamma$ of solutions of (1) with $f = f_\ell$, $\ell = 1, \ldots, N_s$, we seek to determine the medium $u$. Thus, we formulate the inverse problem as a PDE-constrained optimization problem for the standard $L^2$-least-squares misfit functional,

$$\mathcal{J}(u) = \frac{1}{2} \sum_{\ell=1}^{N_s} \int_0^T \| y_\ell - y_\ell^{\text{obs}} \|_{L^2(\Gamma)}^2,$$

where for each $\ell$, $y_\ell = y_\ell(u)$ is the solution of (1) with $f = f_\ell$.

2 Adaptive spectral inversion (ASI)

AS decompositions (ASD) have been proposed as low dimensional search spaces during the iterative process of inverse medium problems; see [1, 2] and the references therein. Here we consider an extension of the ASI approach from [2] to the time-dependent wave equation.

Since the inverse medium problem is in general severely ill-posed, a Tikhonov (TV) regularization term is typically added to the misfit (2). Here, instead, we rely on the regularizing effect of the search space selection, which we adapt iteratively as follows: at the $m$-th iteration we compute $u_m$ by minimizing (2) in a low-dimensional search space $\Psi^m$. Then, based on $u_m$ and $\Psi^m$, we build a new search space $\Psi^{m+1}$ for the next iteration.

To construct $\Psi^{m+1}$, we combine the previous search space $\Psi^m$ with the AS space $\Psi_{K_m} = \text{span}\{\varphi_k\}_{k=1}^{K_m}$ spanned by the first $K_m$ eigenfunctions of the linear elliptic operator [1, 2]

$$L_\varepsilon[u_m]v = -\nabla \cdot (\mu_\varepsilon[u_m] \nabla v),$$

where

$$\mu_\varepsilon[u_m] = \frac{1}{\sqrt{|\nabla u_m|^2 + \varepsilon^2}}, \quad \varepsilon > 0.$$

Thus, for each $k$

$$L_\varepsilon[u_m]\varphi_k = \lambda_k \varphi_k \quad \text{in } \Omega,$$

$$\varphi_k = 0 \quad \text{on } \Gamma,$$

where $(\lambda_k)_{k \geq 1}$ is the nondecreasing sequence of the eigenvalue of $L_\varepsilon[u_m]$, each repeated according to its multiplicity, and $\{\varphi_k\}$ are $L^2$-orthonormal.

3 Error analysis for ASD

So far, the remarkable ability of the ASD to (approximately) decompose piecewise constant
functions has only been supported by numerical evidence. Here we present rigorous $L^2$-error estimates [3] for AS approximations of piecewise constant functions.

For simplicity, suppose that $u : \Omega \to \mathbb{R}$ is piecewise constant with $K$ inclusions,

$$u(x) = \sum_{k=1}^{K} \alpha_k \chi_{A_k}(x), \quad \alpha_k \neq 0, \quad (6)$$

where $\chi_{A_k}$ are the characteristic functions of Lipschitz domains $A_k \subset \subset \Omega$ with connected but mutually disjoint boundaries. Now, let $u_h \in V_h$ be the (standard) interpolant of $u$ in an $H^1$-conforming, piecewise polynomial $P^l$-FE space $V_h$ associated with a mesh $\mathcal{T}_h$ of size $h$, where the family $\{T_h\}_h$ is regular and quasi-uniform.

Suppose $\{\varphi_k\}_{k=1}^{K} \subset V_h$ are the (discrete approximate) eigenfunctions obtained by the Galerkin FE formulation of the eigenvalue problem (5) with $u_m$ replaced by $u_h$. Then the AS projection $\Pi_K^h[u_h] : L^2(\Omega) \to \Phi_K$ into the AS space $\Phi_K = \text{span}\{\varphi_k\}_{k=1}^{K}$ is the standard $L^2$-projection given by

$$\langle v - \Pi_K^h[u_h], \varphi \rangle = 0, \quad \forall \varphi \in \Phi_K. \quad (7)$$

We have the following error estimate [3]:

**Theorem 1** For each $v \in \text{span}\{\chi_{A_k}\}_{k=1}^{K}$, there exists a constant $C = C(v)$, such that for every $\varepsilon, h > 0$ sufficiently small,

$$\|v - \Pi_K^h[u_h]\|_{L^2(\Omega)} \leq C \sqrt{\varepsilon h}. \quad (8)$$

In particular, the above is true for $v = u$.

**Remark 2** The estimate of Theorem 1 holds true in a more general setting [3] where the FE formulation is replaced by a Galerkin formulation in a closed subspace $Y^h \subset H^1$ and the FE-interpolant $u_h$ is replaced by a more general admissible approximation $u_\delta \in Y^h$. Moreover, $u$ also need not be constant near $\Gamma$ and the weight function $4$ can be replaced by a more general function.

Consider the piecewise constant medium $u$ shown in Figure 1 (left), which consists of $K = 3$ characteristic functions (obstacles) in $\Omega = (0, 1)^2$. To verify the convergence rate in Theorem 1 for $h \to 0$ and fixed $\varepsilon = 10^{-8}$, we compute the approximation error (8) using $P^1$-FE on a regular, uniform triangular mesh whose vertices lie on an equidistant Cartesian grid with mesh size $h$. The right frame of Figure 1 corroborates the expected error decay of $O(\sqrt{h})$.

### 4 Numerical Results

Here we apply the ASI approach, described in Section 2, to solve a time-dependent inverse scattering problem for the (unknown) medium $u$ shown in Figure 1, given the scattered wave data on $\Gamma$ from 32 evenly distributed sources near the boundary with 20% added noise. The forward problem (1) is discretized in $\Omega = (0, 1)^2$ until time $T = 1.5$ using $P^2$-FE (with mass-lumping) in space and the (standard, explicit, second-order) leapfrog method in time. In Figure 2, we display the reconstructed medium after 18 ASI iterations, when the discrepancy principle is satisfied: Starting from the homogeneous background, the ASI algorithm recovers $u(x)$ both in shape and magnitude quite accurately. In stead of a grid-based discrete FE representation with $250'000$ unknowns, the dimension of the search space in the ASI approach never exceeds $K_{\text{max}} = 100$ during the entire inversion. At each iteration, the first few eigenfunctions $\varphi_k$ are computed with $P^1$-FE on the same FE mesh using a cheap Lanczos method for symmetric and positive definite eigenvalue problems.

### References


Optimal Transport for Elastic Seismic Source Inversion

Tyler Masthay1,∗, Björn Engquist1

1Oden Institute for Computational Engineering and Sciences, University of Texas at Austin, USA
∗Email: tyler@oden.utexas.edu

Abstract

Full-waveform inversion (FWI) is a state-of-the-art method for imaging the earth’s subsurface. However, FWI is notorious for local-minimum trapping, or “cycle skipping,” and thus requires an accurate initial model ([2]). Cycle skipping is caused by the nonconvex nature of the misfit optimization landscape in its typical least-squares formulation. The Wasserstein-2 distance is convex with respect to shifts and dilations, both of which occur naturally in seismic data. Therefore, we propose using this optimal transport metric as our misfit for FWI. Previous work using optimal transport for source inversion, whose applications include microseismic event detection and deformation mechanics in subduction zones, has shown promise ([1]). However, this work uses the acoustic wave equation, which is less accurate than the elastic wave equation. In this paper, we extend these results to elastic source inversion and show that they translate well to the elastic model.

Keywords: seismic imaging, optimal transport, inverse problems

1 Introduction

FWI is formulated as a PDE-constrained optimization problem with respect to a given misfit functional. Given that time shifts and amplitude dilations occur naturally in seismic data, we would ideally use a misfit functional that is convex with respect to these transformations. The Wasserstein-2 distance, denoted $W_2$, satisfies this property, whereas the industry standard $L^2$ misfit does not ([4]). $W_2(\mu, \nu)$ for probability distributions $\mu, \nu$ on $X = \mathbb{R}^3$ is given by

$$W_2^2(\mu, \nu) := \inf_{T \in \mathcal{M}} \int_X |x - T(x)|^2 d\mu(x)$$  \hspace{1cm} (1)

where

$$\mathcal{M} := \{T | \forall B \in \mathcal{B}(X), \mu(T^{-1}(B)) = \nu(B)\}$$

is the set of feasible transport maps ([3]). $W_2$ is defined between probability distributions, but seismic data are not probability distributions. Thus, we must renormalize our seismic data via some map $R$; we use positive/negative splitting renormalization as outlined in [4]. Figure 1 demonstrates that convexity of $W_2$ under shift is preserved after renormalization as a model elastic wave with a Ricker wavelet source. Directly computing the $L^2$ norm clearly results in a nonconvex optimization landscape. Previous work has applied optimal transport to velocity source inversion but has used the acoustic wave equation as the forward model ([1], [5]). In this paper, we apply optimal transport to seismic source inversion but with the elastic wave equation, a more complete and accurate forward model. We exhibit that the promising results from the acoustic model translate well to the elastic model.

2 Problem Formulation

Our forward model is the isotropic elastic wave equation over domain $\Omega = (a, b) \times (c, d) \times (0, T)$. Our Lamé parameters are given by $\lambda(x)$ and $\mu(x)$. The source signature of a Ricker wavelet with a characteristic timescale $\sigma$ and amplitude $A$. The model parameter is the source location $s$. That is, $u = F(s)$ if and only if

$$\rho \ddot{u} = \left(\lambda + \mu\right) \nabla (\nabla \cdot u) + \mu \nabla^2 u + f_s$$  
$$+ \nabla \lambda (\nabla \cdot u) + \nabla \mu \cdot (\nabla u + (\nabla u)^T)$$  in $\Omega$

$u(z, x, 0) = 0$

$u$ satisfies Sommerfeld condition
where
\[ f_s = AR_\sigma(t) \delta(x - s) \]
\[ R_\sigma(t) := \left(1 - \left(\frac{t}{\sigma}\right)^2\right) e^{-\frac{t^2}{2\sigma^2}}. \]

Given that \( W_2 \) computation has linear cost in 1D and is expensive in higher dimensions, we use the trace-by-trace \( W_2 \) distance, as outlined in [4]. The trace-by-trace \( W_2 \) distance computes the renormalized \( W_2 \) distance between time series at each receiver location and then sums them. Formally, we define an observation map \( O \) by
\[ O(u)(x) := u(0, x, \cdot). \] (2)

Thus our full map from parameter space to observation space is given by
\[ P_s := R[O[F(s)]]. \] (3)

Given observation time series \( \{d_r(t) : t \in (0, T)\}\) at surface coordinates \( \{x_r\}\), we seek a source location \( s^* \) such that
\[ s^* = \arg \min_s \sum_{r=1}^R W_2^2(P_s(x_r), R(d_r)). \]

3 Computational Results

In Figure 3, we compare the optimization landscape of our modified \( W_2 \) distance and the \( L^2 \) norm. Note that the \( W_2^2 \) landscape is much smoother and has a unique global minimum. This contrasts to the many spiky local minima seen for the square of the \( L^2 \) norm. Given an inaccurate initial source location, we would expect convergence to the global minimum for \( W_2 \), but we will likely see convergence to only a local minimum for \( L^2 \). In Figure 3, we directly test this with an initial guess of \((0.8, 0.5)\) with data \( d = F((0.5, 0.5)) \) synthetically generated at the center of the domain. We see convergence to the global minimum for \( W_2 \) in few iterations and only convergence to a local minimum (that is quite far away from the global minimum) for \( L^2 \). Our experiments support our hypothesis that when applied to the elastic wave equation, \( W_2 \) has a smoother optimization landscape with less likelihood of getting trapped in a local minimum.

References


Solving inverse source wave problem: from observability to observer design

Tiphaine Delaunay, Sébastien Imperiale, Philippe Moireau

Abstract

The objective of this work is to propose a practical method using observers to estimate a source term of a wave equation, from internal measurements in a subdomain \( \omega \). The first part of the work consists in proving an identifiability result from classical observability conditions for wave equations. We deduce that the source reconstruction is an ill-posed inverse problem (IP) of order 2. This (IP) is solved using a sequential strategy that is proven to be equivalent to a minimization of a cost functional with Tikhonov regularization.

Keywords: Observer, Identifiability, Control

1 Statement of the problem

Let \( T > 0 \) and \( \Omega \) be a bounded, connected open domain of class \( C^2 \) in \( \mathbb{R}^d \). In the spirit of [1], we consider a scalar wave equation with \( \lambda(t) \theta(x) \) as the source term and \( (u_0, v_0) \) as initial condition. This system can classically be rewritten as a first-order system in the state-space \( Z = H^1_0(\Omega) \times L^2(\Omega), \)

\[
\begin{aligned}
\dot{z} &= A z + B(t) \theta, \quad \text{in } (0, T), \\
z(0) &= z_0,
\end{aligned}
\]

where \( J_\omega \) is the restriction to \( \omega \) bounded operator from \( H^1_0(\Omega) \) to \( H^1_0(\omega) \). With our choice of norm in \( H^1_0(\omega) \), we find \( C^* = (E_\omega \ 0)^\dag \).

Let us then consider an actual wave solution \( \hat{\theta} \) modeled as a mild solution \( \hat{z} \) of (1) for given and known \( (u_0, v_0) \) and \( \lambda(t) \) but an unknown \( \hat{\theta} \) that we want to estimate. This trajectory is subject to measurements a procedure modeled with the observation operator \( C \). The noisy measurements are denoted \( \delta^g \), and typically there exists \( \delta \in \mathbb{R}^+ \) such that

\[ \| y^g - C \hat{z} \|^2_{L^2((0,T); \mathcal{Y})} \leq \delta^2 T, \]

with \( \mathcal{Y} \) the observation space to be specified. In essence, recovering \( \hat{\theta} \) from \( \delta^g \) consists in inverting the input-output linear operator

\[ \Psi_T : \begin{cases} L^2(\Omega) \to L^2((0,T); \mathcal{Y}), \\
\quad \theta \mapsto (t \mapsto y^g - C e^{tA} z_0)
\end{cases} \]

and we will proceed by steps of increasing difficulties: First, we suppose that for all \( t \), the measurements \( y^g(t) \) belong to \( \mathcal{Y} = H^1(\omega) \), before generalizing to \( y^g(t) \in \mathcal{Y} = L^2(\omega) \).

2 Observability condition

Let us first prove an observability result, which by the way, gives the injectivity of \( \Psi_T \).

**Theorem 1** Let \( \lambda(t) \in H^1(0, T) \) with \( \lambda(0) \neq 0 \). There exists \( T_0 \) such that for \( T > T_0 \), there exists a constant \( C^\ast(T) \) such that

\[ \int_0^T \| u \|^2_{H^1(\omega)} \, dt \geq C^\ast(T) \| \theta \|^2_{H^{-1}(\Omega)}. \]

Here, we adapt the strategy proposed in [1] by combining a Volterra equation and initial condition observability in the \( H^{-1} \) weak norm. From this observability inequality, we understand that the observations have to belong to \( H^1(\omega) \) allowing a stable reconstruction only in a \( H^{-1} \) norm. As a consequence, we face an ill-posed problem of order 2.
3 From regularization to observer design

As a first step, let us assume that the measurements belong to $H^1(\omega)$. To overcome the parameter lack of regularity in the observability condition, we need to introduce some a priori with typically $\|\hat{\theta}\|_{H^1(\Omega)} \leq M$. We hence define the following cost functional which corresponds to a generalized Tikhonov regularization strategy for inverting $\Psi_T$:

$$ J(\theta) = \frac{\epsilon^2}{2} \|\theta\|^2_{H^1(\Omega)} + \frac{1}{2} \int_0^T \|y^\delta(t) - u_\theta\|^2_{H^1(\Omega)} \, dt, $$

with $\epsilon = \delta M^{-1}$. We prove using standard Tikhonov regularization arguments:

**Theorem 2** Under the assumptions of Theorem 1, for $\hat{\theta} \in H^1_0(\Omega)$ such that $\|\hat{\theta}\|_{H^1_0(\Omega)} \leq M$, there exists a constant $C^s(T)$ such that

$$ \|\hat{\theta}_T - \hat{\theta}\|_{L^2(\Omega)} \leq C^s(T)\sqrt{M\delta}, $$

where $\hat{\theta}_T = \arg\min_{\theta \in H^1_0(\Omega)} J_T(\theta)$.

In order to avoid solving this minimization with adjoint-based approaches, we propose to rely on a sequential approach based on the following observers,

$$ \begin{cases} \dot{x}(t) = A \theta(t) + B \hat{\theta}(t) + L(t) \hat{\theta}(t), & \text{in } (0, T) \\ \dot{\theta}(t) = \frac{1}{\delta^2} Q L^* C^*(y(t) - C \hat{\theta}(t)), & \text{in } (0, T) \\ \hat{x}(0) = x_0, \hat{\theta}(0) = 0, \end{cases} $$

where the operators $L(t) = \int_0^t e^{(t-s)A} B$ and $Q$ is a compact symmetric positive operator strong solution of the Riccati equation [3, Part IV, Section 1, Theorem 2.1]

$$ \begin{cases} \dot{Q} = -\frac{1}{\delta} Q L^* C^* CLQ, \\ Q(0) = M^2 \Delta_0^{-1}. \end{cases} $$

In fact, we prove the dynamic programming result:

**Theorem 3** The observer $\hat{\theta}$ defined by (4) is an optimal estimator of $\theta$ in the following sense:

$$ \hat{\theta}(t) = \hat{\theta}_t = \arg\min_{\theta \in H^1_0(\Omega)} J_T(\theta). $$

Let us now move to the more general case where the measurements are actually in $L^2(\omega)$. In our observer definition, we then replace the adjoint of the observation operator by $F_\alpha = (E_{\omega\alpha}^0, 0)^T$ where $E_{\omega\alpha}^0 : L^2(\omega) \to D(\Delta_0)$ is a regularizing family for $J_\alpha$ defined by

$$ E_{\omega\alpha}^0 \phi = \arg\min_{u \in H^1_0(\Omega)} \frac{1}{\alpha^2} \|u - \phi\|^2_{L^2(\omega)} + \|\nabla u\|^2_{L^2(\Omega)}. $$

This change is reflected in the definition of the dynamics $Q$ and $\hat{\theta}$ which becomes

$$ \begin{cases} \dot{\theta}(t) = \frac{1}{\delta^2} Q L^* C^*(y(t) - C \hat{\theta}(t)), \\ \dot{Q} = -\frac{1}{\delta^2} Q L^* C^* CLQ. \end{cases} $$

The operator $Q$ can still be defined using Riccati’s theory as $F_\alpha C$ is proved to be a bounded, symmetric and positive operator. Then, we show again that

$$ \hat{\theta}_t = \hat{\theta}(t) = \arg\min_{\theta \in H^1_0(\Omega)} J_T(\theta), $$

where, this time, the functional is modified into

$$ J_T(\theta) = \frac{\epsilon^2}{2} \|\theta\|^2_{H^1(\Omega)} + \frac{1}{2} \int_0^T \|y^\delta(t) - u_\theta\|^2_{H^2,\alpha} \, dt, $$

with $\|\cdot\|_{H^2,\alpha} = \|E_{\omega\alpha}^0 \cdot H^1(\Omega), \alpha = \sqrt{\delta M^{-1}}$. Combining properties about the regularizing family and the observability condition leads this time with $m \in (\frac{1}{4}, \frac{1}{2})$ to

$$ \|\hat{\theta}_T - \hat{\theta}\|_{L^2(\Omega)} \leq C^s(T) M^{1-m} \delta^m. $$

Finally, as a perspective of this work, we will discuss discretization strategies and generalization to the more general case where the source term decomposes into $\lambda(t, x)\theta(x)$.

**References**


Iterative helioseismic holography—Inversions for solar differential rotation

Björn Müller\textsuperscript{1,*}, Laurent Gizon\textsuperscript{1}, Thorsten Hohage\textsuperscript{2}, Damien Fournier\textsuperscript{1}

\textsuperscript{1}Max-Planck-Institute for Solar System research, Göttingen, Germany
\textsuperscript{2}Institut für Numerische und Angewandte Mathematik, Göttingen, Germany
*Email: muellerb@mps.mpg.de

Abstract

Helioseismic inversions are still challenging due to the high level of noise based on the stochastic nature of solar oscillations and the large amount of input data. In order to deal with the immense size of data one usually is in need of some a priori averaging. Traditional helioseismic holography averages the data by backpropagating the surface data to a target location in the solar interior. Therefore holography provides feature maps, but no quantitative reconstructions. We extend helioseismic holography to a full converging regularization method by linking the physically motivated backpropagation operator with the adjoint of the Fréchet derivative of an appropriate operator mapping to the cross-covariance operator.

Keywords: helioseismology, holography, inverse problems

1 Introduction

In helioseismology one analyzes solar oscillations at the surface (e.g. line-of-sight velocities) in order to learn about subsurface properties. Data of the inverse problems are cross-correlations of the observed wavefield $\psi$ between two points $r_1, r_2$ on the solar surface caused by stochastic turbulent convection.

$$C(r_1, r_2, \omega) = \frac{1}{N} \sum_{i=1}^{N} \psi_i(r_1, \omega)\psi_i^*(r_2, \omega),$$

where $\omega$ denotes the frequency. The cross-correlation is a five-dimensional data set of immense size, which is unfeasible to store and invert directly. Therefore, one is generally in need of a priori averaging in space and frequency. Traditional approaches like time distance helioseismology achieve this goal by reducing the cross-correlation to a small number of physically interpretable quantities (for example travel times) with an acceptable signal-to-noise ratio. In contrast to time distance helioseismology, helioseismic holography first propagates the wavefield back to a target location and afterwards locally cross-correlate the backpropagated wave field in order to image the quantity of interest. This way the whole cross-correlation data is used implicitly without computing the cross-correlation explicitly. Despite to the great success of helioseismic holography, it is no quantitative regularization method (see figure 1).

![Image](image_url)

Figure 1: It is shown Lindsey-Braun holography for a uniform medium with wavenumber $k = 100 + i\gamma$. We have chosen 100 receivers uniformly spaced at a circular surface of radius 1. Although the main features are visible for small wave attenuation, the holographic image is wrong on scales.

2 Helioseismic holography

The wavefield can be described by a Helmholtz equation [1]:

$$-(\Delta + k^2)\psi - \frac{2i\omega}{\rho^{1/2}c}\nabla \left( \frac{\psi}{\rho^{1/2}c} \right) = s,$$

where $\mathbf{u}$ is the flow field and $s$ the stochastic source term. The density $\rho$, the sound speed $c$ and the wave attenuation $\gamma$ are modeled by the Solar Model S, smoothly extended to the atmosphere [2]. The local wavenumber $k$ takes the form

$$k^2 = \frac{\omega^2 + 2i\omega\gamma}{c^2} - \rho^{1/2}\Delta\rho^{-1/2}.$$
We use a radiation boundary condition assuming an exponential decay in near-surface layers. The holograms $\phi_\alpha$ can be computed from the measured wavefield on the observable surface:

$$\phi_\alpha(x, \omega) = \int_A H_\alpha(x, y, \omega) \psi(y, \omega) dy,$$

where $H_\alpha$ is a wave propagator (usually defined in terms of the Green function), which back-propagates the wavefield on the surface to a target location in the solar interior. Due to the stochastic nature of solar oscillations and within the holograms we are interested in the hologram intensity:

$$I_{\alpha, \beta}(r, \omega) = \phi_\alpha(r)^* \phi_\beta(r)$$

Perturbations to the solar medium can be expressed in terms of sensitivity Kernels $K_{\alpha, \beta}$:

$$\mathbb{E}[\delta I_{\alpha, \beta}(x, \omega)] = \int_\Omega K_{\alpha, \beta}(x, y) \delta q(x) dx,$$

where $q \in \{\rho, c, \gamma, u\}$. Usually the backpropagators are chosen, such that the sensitivity Kernels become localized.

3 Iterative holography

In contrast to the traditional approach of holography we will fix the wave propagators by the scalar wave equation and improve the holographic images by iterations. The covariance of the Doppler velocities can be written in the form [3]:

$$C(q) := \text{Cov}[v] = TL_q^{-1} \text{Cov}[s](L_q^*)^{-1} T^*,$$

where $T$ is a trace operator acting as projection to the surface and $C$ the covariance operator. The Fréchet derivative is given by:

$$\hat{C}[q] \delta q = -2 \text{Re} \left( H_\alpha^* [\partial_q L_q \delta q] H_\beta \right),$$

$$H_\alpha^* = TL_q^{-1}, \quad H_\beta^* = L_q^{-1} \text{Cov}[s](L_q^*)^{-1} T^*$$

where $\text{Re} A = \frac{1}{2}(A + A^*)$. The adjoint with respect to the Frobenius norm takes the form

$$C[q]^* \hat{C} = -2 [\partial_q L_q]^* \left( (H_\alpha (\text{Re} C) TL_q^{-1} H_\beta \right)$$

The operators $H_\alpha$ and $H_\beta$ can be interpreted as backpropagator, whereas $(\partial_q L_q)^*$ takes the role of a local correlation operator. This setting links the adjoint of the Fréchet derivative of the covariance operator to the wave propagation of traditional seismic holography. In this way we can extend helioseismic holography to a converging iterative regularization method, where the first iteration coincides with the classical holographic image.

4 Differential rotation

Due to the large computational costs for solving the forward problem, caused by the strong gradients close to the solar atmosphere, one usually solves linearized problems in local helioseismology. Our approach allows an application to nonlinear problems like inversions for solar differential rotation or solar convection. Usually differential rotation is measured by the frequency splitting caused by a rotating medium. Although this inversion has led to exciting results as the detection of the tachocline and NSSL, there are still some questions open. In particular frequency splitting does not allow us to invert for the antisymmetric part of the differential rotation. We have achieved very encouraging numerical results for the differential rotation in the solar convection zone (see figure 2).

References


Solution of a non-linear eigenvalue problem for Photonic Crystal Fiber applications

J.-R. Poirier¹*, R. Perrussel¹

¹LAPLACE, Université de Toulouse, CNRS, INPT, UPS, France
*Email: poirier@laplace.univ-tlse.fr

Abstract
A method to solve a non-linear eigenvalue problem coming from boundary integral equations is studied. The equations are provided by photonic crystal fiber applications.

Keywords: Boundary Element Method, Photonic Crystal Fiber, Non-linear eigenvalue problem

1 Introduction
Photonic crystal fibers (PCF) are systems that have been widely used for decades to allow light propagation. The geometry, the dielectric characteristics of the materials and the wavelength of the source are the main parameters to determine the effective refractive index of the medium. The complexity of these optical systems – heterogeneous structure, geometry of the section and the micrometric order of magnitude – makes the numerical methods mandatory to quickly design a PCF for the desired application. The finite-difference time-domain method and the finite element method are common approaches used to solve the problem of propagation in a PCF. However, these methods may require a huge amount of memory and computation time, according to the size of the mesh for a PCF with several inclusions. Solutions based on the Boundary Element Method (BEM) [1] have been proposed to reduce the size of the problem. They allow to consider only the mesh on the boundary of the inclusions but are limited by the resolution of a nonlinear eigenvalue problem. Usually solved by Müller’s method, it requires a rather precise knowledge of the solution as a starting point. We propose as an alternative a search method based on contour integrals and rational interpolation [2] not limited by these difficulties.

2 Boundary Integral Equations
We apply the formulation proposed in [1] but other formulations could be considered. Using the free space Green function

\[
G(r, \tilde{r}) = \frac{1}{4} H_0^{(1)}((k^2 - \beta^2)|r - \tilde{r}|), \quad r \neq \tilde{r}
\] (1)

where \(H_0^{(1)}\) is the Hankel function. Magnetic field components \(u = H_x\) or \(H_y\) can be represented for \(r \notin \partial \Omega_j\) by

\[
u(r) = \int_{\partial \Omega_j} G(r, \tilde{r}) \frac{\partial u(\tilde{r})}{\partial \nu} d\tilde{r} - \int_{\partial \Omega_j} \frac{\partial G(r, \tilde{r})}{\partial \nu}(\tilde{r}) u(\tilde{r}) d\tilde{r}, \quad (2)
\]

where \(\Omega_j\) is an homogeneous inclusion. Expressing continuity conditions on an interface \(\partial \Omega_j\)

\[\left[\frac{\partial H}{n^2} \right] = [E_z] = 0\]

and using Maxwell’s equations

\[ik_0 n^2 E_z = \partial_y H_x - \partial_x H_y,\]

the system can be expressed under the form

\[\mathcal{M} \begin{bmatrix} H_x \\ H_y \end{bmatrix} = 0 \]

with

\[\mathcal{M} = \begin{bmatrix} \frac{1}{\nu_x} (\nu_y \partial_y + \nu_z \partial_z) & \frac{1}{\nu_y} (\nu_x \partial_x - \nu_y \partial_y) \\ \frac{1}{\nu_z} (\nu_x \partial_x + \nu_y \partial_y) & \frac{1}{\nu_z} (\nu_y \partial_y - \nu_z \partial_z) \end{bmatrix} \]

It leads to solve a non-linear eigenvalue problem

\[F(n_{\text{eff}}) \mu^H = 0. \quad (3)\]

Matrix \(F\), coming from continuous operator \(\mathcal{M}\), depends on the effective refractive index \(n_{\text{eff}}\).

3 Algorithm for solving problem (3)
For solving a non-linear eigenvalue problem as (3), approaches exploiting contour integrals have been introduced in [2] and some improved variants have been proposed in several references (see for instance [3]). It consists to numerically compute integrals

\[\frac{1}{2\pi i} \int_C f(z) F(z)^{-1} \hat{V} \, dl\]

where \(C\) is a smooth contour enclosing the eigenvalues of interest, \(f\) an analytic function and \(\hat{V}\)
a random matrix of $L$ columns. Keldysh’ theorem provides us a link with the eigenvalues and right/left eigenvectors; for instance in the case of simple eigenvalues, we can write

$$F(z)^{-1} = \sum_{i=1}^{n(C)} v_k w_k^H \frac{1}{z - \lambda_k} + R(z)$$

where $n(C)$ is the number of eigenvalues inside $C$. $\lambda_k$ are these eigenvalues, $v_k$ and $w_k$ the corresponding right and left eigenvectors and $R$ is an analytic function. Computing contour integrals then enables us to focus only on the contribution of the rational part containing information on the eigenvalues. In most of the proposed algorithms, $f$ is chosen as the moments $z^k$, with $k = 1, \ldots, K$ and it enables to convert the nonlinear eigenvalue problem into a linear generalized eigenvalue problem.

Connections have also been done between this approach and rational interpolation; it leads in [3] to an algorithm called SS-RI (Sakurai-Sugiura method with Rational Interpolation). The proposed modifications enable to provide more numerical stability, in particular for large $K$, and also to choose "quadrature" points not only on the contour $C$ but also inside. This approach is considered for the numerical results.

4 Numerical Results

The tests in this section correspond to several discretisations of the fiber shown Figure 1 with the following physical parameters: free space wavelength is $\lambda = 1.45\mu m$, each hole has a diameter of $5\mu m$ and is discretized by $N = 40$ unknowns. The refractive index of the glass matrix is 1.45 and the medium surrounding the hole is infinite. We have tested several integral contours proposed in [3] but the most convenient is to keep a segment $[a_x, b_x]$ on the real axis discretized with $N_x$ Chebyshev points. It is then interesting to note that without any computation outside the real axis, the method gives a good approximate value of the imaginary part.

Table 1 gives zero(s) obtained for several discretizations and lengths of the segment. As expected, more Chebyshev points are necessary when the size of the segment increases. The main result is that a good approximation can be obtained with few computations. To start the search, a rough interval scan have to be performed and a few Müller iterations are useful to refine the solution. We point out that the algorithm may give several close solutions (two in our example) and that the refinement shows that they are equal. The SS-RI algorithm requires less computations than the brute force Müller algorithm [1] and does not require a very close initial guess. It makes the method more relevant to compute new PCF.

<table>
<thead>
<tr>
<th>$[a_x, b_x]$</th>
<th>$N_x$</th>
<th>$n_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>[1.445,1.4454]</td>
<td>3</td>
<td>(1.4453952345,3.321264e-08)</td>
</tr>
<tr>
<td>[1.445,1.4454]</td>
<td>5</td>
<td>(1.4453952341,3.19389e-08)</td>
</tr>
<tr>
<td>[1.445,1.4454]</td>
<td>10</td>
<td>(1.4453952341,3.19388e-08)</td>
</tr>
<tr>
<td>[1.445,1.4456]</td>
<td>5</td>
<td>(1.4453952335,2.856982e-08)</td>
</tr>
<tr>
<td>[1.445,1.446]</td>
<td>10</td>
<td>(1.4453952341,3.19371e-08)</td>
</tr>
<tr>
<td>[1.445,1.446]</td>
<td>20</td>
<td>(1.4453952341,3.19393e-08)</td>
</tr>
<tr>
<td>[ax,bx]</td>
<td>$N_x$</td>
<td>$n_{\text{eff}}$</td>
</tr>
<tr>
<td>[1.44,1.45]</td>
<td>20</td>
<td>(1.4453952506,4.34323e-08)</td>
</tr>
<tr>
<td>[1.44,1.45]</td>
<td>50</td>
<td>(1.4453952304,3.997883e-08)</td>
</tr>
<tr>
<td>[1.44,1.45]</td>
<td>100</td>
<td>(1.4453952343,3.1748179e-08)</td>
</tr>
</tbody>
</table>

Table 1: SS-RI algorithm Results

References


Modal computation for open waveguides

A. Leclerc\textsuperscript{2,1,∗}, A. Tonnoir\textsuperscript{1}, H. Barucq\textsuperscript{2}, M. Duruflé\textsuperscript{2}, C. Gout\textsuperscript{1}

\textsuperscript{1}LMI, INSA Rouen, 76 000 Rouen France
\textsuperscript{2}INRIA Bordeaux Sud Ouest, EPI Makutu, 64 000 Pau, France
∗Email: augustin.leclerc@insa-rouen.fr

\textbf{Abstract}

In this work, we are interested in mode computation in a three-dimensional open waveguide. We propose some absorbing boundary conditions to compute the modes in a bounded domain.

\textbf{Keywords:} open waveguides, Helmholtz equation, absorbing boundary conditions.

\textbf{1 Introduction}

The study of electromagnetic (EM) wave propagation is essential for considering the impact of Human’s technologies on the environment. For instance, the offshore wind energy is transported through twisted dynamic cables, which armours prevent a significant portion of the waves to irradiate outside the cable. Nevertheless, a remaining and possibly significant part might escape from the cable. Hence, our aim is to look at their scattering in the large stretch of sea water.

To consider this problem, we propose to modelize the cable and the surrounding water by an open 3D waveguide, which is an invariant domain according to the cable direction and which is unbounded in the two other directions. We will then take a modal approach for the resolution. Moreover, although Maxwell equations govern the propagation of EM waves, they will be here simplified to the Helmholtz equation, by considering Transverse Magnetic waves.

Before studying the EM field far away from the cable, we propose to focus on its behavior in its vicinity. Thus, we will use absorbing boundary conditions around the cable. Then, we will discuss about their relevance, especially in a low frequency system.

\textbf{2 The modal problem}

We consider the following Helmholtz problem:

\begin{equation}
- \Delta U - \rho \omega^2 U = 0 \quad \text{in} \quad \mathbb{R}^3
\end{equation}

where $\omega$ is the pulsation and where $\rho = \rho(x, y) \geq \rho_- > 0$ (invariant in $z$) and there is a constant $\rho_{\infty}$ such that $\rho - \rho_{\infty}$ is compactly supported in the plane $\{(x, y) \in \mathbb{R}^2\}$, and $C$ denotes its support. We also consider $\rho_+ = ||\rho||_{\infty}$. We seek for modal solutions of the form $U(x, y, z) = u(x, y) e^{i\beta z}$ where $u \in H^1(\mathbb{R}^2)$ and $\beta \in \mathbb{C}$ is the eigenvalue. Such a decomposition is possible because the domain is a waveguide whose geometry does not vary with $z$. It leads us to the following eigenvalue problem:

\begin{equation}
- \Delta_{x,y} u - (\rho \omega^2 - \beta^2) u = 0 \quad \text{in} \quad \mathbb{R}^2
\end{equation}

where $\Delta_{x,y} = \partial^2_{x^2} + \partial^2_{y^2}$ is the transverse Laplace operator.

\textbf{Lemma 1} If the eigenfunction $u$ is in $H^1(\mathbb{R}^2)$, then the eigenvalue $\beta^2$ is in $\omega^2[\rho_-, \rho_+]$.

This result is proven by contradiction arguments (using arguments of [1]) and will be detailed during the talk. Using radial decomposition of the solution, one can show that the solution $u$ should satisfy the radiation condition, analogous to the Sommerfeld condition:

\begin{equation}
\lim_{r \to +\infty} \partial u \over \partial r - i \sqrt{\rho_{\infty} \omega^2 - \beta^2} u = 0
\end{equation}

where $r = \sqrt{x^2 + y^2}$.

We can approximate this condition by imposing it at finite distance, for instance on a boundary $\partial \Omega$ (typically a circle of center 0 with radius $R$), such that the induced disk $\Omega$ includes the domain $C$ in the plane $Oxy$. It implies that we restrict (3) on $\Omega$, and that we can write:

\begin{equation}
\partial u \over \partial r |_{\partial \Omega} - i \sqrt{\rho_{\infty} \omega^2 - \beta^2} u |_{\partial \Omega} = 0
\end{equation}

Such a condition is called absorbing boundary condition (ABC). The new difficulty of the eigenproblem is in the non-linearity of this condition with the eigenvalue. The next section presents how to handle this.
3 Different sorts of ABC

The first idea to linearize the ABC is to consider that $\beta^2 \sim \rho^2 \omega^2$ (but still lesser). This consideration, with the fact that $\rho = \rho_\infty$ on $\partial \Omega$, leads us to approximate the square-root of the ABC as follows:

$$\frac{\partial u}{\partial r} |_{\partial \Omega} - i \omega \sqrt{\rho_\infty - \rho^2} u |_{\partial \Omega} = 0 \quad (5)$$

This expression is a common Robin boundary condition, independent of $\beta$, which will ease the resolution of the eigenproblem. However, we have to keep in mind that it results from a quite rough approximation. Using (5) might thus reduce the accuracy of the numerical results.

The two other ABCs that we propose come from the first two steps of the Newton-Raphson algorithm, applied to $i \sqrt{\rho_\infty \omega^2 - \beta^2}$. We take a small parameter $\varepsilon_0$, which will be our initial guess for this root. The first step of the algorithm gives us the following expression for the ABC:

$$\frac{\partial u}{\partial r} |_{\partial \Omega} + \left( -\frac{\varepsilon_0}{2} + \frac{\rho_\infty \omega^2 - \beta^2}{2 \varepsilon_0} \right) u |_{\partial \Omega} = 0 \quad (6)$$

This one shall be a more accurate condition, and is linear in $\beta^2$, which does not make the implementation more difficult.

The last ABC is obtained by applying the second step of the Newton-Raphson algorithm:

$$\frac{\partial u}{\partial r} |_{\partial \Omega} + \left( -\frac{\varepsilon_0}{4} + \frac{\rho_\infty \omega^2 - \beta^2}{4 \varepsilon_0} \right) + \left( \frac{\rho_\infty \omega^2 - \beta^2}{\varepsilon_0} + \frac{\rho_\infty \omega^2 - \beta^2}{\varepsilon_0} \right) u |_{\partial \Omega} = 0 \quad (7)$$

This condition is clearly non-linear with $\beta$, but we can linearize it pretty simply. Indeed, let $v$ be a function defined on $\partial \Omega$ such that

$$\left( \varepsilon_0 + \frac{\beta^2 - \rho_\infty \omega^2}{\varepsilon_0} \right) v = u |_{\partial \Omega} \quad (8)$$

This expression is linear with $\beta^2$, and leads to the following condition:

$$\frac{\partial u}{\partial r} |_{\partial \Omega} + \left( -\frac{\varepsilon_0}{4} + \frac{\rho_\infty \omega^2 - \beta^2}{4 \varepsilon_0} \right) u |_{\partial \Omega} + \left( \rho_\infty \omega^2 - \beta^2 \right) v = 0 \quad (9)$$

This condition is more difficult to implement, because of the new variable $v$ which must be taken into account. However, we can reasonably expect better results.

4 Numerical results

To show our first results, we consider $\mathcal{C} = \{ r \leq 0.2 \}$, $\rho = 10 \cdot 1_{\mathcal{C}} + 1_{\Omega \setminus \mathcal{C}}$ and $\omega = 10$. We will compare the results with different size of $\Omega$, that is to say with $R = 0.5$ and $R = 1$.

The modal computation of this example, with those two sizes of domain, gives us ten modes, whose eigenvalues are all in the interval $[100, 1000]$, satisfying the lemma 1. Figure 1 represents the first mode $u(x, y)$ (i.e. with largest $\beta$) for the two radii and with the ABC (5) on $\partial \Omega$.

Figure 1: On the left, the first mode $u$ with $R = 0.5$, and on the right, with $R = 1$, both with $\omega = 10$.

We can see that both radii give similar solutions. The same conclusion holds for the other ABCs. Actually, the frequency $\omega$ is high enough to enable the modes concentration near $\mathcal{C}$, giving few importance to the boundary condition.

Figure 2: On the left, the first mode $u$ with $R = 0.5$, and on the right, with $R = 1$, both with $\omega = 2$.

Let us see what the first ABC gives when the frequency is lower, for instance $\omega = 2$. On Figure 2, we can see that the solutions are no more neglectable on the boundary of the domain, so clearly in this case, the ABC must be well chosen to keep accurate results. This will be discussed in detail during the talk.

References

Adapted contour integration for nonlinear eigenvalue problems in wave-guide coupled resonators

Kersten Schmidt¹*, Philipp Jorkowski², Carla Schenker³, Luka Grubišić⁴, Rolf Schumann²

¹Department of Mathematics, TU Darmstadt, Germany  
²Chair “Theoretische Elektrotechnik”, TU Berlin, Germany  
³Simula Research Laboratory, Oslo, Norway  
⁴Department of Mathematics, Faculty of Science, University of Zagreb, Croatia

∗Email: kersten.schmidt@tu-darmstadt.de

Abstract
The eigenvalue problem for a resonator coupled to an unbounded waveguide is considered which becomes with a Dirichlet-to-Neumann map nonlinear in the eigenfrequency. The nonlinear eigenvalue problem (NEVP) shall be solved by the contour integration method of Beyn. For this a closed contour in the complex plane around the many desired eigenvalues is considered. Typically, contour integration methods are designed for circular (or more generally elliptic) shaped contours and rely on the exponential convergence of the trapezoidal rule applied to periodic functions. At each cut-off frequency of the waveguide the nonlinear operator has a square root singularity leading to branch cuts. For this the integration contours and the quadrature rules have to adapted to reliably find eigenvalues in the vicinity of the branch cuts. We analyze the accuracy of the different contours based on the convergence of filter functions and validate the estimates numerically using the example of the TESLA cavity.

Keywords: contour integration, electromagnetic wave-guide, nonlinear eigenvalue problems

1 The nonlinear eigenvalue problems in a wave-guide coupled resonator

An homogenous infinite wave-guide in 3D with constant cross-section connected to a bounded dielectric body is considered and the resonating behaviour shall be predicted by computing the complex eigenfrequencies with small imaginary part. Discretization of the Maxwell equations in frequency domain by the finite element method or the finite integration techniques with a (truncated) Dirichlet-to-Neumann map for the infinite wave-guide leads to the nonlinear eigenvalue problem

$$T(\omega)e = (A - \omega^2M + i\omega BP(\omega)B^H)e = 0,$$

with the curl-curl stiffness matrix $A \in \mathbb{R}^{n,n}$ and the mass matrix $M \in \mathbb{R}^{n,n}$. The Dirichlet-to-Neumann map leads to the matrix product $i\omega BP(\omega)B^H$, where $B$ represents the wave-guide modes and the $M \times M$ diagonal matrix valued function $P(\omega)$ has diagonal entries proportional to $\sqrt{\omega^2 - \omega_{c,m}^2}$ for transverse magnetic or its reciprocal for transverse electric modes, where $\omega_{c,m}, m = 1, \ldots, M$ are the first $M$ cut-off frequencies. For the finite integration technique the mass matrix is indeed the identity matrix $I$, which we will consider in the following.

2 Contour integration for nonlinear eigenvalue problems

The contour integration method of Beyn [1] can handle general nonlinearities for matrix-valued functions $T(z)$ if they are holomorphic in an open domain $\Omega \subset \mathbb{C}$. The method finds approximations $\lambda_{k,N}, k = 1, \ldots, K$ to all $K$ eigenvalues $\lambda_k, k = 1, \ldots, K$ inside a chosen closed contour $\Gamma \subset \Omega$ if they all are semi-simple and the associated eigenvectors linearly independent. To achieve an high accuracy in general the contour $\Gamma$ has to chosen not too close to any eigenvalue in $\Omega$ and not too close to the boundary $\partial \Omega$ of the holomorphicity domain.

The method is based on representation of

Figure 1: TESLA cavity with waveguide ports at the left and right boundary.
the resolvent by the theorem of Keldysh,
\[ T^{-1}(z) = \sum_{k=1}^{K} v_k w_k^H (z - \lambda_k)^{-1} + R(\Gamma; z). \]

Here, \( v_k \) and \( w_k \) are the left and right eigenvectors and \( R \) is an holomorphic function in a neighbourhood and the interior of the contour \( \Gamma \).

The rectangular matrices \( A_0 \) and \( A_1 \in \mathbb{C}^{n,\ell} \) are defined by the contour integrals along \( \Gamma \)
\[
A_0 := \frac{1}{2\pi i} \int_{\Gamma} T(z)^{-1} V \, dz,
A_1 := \frac{1}{2\pi i} \int_{\Gamma} z T(z)^{-1} V \, dz,
\]
where \( V \in \mathbb{C}^{n,\ell} \) with \( \ell \geq K \) columns has full rank. Here, \( \ell \) is chosen to be at least the number of (expected) eigenvalues in the contour. Approximations \( A_{0,N} \) and \( A_{1,N} \) of the two matrices can be computed by numerical quadrature. Then, a singular value decomposition of \( A_{0,N} \) leads to a small linear eigenvalue problem whose eigenvalues \( \lambda_{k,N} \) approximate those of the non-linear eigenvalue problem \( T(\lambda) v = 0 \).

The error of the method can be analyzed using the error in the filter functions
\[
b_0(\lambda) - b_{0,N}(\lambda) = \frac{1}{2\pi i} \int_{\Gamma} \frac{1}{z - \lambda} - \sum_{j=0}^{N-1} \frac{w_j}{z_j - \lambda} \, dz,
\]
with the abscissa \( z_j \) and weights \( w_j \) of the quadrature rule, evaluated on the approximative eigenvalues and the boundary of the domain of holomorphicity.

3 Adapted contour integration for waveguide coupled resonators

To address the square-root behaviour of the NEVP of the waveguide coupled resonator we first rotate the branch cuts into the negative imaginary plane by a proper definition of the square root.

Then, we compare a conformally mapped circular contour with associated trapezoidal rule with a polygonal contour and Gauss-Legendre rule both with a concentration of quadrature points close to the branch points. For both we observe a very fast decay of the error of the filter functions in the neighbourhood of the branch-points. Hence, even eigenvalues rather close to the branch-points are computed by method to an high accuracy as we observe on a model problem and for the 3D simulation of the TESLA cavity (see Fig. 1). In a post-processing step we select the computed eigenvalues with a very low eigenvalue residual. Both contours achieve very high accuracy, where the polygonal contours turn out to be more flexible when handling areas with several close branch-points.

References


Computing eigenvalues of the Laplacian on rough domains

Frank Rösler1, Alexei Stepanenko1,*
1School of Mathematics, Cardiff University, UK
*Email: stepanenkoa@cardiff.ac.uk

Abstract
We prove sufficient conditions under which the eigenvalues of a sequence of Dirichlet Laplace operators on bounded domains converge to the eigenvalues of a given limit domain. Our hypotheses allow for a wide variety of domains with cusps and fractal boundaries. This result is applied to prove the convergence of a numerical algorithm for computing the eigenvalues of such domains.

Keywords: Mosco convergence, spectral approximation, rough boundaries.

1 Introduction
This short paper focuses on the main technical results of our paper [1], where we study the Solvability Complexity Indices (SCI) [2] of computational eigenvalue problems associated to the Dirichlet Laplacian on bounded domains.

Throughout this paper, we consider a sequence of bounded domains $\mathcal{O}_n \subset \mathbb{R}^2$, $n \in \mathbb{N}$, converging to a bounded domain $\mathcal{O} \subset \mathbb{R}^2$ in the sense that

$$l(n) := \text{dist}_H(\mathcal{O}_n, \mathcal{O}) + \text{dist}_H(\partial \mathcal{O}_n, \partial \mathcal{O}) \to 0$$

as $n \to \infty$, where dist$_H$ denotes the Hausdorff distance. Let $-\Delta_{\mathcal{O}_n}$ and $-\Delta_{\mathcal{O}}$ denote the corresponding Laplace operators, endowed with Dirichlet boundary conditions. We denote the eigenvalues of $-\Delta_{\mathcal{O}_n}$ by $\lambda_k(\mathcal{O}_n)$, $k \in \mathbb{N}$, and the eigenvalues of $-\Delta_{\mathcal{O}}$ by $\lambda_k(\mathcal{O})$, $k \in \mathbb{N}$.

Our main result Theorem 3 concerns Mosco convergence. It implies the following result concerning the convergence of eigenvalues.

Theorem 1 Suppose that $\partial \mathcal{O}$ is a Jordan curve with zero Lebesgue measure and that, for each $n \in \mathbb{N}$, $\partial \mathcal{O}_n$ is locally connected. Then, for each $k \in \mathbb{N}$, we have

$$\lambda_k(\mathcal{O}_n) \to \lambda_k(\mathcal{O}) \quad \text{as} \quad n \to \infty.$$

In fact, this result is proved in [1] under more general hypotheses which allow for multiple boundary components. Note that a Jordan curve need not be locally the map of a continuous function, may contain cusps and may have Hausdorff or upper box-counting dimension of up to two.

2 Mosco convergence

The notion of Mosco convergence can be stated for general Banach spaces, however, here we restrict our attention to $H^1_0$ Sobolev spaces.

Definition 2 We have convergence in the Mosco sense $H^1_0(\mathcal{O}_n) \xrightarrow{M} H^1_0(\mathcal{O})$ as $n \to \infty$ if

(i) For all $u \in H^1_0(\mathcal{O})$, there exists $u_n \in H^1_0(\mathcal{O}_n)$, $n \in \mathbb{N}$, such that $\lim_{n \to \infty} \|u_n - u\|_{H^1} = 0$.

(ii) For any subsequence $H^1_0(\mathcal{O}_{n_j})$, $j \in \mathbb{N}$, and any $u_j \to u$ as $j \to \infty$ in $H^1$ for some $u \in H^1(\mathbb{R}^2)$, we have $u \in H^1_0(\mathcal{O})$.

It is well known that, since the domains $\mathcal{O}_n$ and $\mathcal{O}$ are bounded, $H^1_0(\mathcal{O}_n) \xrightarrow{M} H^1_0(\mathcal{O})$ implies the convergence for the eigenvalues of the Dirichlet Laplace operators. Hence, the next result implies Theorem 1.

Theorem 3 Under the hypotheses of Thm. 1, we have

$$H^1_0(\mathcal{O}_n) \xrightarrow{M} H^1_0(\mathcal{O}) \quad \text{as} \quad n \to \infty. \quad (1)$$

Let us now outline the main steps of the proof, assuming all stated hypotheses.

A) From uniform Poincaré to Mosco
Firstly, we are able to reduce Mosco convergence to the verification of certain Poincaré-type inequalities on neighbourhoods of the boundary of the form

$$\partial^c \mathcal{O} := \{x \in \mathcal{O} : \text{dist}(x, \partial \mathcal{O}) < r\}, \quad r > 0.$$

Proposition 4 Suppose that there exists a sequence $\epsilon(n) \geq 2l(n)$, $n \in \mathbb{N}$, with $\epsilon(n) \to 0$ as $n \to \infty$ and constants $C, \alpha > 0$ such that

$$\|u\|_{L^2(\partial^c \mathcal{O})} \leq C(n)\|\nabla u\|_{L^2(\partial \mathcal{O}_n \setminus \partial \mathcal{O})}, \quad (2)$$

$$\|v\|_{L^2(\partial^c \mathcal{O}_n \setminus \partial \mathcal{O})} \leq C(n)\|\nabla v\|_{L^2(\partial \mathcal{O}_n \setminus \partial \mathcal{O})}, \quad (3)$$

for all $n \in \mathbb{N}$, $u \in H^1_0(\mathcal{O})$ and $v \in H^1_0(\mathcal{O}_n)$. Then, (1) holds.

It therefore suffices to prove (2) and (3).
B) Poincaré for a single domain

Inequality (2) follows from the following result.

**Theorem 5** For \( r \in (0, r_0) \) and \( u \in H_1^1(\mathcal{O}) \),

\[
\|u\|_{L^{2}(\partial \mathcal{O})} \leq 5r\|\nabla u\|_{L^{2}(\partial \mathcal{O}, \mathbb{R}^2)}
\]

where \( r_0 = (4\sqrt{2})^{-1}Q(\partial \mathcal{O}) \) and

\[
Q(\partial \mathcal{O}) := \inf \left\{ \text{diam}(\Gamma) : \Gamma \subset \partial \mathcal{O} \text{ path component} \right\}.
\]

Here, the path components refer to the equivalence classes under the relation \( x \sim y \iff x \) connected by a path to \( y \). In fact, Theorem 5 holds for an arbitrary open set \( \mathcal{O} \subset \mathbb{R}^2 \) with \( Q(\partial \mathcal{O}) > 0 \). We prove this result by a geometric method involving explicitly constructing a certain type of bundle of paths from points in \( \partial \mathcal{O} \) to the boundary \( \partial \mathcal{O} \).

C) Poincaré for a sequence of domains

Under our hypotheses, we can provide a geometric description of \( \partial \mathcal{O}_n \) for large \( n \). More precisely, we show that there exists a sequence \( \epsilon(n) \) as in Proposition 4 such that, for all large enough \( n \), \( \partial \mathcal{O}_n \) has a path-connected subset \( \Gamma_n \) whose diameter exceeds \( \text{diam}(\partial \mathcal{O}) - \epsilon(n) \) and such that any other point in \( \partial \mathcal{O}_n \) lies within a distance \( \epsilon(n) \) to \( \Gamma_n \).

As it turns out, by applying Theorem 5 to the domain \( \mathcal{V}_n = \Gamma_n \), we are able to verify inequality (3) with \( C = 10 \) and \( \alpha = 4\sqrt{2} \).

3 Pixelated domain algorithm

\[ p_{30}(\mathcal{O}) \]

Figure 1: A pixelated domain approximation for the interior of a Koch snowflake.

Consider any domain \( \mathcal{O} \) satisfying the hypotheses of Theorem 1. Suppose we have access to the information of whether or not a given point \( x \in \mathbb{R}^2 \) is in \( \mathcal{O} \). Using the above results, we are able to construct a simple numerical method for the eigenvalues of \( -\Delta_{\mathcal{O}} \).

This numerical method is based on pixelated domain approximations, which are defined by

\[
p_n(\mathcal{O}) := \text{int} \left( \bigcup_{j \in L_n(\mathcal{O})} \left( j + [-\frac{1}{2n}, \frac{1}{2n}]^2 \right) \right)
\]

where

\[
L_n(\mathcal{O}) := \{ j \in (n^{-1}\mathbb{Z})^2 : j \in \mathcal{O} \}.
\]

Under the stated hypotheses for \( \mathcal{O} \), we are able to prove that pixelated domains converge in the sense that

\[
\text{dist}_H(p_n(\mathcal{O}), \mathcal{O}) + \text{dist}_H(\partial p_n(\mathcal{O}), \partial \mathcal{O}) \to 0
\]

as \( n \to \infty \). Consequently, Theorem 1 guarantees that the eigenvalues of \( -\Delta_{p_n(\mathcal{O})} \) converge to the eigenvalues of \( -\Delta_{\mathcal{O}} \).

Due to their regular shape, pixelated domains may be easily triangulated, for instance with a uniform mesh. Hence the eigenvalues of \( -\Delta_{p_n(\mathcal{O})} \) may be approximated using a finite element scheme, in turn providing an approximation for the eigenvalues of \( -\Delta_{\mathcal{O}} \).

4 Examples

**Example 6** Let \( f_c(z) = z^2 + c \), where \( |c| < \frac{1}{4} \), and consider the compact set

\[
K(f_c) := \{ z_0 \in \mathbb{C} : (f^n(z_0))_{n \in \mathbb{N}} \text{ bounded} \}.
\]

Then, the bounded domain \( \text{int}(K(f_c)) \) satisfies the hypotheses of Thm. 1.

References


Maximum norm error bounds for the full discretization of non-autonomous wave equations

Benjamin Dörich\textsuperscript{1,}\textsuperscript{*}, Jan Leibold\textsuperscript{1}, Bernhard Maier\textsuperscript{1}
\textsuperscript{1}Institute for Applied and Numerical Mathematics, Karlsruhe Institute of Technology, 76149 Karlsruhe, Germany
\textsuperscript{*}Email: benjamin.doerich@kit.edu

Abstract
In this talk, we consider a specific class of non-autonomous wave equations on a smooth, bounded domain and their discretization in space by isoparametric finite elements and in time by the implicit Euler method. Building upon the work of Baker and Dougalis (1980), we prove maximum norm estimates for the semi discretization in space and the full discretization. The key tool is the gain of integrability coming from the inverse of the spatially discretized differential operator. For this, we have to bound differentiated initial errors in the energy norm.

Keywords: error analysis, full discretization, wave equation, maximum norm error bounds, nonconforming space discretization, isoparametric finite elements, a-priori error bounds.

1 Introduction
We consider non-autonomous wave equations of the form
\[
\partial_t u(t) = \lambda(t)^{-1} \Delta u(t) + f(t),
\]
subject to homogeneous Dirichlet boundary conditions for \( t \in [0,T] \) on a domain \( \Omega \subset \mathbb{R}^N \), \( N = 2,3 \), with sufficiently regular boundary \( \Gamma \). In space, we employ isoparametric finite elements and in time the implicit Euler scheme. Following the approach in [1], we derive maximum norm error bounds for the semi- and full discretization. The main application we have in mind is the quasilinear wave equation
\[
\partial_t u(t) = \lambda(u(t))^{-1} \Delta u(t) + f(t,u(t)).
\]
In order to guarantee well-posedness of (2), one exploits a pointwise lower bound on \( \lambda(u) \) and this property has to be conserved in the discretization. Up to now, this is ensured via inverse estimates that either lead to a CFL conditions or to a restriction on the minimal polynomial degree of the ansatz space. By our linear results, we hope to show that these constraints are only of theoretical nature and can be removed.

2 Discretization in space
We consider the unified error analysis introduced in [3] and reformulate (1) as a first-order system
\[
\partial_t y(t) = A(t)^{-1} y(t) + F(t),
\]
in the product space \( X = H_0^1(\Omega) \times L^2(\Omega) \), with \( y = (u, \partial_t u) \) and initial value \( y(0) = y^0 \), operators
\[
A(t) = \begin{pmatrix} \text{Id} & 0 \\ 0 & \lambda(t) \end{pmatrix}, \quad \Lambda = \begin{pmatrix} 0 & \text{Id} \\ \Delta & 0 \end{pmatrix},
\]
and \( F(t) = (0, f(t)) \). Further, we consider the spatially discretized version on a finite dimensional space \( X_h \)
\[
\partial_t y_h(t) = A_h(t)^{-1} A_h y_h(t) + F_h(t),
\]
on the computational domain \( \Omega_h \approx \Omega \). In order to relate functions on the two (in general) different domains, we introduce a lift operator \( L_h \) mapping functions on \( \Omega_h \) to functions on \( \Omega \).

For technical reasons, we have to make the following assumption on \( \lambda \), which ensures the preservation of boundary conditions.

\textbf{Assumption 1} There is some \( \ell_{\text{max}} \geq 4 \) such that for \( 0 \leq \ell \leq \ell_{\text{max}} \) and \( u \in \mathcal{D}((-\Delta)^{\ell/2}) \) it holds
\[
\lambda u, \lambda^{-1} u \in \mathcal{D}((-\Delta)^{\ell/2}).
\]

A sufficient conditions for this assumption is for example given by
\[
\nabla \lambda |_{\Gamma} = 0.
\]
In [2], we obtained the following semidiscrete error bound.

\textbf{Theorem 2} Let \( \partial \Omega \in C^{k+1,1,} \), \( \ell_{\text{max}} \geq 2 \), and let \( u \) and \( \lambda \) be sufficiently regular. If the discrete initial value \( y_h(0) \) is chosen appropriately, then it holds
\[
\|y(t) - L_h y_h(t)\|_{L^\infty \times L^\infty} \leq C h^k,
\]
where \( C \) is independent of \( h \).
3 Discretization in space and time
We denote the time step by $\tau > 0$ and write the implicit Euler method in the form

$$\partial_t y_h^n = (A_h^n)^{-1} A_h y_h^n + F_h^n, \quad (4)$$

where we use the discrete derivative

$$\partial_t \varphi^n = \frac{1}{\tau} (\varphi^n - \varphi^{n-1}).$$

For the fully discrete solution (4), we show the following error bound, see [2].

**Theorem 3** Let $\partial \Omega \in C^{k+1,1}$, $\ell_{\text{max}} \geq 4$, and let $u$ and $\lambda$ be sufficiently regular. If the discrete initial value $y_h^0$ is chosen appropriately, then there is $\tau_0 > 0$ such that for $\tau \leq \tau_0$ and $n \geq 3$ we have the error bound

$$\|y(t^n) - \mathcal{L}h_{y_h}^n\|_{L^\infty \times L^\infty} \leq C \tau + Ch^\min\{k, \ell_{\text{max}} - 2\},$$

where $C$ is independent of $h$ and $\tau$, and $\tau_0$ is independent of $h$.

We note that by a slightly different approach, we prove similar convergence rates for the first approximations $y_h^j$, $j = 0, 1, 2$.

4 Strategy of the proof
In the continuous case, one can employ Sobolev’s embedding $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$ to obtain maximum norm bounds on the solution $u$. However, this is not possible for $u_h$ since the Lagrangian finite elements are not $H^2$-conforming.

Denoting the inverse of the discretized differential operator $A_h^{-1}$, we can generalize the following result from [1], and still obtain integrability in the discrete case.

**Lemma 4** Let $\partial \Omega \in C^{1,1}$ and $p, q, r \geq 2$ with $0 \leq \frac{1}{r} - \frac{1}{p} < \frac{1}{N}$. Then, it holds for $\xi_h \in X_h$

$$\|A_h^{-1} \xi_h\|_{L^p \times L^q} \leq C \|\xi_h\|_{L^r \times L^s}.$$ 

Together with a Sobolev’s embedding, a direct consequence of Lemma 4 is the continuity of the map

$$X_h \hookrightarrow L^4(\Omega_h) \times L^2(\Omega_h) \xrightarrow{A_h^{-1}} L^\infty(\Omega_h) \times L^\infty(\Omega_h).$$

Together with the reformulation of (3) as

$$y_h = A_h^{-1} A_h(t) \partial_t y_h - A_h^{-1} A_h(t) F_h(t), \quad (5)$$

we exchange integrability for time derivatives. Denoting the discrete error by $e_h(t)$, the maximum norm is bounded by

$$\|e_h(t)\|_{L^\infty \times L^\infty} \leq C \sum_{j=1}^3 \|\partial_t^j e_h(t)\|_{X_h} + Ch^k.$$

In the second step, we use energy techniques to bound the time derivatives of the error by further defects and the discrete initial errors

$$\|\partial_t^j e_h(0)\|_{X_h}, \quad j = 1, 2, 3.$$

An appropriately chosen initial value yields the desired order of convergence.

With the implicit Euler scheme given in the form (4), we derive analogously to (5) a representation for the fully discrete scheme. This allows us to mimic the proof of the semi discretization with some calculus for discrete derivatives and obtain the assertion of Theorem 3.

5 Acknowledgement
Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 25874477 – SFB 1173.

References


Order-preserving non-conforming grid interfaces for boundary-optimized summation-by-parts operators

Vidar Stiernström1,*, Martin Almquist1
1Department of Information Technology, Uppsala University, Uppsala, Sweden
*Email: vidar.stiernstrom@it.uu.se

Abstract
We present new operators for coupling boundary-optimized summation-by-parts (SBP) finite difference methods with non-equispaced grid points across non-conforming grid interfaces. The coupling utilizes projection operators that move grid functions across the non-conforming interface by projecting them to an intermediate piecewise polynomial space. We demonstrate that the new operators can be used to construct order-preserving interpolation operators for equations with second derivatives in space. The results are corroborated by solving the acoustic wave equation on a grid with a non-conforming interface. In addition, we demonstrate the superior accuracy of the boundary-optimized operators compared to the traditional SBP finite difference operators by solving the Euler vortex problem on a curvilinear grid with a non-conforming interface.

Keywords: high-order finite difference methods, summation-by-parts, non-conforming interfaces

1 Introduction
High-order SBP finite differences have proven to be an efficient and robust method for solving hyperbolic partial differential equations. For linear well-posed problems, the SBP property in combination with stable boundary treatment, such as simultaneous approximation terms (SAT), allows for the construction of provably energy-stable schemes. The SBP property however comes at the cost of a reduction in the order of accuracy of the operator in the boundary region. To alleviate the issue, boundary-optimized SBP operators were derived in [1]. The operators utilize non-equispaced grid points in the boundary region in order to reduce the leading order error. However, the non-equispaced grid points complicate coupling of grids with non-conforming interfaces. Traditionally, non-conforming interfaces are treated by the use of SBP-preserving interpolation operators, first presented in [2]. The interpolation operators transfer grid functions directly from one side of the interface to the other, and are constructed to adhere to a specific grid-spacing ratio across the interface (e.g 1:2). With non-equispaced grid points, no fixed ratio exists. We therefore turn to methods capable of coupling general grids and utilize the method presented in [3], where the grid functions are projected to and from a so-called glue grid, i.e., a piecewise polynomial space, in such a way that accuracy and stability is preserved.

The interpolation and glue projection operators in [2,3] all have order $p$, leading to a reduction in global convergence rate from $p+2$ to $p+1$ for equations with second derivatives in space discretized using SBP operators of interior order $2p$, and boundary order $p$, denoted SBP($2p,p$). In [4], order-preserving interpolation operators were presented. The authors showed that by combining operator pairs of orders $p+1,p$ one can construct an interface coupling such that the reduction in global convergence rate is avoided. Here, we present glue projection operators of orders $p+1,p$ and use these to construct order-preserving couplings of non-conforming grids.

2 Glue projection operators
Consider two finite difference grids $\bar{\Omega}_a$ and $\bar{\Omega}_b$ sharing a common interface. The idea presented in [3] is to construct operators $P_{2a,2b}$, $P_{2a,2a}$, where $P_{2a,2b}$ accurately projects grid functions from the interface of $\bar{\Omega}_a$ to a glue grid $\bar{\Omega}_b$, and vice versa for $P_{2a,2a}$. The piecewise polynomial space on $\bar{\Omega}_a$ is such that the interval edges coincide with the interface points of $\bar{\Omega}_a$. Once the grid function is projected to the glue grid, going between polynomial spaces is done by standard $L^2$ projection. That is, for a glue grid $\bar{\Omega}_b$ aligned with $\bar{\Omega}_a$ one may construct $P_{2a,2b}$ going from $\bar{\Omega}_a$ to $\bar{\Omega}_b$ by $L^2$ projection. Given glue projection operators $P_{2a,2b}$ and $P_{2a,2a}$, the interpolation operator $I_{2a}$ moving grid functions from $\bar{\Omega}_a$ to $\bar{\Omega}_b$ is formed as $I_{2a} = P_{2a,2a} P_{2a,2b} P_{2b,2a}$. The construction of $I_{2a}$ is analogous. As previously mentioned, the operators presented in [3] corre-
sponding to SBP(2p, p) operators are of order p.
In this work, we construct operator pairs where the order is raised to p + 1 in one of the projection directions. That is, we construct pairs of operators \((P_{a2p}, P_{b2p})\) of orders \((p + 1, p)\), and \((P_{b2p}, P_{a2p})\) of orders \((p, p + 1)\). Following the terminology of [4], this allows us to construct a 'good' \(I_{a2p}\) of order \(p + 1\) and 'bad' \(I_{b2p}\) of order \(p\). By exchanging the orders, one may also construct a 'bad' \(I_{a2p}\) and a 'good' \(I_{b2p}\). With this set of 'good' and 'bad' operators, the order-preserving interpolation presented in [4] is realized.

3 Numerical results

Consider the following wave equation

\[
\begin{align*}
  u_{tt} - c_a^2 \Delta u &= 0, \quad \bar{x} \in \Omega_a, \quad t > 0, \\
  v_{tt} - c_b^2 \Delta v &= 0, \quad \bar{x} \in \Omega_b, \quad t > 0, \\
  u - v &= 0, \quad \bar{x} \in \Omega_a \cap \Omega_b, \quad t > 0, \\
  c_a^2 u_x - c_b^2 v_x &= 0, \quad \bar{x} \in \Omega_a \cap \Omega_b, \quad t > 0,
\end{align*}
\]

where \(c_a = 1\), \(c_b = 1/3\), \(\Omega_a = [-10, 0] \times [0, 10]\) and \(\Omega_b = [0, 10]^2\). We discretize (1) as in [4] using boundary-optimized SBP operators and our new glue projection operators, with \(N^2\) grid points on \(\Omega_a\) and \((3N)^2\) grid points on \(\Omega_b\), such that the number of grid points per wavelength is constant. Convergence is measured against the solution \(u = \cos(x + y - \sqrt{2}c_at) + k_2 \cos(x - y + \sqrt{2}c_at), \ v = (1 + k_2) \cos(k_1 x + y - \sqrt{2}c_at), \ k_1 = \sqrt{2c_a/c_b^2 - 1}, \ k_2 = (c_a^2 - c_b^2k_1)/(c_a^2 + c_b^2k_1)\) at \(t = 2\) in the SBP \(H\)-norm, and the expected order-preserved rate is observed. See Figure 1.

![Figure 1: Error plot for the wave equation.](image1)

Next, consider the Euler vortex problem on a non-conforming grid with periodic boundaries discretized using SBP(4, 2) operators. See Figure 2 in which the grid is outlined and [1, 2] where the problem is presented in detail. The vortex is initialized in the center of the domain and propagated to the right along the interface. The solution using traditional SBP op-

erators and the interpolation operators in [2] is clearly distorted while similar errors are not visible when using the boundary-optimized operators and the newly developed glue projection operators.

![Figure 2: Pressure at \(t = 8.8\).](image2)

References


Linearly implicit energy consistent time discretisation for nonlinear wave equations

Guillaume Castera\(^1\), Juliette Chabassier\(^1\)
\(^1\)MAKUTU team, LMAP (UMR 5142, UPPA–Inria BSO)
*Email: guillaume.castera@inria.fr

Abstract
Nonlinear phenomena can occur in vibrating structures, as for instance piano strings, due to large deformations or nonlinear constitutive state laws. Integrating the nonlinear models in space and time can be done accurately in many ways, but preserving an energy identity at the discrete level is an efficient way to address numerical stability when coupling with other systems (as in the case of the piano). Gradient based integrators achieve this purpose at the cost of solving a nonlinear system at every time step. New formulations called Invariant Energy Quadratization (IEQ) and Scalar Auxiliary Variable (SAV) \([2–4]\) only require the inversion of a linear system while still preserving a discrete energy identity. This work presents a convergence analysis of an interleaved time integrator based on IEQ and \(\theta\)-scheme as well as numerical illustrations.

Keywords: nonlinear wave equation, energy identity, linearly implicit scheme

1 Introduction
Let \(x \in \Omega = [0, L] \) and \( t \in [0, T] \), a system of wave equations is considered under the form:

\[
M\ddot{q} + (R_1 \dot{q} - \partial_x (R_2 \partial_x q)) - \partial_x \left(K \partial_x q + Bq\right) + \nabla U(\partial_x q) + Cq + \mathbf{1}B \partial_x q = S(x, t) \tag{1}
\]

where \(q(x, t) \in \mathbb{R}^N\), \(M\), \(R_1\), \(R_2\), \(K\), \(B\), \(C\) are matrices with physical coefficients, \(U : \mathbb{R}^N \to \mathbb{R}^+\) is a nonlinear application and \(S\) is the source term. Boundary and initial conditions are given by \(q(0, t) = q(L, t) = q(x, 0) = 0\). The piano string enters this general framework, see \([1]\). Any regular solution to (1) satisfies an energy identity that states

\[
\frac{dE}{dt} = \int_0^L S \cdot \dot{q} - \int_0^L \dot{R}_1 \dot{q} \cdot \dot{q} - \int_0^L \partial_x R_2 \partial_x \dot{q} \cdot \partial_x \dot{q} \tag{2a}
\]

\[
E = \frac{1}{2} \int_0^L M \ddot{q} \cdot \dot{q} + \int_0^L U(\partial_x q) + \frac{1}{2} \int_0^L \begin{pmatrix} C & \mathbf{1}B \end{pmatrix} \begin{pmatrix} q \end{pmatrix} \cdot \begin{pmatrix} \partial_x q \end{pmatrix} \tag{2b}
\]

2 Energy compliant formulation of a nonlinear system of wave equations
Following the Invariant Energy Quadratization technique \([2–4]\) an auxiliary variable is introduced as \(\zeta(x, t) = \sqrt{2U(\partial_x q(x, t))} + c\), where \(c\) is chosen so that the square root is real. Hence the term \(\nabla U(\partial_x q)\) in (1) is equal to \(\zeta \mathcal{H}(\partial_x q)\) where

\[
\mathcal{H}(p) = \frac{\nabla U(p)}{\sqrt{2U(p)} + c} \tag{3}
\]

so (1) becomes

\[
\begin{cases}
M\ddot{q} + (R_1 \dot{q} - \partial_x (R_2 \partial_x q)) - \partial_x \left(K \partial_x q + Bq\right) + \zeta \mathcal{H}(\partial_x q) + Cq + \mathbf{1}B \partial_x q = S(x, t) \\
\dot{\zeta} = \mathcal{H}(\partial_x q) \cdot \partial_x q \tag{4}
\end{cases}
\]

and this new system satisfies the previous energy identity (2a) with

\[
\mathcal{E}_c = \frac{1}{2} \int_0^L M \ddot{q} \cdot \dot{q} + \frac{1}{2} \int_0^L \zeta^2 + \frac{1}{2} \int_0^L \begin{pmatrix} C & \mathbf{1}B \end{pmatrix} \begin{pmatrix} q \end{pmatrix} \cdot \begin{pmatrix} \partial_x q \end{pmatrix} \tag{5}
\]

3 Space and time approximations
After performing a variational formulation of (4) with \(q(t) \in (H^1(\Omega))^N\) and \(\zeta(t) \in L^2(\Omega)\) and restricting to adequate finite-elements approximation spaces, a semi-discrete system is obtained

\[
\begin{align*}
M_h \ddot{\tilde{q}}_h + R_h \dot{\tilde{q}}_h + \mathcal{H}(Q_h)Z_h = S_h \\
A_h \ddot{Z}_h = \mathcal{H}(Q_h) \cdot \dot{\tilde{q}}_h
\end{align*} \tag{6}
\]

where \(M_h\), \(A_h\), \(R_h\) and \(K_h\) are usual FEM matrices, \(S_h\) the source vector, and \(\mathcal{H}(Q_h)\) is a matrix whose values depend on \(Q_h\).

Following \([4]\), an interleaved time scheme is proposed:

\[
\begin{align*}
M_h \left[Q_h^{n+1} - Q_h^n\right]_{\Delta t^2} &+ R_h \left[Q_h^{n+1} - Q_h^n\right]_{2\Delta t^2} + K_h \left[Q_h^{n+1}\right]_{\Delta t^2} + \\
\mathcal{H}(Q_h^{n+1})Z_h^{n+1/2} + Z_h^{n-1/2} &= S_h^{n+1/2} + S_h^{n-1/2} \\
\left[Q_h^{n+1} - Q_h^{n+1/2}\right]_{\Delta t^2} + Z_h^{n+1/2} - Z_h^{n-1/2} &= S_h^{n+1/2} - S_h^{n-1/2} \tag{7}
\end{align*}
\]
where \([Q_h]_{n\Delta t^2} = (Q_{n+1}^h - 2Q_n^h + Q_{n-1}^h) / \Delta t^2\) and \({Q_h}\)\(_\theta = \theta Q_{n+1}^h + (1 - 2\theta) Q_n^h + \theta Q_{n-1}^h\).

### 3.1 Energy consistency

This space/time discretisation satisfies a discrete equivalent of (2a)

\[
- \frac{\mathcal{E}_h^{n-1/2}}{\Delta t} = S_h Q_h^{n+1} - 2Q_h^n + Q_h^{n-1} / 2 \Delta t
\]

where the modified mass matrix writes \(\tilde{M}_h = M_h + \Delta t^2 (\theta - \frac{1}{4}) K_h\).

### 3.2 Stability

The scheme (7) is shown to be stable if the modified mass matrix \(\tilde{M}_h\) is definite positive, which is the classical CFL condition of the \(\theta\)-scheme. The treatment of nonlinear terms does not impact the stability properties.

### 3.3 Complexity

An interesting property of scheme (7) is that for each time step, knowing \((Q_h^{n-1}, Q_h^n, Z_h^{n-1/2})\), the computation of \((Q_h^{n+1}, Z_h^{n+1/2})\) only requires the evaluation of \(\mathcal{H}(Q_h^n)\) and the solution of one linear system of size \(N \times N_h^n + N_h^n\).

### 4 Convergence analysis

Let \(e_Q^n = Q_h^n - Q_h(t^n)\) and \(e_Z^n = Z_h^n - Z_h(t^n)\) where \(Q_h, Z_h\) are solutions of (6). We will show that:

\[
\|e_Q^n\|_p \lesssim T R \quad \text{and} \quad \|e_Z^{n+1/2}\|_p \lesssim R,
\]

where

\[
R = e^{K^- T} \left[ \frac{\Delta t}{\sqrt{M^-}} \sum_{j=1}^{n_0} \|e^j_{h,1}\|_p + \frac{\Delta t}{\sqrt{A^-}} \sum_{j=1}^{n_0} \|e^j_{6,2}\|_p \right]
\]

and \(K^-, M^-, A^-\) are the strictly positive minimal eigenvalues of \(K_h, \tilde{M}_h\) and \(A_h\) which are supposed definite positive.

Truncation errors \(e_{h,n}\) are \(O(\Delta t^2)\) if the semi-discrete solution is regular enough in time (\(Q_h\) must be \(C^4\) and \(Z_h\) must be \(C^3\)).

### 5 Numerical illustration

A piano string is modeled (see [1]) and forced with a \(C^\infty\) in space and time compactly supported source. Fig. 1 shows the relative \(L^2\) in space and \(L^\infty\) in time relative error between the solution computed with a time step \(\Delta t\) and the refined one with step \(\Delta t/2\), using second order FEM. As expected the presented IEQ scheme shows quadratic convergence.

Figure 1: \(L^2\) in space and \(L^\infty\) in time relative error of several schemes

### 6 Prospects

Another promising idea [3] is to define \(\zeta\) as

\[
\zeta(t) = \sqrt{2 \int_0^L U(\partial_x q)(x, t) dx + c} \quad (8)
\]

This auxiliary variable is now a scalar and the new system equivalent to (7) is only of size \(N \times N_h^Q + 1\). This SAV scheme is faster than IEQ and the relative error between the two obtained solutions is only \(10^{-8}\). Convergence is also quadratic (see Fig. 1).

### References


Non-conforming and moving grids for the simulation of waves in viscous fluids

Manfred Kaltenbacher\textsuperscript{1,*}, Dominik Mayrhofer\textsuperscript{1}, Hamideh Hassanpour Guivaise\textsuperscript{2}, Florian Toth\textsuperscript{2}

\textsuperscript{1}Institute of Fundamentals and Theory in Electrical Engineering, TU Graz, Austria
\textsuperscript{2}Institute of Mechanics and Mechatronics, TU Wien, Austria

Email: manfred.kaltenbacher@tugraz.at

Abstract

We present a Finite Element (FE) formulation for waves in viscous, compressible fluids coupled to solid bodies described by linear elasticity. In doing so, we allow for non-conforming grids based on the Nitsche-type mortaring.

Keywords: waves in viscous compressible fluids, grids based on the Nitsche-type mortaring.

1 Formulation

We consider an elastic solid coupled to a viscous, compressible fluid along with a common interface as displayed in Fig. 1. The behavior of the solid is described by the balance of momentum and a suitable constitutive law (Hooke’s law). The governing equations in the fluid domain $\Omega_f$ are the balance of mass and momentum as well as an equation of state and constitutive law (Newtonian fluid). By applying a perturbation ansatz via a splitting of the total quantities (pressure, density and velocity) into a mean part and a fluctuating one, neglecting the non-linear terms and using the linearized equation of state between density perturbation $\rho$ and pressure $p$ via $\rho = \frac{\rho_0}{c_s^2}$ (c denotes the isentropic speed of sound), we arrive at

\begin{align}
\frac{1}{c_s^2} \frac{\partial p}{\partial t} + \rho_0 \nabla \cdot \mathbf{v} &= 0 \quad \text{in } \Omega_f, \quad (1) \\
\rho_0 \frac{\partial \mathbf{v}}{\partial t} - \nabla \cdot \mathbf{\sigma}_f &= 0 \quad \text{in } \Omega_f. \quad (2)
\end{align}

In (1), (2) $p$ denotes the acoustic pressure, $\mathbf{v}$ the acoustic particle velocity, and $\mathbf{\sigma}_f$ the fluid stress tensor, which computes for an isotropic Newtonian fluid by

\begin{align}
\mathbf{\sigma}_f &= -p \mathbf{I} + \mu (\nabla \mathbf{v} + (\nabla \mathbf{v})^T) + (\lambda - \frac{2}{3} \mu) (\nabla \cdot \mathbf{v}) \mathbf{I}, \quad (3)
\end{align}

where $\mu$ is the dynamic (shear) viscosity and $\lambda$ the bulk viscosity. The elastic solid in $\Omega_s$ is governed by the conservation of momentum

\begin{align}
\rho_s \frac{\partial^2 \mathbf{u}}{\partial t^2} - \nabla \cdot \mathbf{\sigma}_s &= 0 \quad \text{in } \Omega_s, \quad (4)
\end{align}

where the solid density is denoted by $\rho_s$, $\mathbf{u}$ is the mechanical displacement vector and $\mathbf{\sigma}_s$ is the mechanical stress tensor. At the interface $\Gamma_{sf}$ between solid and fluid, one needs to enforce the dynamic and kinematic conditions requiring continuity of traction and velocity, respectively. Traction continuity is enforced by requiring

\begin{align}
\mathbf{\sigma}_s \cdot \mathbf{n}_s - \mathbf{\sigma}_f \cdot \mathbf{n}_f &= 0 \quad \text{on } \Gamma_{sf}, \quad (5)
\end{align}

where $\mathbf{n}_f$ and $\mathbf{n}_s$ are the outer normal of the fluid and solid domain, respectively (see Fig. 1). The second interface condition is velocity continuity at the interface, which requires

\begin{align}
\frac{\partial \mathbf{u}}{\partial t} &= \mathbf{v} \quad \text{on } \Gamma_{sf}. \quad (6)
\end{align}

To obtain the Nitsche coupled formulation, we combine the weak forms of the partial differential equations (PDEs) for the viscous fluid and elastic solid and incorporate (6), (7) to arrive at

\begin{align}
\int_{\Omega_f} \rho_0 \mathbf{v} \cdot \frac{\partial \mathbf{v}}{\partial t} \, d\Omega + \int_{\Omega_f} \nabla \mathbf{v} \cdot \mathbf{\sigma}_f \, d\Omega + \int_{\Gamma_{sf}} \left( \mathbf{u}' \cdot \mathbf{n}_s \cdot \frac{\partial \mathbf{u}}{\partial t} - \mathbf{\sigma}_s \cdot \mathbf{n}_s \right) \, d\Gamma \\
= \int_{\Gamma_{sf}} \left( \mathbf{u}' \cdot \mathbf{n}_s \right) \cdot \left( \mathbf{\sigma}_f \cdot \mathbf{n}_f \right) \, d\Gamma - \int_{\Gamma_{sf}} \mathbf{t} \cdot \mathbf{v} \, d\Gamma + \int_{\Omega_f} \rho_0 \mathbf{v} \cdot \frac{\partial \mathbf{v}}{\partial t} \, d\Omega + \int_{\Omega_f} \nabla \mathbf{v} \cdot \mathbf{\sigma}_f \, d\Omega + \int_{\Gamma_{sf}} \left( \mathbf{u}' \cdot \mathbf{n}_s \cdot \frac{\partial \mathbf{u}}{\partial t} - \mathbf{\sigma}_s \cdot \mathbf{n}_s \right) \, d\Gamma \quad \text{(traction consistency)}
\end{align}

\begin{align}
+ \beta \rho_s \frac{\partial^2 \mathbf{u}}{\partial t^2} \frac{\partial \mathbf{u}}{\partial t} \mathbf{n}_s \, d\Gamma = 0. \quad (8)
\end{align}
To meet the inf-sup (Ladyzhenskaya-Babuška-Brezzi) condition, we use a one-order higher polynomial basis function for particle velocity \( v \) than that for the acoustic pressure \( p \) \cite{1, 2}.

\section{Validation}

To validate our formulation for a viscous fluid, we consider a Stokes boundary layer generated by an infinitely long plate, which oscillates with a velocity \( \hat{v} \cos(\omega t) \) in \( x \)-direction and fulfilling the solution

\[ v_y = \hat{v} \text{Re} \left\{ \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{\rho \omega}} \right)^{1/2} \right\}. \tag{9} \]

The computational domain is displayed in Fig. 2 for a graded mesh and the convergence behavior of the error both for \( h^- \) and \( p^- \) refinement is shown in Fig. 3. The results clearly demonstrate the superiority of \( p^- \)-FEM on a graded mesh.

\section{Application}

As a practical application, we consider a micro-electro-mechanical system (MEMS) speaker as displayed in Fig. 4. To further decrease the computational time, we apply the linearized balance of mass and momentum of the viscous fluid (viscous PDEs) just in the channel and in a small region surrounding the ambient air, and then couple it to the standard wave equation again via a non-conforming grid to compute the radiated sound (see Fig. 5). The computational results are displayed in Fig. 6 both scaled for the channel part, where the viscous effect is strongly present and for the ambient air.

Currently, we extend our formulation to include also moving structures via an ALE (Arbitrary Lagrangian - Eulerian) formulation and apply it to a MEMS speaker based on digital sound reconstruction using moving shutter gates.

\section{References}

\begin{enumerate}
\end{enumerate}
Thursday, July 28, First Afternoon Session
An Efficient Iterative High Order Numerical Method for Multiple Scattering

Vianey Villamizar1,* , Tahsin Khajah2, Jonathan Hale1, Monu Jaiswal2

1Department of Mathematics, Brigham Young University, Utah, USA
2Department of Mechanical Engineering, University of Texas at Tyler, Texas, USA
*Email: Vianey@mathematics.byu.edu

Abstract

We have developed a highly accurate, efficient, and high order numerical iterative method for multiple scattering by coupling finite differences (FD) and an isogeometric finite element method (IGA) with local high order ABC, based on Karp’s farfield expansions.

Keywords: Multiple Scattering, High Order Method, Absorbing Boundary Conditions

1 Formulation of the Iterative Multiple Scattering Problem Combined with Karp’s Farfield Expansion ABC

Our problem consists of finding the scattered wave, u, obtained from the scattering of a time-harmonic incident plane wave, uinc, from M multiple obstacles. The boundary of each obstacle is denoted as Γm and the unbounded region in the exterior of Γm by Ωm, for m = 1, . . . , M. Therefore, the common scattered region is Ω = ∪m=1MΩm and the boundary of the full problem is Ω = ∪m=1MΓm. Hence, our problem can be formulated as

\[ \Delta u + k^2 u = 0, \quad \text{in} \; \Omega, \]  
\[ B u = \left[ Z \frac{\partial u}{\partial r} + (1 - Z)u \right] + \frac{Z \partial u_{inc}}{\partial r} + (1 - Z)u_{inc}, \quad \text{in} \; \Gamma, \]  
\[ \lim_{r \to \infty} r^{1/2} (\partial_r u - ik u) = 0, \]  

where Z represents the acoustic hardness Z ∈ [0, 1]. In this work, we adopt a formulation, proposed by Guizane et al. [1], which consists of considering M single scattering problems in each Ωm coupled at their scatterer boundaries. Each scattered wave um is obtained from the scattering of the incident wave, uinc, and the waves um emanating from the other scatterers (\( m \neq n \)). Balaban [4] proved that the solution u of the multiple scattering problem can be uniquely decomposed as, \( u = \sum_{m=1}^{M} u_m \), in Ω. As a consequence, we approximate u by numerically solving a family of single scattering problems for um coupled at their scatterer boundaries, Γm. Since our purpose is to apply finite differences and finite element methods, we introduce a circular artificial boundary Cm of radius Rm enclosing the m-th obstacle, which reduces each infinite domain Ωm to a bounded one, Ω+m. Next, we define an appropriate ABC on Cm. For this purpose, we employ a high order local ABC derived by Villamizar, Acosta and Dastrup [2], and adopted by Khajah et al., [3] to derive an overall high order technique, based on IGA.

Governing equations and scatterer boundary conditions for obstacle m:

\[ \Delta u_m + k^2 u_m = 0, \quad \text{in} \; \Omega_m, \]  
\[ B u_m = -B \left( u_{inc} + \sum_{\hat{m}=1, \hat{m} \neq m}^{M} u_{\hat{m}} \right) \quad \text{on} \; \Gamma_m. \]

High order local farfield expansion ABC on the circular artificial boundary, Cm of radius Rm:

\[ u_m(R_m, \theta_m) = K_{m,L}(R_m, \theta_m), \quad \text{in} \; C_m, \]  
\[ \frac{\partial u_m}{\partial r_m}(R_m, \theta_m) = \frac{\partial K_{m,L}}{\partial r_m}(R_m, \theta_m) \quad \text{in} \; C_m, \]  
\[ H_0(kr_m) \left[ (L - 1)^2 F_{m,L-1} + \frac{d_{m,L-1}^2}{d_{m,L-1}^2} F_{m,L-1} \right] + H_1(kr_m) \left[ L^2 G_{m,L-1} + \frac{d_{m,L-1}^2}{d_{m,L-1}^2} G_{m,L-1} \right] = 0, \]  
\[ 2l F_{m,l-1} + \frac{d_{m,L-1}^2}{d_{m,L-1}^2} F_{m,L-1} \right] + H_1(kr_m) \left[ l^2 G_{m,L-1} + \frac{d_{m,L-1}^2}{d_{m,L-1}^2} G_{m,L-1} \right] = 0, \]  
\[ 2l F_{m,l} = -l F_{m,l-1}(\theta) - \frac{d_{m,L-1}^2}{d_{m,L-1}^2} G_{m,L-1}, \]  
\[ \text{on} \; C_m, \; \text{for} \; m = 1, \ldots, M \; \text{and} \; l = 1, \ldots, L - 1, \]

where \( \theta_m \) is the angle along \( C_m \). The symbol \( K_{m,L} \) designates a truncated version of the Karp farfield expansion,

\[ K_{m,L}(r_m, \theta_m) = H_0(kr_m) \sum_{l=0}^{L-1} \frac{F_{m,l}(\theta_m)}{(kr_m)^l} + H_1(kr_m) \sum_{l=0}^{L-1} \frac{G_{m,l}(\theta_m)}{(kr_m)^l}, \quad \text{in} \; \Omega_m^+, \]

which is an exact representation of the solution um in the unbounded exterior region \( \Omega_m^+ = \mathbb{R}^2 \setminus \Omega_m \). The angular functions \( F_{m,l}(\theta_m) \) and
$G_{m,l}(\theta_m)$ are additional unknowns. They depend on the geometry of the scatterers and the physical properties of the bounded regions $\Omega_m^-$. Once that approximations for $F_{m,l}$ and $G_{m,l}$ are obtained, we can compute the values of $u_m$ anywhere in the exterior region $\Omega_m^+$, in particular, at the other scatterers boundaries.

The computation of the solutions $u_m$ of the family of multiple scattering problems (4)-(10) can be greatly simplified by adopting an iterative Jacobi- or Gauss-Seidel-type formulation, similar to the one found in [1]. Assuming that the outgoing waves from other scatterers are known from a previous iteration, it is possible to reduce the multiple scattering problem (4)-(10) to a family of single scattering problems. They can be solved individually in their respective local coordinate systems to obtain $u_m$ and then adding these $u_m$, we obtain the total scattered field $u$ from all scatterers.

![Figure 1: Total field numerical solution](image)

## 2 Numerical Results

We obtain numerical approximations to the original multiple scattering problem by applying two different numerical methods to the iterative problems: 1) a second order finite difference, and 2) a high order isogeometric finite element method. A key aspect of the proposed numerical techniques is that each of the ultimate matrices $A_m$, which are obtained from the numerical method (either FD or IGA) when solving the BVP for $u_m$, do not change during all iteration-steps. Hence, only one matrix inversion is needed during the iteration process. This represents a significant saving of computational time. In Table 1, we show the second order of convergence expected for our second order FD method. As seen, it requires very few iterations. In Table 2, we show a much higher accuracy for the same grid sizes. Also, the higher order of convergence of the IGA method combined with the farfield ABC is clearly shown. In both cases, we are only using 10 terms in the Karp’s farfield expansion.

We have performed a great number of numerical experiments including complex configuration of several obstacles of arbitrary shape that show the high accuracy, high order of convergence, and efficiency of our numerical methods. We will discuss them during our presentation at Waves 2022.

<table>
<thead>
<tr>
<th>PPW</th>
<th>$h$</th>
<th>Iters</th>
<th>Error</th>
<th>Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>6.67-02</td>
<td>8</td>
<td>8.93-03</td>
<td>—</td>
</tr>
<tr>
<td>20</td>
<td>5.00-02</td>
<td>6</td>
<td>4.71-03</td>
<td>2.23</td>
</tr>
<tr>
<td>25</td>
<td>4.00-02</td>
<td>5</td>
<td>2.91-03</td>
<td>2.15</td>
</tr>
<tr>
<td>30</td>
<td>3.33-02</td>
<td>5</td>
<td>1.98-03</td>
<td>2.12</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>PPW</th>
<th>$h$</th>
<th>Iters</th>
<th>Error</th>
<th>Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>6.67-02</td>
<td>16</td>
<td>9.27-07</td>
<td>—</td>
</tr>
<tr>
<td>20</td>
<td>5.00-02</td>
<td>16</td>
<td>2.61-07</td>
<td>4.33</td>
</tr>
<tr>
<td>25</td>
<td>4.00-02</td>
<td>16</td>
<td>1.05-07</td>
<td>4.03</td>
</tr>
<tr>
<td>30</td>
<td>3.33-02</td>
<td>16</td>
<td>5.39-08</td>
<td>3.60</td>
</tr>
</tbody>
</table>

**References**


Asymptotic analysis for sound-hard acoustic scattering by two closely-situated spheres

Camille Carvalho$^{2,1}$, Arnold Kim$^2$, Cory McCullough$^{2,*}$

$^1$Univ Lyon, INSA Lyon, UJM, UCBL, ECL, CNRS UMR 5208, ICJ, F-69621, France
$^2$Department of Applied Mathematics, University of California Merced, United States

Email: cmccullough2@ucmerced.edu

Abstract

We consider acoustic binding of particles resulting from radiation forces created through multiple scattering. This problem has potential for developing methods for assembling novel metamaterials. A key consideration in acoustic binding is when two or more particles are closely situated to one another and form a cluster. For that case, the near-field scattering by the particles becomes important. Here, we study multiple scattering by two closely-situated sound-hard spheres. Using boundary integral equation (BIE) methods, we find that a close evaluation problem arises leading to a nearly singular system of BIEs governing the surface fields. An asymptotic analysis of the problem reveals that this nearly singular behavior will lead to large error in the numerical solution unless it is explicitly addressed.

Keywords: Boundary integral methods, asymptotics, nearly-singular integrals.

1 Problem Description

We consider the plane wave $u^{\text{inc}} = e^{i k z}$ scattered by two sound-hard spheres (denoted $D_i$, with boundary $B_i$, $i = 1, 2$). The total field $u = u^{\text{ sca}} + u^{\text{ inc}}$ satisfies

$$\Delta u + k^2 u = 0, \quad u = 0, \quad \text{on } \partial E := B_1 \cup B_2,$$

and $u^{\text{sca}}$ satisfies the Sommerfeld radiation condition. Upon solution of (1), we compute the acoustic radiation forces,

$$F_i = -\int_{B_i} \left\{ \left[ \frac{1}{2} \delta_0 (p_i^2) - \frac{1}{2} \delta_0 (u_i^2) \right] \hat{n} + \rho_0 \left( \hat{n} \cdot \vec{v}_i \right) \hat{v}_i \right\} dS, \quad i = 1, 2,$$

where $\vec{v}_i = \nabla u_i$, $p_i = i \rho_0 \omega u_i$, with $\rho_0$ the density of the spheres, $\omega$ the angular frequency, $\hat{n}$ the unit outward normal of each sphere, and $u_i$ the surface field on each sphere: $u_i = u|_{B_i}$, $i = 1, 2$. It has been shown recently that this force can be significant when the size of the spheres is comparable to the wavelength and lead to so-called acoustic binding of particles [1]. An important case in acoustic binding is when the spheres are situated closely to one another. To study this problem, let $x_1$ and $x_2$ denote the centers of the two spheres both with radius $a$ (with $ka = O(1)$), and consider $|x_1 - x_2| = 2a + \varepsilon$ in the asymptotic limit, $\varepsilon \to 0^+$ (see Fig. 1).

This scattering problem is challenging due to strong near-fields interactions.

Figure 1: (Left) Sketch of the problem and notations. (Right) Plot of the expansion coefficients $(C^{(0)}_{\ell k})_{-0,32}$ in (5) for $k = 7.33$, $a = 0.16$, $x_1 = (0,0,0)$, $x_2 = (0,0,2a + 1)$. The blue curve represents obtained $(C^{(0)}_{\ell k})_k$ when approximating (4) using Gaussian Product Quadrature rule (GPQ), the yellow curve refers to $(C^{(0)}_{\ell k})_k$ obtained analytically when there is only $D_1$.

2 Boundary integral equations

Note that (2) only requires the surface fields. For this reason, boundary integral equation methods are natural for studying this problem. Additionally, since the scatterers are spheres, we use a Galerkin projection method to study the governing boundary integral equations (BIEs) that we discuss below. We write

$$u^{\text{sca}}(x) = \sum_{i=1}^{2} S_i [\partial_n u^{\text{inc}}_i] + D_i [u^{\text{sca}}_i], \quad x \in E, \quad (3)$$

where $D_i$ and $S_i$, $i = 1, 2$ are the double- and single-layer potentials, respectively, for each of the two spheres indexed by $i$. In (3), $S_i$ is applied to the normal derivative of the known incident field on $B_i$, which we denote by $\partial_n u^{\text{inc}}_i$, and $D_i$ is applied to the unknown scattered field on $B_i$, which we denote by $u^{\text{sca}}_i$. Upon projecting (3) onto $B_1$ and $B_2$, we obtain the following system of BIEs,
\[
\begin{bmatrix}
\frac{1}{2} - D_{11} & -D_{12} \\
-D_{21} & \frac{1}{2} - D_{22}
\end{bmatrix}
\begin{bmatrix}
u_{1}^{sca} \\
u_{2}^{sca}
\end{bmatrix} = 
\begin{bmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{bmatrix}
\begin{bmatrix}
\partial_{\nu_{1}} u_{1}^{inc} \\
\partial_{\nu_{2}} u_{2}^{inc}
\end{bmatrix},
\]
where \(D_{ij}\) and \(S_{ij}\) are the double- and single-layer potentials for sphere \(i\) evaluated on sphere \(j\), respectively.

3 Galerkin method

To solve (4), we substitute
\[
u_{i}^{sca} = \sum_{\ell m} C_{\ell m}^{(i)} h_{\ell}^{(1)}(kr) Y_{\ell m}^m(\theta, \phi), \quad i = 1, 2,
\]
with \(h_{\ell}^{(1)}\) denoting the spherical Hankel functions of the first kind, and \(Y_{\ell m}^m(\theta, \phi)\) the spherical harmonics. Similarly, one can write a spherical harmonic expansion of the layer potential kernels. Using the orthogonality of spherical harmonics, we derive a linear system for the expansion coefficients \(C_{\ell m}^{(i)}\), \(i = 1, 2\). We truncate this system at some fixed order \(\ell^*\), solve that system, and use the corresponding truncation of (5) to approximate the solution.

We solve this truncated system for the expansion coefficients with \(\ell = 1\). The expansion coefficients \(C_{\ell m}^{(i)}\) for \(B_1\) as a function of order \(\ell\) are shown as a blue dotted curve in the right plot in Fig. 1. For comparison, we plot the expansion coefficients for a single sphere as a yellow dotted curve (analytic result). The decay of \(C_{\ell m}^{(1)}\) with \(\ell\) is substantially slower than that for a single sphere. Thus, one needs to consider large values of \(\ell^*\) in comparison to the single sphere problem to achieve a comparable accuracy.

The slower decay of expansion coefficients is due to the off-diagonal blocks in (4). Those off-diagonal blocks model the coupling of scattered fields between the two spheres. In particular they involve the evaluation of the double-layer potential from one sphere on the other. In the limit \(\epsilon \to 0^+\), we find that these off-diagonal blocks involve a close evaluation of the double-layer potential thereby yielding nearly singular behavior. The results shown in Fig. 1 indicate that even when the spheres are not too close, the coupling effects are strong and affect the accuracy of the numerical approximation.

4 Asymptotic Analysis

Without addressing the close evaluation problem explicitly, one will need large computational resources to maintain accuracy [2,3]. To identify the main cause and address this problem, we propose an asymptotic analysis of the off-diagonal blocks in (4). Below, we identify the main mechanism resulting in the nearly singular behavior of those off-diagonal blocks.

At close evaluation distance \(r = a(1 + \epsilon)\), by expanding about \(\epsilon = 0\) one can show that
\[
h_{\ell}^{(1)}(ka(1 + \epsilon)) = \left[1 - \epsilon^2 \frac{(ka)^2}{2}\right] \frac{\ell(\ell + 1)}{2} h_{\ell}^{(1)}(ka) + \epsilon(1 + \epsilon)(ka) h_{\ell + 1}^{(1)}(ka) + O(\epsilon^3).
\]

Using (6), one can show that the close evaluation of the double-layer potential involves two operators: the spherical Laplacian \(\Delta_{S2}\) which satisfies \(\Delta_{S2} Y_{\ell m}^{m} = -\ell(\ell + 1) Y_{\ell m}^{m}\), and
\[
L_{3/2}[u] = \frac{1}{4\pi\sqrt{2}} \int_{S^2} \frac{u(s') - u(s)}{(1 - s \cdot s')^{3/2}} ds',
\]
which satisfies \(L_{3/2} Y_{\ell m}^{m} = -\ell Y_{\ell m}^{m}\) [4]. These operators account for the slow decay of expansion coefficients at close separation distance (causing large errors). In the spirit of [3], one can derive asymptotic approximations of the operators above, allowing to design an adapted quadrature rule for the off-diagonal terms that addresses the close evaluation problem. Extensions to the scattering by multiple spheres and comparison of computed acoustic radiation forces with experiments will be considered.

Acknowledgement This work was partially funded by the National Science Foundation Grants: DMS-1819052 and DMS-1840265.

References

Analysis and Approximation of Electromagnetic Surface Waves in Nonlinear Dispersive Media

Mathias Ionescu-Tira$^{1,*}$, Tomáš Dohnal$^1$, Marcus Waurick$^2$

$^1$Department of Mathematics, Martin-Luther-Universität Halle, Germany
$^2$Technische Universität Bergakademie Freiberg, Germany
*Email: mathias.ionescu-tira@mathematik.uni-halle.de

Abstract

We discuss well-posedness and stability results for nonlinear Maxwell equations, at an interface between dispersive media, based on evolutionary operator equations. Within this framework we propose a method for obtaining a justification of a wave packet approximation on long time intervals.

Keywords: Maxwell equations, evolutionary equations, dispersive waves

1 Maxwell system at an interface

Wave phenomena in nonlinear and interface optics are explained using the macroscopic Maxwell equations, where the material response (electric permittivity and magnetic permeability) is frequency-dependent, i.e., non-instantaneous. In physics, EM surface waves like surface plasmon polaritons at an interface are documented for a number of configurations. These are formal solutions of the linear Maxwell system and given by a plane-wave ansatz of the form

$$
\varphi(x_1) e^{ikx_2 - \omega t},
$$

where $\varphi : \mathbb{R} \to \mathbb{R}^6$ is exponentially decaying, and $k \in \mathbb{R}$ and $\omega \in \mathbb{C}$ are related by a dispersion relation $\omega(k)$. These evanescent linear modes serve as building blocks for the approximation of solutions of the nonlinear Cauchy problem.

2 Evolutionary operator equations

The initial value problem for the Maxwell system is an evolutionary problem with memory and can be formulated as an operator equation

$$
\partial_t M(\partial_t) u + Au = F(u) + g
$$

(in the sense of [1]) in the weighted Hilbert space

$$
L^2_\phi(\mathbb{R}, \mathcal{H}) = \{ u \in L^2_{\text{loc}}(\mathbb{R}, \mathcal{H}) : \|e^{-\phi t} u(t)\|_{L^2(\mathcal{H})} < \infty \}. 
$$

where $\mathcal{H} = L^2(\Omega)^6$. Here $A = (\begin{smallmatrix} 0 & -\text{curl} \\ \text{curl} & 0 \end{smallmatrix})$ is the Maxwell operator, $\partial_t$ denotes the time derivative, and $F$ is a (uniformly) Lipschitz continuous map on $L^2_\phi(\mathbb{R}, \mathcal{H})$. The operator $M(\partial_t)$ is called a linear material law and is related through the unitary Fourier-Laplace transform $L_\phi : L^2_\phi(\mathbb{R}, \mathcal{H}) \to L^2_\phi(\mathbb{R}, \mathcal{H})$ to an analytic map $M : \mathbb{C}_{\Re \geq \gamma_0} \to \mathcal{B}(\mathcal{H}, \mathcal{H})$ via $M(\partial_t) = L_\phi M(z)L_\phi$. The well-posedness of the (linear) problem, as well as properties like exponential stability, follow from (accretivity) conditions of the map $z \mapsto M(z)$, see [2,3].

![Figure 1: Schematic depiction of the electric field of a surface wave at the planar interface $\Gamma$ between two media $\Omega^+$ and $\Omega^-$ in $\mathbb{R}^3$.](image)

3 Approximation of surface waves

Assume the setting in Figure 1 with $\Omega = \Omega^+ \cup \Gamma \cup \Omega^-$, let $\mathcal{H} = L^2(\Omega)^6$ and consider the linear material law

$$
M(z) = M_0 + \frac{\alpha}{z} + \sum_{j=1}^N \frac{\beta_j}{z + \gamma_j},
$$

on $\mathcal{H}$, where $\alpha > 0$, $\beta_j, \gamma_j \geq 0$ and $M_0$ is symmetric and positive definite. There exists $\nu_0 > 0$ such that $\Re z > -\nu_0 \implies \Re zM(z) \geq c$ holds for some $c > 0$. Thus, $M$ satisfies the condition of exponential stability of the linear system $(\partial_t M(\partial_t) + A)u = g$ from [3], i.e., the solution operator $(\partial_t M(\partial_t) + A)^{-1}$ is bounded and causal on $L^2_\phi(\mathbb{R}, \mathcal{H})$ for large $g > 0$, and, for small $\nu < \nu_0$, maps $L^2_{\nu}(\mathbb{R}, \mathcal{H})$ into itself. The question whether exponential stability can be expected also for the nonlinear system (2) can be answered in part by imposing local Lipschitz...
continuity of $F$ (with small Lipschitz constant on small sets) in $L^2_{-\nu}(\mathbb{R}, \mathcal{H})$ and using a fixed-point argument on a small ball.

Now let $\Phi_k$ for fixed $k$ denote a linear mode as in (1). We model a wave packet propagating in $x_2$-direction by the multiple-scale ansatz

$$u_\varepsilon(t, x) = \varepsilon a(\varepsilon^2 t, \varepsilon(x_2 - c_g t), \varepsilon^2 x_3)\Phi_k(t, x),$$

where $0 < \varepsilon \ll 1$ is a small parameter and $a$ is a complex-valued amplitude. From (2) we obtain an equation for the error $R = u - u_\varepsilon$ of a similar form,

$$(\partial_t M_\varepsilon(\partial_t) + A)R + \text{Res}(u_\varepsilon) = F_\varepsilon(R) + \tilde{g},$$

where $\text{Res}(u_\varepsilon) = (\partial_t M(\partial_t) + A)u_\varepsilon - F(u_\varepsilon)$, with the linear material law $M_\varepsilon$ depending on $u_\varepsilon$, and where $F_\varepsilon$ is nonlinear. Our aim here is to obtain a small global solution of (3) by applying the previous argument, which in turn justifies a long-time approximation of solutions of the initial Maxwell system (2). We give an outline of the conditions needed.

(a) Exponential stability of the linearized system. The necessary condition can be (for small $\varepsilon$) inherited from the material law $M$.

(b) Local Lipschitz-continuity of $F_\varepsilon$ in the space $L^2_{-\nu}(\mathbb{R}, \mathcal{H})$ with small Lipschitz constant. An example can be provided by a fully nonlocal model.

(c) Smallness of the residual, $\text{Res}(u_\varepsilon) = o(\varepsilon)$ in $L^2_{-\nu}(\mathbb{R}, \mathcal{H})$. Expanding into powers of $\varepsilon$, formally $\text{Res}(u_\varepsilon) = O(\varepsilon^4)$ can be achieved through refinement of the ansatz, and demanding that $a$ is a solution of an amplitude equation of complex Ginzburg-Landau type. Rigorous estimates can be obtained by imposing higher regularity on $a$, yielding $\text{Res}(u_\varepsilon) = O(\varepsilon^{3/2})$ in $L^2_{-\nu}(\mathbb{R}, \mathcal{H})$.

A fixed-point argument in $L^2_{-\nu}(\mathbb{R}, \mathcal{H})$ finally yields small solutions $R$ of (3) for small data $\tilde{g}$.

4 Future work

Electro-magnetic surface waves are often treated in the non-magnetic setting, where the magnetic permeability is constant. In this case the linear material law does not meet the requirements for exponential stability. Still, similar results can be obtained for the Maxwell system on a bounded domain [4].

References


Wave power farm made of many rigid floating structures in Boussinesq regime

Geoffrey Beck\textsuperscript{1,*}, David Lannes\textsuperscript{2}, Lisl Weynans\textsuperscript{2}

\textsuperscript{1}Département de Mathématiques et applications, ENS, Paris, France
\textsuperscript{2}Institut de Mathématiques de Bordeaux, Bordeaux, France

*Email: geoffrey.beck@ens.fr

Abstract

This work deals with the interaction of waves governed by a Boussinesq system with some floating structures. The full system can be reduced to coupled boundary problems for the Boussinesq equations with boundary conditions given in terms of the vertical displacement of the objects, the average horizontal discharge beneath it and the traces of the water-column. The latter quantities are determined by nonlinear ODEs with forcing terms coming from the exterior waverfield.

Keywords: Fluid-structure interaction, Dispersive perturbation of hyperbolic problems, Wave Energy Converters in shallow water regime.

1 Modelling floating bodies

The mathematical study of floating structures is a keystone to understand wave power facilities. Consider N partially immersed rigid rectangles in a 2D fluid allowed to move vertically (see figure above). We denote by \(2\ell_i\) and \(x_i\) the horizontal length and the abscissa of the center of the \(i\)-body. The domain of wave propagation \(\mathbb{R}\) is divided into "congested" areas \(\mathcal{Z} = \bigcup_{i=1}^{N} (x_i - \ell_i, x_i + \ell_i)\) where the floating bodies are located and free areas \(\mathcal{E} = \mathbb{R}/\mathcal{Z}\). We will denote by \(d_{i+\frac{1}{2}} = x_{i+1} - x_{i+1} - x_i - \ell_i\) the distance between the \(i\)-th body and \(i+1\)-th body.

The dynamics of each body is given by the Newton equation

\[
m \ddot{z}_i + g z_i = \int_{x_i - \ell_i}^{x_i + \ell_i} P \quad (1)
\]

where the unknowns \(z_i\) denote the vertical displacement of the center of mass of the \(i\)-th body and \(\ddot{\cdot}\) is the second derivative with respect to time. The source term \(P\) is the pressure exerted by the fluid under each body. At equilibrium the water column is piecewise constant

\[
h_{eq} = \begin{cases} h_0 & \text{in } \mathcal{E} \\ h_0 - L_{w,i} & \text{in } (x_i - \ell_i, x_i + \ell_i) \end{cases}
\]

where \(L_{w,i}\) is the length of the immersed part of the vertical wall at equilibrium. The dynamics of the waves in \(\mathbb{R}\) is described by the Boussinesq-Abbott system which is the following dispersive PDE

\[
\begin{align*}
\partial_t h + \partial_x q &= 0 \\
(1 - \frac{h_{eq}^2}{3} \partial_x^2) \partial_t q + \partial_x \left( \frac{h^2}{2} + \frac{q^2}{h} \right) &= -h \partial_x P
\end{align*}
\]

where \(q\) refers to the fluid horizontal discharge and \(h\) to the water-column. The latter is

- unknown in the free areas,
- should fit the wetted surface \(h_{w,i} := h_{eq} + z_i - h_{eq}\) under any body \((x_i - \ell_i, x_i + \ell_i)\).

In particular, this implies that

\[
q_{w,i} := q_{(x_i - \ell_i, x_i + \ell_i)} = - (x - x_i) \ddot{z}_i + q_i
\]

where the average is defined by

\[
q_i = \frac{1}{2} (q_{w,i}(x_i + \ell_i) + q_{w,i}(x_i - \ell_i)).
\]

2 Pressure term

The pressure \(P\) is

- equal to the constant atmospheric one,
- unknown under any body and can be seen as Lagrangian multipliers \(\partial_h P_{(x_i - \ell_i, x_i + \ell_i)}\) associated to the constraints \(h = h_{w,i}\).

The system is not complete. Indeed one needs transmission conditions at each contact point \(x_i \pm \ell_i\) between the free and "congested" areas.
The first transmission condition is associated to fluid volume conservation which implies that
\[ q_E(x_i \pm \ell_i) = q_E(x_i \pm \ell_i) = \mp \ell_i \dot{z}_i + q_i, \]

The second one is associated to the conservation of energy of the full system. This is satisfied if we assume that
\[ P = g[h_E - h_{w,i}] + \frac{1}{2} \left( \frac{q_E^2}{h_E} - \frac{\ell_i q_E}{h_{w,i}} \right) + \frac{h_{E0}^2 h_E}{3 h_E} - \frac{h_{eq}^2}{3 h_{w,i}} \]
at each contact point \((x_i \pm \ell_i)\).

Taking the space derivative of the second equation in (2), one gets an elliptic equation for the pressure \( P \) on \((x_i - \ell_i, x_i + \ell_i)\) with Dirichlet boundary conditions and source depending on \( \gamma = (q_i, z_i, \dot{z}_i) \)
and its time derivative. If we use this elliptic problem in (1) and the second equation of (2) to eliminate \( P \), we get nonlinear ODEs
\[ m(\gamma, h_i, \dot{h}_i) + \gamma(\gamma, h_i) = \bar{f}(h_i, \dot{h}_i), \quad (3) \]

with forcing term \( \bar{f}(h_i, \dot{h}_i) \) coming from the wavefield in free areas
\[ h_i = (h_E(x_i - \ell_i), h_E(x_i + \ell_i)). \]

The coefficients \( m(\gamma, h_i), \gamma(\gamma, h_i) \) and the forcing term \( \bar{f}(h_i, \dot{h}_i) \) are similar to the ones given in [1]. The equations of wave-structure system are now complete.

3 An augmented formulation

Taking advantage of the dispersion terms, we can introduce a hidden equation for the traces of the water-column on each wall of floating solid. Firstly, we introduce the unknowns
\[ u_{i+\frac{1}{2}}(x) = (h_E, q_E)(x_i + \ell_i + d_{i+\frac{1}{2}} x) \]
that are cast on the unit cell \((0,1)\) for \( i = 1...N-1 \) and
\[ \begin{cases} u_-(x) = (h, q)(x_1 - \ell_1 - x) \\ u_+(x) = (h, q)(x - x_N - \ell_N) \end{cases} \]

that are cast on \((0,\infty)\). Secondly, we introduce \( \kappa_{i+\frac{1}{2}} := \frac{d_{i+\frac{1}{2}}}{\sqrt{\ell_i}} \) the regularizing operators
\[ R^{i+\frac{1}{2}} : H^n(0,1) \to H^{n+2}(0,1) \]

which are the inverse operators of \((1 - \kappa_{i+\frac{1}{2}} \partial_x^2)\) with homogeneous Neumann boundary conditions and \( R^0 \) the inverse operator of \((1 - \kappa_{i+\frac{1}{2}} \partial_x^2)\) on \((0,\infty)\) with homogeneous Neumann boundary condition at \(\{0\} \). Therefore, equations (2) can be rewritten on the conservative form on \((0,1)\)
\[ \partial_t u_{i+\frac{1}{2}} + d_{i+\frac{1}{2}} \partial_x \bar{f}_{i+\frac{1}{2}} = \left( \frac{0}{\kappa_{i+\frac{1}{2}}} \right) e^{-\frac{x}{\kappa_{i+\frac{1}{2}}}} + \left( \frac{0}{\kappa_{i+\frac{1}{2}}} \right) e^{-\frac{x}{\kappa_{i+\frac{1}{2}}}} \]

and on \((0,\infty)\)
\[ \partial_t u_{i+\frac{1}{2}} + \partial_x \left( \frac{\kappa_{i+\frac{1}{2}}}{R^0 f_{i+\frac{1}{2}}} \right) = \left( \frac{0}{\kappa_{i+\frac{1}{2}}} \right) e^{-\frac{x}{\kappa_{i+\frac{1}{2}}}} \]

with boundary conditions
\[ q_{i+\frac{1}{2}}(0) = -\ell_i \dot{z}_i + q_i, \quad q_{i+\frac{1}{2}}(1) = \ell_{i+1} \dot{z}_{i+1} + q_{i+1}, \quad q_-(0) = \ell_i \dot{z}_i + q_i, \quad q_+(0) = -\ell_i \dot{z}_i + q_i. \]

In the previous equations, the flux terms are
\[ \bar{f}_{i+\frac{1}{2}} = \left( \frac{q_{i+\frac{1}{2}}}{R^{i+\frac{1}{2}} f_{i+\frac{1}{2}}} \right), \quad f_{i+\frac{1}{2}} = \frac{g}{2} \left( h_{E0}^2 - h_{Ei}^2 \right) \frac{q_{i+\frac{1}{2}}^2}{h_{Ei}^2} \]

and the source terms are
\[ \kappa_i \left( \frac{\kappa_i q_{i+\frac{1}{2}}}{R^0 f_{i+\frac{1}{2}}} \right) = \left( \frac{\kappa_i q_{i+\frac{1}{2}}}{R^0 f_{i+\frac{1}{2}}} \right) \left( \frac{\kappa_i q_{i+\frac{1}{2}}}{R^0 f_{i+\frac{1}{2}}} \right) \]

Taking the spatial derivative of the second equation in (4), one gets a hidden equation on the water-column
\[ \kappa_{i+\frac{1}{2}} \partial_t \bar{f}_{i+\frac{1}{2}} + f_{i+\frac{1}{2}} = R^{i+\frac{1}{2}} f_{i+\frac{1}{2}} + \]
\[ \kappa_{i+\frac{1}{2}} \left( \frac{\kappa_{i+\frac{1}{2}}}{R^0 f_{i+\frac{1}{2}}} \right) \left( \frac{\kappa_{i+\frac{1}{2}}}{R^0 f_{i+\frac{1}{2}}} \right) \]

that can be taken at each contact point \( x_i \pm \ell_i \) in order to be coupled with (3) to make an ODE in which the exterior wave-fields \( R^{i+\frac{1}{2}} f_{i+\frac{1}{2}} \) acts as a forcing term. The full equations (3,6,4,5) are used to show local well-posedness theory and perform simulations with the finite volume method.

References
[1] G. Beck, D. Lannes, Freely Floating Objects on a Fluid Governed by the Boussinesq Equations. (hal-03122015)
Log-stability results for inverse coefficients problem associated with time harmonic magnetic Schrödinger operator

Mourad Bellassoued$^1$, Housssem Haddar$^2$, Amal Labidi$^2,*$

$^1$ENIT-LAMSIN, National Engineering School of Tunis, University of Tunis El Manar, Tunis, Tunisia
$^2$INRIA, ENSTA Paris Tech (UMA), Polytechnic Institute of Paris, Palaiseau, France

*Email: amal.abidi@enit.utm.tn

Abstract

We derive conditional stability estimates for inverse scattering problems related to time harmonic magnetic Schrödinger equation. We prove logarithmic type estimates for retrieving the magnetic (up to a gradient) and electric potentials from near field or far field maps. Our approach combine techniques from similar results obtained in the literature for inhomogeneous inverse scattering problems based on the use of geometrical optic solutions.

Keywords: Inverse problems, stability estimate, magnetic potential.

1 Introduction

Let $D \subset \mathbb{R}^3$ be a bounded open set with smooth boundary such that $(\mathbb{R}^3 \setminus D)$ is connected and let the magnetic potential $A \in W^{1,\infty}(\mathbb{R}^3)^3$ be a real valued vector and the electric potential $q \in L^\infty(\mathbb{R}^3)$ be a complex valued function with non negative imaginary part such that $\text{Supp}(A) \subset D$ and $\text{Supp}(q) \subset D$. We introduce with the magnetic Schrödinger operator in three-dimensional case

$$\mathcal{H}_{A,q} := -(\nabla + iA)^2 + q = -\Delta - Q_{A,q},$$

where $Q_{A,q}$ is the first order operator given by

$$Q_{A,q}v(x) := i \text{div}(A(x)v(x)) + iA(x) \cdot \nabla v(x) - (|A(x)|^2 + q(x))v(x).$$

The direct scattering problem in the near field setting can be considered as follows. Let $B$ be a smooth bounded domain containing $D$ with outward normal denoted by $\nu$ and let $y \in \partial B$ be the location of a point source. The total field $u(\cdot, y)$ generated by the point source satisfies

$$\mathcal{H}_{A,q}u(\cdot, y) - k^2u(\cdot, y) = \delta_y \quad \text{in} \ \mathbb{R}^3,$$

with $\delta_y$ denoting the Dirac distribution at $y$ and $k > 0$ is the wave number. The total field is decomposed into

$$u_{A,q}(\cdot, y) = \Phi(\cdot, y) + u^s_{A,q}(\cdot, y) \quad \text{in} \ \mathbb{R}^3,$$

where the scattered field $u^s_{A,q}(\cdot, y) \in H^2_{\text{loc}}(\mathbb{R}^3)$ and satisfies the Sommerfeld radiation condition

$$\lim_{r \to \infty} r \left( \partial_r u^s - iku^s \right) = 0, \quad r = |x|$$

uniformly with respect to $\hat{x} = \frac{x}{|x|}$. The incident field is given by

$$\Phi(x, y) := \frac{1}{4\pi |x - y|}, \quad x \neq y,$$

and is the fundamental solution of the Helmholtz equation, i.e. satisfying (3) for $A = q = 0$ together with the Sommerfeld radiation condition.

2 The inverse problem

The inverse scattering problem we are interested in is reconstruction the coefficients of the first order operator $Q_{A,q}$ from the knowledge of $u_{A,q}(x, y)$ for all $(x, y) \in \partial B \times \partial B$.

Let us first indicate that there is an obstruction to uniqueness for near field settings. Namely, given $\varphi \in W^{2,\infty}(\mathbb{R}^3)$ with support compactly embedded in $B$ and letting $\tilde{u} = u(x)e^{-i\varphi(x)}$ one easily observes that

$$\mathcal{H}_{A+\nabla \varphi,q}\tilde{u} = e^{-i\varphi(x)}\mathcal{H}_{A,q}u.$$

Since $\varphi = 0$ outside $B$, $\tilde{u}$ then satisfies the same equation as $u$, namely (4) with $\mathcal{H}_{A,q}$ replaced by $\mathcal{H}_{A+\nabla \varphi,q}$.

Let us denote by $u^s_{A+\nabla \varphi,q}$ the scattered field associated with the potentials $A + \nabla \varphi$ and $q$. One then can deduce (from uniqueness of solutions to the above stated scattering problem) that for all $y \in \partial B$

$$u^s_{A+\nabla \varphi,q}(\cdot, y) = (e^{-i\varphi} - 1)\Phi(\cdot, y) + e^{-i\varphi}u^s_{A,q}(\cdot, y),$$

in $\mathbb{R}^3$. This clearly shows that $u^s_{A+\nabla \varphi,q}(\cdot, y) = u^s_{A,q}(\cdot, y)$ outside $D$ and therefore, the magnetic potential $A$ cannot be uniquely determined from near field measurements on $\partial B$. This indicates that the best we can expect is to identify $(A, q)$ modulo a gauge transformation of $A$. Since $\text{Supp}(A) \subset D$, the problem may be equivalently
reformulated as whether the magnetic field defined by the 2-form associated with the vector field
\[ \text{curl } A := \frac{1}{2} \sum_{i,j=1}^{3} \left( \partial_{x_i} a_j - \partial_{x_j} a_i \right) dx_j \wedge dx_i, \] 
(8)
and the electric potential \( q \) can be retrieved from the knowledge of \( u^s_{A_j,q}(x,y) \) for all \((x,y) \in \partial B \times \partial B \).

3 The main stability result

Let us first indicate the set of admissible compactly supported magnetic potentials \( A \) and electric potentials \( q \). Let \( M > 0 \) and \( \sigma > 0 \) be given. We define the set of admissible magnetic potentials \( A_\sigma(M) \) by
\[ A_\sigma(M) := \left\{ A \in W^{2,\infty}(D, \mathbb{R}), \text{Supp}(A) \subset D, \right. \]
\[ \left. \|A\|_{W^{2,\infty}} \leq M, \right. \]
\[ \left. \|\text{curl } A\|_{L^2_b(\mathbb{R}^3)} \leq M \right\}, \]
(9)
where \( \widehat{\nu} \) denotes the Fourier transform of \( v \) and \( L^2_b(\mathbb{R}^3), \tau > 0 \) is the weighted \( L^2(\mathbb{R}^3) \) space with norm
\[ \|v\|_{L^2_b(\mathbb{R}^3)} = \int_{\mathbb{R}^3} (1 + |\xi|^2)^{\tau/2} |\hat{v}(\xi)| d\xi. \]

Given \( M > 0 \) and \( \gamma > 0 \), we define the set of admissible electric potentials \( Q_\gamma(M) \) by
\[ Q_\gamma(M) := \left\{ q \in L^\infty(D, \mathbb{C}), \text{Supp}(q) \subset D, \right. \]
\[ \left. \exists \gamma > 0, \|q\|_{L^\infty(D)} \leq M \right. \]
\[ \left. \|\hat{q}\|_{L^1_b(\mathbb{R}^3)} \leq M \right\}. \]
(10)
The main result can be stated as follows.

**Theorem 1** Let \( M > 0, \sigma > 0 \) and \( \gamma > 0 \). Then there exists a constant \( C > 0 \) such that for any \((A_j, q_j) \in A_\sigma(M) \times Q_\gamma(M), j = 1, 2, \) we have
\[ \|\text{curl } (A_1) - \text{curl } (A_2)\|_{L^\infty(D)} \]
\[ \leq C(\kappa^{1/2} + (\log^{-}(\kappa))^{-\sigma/(\sigma+3)}), \]
(11)
and
\[ \|q_2 - q_1\|_{L^\infty(D)} \]
\[ \leq C(\kappa^{1/2} + (\log^{-}(\kappa))^{-\gamma\sigma/(\sigma+3)(2\gamma+3)}), \]
(12)
where \( \kappa = \|u^s_{A_1,q_1} - u^s_{A_2,q_2}\|_{L^2(\partial B \times \partial B)} \) and \( \log^{-}(t) := \max(-\log(t), 0) \) for \( t > 0 \). Here \( C \) depends only on \( B, M, \sigma \) and \( \gamma \).

Let us point out that Theorem 1 implies the following uniqueness result.

**Corollary 2** Let \( A_1 \) and \( A_2 \in A_\sigma(M) \) two vector fields, \( q_1 \) and \( q_2 \in Q_\gamma(M) \) and \( B \supset D \). Then, we have
\[ u^s_{A_1,q_1}(x,y) = u^s_{A_2,q_2}(x,y), \quad \forall (x,y) \in \partial B \times \partial B, \]
implies \( q_1 = q_2 \) and \( \text{curl } A_1 = \text{curl } A_2 \) in \( D \).

The first step in the proof is the derivation of the following orthogonality identity,
\[ \left| \int_B \left[ i(A_1 - A_2) \cdot (u_1 \nabla u_2 - u_2 \nabla u_1) \right. \right. \]
\[ \left. \left. - (|A_1|^2 - |A_2|^2 + (q_1 - q_2))u_1u_2 \right] dx \right| \]
\[ \leq C\|u^s_{A_1,q_1} - u^s_{A_2,q_2}\|_{H^2(D)}\|u_1\|_{H^2(D)}\|u_2\|_{H^2(D)} \]
for all \( u_1 \in H^2(D) \) satisfying \( \mathcal{H}_{A_1,q_1} u_1 = k^2 u_1 \) in \( B \) and all \( u_2 \in H^2(D) \) satisfying \( \mathcal{H}_{A_2,q_2} u_2 = k^2 u_2 \) in \( B \). We then use complex geometrical optics solutions \([4]\) to estimate the Fourier coefficients of the difference of two magnetic fields. The stability estimate for electric potential is obtained thanks to the use of an appropriate Helmholtz decomposition.

We shall also explain how to exploit Theorem 1 to obtain similar stability results using far field measurements following the arguments in \([3]\).

**References**


Numerical methods for a Schrödinger equation inverse eigenvalue problem

K. Wright1,∗, R. Marcia1, B. Ilan1

1Department of Applied Mathematics, University of California Merced, Merced, CA
∗Email: kwright11@ucmerced.edu

Abstract

We seek to solve for the potential function that satisfies the one-dimensional time-independent Schrödinger equation for a given set of eigenvalues. A variety of formulations are considered, which are all based on a discretization of this problem. The resulting systems of equations are solved using root-finding and optimization-based methods. Our results show that the success of these approaches depends on the distance between the eigenvalues.

Keywords: Quantum mechanical waves

1 Problem Setting

The Schrödinger equation plays a central role in the description of waves in quantum mechanics. It is of great practical interest to design physical systems with prescribed energy levels. Inspired by this, we consider the one-dimensional time-independent Schrödinger equation

\[ -\psi''(x) + V(x)\psi(x) = \lambda \psi(x), \]  

(1)

where \(\psi(x), V(x),\) and \(\lambda\) correspond to the wave function, potential function, and energy level in quantum mechanics, respectively. We seek to solve for the potential function given a set of real eigenvalues. To this end, discretization of \(x\) on a grid allows the problem to be approximated as \((T + D)\tilde{\psi} = \lambda\tilde{\psi}\), where \(T\) is a \((-1, 2, -1)\) tridiagonal \(n \times n\) matrix representing the discretized second-derivative operator and \(D = \text{diag}(d_i)\) is a diagonal matrix, representing \(V(x)\). Let \(A = T + D\), where \(a_i = 2 + d_i\) \((i = 1, \ldots, n)\) are the diagonal elements of \(A\). Given a set of eigenvalues, \(\tilde{\lambda} = [\lambda_1 \cdots \lambda_n]^T \in \mathbb{R}^n\), we seek to find \(\tilde{a} = [a_1 \cdots a_n]^T \in \mathbb{R}^n\), such that the eigenvalues of \(A\) are \(\tilde{\lambda}\), that is,

\[ A\tilde{\psi} = \tilde{\lambda} \tilde{\psi}, \]  

(2)

where \(\tilde{\psi}\) is the corresponding eigenvector. Our objective is to develop efficient numerical approaches for solving this inverse-eigenvalue problem (IEP). IEPs come in many different forms, cf. [1], which describes both theory and numerical techniques. For several classes of IEPs, when there are repeated eigenvalues the IEP is unsolvable almost everywhere (Theorems 3.4 and 3.10 in [1]). Hence, we require the eigenvalues to be real and distinct and assume that \(\tilde{\lambda}\) is ordered in increasing values.

2 System of equations formulations

There are a variety of systems of equations that can be used to solve this problem. We construct vector-valued functions for these systems of equations. The roots of these functions are solutions to (1). Formulations 1 and 2 described below are obtained using the characteristic polynomial of \(A\). Formulation 3 involves simultaneously for \(\tilde{a}\) with the set of eigenvectors of \(A\).

Formulation 1: The eigenvalues of \(A\) are the roots of its characteristic polynomial. In this study we consider the \(n = 3\) case, where

\[ \det(A - \lambda I_3) = -\lambda^3 + c_1(\tilde{a})\lambda^2 + c_2(\tilde{a})\lambda + c_3(\tilde{a}), \]  

(3)

where \(c_1(\tilde{a}) = a_1 + a_2 + a_3,\) \(c_2(\tilde{a}) = -(a_1a_2 + a_1a_3 + a_2a_3) - 2\), and \(c_3(\tilde{a}) = a_1a_2a_3 - (a_1 + a_3)\). As \(\det(A - \lambda I) = 0\) for each \(\lambda_i \in \tilde{\lambda}(A)\), the requisite vector of diagonal elements, \(\tilde{a}\), must be a root of the vector function

\[ f_1(\tilde{a}) = \begin{bmatrix} \det(A - \lambda_1 I_3) \\ \det(A - \lambda_2 I_3) \\ \det(A - \lambda_3 I_3) \end{bmatrix}. \]

More generally this would be a system of \(n\) polynomial equations of degree \(n\) for the the \(n\) unknowns in \(\tilde{a}\).

Formulation 2: Alternatively, the characteristic polynomial can be factored as

\[ \det(A - \lambda I) = (\pm 1)^{n-1}(\lambda_1 - \lambda)\cdots(\lambda_n - \lambda). \]  

(4)

Equating the coefficients in (3) and (4) yields our second vector function,

\[ f_2(\tilde{a}) = \begin{bmatrix} c_1(\tilde{a}) - (\lambda_1 + \lambda_2 + \lambda_3) \\ c_2(\tilde{a}) - (\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3) \\ c_3(\tilde{a}) - \lambda_1\lambda_2\lambda_3 \end{bmatrix}. \]

Formulation 3: Since \(A\) is symmetric, it follows that \(A = P\Delta P^T\) where \(\Delta = \text{diag}(\tilde{\lambda})\) and \(P\)
is an orthogonal matrix whose columns are the eigenvectors of $A$. It follows that

$$AP - PA = 0 \quad \text{and} \quad PP^T = I,$$

(5)

Let $\vec{p} \in \mathbb{R}^{n^2}$ denote the elements of $P$. Using the upper triangular part of (5) yields the vector $f_3(\vec{a}, \vec{p})$, which corresponds to $n(n+1)$ quadratic equations for the $n(n+1)$ unknowns $\vec{a}$ and $\vec{p}$.

3 Algorithms

With the goal of solving for $\vec{a}^*$ with $f_i(\vec{a}^*) = 0$, we employ two approaches. Method I is a root-finding approach based on Newton’s Method, which uses the Jacobian of $f_i(\vec{a})$ for determining the iterations. Method II is an optimization approach that minimizes the objective function $g_i(\vec{a}) = \frac{1}{2}\|f_i(\vec{a})\|^2$. Method II uses a quasi-Newton approach, which approximates the Hessian matrix using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) update.

4 Initial Iterate

Root finding and optimization methods are often sensitive to the choice of initial point. To this end, the Gershgorin Circle Theorem ensures that every eigenvalue of $A$ lies within at least one of the Gershgorin discs [2]. Applying this to the matrix $A$, we conclude that there exists at least one permutation of the eigenvalues such that if initial point $\vec{a}_0$ is equal to this permutation, then there is a “nearby” root with $\|\vec{a}^* - \vec{a}_0\|_\infty \leq 2$. As discussed below, this theorem also provides insight into the success of the numerical methods.

5 Results

To test our methods, we first generate a set of 10,000 $A$ matrices, whose eigenvalues are real and distinct. Then, using permutations of those eigenvalues as initial points, we implemented and compared the performance of the above formulations and algorithms. These experiments show that, for all sets of eigenvalues, every combination of formulations and algorithms converge to a solution for at least one permutation of the eigenvalues as initial point. In addition, Table 1 shows the percentage of such permutations that converge to a solution for two categories of eigenvalue separation. These results show that there is a notable difference in success dependent on the minimum distance between the eigenvalues. In particular, when the eigenvalues are well separated, i.e., if $(\Delta \lambda)_{\min} \geq 2$, where $(\Delta \lambda)_{\min} = \min_{i \neq j} |\lambda_i - \lambda_j|$, the algorithms find a solution for all permutations of eigenvalues as initial points. In contrast, when $(\Delta \lambda)_{\min} < 2$, solutions are obtained for only a subset of such permutations. In addition, when $(\Delta \lambda)_{\min} < 2$ more iterations are needed to find a solution. Method I (Newton’s method) finds a solution for a noticeably larger percentage of initial points than Method II (Quasi-Newton Method). For both Methods I and II, Formulations 1 and 2 perform similarly. For Method I, Formulation 3 ($f_3(\vec{a}, \vec{p})$) finds a solution for a lower percentage of permutations, generally requires a larger number of iterates, and takes substantially more time to converge. This is likely due to the higher dimensionality of $f_3(\vec{a}, \vec{p})$.

<table>
<thead>
<tr>
<th>Method</th>
<th>Formulation</th>
<th>$(\Delta \lambda)_{\min} &lt; 2$</th>
<th>$(\Delta \lambda)_{\min} \geq 2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>$f_1(\vec{a})$</td>
<td>87.63%</td>
<td>100.00%</td>
</tr>
<tr>
<td>I</td>
<td>$f_2(\vec{a})$</td>
<td>87.20%</td>
<td>100.00%</td>
</tr>
<tr>
<td>I</td>
<td>$f_3(\vec{a}, \vec{p})$</td>
<td>63.14%</td>
<td>100.00%</td>
</tr>
<tr>
<td>II</td>
<td>$g_1(\vec{a})$</td>
<td>66.97%</td>
<td>100.00%</td>
</tr>
<tr>
<td>II</td>
<td>$g_2(\vec{a})$</td>
<td>67.05%</td>
<td>100.00%</td>
</tr>
<tr>
<td>II</td>
<td>$g_3(\vec{a}, \vec{p})$</td>
<td>68.34%</td>
<td>100.00%</td>
</tr>
</tbody>
</table>

Table 1: Percentage of initial iterates converging to a solution using Method I (Newton’s Method for finding the roots of $f_i(\vec{a})$) and Method II (Quasi-Newton Method for minimizing $g_i(\vec{a})$). Here, $(\Delta \lambda)_{\min} = \min_{i \neq j} |\lambda_i - \lambda_j|$.  

6 Conclusions

We investigated numerical methods for solving an inverse eigenvalue problem associated with a 1-D time-independent Schrödinger equation. We note that all the formulations and algorithms become more sensitive to the initial point when the minimum distance between the eigenvalues is less than 2.

Acknowledgments. This work was supported by NSF Grants IIS 1741490 and DGE 2125510.

References

Acoustic passive cloaking using thin resonant ligaments

Lucas Chesnel¹, Jérémy Heleine¹,*, Sergei A. Nazarov²

¹Inria, Ensta Paris, Institut Polytechnique de Paris, Palaiseau, France
²Saint-Petersburg State University, St. Petersburg, Russia
*Email: jeremy.heleine@ensta-paris.fr

Abstract

We consider the propagation of acoustic waves in a 2D waveguide unbounded in one direction and containing a bounded obstacle. The goal of this work is to propose a method to cloak the obstacle at infinity, that is to retrieve the reflection and transmission coefficients as in the reference strip.

Keywords: acoustic waveguide, passive cloak- ing, asymptotic analysis, thin resonators, scattering coefficients, complex resonance

1 Introduction

Let Ω denote a 2D waveguide, unbounded in the (Ox) direction and containing a compact obstacle (rigid or penetrable inclusion, deformation of the wall, ...). In other words, the obstacle is located inside a region \{(x, y) ∈ Ω; |x| < L\}, for a given \(L > 0\), and Ω coincides with the reference guide \(Ω₀ = \mathbb{R} \times (0, 1)\) outside of this region. Considering the propagation of acoustic waves in Ω leads us to study the problem

\[
\begin{align*}
\Delta u + k^2 u &= 0, \quad \text{in } \Omega, \\
\partial_n u &= 0, \quad \text{on } \partial \Omega,
\end{align*}
\]

where \(n\) denotes the outer unit normal to Ω. We fix the wavenumber \(k \in (0, \pi)\) so that only the modes \(w^\pm; (x, y) \mapsto e^{\pm ikx}\) can propagate. We are interested in the solutions \(u^\pm\) to (1) generated by the waves \(w^\pm\) coming from ±∞. They admit the decompositions

\[
\begin{align*}
    u^+ &= w^+ + R^+ w^- + \ldots, \quad x \to -\infty, \\
    u^- &= w^- + T w^- + \ldots, \quad x \to +\infty,
\end{align*}
\]

where the ellipsis stand for evanescent terms and \(R^\pm, T \in \mathbb{C}\) are reflection and transmission coefficients.

In the reference guide, the solution is simply \(u = w^+\) so that we have zero reflection and a transmission coefficient equal to one. The goal of this work is to explain how to cloak the obstacle by perturbing the geometry.

The difficulty in this task lies in the fact that in general the dependence of the scattering coefficients with respect to the geometry is implicit and not linear. Our approach consists in adding thin ligaments of width \(\varepsilon \ll 1\) (see Figure 1). We then create a new geometry \(\Omega^\varepsilon\) where we denote by \(u^\varepsilon\) the solution to (1) and by \(R^\varepsilon, T^\varepsilon\) its scattering coefficients. We will see that, since ligaments are almost 1D objects, we can get relatively explicit formulas allowing us to find situations where, as \(\varepsilon \to 0\):

\[
R^\varepsilon = o(1), \quad T^\varepsilon = 1 + o(1),
\]

as if, approximately, there were no obstacle.

2 Asymptotic analysis

Attach the ligament \(\mathcal{L}^\varepsilon = (p - \frac{\varepsilon}{2}, p + \frac{\varepsilon}{2}) \times (1, 1 + \ell')\) at the point \(A = (p, 1), p \in \mathbb{R}\). We assume that its length is equal to \(\ell' = \ell + \varepsilon \ell'\). Here \(\ell, \ell'\) will be fixed later to obtain interesting phenomena.

The first step is to derive an asymptotic expansion of \(u^\varepsilon, R^\varepsilon\) and \(T^\varepsilon\), as \(\varepsilon \to 0\). We employ the technique of matched asymptotic expansions. In the process, the following 1D problem plays a key role:

\[
\begin{align*}
v'' + k^2 v &= 0, \quad \text{in } (1, 1 + \ell), \\
v(1) &= v'(1 + \ell) = 0.
\end{align*}
\]

It is obtained by considering the restriction of the Helmholtz problem to the ligament. We choose \(\ell\) as a resonant length of (2), i.e. such that \(k \ell = \frac{\pi}{2} + m\pi, m \in \mathbb{N}\). In this case, (2) admits non zero solutions.

Theorem 1 When \(\varepsilon\) tends to zero, we have :

\[
\begin{align*}
u^\varepsilon &= u^+ + o(\varepsilon)k\gamma + o(1) \quad \text{in } \Omega, \\
u^\varepsilon &= \varepsilon a(\ell')\sin(k(-1)) + O(1) \quad \text{in } \mathcal{L}^\varepsilon, \\
R^\varepsilon &= R^+ + \frac{i a(\ell')}{2} u^+(A) + o(1), \\
T^\varepsilon &= T + \frac{i a(\ell')}{2} u^-(A) + o(1),
\end{align*}
\]
where $a(\ell') \in \mathbb{C}^*$ and $\gamma$ is a certain Green function centered at $A$.

### 3 Zero reflection

When $\ell'$ varies around the resonant length ($\ell' \in \mathbb{R}$), the main terms in the asymptotics of $R^\varepsilon$, $T^\varepsilon$ run on circles whose features depend in an explicit way on the position $A$ of the ligament. We can then find out situations where one can cancel asymptotically the reflection (see Figure 1).

![Figure 1: Top: the obstacle generates a rather large reflection. Middle: a thin ligament is added and tuned to get $R^\varepsilon \approx 0$.](image)

**Theorem 2** Assume that $R^+ \neq 0$ and $T \neq 0$. Then there are some positions at which one can place the ligament and tune its length to get $R^\varepsilon = o(1)$.

The relation of conservation of energy $|R^\varepsilon|^2 + |T^\varepsilon|^2 = 1$ implies that if $R^\varepsilon = o(1)$, we get $|T^\varepsilon| = 1 + o(1)$. As a consequence, in general we only have $T^\varepsilon = e^{i\varphi} + o(1)$ for some $\varphi \neq 0$: there is a phase shift in the transmission (see the right part of the guides in Figure 1).

### 4 Phase shifter

To compensate this phase shift, let us create a phase shifter. To proceed, we perturb the reference guide $\Omega_0 = \mathbb{R} \times (0, 1)$ by adding two ligaments.

**Theorem 3** Let $\mu \in (-\pi, \pi)$. Then one can place two ligaments and tune their lengths to get $R^\varepsilon = o(1)$ and $T^\varepsilon = e^{i\mu} + o(1)$.

Now, by combining both Theorem 2 and Theorem 3, one can approximately cloak an obstacle appealing to the following procedure:

1. cancel the reflection with one ligament; this leads to $T^\varepsilon = e^{i\varphi} + o(1)$;
2. far to the right of the obstacle (to neglect the evanescent terms), place two ligaments that do not produce reflection and create a phase shift equal to $-\varphi$.

### 5 Cloaking with only two ligaments

The previous procedure guarantees that one can cloak an obstacle with three ligaments. Actually, it is also possible to show that cloaking is achievable with only two resonators. For that, the following result is necessary.

**Theorem 4** Assume that $T$ is located on the circle of center $1/2$ and of radius $1/2$. Then, there are some positions at which one can place the ligament and tune its length to get $R^\varepsilon = o(1)$ and $T^\varepsilon = 1 + o(1)$.

This shows that, for a specific class of obstacles, only one ligament is necessary to achieve cloaking. Now, the following procedure can be used to cloak any obstacle with two ligaments:

1. place a ligament and tune its length to get a transmission coefficient on the circle of center $1/2$ and of radius $1/2$;
2. place another ligament and tune its length to cancel the new reflection.

This procedure has been used in Figure 2. We observe that, both on the left and right of the guide, the wave has the same behavior as in the reference guide. For more details, we refer the reader to [1].

![Figure 2: Top: scattering of $w^+$ in presence of the initial obstacle. Middle: two ligaments have been added and tuned to get $R^\varepsilon \approx 0$ and $T^\varepsilon \approx 1$.](image)

### References

The Weyl Law of transmission eigenvalues and the completeness of the generalized transmission eigenfunctions without the complementing conditions

Jean Fornero1,*, Hoai-Minh Nguyen2
1Groupe Picasso, EPFL, Lausanne, Suisse
2Laboratoire Jacques Louis Lions, Sorbonne Université, Paris, France
*Email: jean.fornero@epfl.ch

Abstract
The transmission eigenvalue problem is a system of two second-order elliptic equations of two unknowns equipped with the Cauchy data on the boundary. In this talk we discuss the Weyl law for the eigenvalues and the completeness of the generalized eigenfunctions for the system without complementing conditions, i.e., the two equations of the system have the same coefficients for the second order terms. These coefficients are allowed to be anisotropic and are assumed to be of class \( C^2 \) only. This is based on a recent joint work with Hoai-Minh Nguyen.

Keywords: Transmission eigenvalue problem, inverse scattering, Weyl law, completeness, generalized eigenfunctions, Hilbert-Schmidt operators

1 Introduction
The transmission eigenvalue problem plays a role in the inverse scattering theory for inhomogeneous media. After four decades of extensive study, the spectral properties are known to depend on a type of contrasts of the media near the boundary. We refer the reader to [1] for a recent, self-contained introduction to the transmission eigenvalue problem and its applications.

Natural and interesting questions on the interior transmission eigenvalue problem include: the discreteness of the spectrum, the location of transmission eigenvalues, the Weyl law of transmission eigenvalues and the completeness of the generalized eigenfunctions.

Let us describe the mathematical settings of the problem under consideration. Let \( \Omega \) be a bounded, simply connected, open subset of \( \mathbb{R}^d \) of class \( C^2 \) with \( d \geq 2 \). Let \( A_1, A_2 \) be symmetric, uniformly elliptic and continuous matrices in \( \overline{\Omega} \) and let \( \Sigma_1, \Sigma_2 \) be two positive and continuous functions bounded from below by a positive constant.

A complex number \( \lambda \in \mathbb{C} \) is called a transmission eigenvalue if there is a non-zero pair of functions \( (u_1, u_2) \in [H^1(\Omega)]^2 \) such that

\[
\begin{aligned}
\text{div}(A_1 \nabla u_1) - \lambda \Sigma_1 u_1 &= 0 & \text{in } \Omega, \\
\text{div}(A_2 \nabla u_2) - \lambda \Sigma_2 u_2 &= 0 & \text{in } \Omega, \\
u_1 &= u_2, & A_1 \nabla u_1 \cdot \nu = A_2 \nabla u_2 \cdot \nu & \text{on } \Gamma.
\end{aligned}
\]

Here and in what follows \( H^1(\Omega) \) denotes the standard Sobolev of functions in \( L^2(\Omega) \) with derivatives belonging to \( L^2(\Omega) \), \( \Gamma \) denotes \( \partial \Omega \) and \( \nu \) denotes the unit outward vector normal on \( \Gamma \).

This problem has been studied under various conditions on the media \( (A_1, \Sigma_1) \) and \( (A_2, \Sigma_2) \). Recently, (Q.H.) Nguyen and (H.M.) Nguyen established the Weyl law of eigenvalues and the completeness of the generalized eigenfunctions under the complementing conditions adapted to this problem [3]. The complementing conditions for elliptic systems are originally due to Agmon et al. in the ’60.

Concerning the degenerate case

\[ A_1 = A_2 = A \text{ in } \Omega \]  \hspace{1cm} (2)

and under the condition

\[ \Sigma_1 \neq \Sigma_2 \text{ on } \partial \Omega \]  \hspace{1cm} (3)

it was also shown by (Q.H.) Nguyen and (H.M.) Nguyen in [3] that the discreteness of the transmission eigenvalues holds. In this talk, we present recent results establishing the completeness of the generalized eigenfunctions and the Weyl law for the transmission eigenvalues under the additional assumption that for some \( \Lambda > 0 \)

\[ \|A\|_{C^0(\overline{\Omega})} + \|(\Sigma_1, \Sigma_2)\|_{C^1(\overline{\Omega})} \leq \Lambda. \]  \hspace{1cm} (4)

Previous results concerning the transmission eigenvalue problem under the condition (2) were obtained in [5].
2 Main results

Let \((\lambda_j)\) be the set of transmission eigenvalues associated with the transmission eigenvalue problem (1).

**Theorem 1 (Fornero d & Nguyen [2])** Assume that (2), (3) and (4) hold. Let \(\mathcal{N}(t)\) denote the counting function i.e.

\[ \mathcal{N}(t) = \# \{ j \in \mathbb{N} : |\lambda_j| \leq t \}. \]

Then

\[ \mathcal{N}(t) = ct^\frac{d}{2} + o(t^\frac{d}{2}) \quad \text{as} \quad t \to +\infty, \]

where

\[ c := \frac{1}{(2\pi)^d} \sum_{\ell=1}^{2} \left| \mathbb{E} \{ \xi \in \mathbb{R}^d; \langle A_\ell(x)\xi, \xi \rangle < \Sigma_\ell(x) \} \right| dx. \]

Concerning the completeness of the generalized eigenfunction we have

**Theorem 2 (Fornero d & Nguyen [2])** Assume that (2), (3) and (4) hold. The set of generalized eigenfunction pairs associated to the problem (1) is complete in \(L^2(\Omega) \times L^2(\Omega)\).

The analysis is based on the well-posedness and the regularity of the following Cauchy problem. Let \(\gamma > 0\). There exists \(\lambda_0 > 0\) such that for every \(\lambda \in \mathbb{C} \) with \(|\Im(\lambda)| \geq \gamma |\lambda|\) and \(|\lambda| > \lambda_0\) for every \((f_1, f_2) \in [L^2(\Omega)]^2\) there exists a unique solution \((u_1, u_2) \in [L^2(\Omega)]^2\) with \(u_1 - u_2 \in H^2(\Omega)\) of

\[
\begin{cases}
\text{div}(A\nabla u_1) - \lambda \Sigma_1 u_1 = f_1 & \text{in } \Omega, \\
\text{div}(A\nabla u_2) - \lambda \Sigma_2 u_2 = f_2 & \text{in } \Omega, \\
u_1 - u_2 = A(\nabla u_1 - \nabla u_2) \cdot \nu = 0 & \text{on } \Gamma.
\end{cases}
\]

(5)

It is worth noting that the Cauchy problem (5) is degenerate due to the condition (2). One of the key steps in order to overcome this difficulty is to derive a priori estimate in a half space. Due to (2) the situation is non-standard and the analysis requires the stability of the Cauchy problem with regularity on the data up to the second derivatives. The regularity of the solution \((u_1, u_2)\) of (5) can be improved only by improving the one of the difference \(f_1 - f_2\). This is distinct from the complementing conditions on \((A_1, \Sigma_1)\) and \((A_2, \Sigma_2)\) considered in [4].

In order to obtain Theorem 1 and Theorem 2 we associate an operator to a system which is equivalent to (5). This procedure is standard in the literature and has been initiated in [5]. Then, we deduce that a certain power of this operator is in fact a Hilbert-Schmidt operator. This allows to obtain Theorem 1 and Theorem 2 by using the theory of Hilbert-Schmidt operators. We follow the approach of [4], but with extra observations and new ideas to solve the problems due to the degenerate condition (2).

3 Outline of the talk

In this talk we will present the proofs of Theorem 1 and Theorem 2. This will be divided into two parts. The first one is devoted to the study of the Cauchy problem associated with the interior transmission problem. Precisely, we will focus on the existence, the uniqueness and the regularity of the solution to the Cauchy problem (5), with a particular care on the new material used in the proof of these results. The second part is devoted to Theorem 1 and Theorem 2.

**References**


Low-order Absorbing Boundary Conditions in HDG discretization of the convected Helmholtz equation

Nathan Rouxelin$^{1,2,*}$, Hélène Barucq$^2$, Sébastien Tordeux$^2$

$^1$Laboratoire de Mathématiques de l’INSA, INSA Rouen–Normandie, France
$^2$MAKUTU, Inria Bordeaux–Sud-Ouest, Université de Pau et des Pays de l’Adour, TotalEnergies, France

*Email: nathan.rouxelin@insa-rouen.fr

Abstract

We describe how low-order boundary conditions for the convected Helmholtz equation can be constructed using the Lorentz transformation that maps the convected Helmholtz equation to the standard Helmholtz equation. The new ABCs are derived from the classical Bayliss-Turkel ABCs and are valid for a carrier flow that varies in the exterior domain. They are easy to implement in an existing finite-element or discontinuous Galerkin solver and lead to accurate numerical results for both low and intermediate Mach numbers.

Keywords: Absorbing Boundary Conditions, convected Helmholtz equation, Lorentz transformation

1 Introduction

In many applications, the waves propagate in an infinite domain, which should be truncated in order to perform numerical simulations. Domain truncation is therefore an important part of computational wave dynamics and various techniques have been developed over the years. In this paper, we focus on the construction of low-order ABCs for the convected Helmholtz equation that can be easily implemented in a discontinuous Galerkin solver.

2 Convected Helmholtz equation

We consider the convected Helmholtz equation in an infinite domain

\[ (-i\omega + \vec{v}_0 \cdot \nabla)^2 p - \text{div} \left( \frac{c_0^2}{\alpha} \nabla p \right) = s, \quad \text{in} \ R^N. \tag{1} \]

The finite computational domain is \( \Omega \subset R^N \), and we denote by \( \Sigma \) its boundary.

To construct new ABCs we make the following assumptions on the carrier flow:

A-1) \( \vec{v}_0 \) is incompressible, i.e. \( \text{div} (\vec{v}_0) = 0 \),

A-2) \( \vec{v}_0 \) is subsonic, i.e. \( |\vec{v}_0| < c_0 \),

(A-3) \( \vec{v}_0 \) and \( c_0 \) are uniform in \( R^N \setminus \Omega \).

Assumptions (A-1) and (A-2) are used to ensure that (1) leads to a well-posed variational problem, whereas (A-3) is used to ease the construction of ABCs.

3 HDG discretization

Hybridizable Discontinuous Galerkin (HDG) methods are mixed DG methods that rely on a static condensation process to reduce the numerical cost. Using HDG methods allows to construct numerical solvers with all the advantages of DG methods (such as high-order, \( hp \)-adaptivity, natural parallelization,…) for a numerical cost similar to a continuous finite-element solver.

As detailed in [3], we need to rewrite (1) as a first-order system to construct a HDG method. We consider the following formulation

\[ \vec{\sigma} + K_0 \nabla p + 2i\omega p\vec{v}_0 = 0, \tag{2} \]
\[ -\omega^2 p + \text{div} (\vec{\sigma}) = s, \tag{3} \]

where \( K_0 = c_0^2 I + \vec{v}_0 \vec{v}_0^T \) and \( \vec{\sigma} \) is the so-called total flux.

To work with the formulation (2)–(3), we want to construct an operator \( \mathcal{Z} \) so that the ABC reads

\[ \vec{\sigma} \cdot \vec{n} + \mathcal{Z} p = 0, \quad \text{on} \ \Sigma, \tag{4} \]

where \( \vec{n} \) is a unit normal vector to \( \Sigma \).

4 Lorentz transformation

Following [2], we introduce the frequency-domain Lorentz transform

\[ \vec{x} = Ax = \left( I + \frac{1}{\alpha (1 + \alpha)} \vec{M}_0 \vec{M}_0^T \right) x, \quad \vec{\omega} = \frac{\omega}{\alpha}, \tag{5} \]

where \( \alpha = \sqrt{1 - |\vec{M}_0|^2} \) is the Lorentz factor and \( \vec{M}_0 = \vec{v}_0/c_0 \) is the Mach vector. For uniform carrier flows, this change of coordinates maps the convected Helmholtz equation to the standard one. More precisely, we have the
Theorem 1 If $\vec{v}_0$ and $c_0$ are uniform and if $p(x, \omega)$ is a solution to (1) then
\[
\tilde{p}(\tilde{x}, \tilde{\omega}) = \alpha \exp \left[ \frac{i}{\alpha c_0} \vec{M}_0 \cdot \tilde{x} \right] p(x, \omega) \tag{6}
\]
is a solution to the standard Helmholtz equation
\[
-\tilde{\omega}^2 \tilde{p} - c_0^2 \Delta \tilde{p} = \tilde{s}, \tag{7}
\]
where $\tilde{\Delta}$ is the Laplace operator in Lorentz coordinates.

5 Transformation of ABCs

We denote by $\tilde{\Sigma}$ the artificial boundary in Lorentz coordinates. As we will transform an ABC for $\tilde{p}(\tilde{x}, \tilde{\omega})$ on $\tilde{\Sigma}$ into an ABC for $p$ on $\Sigma$, it is convenient to chose $\tilde{\Sigma}$ circular, i.e.
\[
\tilde{\Sigma} = \{ \tilde{x} \mid |\tilde{x}| = R^2 \}. \tag{8}
\]
With this choice of $\tilde{\Sigma}$ the artificial boundary in physical coordinates is the following ellipse
\[
\Sigma = \{ x \mid |Ax|^2 = R^2 \}. \tag{9}
\]
Then, we write an ABC for the standard Helmholtz equation (7) on $\tilde{\Sigma}$ as
\[
\partial_n p + \tilde{Z} p = 0, \text{ on } \tilde{\Sigma}. \tag{10}
\]
It can be transformed into an ABC for $p$ using the

Theorem 2 If $\vec{v}_0$ and $c_0$ are uniform in a neighborhood of $\Sigma$ and if $Z$ is defined as
\[
Z(x, \omega) = -c_0^2 A^{-1} n \tilde{Z}(\tilde{x}, \tilde{\omega}) + i \omega \vec{v}_0 \cdot \vec{n}, \tag{11}
\]
then
\[
\hat{\sigma} \cdot \hat{n} + \tilde{Z} p = 0, \text{ on } \Sigma, \tag{12}
\]
is an ABC for the convected Helmholtz equation.

Notice that the local uniformity of the carrier flow is ensured through assumption (A-3).

6 Numerical results

In Table 1, the error between the numerical solution and an analytic solution is given for various sizes of domains and for three ABCs: the transformation of the 0th and 1st order Bayliss-Turkel ABCs of [1], and an ABC that selects the outgoing plane waves that are locally orthogonal to $\Sigma$. Clearly (ABC-1) outperforms the two other ABCs. In Figure 1 and Figure 2, we give two illustrative examples using (ABC-1).

References


Solving the water-waves problem with Laplace’s free-space Green’s function

Alexis Anne¹, Anne-Sophie Bonnet-BenDhia¹, Luiz M. Faria¹,⋆
¹POEMS Laboratory, IPP, Palaiseau, France
⋆Email: luiz.maltez-faria@inria.fr

Abstract
We present a novel boundary integral equation (BIE) formulation for the water-waves problem based solely on the free-space Green’s function for Laplace’s equation. The method relies on a complex coordinate-stretching to render the propagative waves exponentially decaying, and thus more amenable to truncation. The formulation uses only simple function evaluations (e.g. complex logarithms and square roots) and thus avoids the computation of the expensive problem-specific Green’s function. We show through a numerical example that the truncation errors are exponentially small with respect to a truncation parameter ℓ.

Keywords: Boundary integral equations, perfectly matched layers, water waves, surface waves

1 Introduction
We consider the time-harmonic water waves problem [1], expressed in terms of the velocity potential ϕ:

\[ \Delta \varphi = 0 \quad (\Omega) \]
\[ \frac{\partial \varphi}{\partial \nu} - \frac{\omega^2}{g} \varphi = 0 \quad (\Gamma_{FS}) \]
\[ \frac{\partial \varphi}{\partial \nu} = f \quad (\Gamma_O \cup \Gamma_B) \]

where \( \Gamma_{FS} = \{(x_1, x_2) : x_1 \in \mathbb{R}, x_2 = 0\} \) denotes the free-surface, \( \Gamma_B \) denotes the bottom topography, \( \Gamma_O \) represents immersed obstacles, and \( f \) is compactly supported source term. It is assumed that the bottom is of constant depth \( d \) except for a compactly supported perturbation. Finally, the domain \( \Omega \) is the region outside \( \Gamma_O \) lying between \( \Gamma_{FS} \) and \( \Gamma_B \). As is well known, an additional radiation condition has to be imposed to recover uniqueness of the solutions (and to guarantee that the waves are “outgoing”). This condition may be expressed as

\[ \int_{|x_1|=R} |\varphi,1 - i k \varphi|^2 \ dS = o(1) \text{ as } r \to \infty, \]

with \( k \in \mathbb{R}^+ \) the solution of \( k \tanh(kd) = \omega^2/g \).

Because \( \Gamma_{FS} \) and \( \Gamma_B \) are unbounded curves, solving the water waves problem by boundary integral equation methods usually requires the use of a problem specific Green’s function \( G \). Expressions for such Green’s function involve expensive integrals which must be approximated numerically [1, Chapter 1]. In this work we show that it is possible to use the inexpensive free-space Green’s function for Laplace’s equation, \( G_\Delta \), together with the perfectly matched layer (PML) truncation technique, to obtain an efficient boundary integral formulation of (1) . This is essentially a PML-BIE technique, as recently put forward by Wangtao Lu and collaborators [2].

2 PML-BIE method
Adopting the change-of-variables point of view for PMLs, we consider a vector-valued transformation \( \tau : \mathbb{R}^2 \to \mathbb{C}^2 \) mapping physical points in \( \mathbb{R}^2 \) into complex points in \( \mathbb{C}^2 \). Letting \( J_{ij} = \frac{\partial \tau_i}{\partial x_j} = \tau_{i,j} \) be the Jacobian of the transformation, it follows that \( \tilde{\varphi}(x) = \varphi(\tau(x)) \) satisfies

\[ \nabla \cdot \left( A(x) \nabla \tilde{\varphi}(x) \right) = 0, \quad \text{for } x \in \Omega, \]

where \( A = |J|J^{-1}(J^{-1})^t \). Interestingly, under some reasonable assumptions on \( \tau \), equation (3) is strongly-elliptic, and its free-space Green’s function \( \tilde{G} \) is simply the composition of \( G_\Delta \) with \( \tau \); i.e. \( \tilde{G}(x,y) = G_\Delta(\tau(x), \tau(y)) \). This suggests a method for solving the PML-transformed problem based on \( \tilde{G} \), the computation of which involves only the evaluation of a (complex) logarithm. In what follows we take

\[ \tau(x) = (\tau(x_1), x_2) \]

for concreteness, where

\[ \tau(x_1) = \begin{cases} x_1 & |x_1| < a \\ \pm a + (\pm x_1 \mp a)e^{i\theta} & (\pm x_1 > a) \end{cases} \]

for some fixed parameters \( a \) and \( \theta \).

Upon this change of variables, the boundary conditions (1b-1c) remain unchanged (provided \( a \) is large enough), and the requirement that \( \varphi \) be ‘outgoing’ translates into the requirement that \( \tilde{\varphi} \) be exponentially decreasing. This
in turn allows for the following boundary integral representation of $\tilde{\varphi}$ (despite the unbounded interfaces):

$$\tilde{\varphi}(r) = S[\gamma_1 \tilde{\varphi}](r) - D[\tilde{\varphi}](r)$$  \hspace{1cm} (5)

where $S[\sigma](r) := \int_{\Gamma} \tilde{G}(r, y) \sigma(y) ds_y$ and $D[\sigma](r) := \int_{\Gamma} \sigma(y) \gamma_1 \tilde{G}(x, y) ds_y$ are the single- and double-layer potentials, and where $\gamma_1 \tilde{\varphi} := \nabla \tilde{\varphi} \cdot \hat{A}t_n$ denotes the conormal derivative.

Using classical jump conditions (see [3]), one finally derives the following second-kind integral equation:

$$\frac{\tilde{\varphi}(x)}{2} + D[\tilde{\varphi}](x) - \frac{\omega^2}{\gamma} S_{\Gamma_r}[r'\tilde{\varphi}](x) = S_{\Gamma \cup \Gamma_B}[f](x),$$  \hspace{1cm} (6)

where the underscript notation on the single-layer operator denotes the surface over which the integration is performed.

In order to obtain a numerical method, the unbounded interfaces in the equation above are truncated, and the integrals are discretized using a Nyström scheme. In the next section we present some numerical results of the proposed methodology.

**Remark 1** Because $\tilde{\varphi}$ decays exponentially as $|x_1| \to \infty$, and $\tilde{G}$ grows no faster than logarithmically, truncating the infinite domains in the equation above leads to exponentially small errors for the exact solution. This, however, is not sufficient to show that the truncation errors of the approximate solution, obtained by solving the truncated equation, are also exponentially small. Although numerical examples appear to indicate that this is the case, a stability result is still lacking in order to have a rigorous proof.

3 Numerical results

To validate the method, we consider first an example with a known $f$ and no other obstacles. A representation for the exact solution can then be obtained by a Fourier series method, and the analytical formula is compared to the numerical solution in figure 1. As can be seen, the solutions agree on the interval $-10 < x_1 < 10$, which is precisely where the PML begins. Inside the PML, a fast decay in the numerical solution is observed, as expected.

In order to better assess the truncation error of the PML-BIE technique, we show in figure 2 a self-convergence study in the presence of obstacles as the size of the PML layer is increased. An exponential convergence is observed; furthermore, the decay rate seems to agree with a theoretical prediction error $\sim \exp(-k \cos(\theta) \ell)$, where $\ell$ is the length of the PML layer, and $\theta$ is the angle parameter in (4). This validates the methodology, and opens the venue for interesting theoretical and computational questions regarding the application of the PML-BIE technique to problems where the Green’s function does not oscillate.

**References**


Thursday, July 28, Second Afternoon Session
Nonlinear Helmholtz equations with sign-changing diffusion coefficient

Rainer Mandel¹, Zoïs Moitier¹,*, Barbara Verfürth²

¹Institute for Analysis, Karlsruhe Institute of Technology, Karlsruhe, Germany
²Institute for Applied and Numerical Mathematics, Karlsruhe Institute of Technology, Karlsruhe,
Germany
*Email: zois.moitier@kit.edu

Abstract

We study nonlinear Helmholtz equations with sign-changing diffusion coefficients on bounded domains. The existence of an orthonormal basis of eigenfunctions is established making use of weak T-coercivity theory. All eigenvalues are proved to be bifurcation points and the bifurcating branches are investigated both theoretically and numerically. In one-dimensional model example we obtain the existence of infinitely many bifurcating branches that are mutually disjoint, unbounded, and consist of solutions with a fixed nodal pattern. We also extend the numerics to a Drude model.

Keywords: Helmholtz equation; Bifurcation Theory; Sign-changing; T-coercivity.

1 Problem setting

We are interested in the nonlinear Helmholtz equations in dimension $N \in \{1, 2, 3\}$ of the form:

$$-\text{div} (\sigma(x) \nabla u) - \lambda c(x) u = \kappa(x) u^3, \quad \text{in } \Omega, \tag{1}$$

for $(\lambda, u) \in \mathbb{R} \times H^1_0(\Omega)$ where $\Omega$ is a bounded open domain of $\mathbb{R}^N$, the diffusion coefficient $\sigma \in L^{\infty}(\Omega)$ is sign-changing, $0 < c \in L^{\infty}(\Omega)$, and $\kappa \in L^{\infty}(\Omega)$. Being sign-changing means that the domain $\Omega$ is partitioned in two open subdomains $\Omega_{\pm}$ such that $\Omega_{-} \cup \Omega_{+} = \Omega$, $\Omega_{-} \cap \Omega_{+} = \emptyset$, and the function $\sigma$ is negative on $\Omega_{-}$ and positive on $\Omega_{+}$. The main goal is to detect nontrivial solutions of Eq. (1) that bifurcate from the trivial solution family $\{(\lambda, 0) \mid \lambda \in \mathbb{R}\}$.

Equation (1) occurs in the study of time-harmonic wave propagation across an interface between a dielectric and a metamaterial with negative permeability and nonlinear Kerr-type permittivity [3]. Those two effects have been studied separately. The term $\kappa u^3$ is a classic manifestation of the nonlinear Kerr-type permittivity. In the case of positive diffusion coefficients $\sigma$ on the whole domain, it is well known that all the eigenvalues give rise to bifurcation branches. The metamaterial property manifests by having $\sigma$ negative on the subdomain $\Omega_{-}$. The linear theory dealing with the well-posedness of such problems for right-hand sides $f(x)$ instead of $\kappa(x) u^3$ has been studied both analytically and numerically [1]. The main difficulty with the indefinite operator $u \mapsto -\text{div} (\sigma(x) \nabla u)$ is that the standard theory for elliptic boundary value problems based on the Lax-Milgram Lemma does not apply. The (weak) T-coercivity has been introduced to recover a linear theory in the Fredholm sense. We assume that the operator $u \mapsto -\text{div} (\sigma(x) \nabla u)$ is weakly T-coercive, which means that there exists an isomorphism $T : H^1_0(\Omega) \rightarrow H^1_0(\Omega)$ and a compact operator $K : H^1_0(\Omega) \rightarrow H^1_0(\Omega)$ such that

$$(u, v) \mapsto \int_{\Omega} \sigma \nabla u \cdot \nabla (Tv) + \int_{\Omega} \nabla (Ku) \cdot \nabla v$$

is coercive. Being weakly T-coercive depends on the precise shape of the interface $\partial \Omega_{-} \cap \partial \Omega_{+}$ and jumps of $\sigma$ across the interface but, in dimension 1 and 2, it is known to be the case in many settings.

2 Main results

The weak T-coercivity ensured the existence of an orthonormal basis $(\phi_j)_{j \in \mathbb{Z}}$ consisting of eigenfunctions associated to the linear differential operator $u \mapsto -c^{-1} \text{div} (\sigma \nabla u)$. Due to the sign-change of $\sigma$ the corresponding sequence of eigenvalues $(\lambda_j)_{j \in \mathbb{Z}}$ satisfy $\lambda_j \rightarrow \pm \infty$ as $j \rightarrow \pm \infty$. Using some recent bifurcation result for strongly indefinite operators needed because of the sign-change of $\sigma$, we can show [3]:

Theorem 1 Each eigenpair $(\lambda_j, \phi_j)$ is a bifurcation point of Eq. (1). If $\lambda_j$ has an odd geometric multiplicity then the connected component $C_j \subset \mathbb{R} \times H^1_0(\Omega)$ containing $(\lambda_j, 0)$ satisfies Rabinowitz’ alternative:

(1) $C_j$ is unbounded in $\mathbb{R} \times H^1_0(\Omega)$;

(2) $C_j$ contains another trivial solution $(\lambda, 0)$. 

In a 1D setting with the subdomain \( \Omega^- = (a^-, 0) \) and \( \Omega^+ = (0, a^+) \), and piecewise constant functions \( \sigma, c \), we can strengthen our result. Using the almost explicit expression of the eigenvalues, we can use the distribution of zeros of the eigenfunction to show:

**Corollary 2** The connected component \( C_j \subset \mathbb{R} \times H^0_0(\Omega) \) is unbounded and \( C_j \cap C_i = \emptyset \) for \( i \neq j \).

Using additional assumptions, see [3, Theorem 6.3], which has been verified in the 1D settings, we can show a variational result for our problem. Meaning, for a fix \( \lambda \in \mathbb{R} \), there exists infinitely many solutions of Eq. (1).

### 3 Bifurcation visualization

We consider \( \Omega^- = (-5, 0) \), \( \Omega^+ = (0, 5) \), the diffusion coefficient is chosen piecewise constant \( \sigma|_{\Omega^-} \equiv -1.005 \) and \( \sigma|_{\Omega^+} \equiv 1 \), \( c \equiv 1 \), and \( \kappa \equiv 1 \). The numerics have been done using a finite element discretization and the Matlab package *pde2path* [4]. The finite element discretization use a \( T \)-conform mesh which is refined close to the interface \( \{0\} \) to faithfully represent the interface behavior. Figure 1 is the 2D bifurcation diagram (abscissa \( \lambda \) and ordinate \( \|u\|_{L^2(\Omega)} \)) where \( \lambda \) is initialized in \([-10, 15]\). All branches are unbounded and seemingly do not contain points of secondary bifurcation.

![Bifurcation diagram](image1)

**Figure 1:** Bifurcation diagram.

### 4 Extension: The Drude model

A simple known model to have negative diffusion parameter is the Drude model, however in that model the coefficients \( \sigma, c \) depend on the spectral parameter \( \lambda \). In [2], the diffusion coefficient \( \sigma \) and coefficient \( c \) are now given by

\[
\sigma_\lambda(x) = \frac{1}{1 - 1_{\Omega_-}(x) \frac{\Lambda_c}{\Lambda}} \quad \text{and} \quad c_\lambda(x) = 1 - 1_{\Omega_-}(x) \frac{\Lambda_x}{\Lambda}
\]

where \( 1_{\Omega_-}(x) \) is the indicator function of \( \Omega_- \) and with \( 0 < \Lambda_c < \Lambda_x \) constants.

For the numerical study, we use the same 1D subdomain \( \Omega^- = (-5, 0) \) and \( \Omega^+ = (0, 5) \), and \( \Lambda_c = 4 \), \( \Lambda_x = 7 \), and \( \kappa \equiv 1 \). Using the same numerical method as before, Figure 2 we show the 2D bifurcation diagram (abscissa \( \lambda \) and ordinate \( \|u\|_{L^2(\Omega)} \)) where \( \lambda \) is initialized in \([0.1, 9]\). We observe that the branches seems to accumulate at \( \lambda = 0 \) and, around \( \lambda = \Lambda_x \), we see a branch that seems to have a vertical asymptote and another that non-smoothly cross the values \( \Lambda_x \). We expect more intricate branch behavior around the values \( \lambda = 0 \) or \( \Lambda_x \) as either \( c_\lambda \) or \( \Lambda_x \) blow-up around those points but a more rigorous study is needed.

![Drude model: bifurcation diagram](image2)

**Figure 2:** Drude model: bifurcation diagram.

### References


**Acknowledgment.** Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) — Project-ID 258734477 — SFB 1173.
3D scalar transmission problem in presence of a conical tip of negative material.

Anne-Sophie Bonnet-Ben Dhia¹, Lucas Chesnel², Mahran Rihani³∗
¹ POEMS (CNRS-INRIA-ENSTA Paris), Palaiseau, France
² IDEFIX (INRIA-ENSTA Paris-EDF), Palaiseau, France
³ CMAP (CNRS, École polytechnique), Palaiseau, France
∗Email: mahranrihani@gmail.com

Abstract
In this work, we study a diffusion like scalar problem between a positive and a negative material in \( \mathbb{R}^3 \). The interface \( \Sigma \) between the two media is assumed to be smooth everywhere except at \( O \) where it has a conical tip. We prove that the problem is well-posed iff what we call propagating (or black hole) singularities do not exist. When there are such singularities, we explain how to recover well-posedness in an appropriate functional framework, which is consistent with the limiting absorption principle. Our results can be seen as an extension of the ones obtained in [1] for the case of 2D interfaces with corners.

Keywords: Kondratiev theory, T-coercivity, Mellin transform, black hole waves, limiting absorption principle, the Mandelshtam radiation principle.

1 Introduction
Let \( \Omega \) be a bounded domain of \( \mathbb{R}^3 \) which contains an inclusion \( \mathcal{M} \) of a negative material. We assume that \( \mathcal{M} \) is \( \mathcal{C}^3 \)− smooth except at the origin \( O \) where it coincides locally with a conical tip (see Figure 1): there exists \( \sigma \in (0,1) \) such that \( \mathcal{M} \cap B_\rho = \mathcal{K} \cap B_\rho \) where \( B_\rho := \{ x \in \mathbb{R}^3 | |x| < \rho \} \) and \( \mathcal{K} := \{ x \in \mathbb{R}^3 | x/|x| \in \mathcal{A} \} \), where \( \mathcal{A} \) is a smooth \( \mathcal{C}^2 \) subdomain of \( \mathbb{S}^2 \). Let \( \sigma \) be a piecewise constant function s.t. \( \sigma = \sigma^- \in \mathbb{R}^- \) in \( \mathcal{M} \) and \( \sigma = \sigma^+ \in \mathbb{R}^+ \) in \( \Omega \setminus \mathcal{M} \). We consider the problem of finding \( u \in H^1_0(\Omega) \) s.t.

\[-\text{div}(\sigma \nabla u) = f \in (H^1_0(\Omega))^*. \tag{1}\]

The study of (1) is related to the one of the operator \( A_{\sigma} : H^1_0(\Omega) \to (H^1_0(\Omega))^* \) s.t. for all \( u,v \in H^1_0(\Omega) \), we have

\[\langle A_{\sigma}u,v \rangle := \int_\Omega \sigma \nabla u \cdot \nabla v dx. \]

Classically, when \( \sigma \) is positive we know that \( A_{\sigma} \) is an isomorphism. But, since \( \sigma \) changes sign and given that \( \Sigma \) is singular at \( O \) (following what has been done in [1]), the operator \( A_{\sigma} \) may be not of Fredholm type. In the sequel, we denote by \( I_\Sigma \) the set of critical values of the contrast \( \kappa_\sigma = \sigma^-/\sigma^+ \) for which \( A_{\sigma} \) is not of Fredholm type, which is called the critical interval [2].

Figure 1: An example of geometry.

2 Characterization of \( I_\Sigma \)
Denote by \( \mathcal{L}_\sigma \) the Mellin symbol generated by the problem (1) near \( O \). For all \( \lambda \in \mathbb{C}, \mathcal{L}_\sigma(\lambda) : H^1(\mathbb{S}^2) \to H^1(\mathbb{S}^2)^* \) is such that

\[\forall u,v \in H^1(\mathbb{S}), \quad \langle \mathcal{L}_\sigma(\lambda)u,v \rangle = \int_{\mathbb{S}} \sigma(\rho \omega)|\nabla_S u \cdot \nabla_S v - \lambda(\lambda + 1)u\rho\omega|d\omega. \]

Above, \( \nabla_S \) stands for the surface gradient operator. By using localization techniques (on \( \mathbb{S}^2 \)) and the T-coercivity approach, we show the

Lemma 1 Assume that \( \kappa_\sigma \neq 0 \). Then \( \Lambda(\mathcal{L}_\sigma) \), the spectrum of \( \mathcal{L}_\sigma \), is composed by isolated eigenvalues which can accumulate only at infinity.

Note that if \( (\lambda,\psi) \in \mathbb{C} \times H^1(\mathbb{S}^2) \) is an eigenpair of \( \mathcal{L}_\sigma \), then \( \psi(x) := r^\alpha \psi_\alpha(x/|x|) \) satisfies \( \text{div}(\sigma \nabla \psi_\alpha) = 0 \) in \( B_\rho \). The function \( \psi_\alpha \) is called a singularity of (1) of exponent \( \alpha \). If \( \lambda \in \Lambda(\mathcal{L}_\sigma) \cap \ell_{-1/2} \) with \( \ell_{-1/2} := \{ \lambda \in \mathbb{C} | \Re(\lambda) = -1/2 \} \), the singularities \( \psi_\alpha \) are not locally in \( H^1 \), they are called propagating (see Figure 2).

Theorem 2 Assume that \( \kappa_\sigma \neq 0 \). Then \( A_{\sigma} \) is of Fredholm type if and only if the problem (1) has no propagating singularity.

Lemma 3 For the circular conical tip of opening angle \( 2\alpha \), we have \( I_\Sigma = [-1, -\alpha_\alpha] \) where \( \alpha_\alpha \) is known explicitly in terms of hypergeometric functions [2].
3 New framework for critical contrasts

Contrary to the case of a smooth $\Sigma$ where $I_{2\Sigma} = \{-1\}$, in our configuration $I_{2\Sigma}$ is an interval that contains the value $-1$ (this is due to surface plasmons that can propagate along the smooth part of $\Sigma$). In order to focus our attention on the effect of the conical singularity, we suppose that $\kappa_\sigma \in I_{2\Sigma}\setminus\{-1\}$. Owing to Theorem 2, we deduce that $\Lambda_{-1/2} := \Lambda(\mathcal{Z}_\sigma) \cap \ell_{-1/2} \neq \emptyset$.

Now, for $\beta \in \mathbb{R}$, we introduce the weighted Sobolev spaces $\tilde{V}_\beta^1(\Omega)$ defined as the closure of $\mathcal{D}(\Omega\setminus\{\Omega\})$ for the norm

$$||u||_{\tilde{V}_\beta^1(\Omega)} := \left( \sum_{|\alpha| \leq 1} ||\nabla^\alpha u||_{L^2(\Omega)}^2 \right)^{1/2}.$$

Note that for all $\beta > 0$ we have

$$\tilde{V}_\beta^1(\Omega) \subset \tilde{V}_0^1(\Omega) \subset \tilde{V}_\beta^1(\Omega).$$

Finally, for $\beta \in \mathbb{R}$, we define the operator $A_\beta^+ : V_\beta^1(\Omega) \to (\tilde{V}_\beta^1(\Omega))^* s.t.$ for $u \in \tilde{V}_\beta^1(\Omega)$ and $v \in \tilde{V}_\beta^1(\Omega)$, we have

$$\langle A_\beta^+ u, v \rangle := \int_\Omega \sigma \nabla u \cdot \nabla v.$$

**Lemma 4** There exists $\beta_0 > 0$ such that for $\beta \in (0; \beta_0)$, the operators $A_{\gamma}^{+\beta}$ are of Fredholm type. Furthermore, $\ker(A_{\gamma}^{+\beta})$ is independent of $\gamma \in (0; \beta_0)$.

Set $T_\sigma := \text{card}(\Lambda_{-1/2})$, and denote by $\lambda_1, \ldots, \lambda_{T_\sigma}$ the elements of $\Lambda_{-1/2}$. Note that contrary to the 2D case of interfaces with corners [1], $T_\sigma$ can be greater than 2. For each $p = 1, \ldots, T_\sigma$, we introduce $(\varphi_{j,k}^p)_{j=1,\ldots,T_\sigma; k=0,\ldots,v_j^p - 1}$ a conical system of Jordan chains corresponding to $\lambda_p$ $(v_j^p$ is the geometric multiplicity of $\lambda_p$ and $v_j^p$ the partial multiplicity of $\varphi_{j,k}^p$). Then, we define the general propagating singularities

$$s_{p,j,k}(x) = \psi(r)^{1/\lambda_p} \sum_{k=0}^{v_j^p} \frac{\log(r)^{s}}{s!} \varphi_{j,k-s}^p \left( \frac{x}{|x|} \right)$$

where $\psi$ is a cutoff function equal to 1 near $r = 0$. One shows that the dimension of $S_\sigma := \text{span}(s_{p,j,k})$ is even ($\dim(S_\sigma) = 2N_\sigma$). Observe that $S_\sigma \subset L^2(\Omega) \setminus H^1(\Omega)$ and that $\text{div}(\sigma \nabla u) \subset L^2(\Omega)$ for all $u \in S_\sigma$. With this in mind, we define the symplectic form $q : S_\sigma \times S_\sigma \to \mathbb{C}$ s.t.

$$q(u, v) = \int_\Omega \text{div}(\sigma \nabla u) - \text{div}(\sigma \nabla v) \cdot \nabla u.$$

Following [3], it has been proved in [2] that there exists $(s_{j}^\pm)_{j=1,\ldots,N_\sigma}$, a basis of $S_\sigma$ such that

$$q(s_{j}^+, s_{k}^-) = 0.$$

The functions $s_{j}^+$ (resp. $s_{j}^-$) are said to be outgoing (resp. incoming) with respect to the Mandelstam radiation principle [3].

Let us mention that the choice of such a basis is not unique. Now for a fixed basis, set $S_\sigma^+ := \text{span}(s_{j}^+)$ and introduce the space

$$\tilde{V}_\beta^\text{out}(\Omega) := \tilde{V}_\beta^1(\Omega) \oplus S_\sigma^+.$$

Then we define the operator

$$A_{\sigma}^{\text{out}} : \tilde{V}_\beta^\text{out}(\Omega) \to (\tilde{V}_\beta^1(\Omega))^* s.t. \forall u = \tilde{u} + s_{j}^+ \in \tilde{V}_\beta^\text{out}(\Omega) \text{ (with } \tilde{u} \in \tilde{V}_\beta^1(\Omega) \text{ and } s_{j}^+ \in S_\sigma \text{) and } \forall v \in \tilde{V}_\beta^1(\Omega) :$$

$$\langle A_{\sigma}^{\text{out}} u, v \rangle := \int_\Omega \sigma \nabla u \cdot \nabla v - \int_\Omega \text{div}(\sigma \nabla s^+ \cdot \nabla u).$$

**Theorem 5** Assume that $\kappa_\sigma \neq -1$. Then for all $\beta \in (0; \beta_0)$, $A_{\sigma}^{\text{out}}$ is a Fredholm operator of index zero. Moreover, $\ker(A_{\sigma}^{\text{out}}) = \ker(A_\sigma^{-\gamma})$, for all $\gamma \in (0; \beta_0)$.

Under some particular assumptions [2] (that are valid for the case of circular conical tips), one can construct a basis $(s_{j}^\pm)$ of $S_\sigma$ satisfying (2) and such that the corresponding framework $\tilde{V}_\beta^\text{out}$ (with $\beta \in (0; \beta_0)$) is consistent with the limiting absorption principle.

**References**


Maxwell’s equations in presence of a tip of material with negative permittivity

Anne-Sophie Bonnet-Ben Dhia\textsuperscript{1,*}, Lucas Chesnel\textsuperscript{2,}, Mehran Rihani\textsuperscript{1,2}

\textsuperscript{1}POEMS (CNRS-INRIA-ENSTA Paris), Palaiseau, France
\textsuperscript{2}IDEX (INRIA-ENSTA Paris-EDF), Palaiseau, France

\textsuperscript{*}Email: anne-sophie.bonnet-bendhia@ensta-paris.fr

Abstract

This work is devoted to the analysis of time-harmonic Maxwell’s equations in presence of a conical tip of a material with negative dielectric permittivity $\varepsilon$ and/or negative magnetic permeability $\mu$. When these constants $\varepsilon$ and $\mu$ belong to some critical range, the electromagnetic field exhibits strongly oscillating singularities, such that Maxwell’s equations are not well-posed in the classical $L^2$ framework. Following what has been done for the 2D scalar case \cite{1}, we show how to provide an appropriate functional setting, adding to weighted Sobolev spaces the so-called outgoing propagating singularities.

Keywords: time-harmonic Maxwell’s equations, metamaterial, singularities, Kondratiev weighted Sobolev spaces, $\mathcal{T}$-coercivity, compact embeddings, vector potentials

1 Setting of the problem

Let $\Omega$ be a bounded domain of $\mathbb{R}^3$ which contains an inclusion $\mathcal{M}$ of a particular material (metal at optical frequency, negative index metamaterial). We assume that $\partial \mathcal{M}$ is of class $C^2$ except at the origin $O$ where $\mathcal{M}$ coincides locally with a conical tip. For simplicity, we suppose that only $\varepsilon$ has a sign-change ($\mu = 1$ everywhere): $\varepsilon$ takes the constant value $\varepsilon_- < 0$ (resp. $\varepsilon_+ > 0$) in $\mathcal{M}$ (resp. $(\Omega \setminus \mathcal{M})$).

![Figure 1: The geometry.](image)

We consider the Maxwell’s problem

\begin{equation}
\begin{aligned}
\begin{bmatrix}
\text{curl} \text{curl} E - \omega^2 \varepsilon(x) E \\
E \times \nu = 0
\end{bmatrix} & = i \omega J & (\Omega) \\
\end{aligned}
\tag{1}
\end{equation}

where the current density $J \in L^2(\Omega)$ satisfies $\text{div} \ J = 0$. Let us introduce the scalar operator $A_\varepsilon : H_0^\varepsilon(\Omega) \rightarrow (H_0^\varepsilon(\Omega))^*$ defined by

$$
\langle A_\varepsilon \varphi, \varphi' \rangle = \int_{\Omega} \varepsilon \nabla \varphi \cdot \nabla \varphi' \, dx
$$

for all $\varphi, \varphi' \in H_0^\varepsilon(\Omega)$. It has been proved in \cite{2} that if $A_\varepsilon$ is an isomorphism, then problem (1) has the following equivalent variational form which satisfies the Fredholm property:

Find $E \in X_N$ such that $\forall F \in X_N$

$$
\int_{\Omega} \text{curl} E \cdot \text{curl} F \, dx - \omega^2 \int_{\Omega} E \cdot F \, dx = i \omega \int_{\Omega} J \cdot F \, dx
$$

where $X_N := \{ E \in H_N : \text{div}(\varepsilon E) = 0 \}$, with $H_N := \{ E : \text{curl} E \in L^2(\Omega), (E \times \nu)|_{\partial \Omega} = 0 \}$.

A similar result holds, replacing $X_N$ by a larger space $\mathcal{X}_N$ when $A_\varepsilon$ is a non-injective Fredholm operator.

The purpose of the present work is to study Maxwell’s problem when $A_\varepsilon$ is not a Fredholm operator, which arises when $\varepsilon_- / \varepsilon_+ \in I_c$, where $I_c$ (a bounded subset of $(-\infty, 0)$) is the so-called critical interval.

2 Scalar propagating singularities

For such critical contrasts, propagating singularities exist, that are of the form

$$
\varphi(x) = \chi(r) r^{-1/2 + i\eta} \varphi(\omega) \quad \text{with } \eta \in \mathbb{R}.
$$

Here $x = r \omega$ with $r = |x|$ and $\chi \in \mathcal{S}(\Omega)$ is a cutoff function equal to 1 near the origin. These singular functions satisfy $\text{div}(\varepsilon \nabla \varphi) = 0$ near the origin. Their span is a vector space $\mathcal{S}_c$ of finite dimension $2N_c$. Then, thanks to a limiting absorption principle, one can define the subspace of outgoing singularities $\mathcal{S}_{\text{out}} = \text{span}\{ \varphi_j : j = 1, \cdots, N_c \}$ such that $q(\varphi_j, \varphi_k) = i \delta_{j,k}$ where $q(u, v) = \int_{\Omega} \text{div}(\varepsilon \nabla u) \nabla v - \text{div}(\varepsilon \nabla v) \nabla u$.

For $\beta \in \mathbb{R}$ and $m \in \mathbb{N}$, recall that the weighted Sobolev (Kondratiev) space $V_{\beta}^m(\Omega)$ is defined as the closure of $\mathcal{S}(\Omega \setminus \{O\})$ for the norm

$$
\| \varphi \|_{V_{\beta}^m(\Omega)} = \left( \sum_{|\alpha| \leq m} \| r^{\frac{|\alpha|}{2}} \partial_x^\alpha \varphi \|_{L^2(\Omega)}^2 \right)^{1/2}
$$
and \( \hat{V}^1_{\beta}(\Omega) = \{ \varphi \in V^1_{\beta}(\Omega) | \varphi|_{\partial \Omega} = 0 \} \). Next for \( \beta > 0 \), setting \( \hat{V}^{\text{out}}_{\beta}(\Omega) = \hat{V}^1_{\beta}(\Omega) \supset S^{\text{out}}_{\beta}(\Omega) \), define the operator \( A^{\text{out}}_{\beta} : \hat{V}^{\text{out}}_{\beta}(\Omega) \to (\hat{V}^1_{\beta}(\Omega))^* \) such that for all \( u = \tilde{u} + \sum_j a_j \tilde{s}_j \in \hat{V}^{\text{out}}_{\beta}(\Omega) \) and \( v \in \hat{V}^1_{\beta}(\Omega) \) \((A^{\text{out}}_{\beta} u, v) = \int_{\Omega} \varepsilon \nabla u \cdot \nabla v \) where we have set
\[
\int_{\Omega} \varepsilon \nabla s_j \cdot \nabla v = -\int_{\Omega} \text{div}(\varepsilon \nabla s_j) v
\]
(note that this integral coincides with the usual one for \( v \in V^1_{\beta}(\Omega) \)).

A main result established in [3] is the existence of \( \beta_D > 0 \) such that the operator \( A^\varepsilon_{\text{out}} \) is Fredholm for all \( \beta \in (0, \beta_D) \), and an isomorphism as soon as \( A^\varepsilon \) is injective (which is assumed in what follows).

### 3 A new framework for Maxwell’s equations

The above results for the scalar problem lead to look for the solution of problem (1) in the space
\[
X^{\text{out}}_N := \{ E = \sum j a_j \nabla s_j + \tilde{E} : \tilde{E} \in H_N, \ a_j \in C, \ \text{div}(\varepsilon E) = 0 \}.
\]

Note that \( X_N \subset X^{\text{out}}_N \). Using the fact that \( A^\varepsilon_{\text{out}} \) is an isomorphism, one can check that a solution of
\[
\int_{\Omega} \varepsilon \nabla s_j \cdot \nabla v = -\int_{\Omega} \text{div}(\varepsilon \nabla s_j) v
\]
is indeed a solution of (1). This result and the analysis of (3) rely on the key following regularity result. If \( E = \sum a_j \nabla s_j + \tilde{E} \in X^{\text{out}}_N \), then for any \( \beta < \min(\beta_D, 1/2) \), \( \tilde{E} \in V^0_{\beta-\varepsilon}(\Omega) \). Moreover there is a constant \( C > 0 \) independent of \( E \) such that
\[
\sum a_j |a_j| + \| \tilde{E} \|_{V^0_{\beta-\varepsilon}(\Omega)} \leq C \| \text{curl} \ E \|_{\Omega}.
\]

As a consequence, \( \| \text{curl} \|_{\Omega} \) is a norm in \( X^{\text{out}}_N \). Besides, one can prove the following compactness result: for any bounded sequence \( E^{(n)}_\varepsilon = \sum a^{(n)}_j \nabla s_j + \tilde{E}^{(n)} \) of \( X^{\text{out}}_N \), there exists a subsequence such that \( a^{(n)}_j \) converges in \( C \) and \( \tilde{E}^{(n)} \) converges in \( V^0_{\beta-\varepsilon}(\Omega) \). Summing up, one can prove the

**Theorem 1** Fredholm alternative holds for problem (3): if uniqueness holds, then the problem is well-posed.

Concerning uniqueness, note that if \( E \) is a solution of (3) for \( J = 0 \), then taking \( F = E \), we get \( \exists \mu \left( \int_{\Omega} \varepsilon \varepsilon E \cdot E \ dx = \sum |a_j|^2 = 0 \right. \). This proves that any solution \( E \) of the homogeneous problem (3) belongs to the classical space \( X_N \). Such a solution is called a trapped mode by analogy with waveguides problems.

### 4 Some concluding remarks

Since \( X_N \) is a closed subset of \( X^{\text{out}}_N \), we see by previous theorem that Fredholm alternative also holds for problem (2) set in the classical framework. But what is wrong with this formulation is that a solution of (2) is not, in general, a solution of Maxwell’s equation (1).

If \( \mu \) is also negative in the inclusion \( \mathcal{M} \), we have to consider another scalar operator. Let \( H^{\mu}_N(\Omega) \) be the subset of \( H^1(\Omega) \) of functions with zero mean value. Consider the operator \( A^\mu : H^{\mu}_N(\Omega) \to (H^{\mu}_N(\Omega))^* \) defined by
\[
\langle A^\mu \varphi, \varphi' \rangle = \int_{\Omega} \mu \nabla \varphi \cdot \nabla \varphi' \ dx
\]
for all \( \varphi, \varphi' \in H^{\mu}_N(\Omega) \). If \( A^\mu \) is a Fredholm operator, the previous results can be easily extended, using \( T \)-coercivity arguments. But if it is not, not only \( E \) has to be singular, but also \( \text{curl} E \) (and therefore the magnetic field). For this case where both contrasts in \( \varepsilon \) and \( \mu \) are critical, an appropriate functional framework is given in [3] in which Fredholmness is restored.

### References


Exponentially Convergent Spectral Galerkin BEM for Elastic Wave Scattering of Cracks.

Carlos Jerez-Hanckes 1, Jose Pinto1,*, Tao Yin2

1Facultad de Ingeniería y Ciencias, Universidad Adolfo Ibáñez, Santiago, Chile
2Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing, China

*Email: jose.pinto@uai.cl

Abstract

In this work, we extend the spectral Galerkin boundary integral solver for Helmholtz presented in [1] to elastic wave scattering by multiple two-dimensional cracks. We rigorously prove the exponential convergence rate of our proposed approximations for Dirichlet and Neumann problems. We show that solutions of the associated standard first-kind boundary integral formulations take the form of a singular function times an analytic one. Then, our method focuses on only approximating the analytic part by the spectral method. Several numerical experiments confirm our claims.

Keywords: Boundary Integral Equations, Elastic wave scattering, Spectral Methods

1 Introduction

We consider an impinging elastic wave \( u^{\text{inc}} \) in a homogeneous isotropic and infinite two-dimensional medium \( \Omega \) containing \( M \) cracks, jointly denoted by \( \Gamma \). The direct problem consists on finding the scattered wave \( u \) under the assumption that either the cracks are rigid (Dirichlet) or traction free (Neumann). The volume problems read

\[
\Delta^* u + \rho \omega^2 u = 0 \quad \text{in} \quad \mathbb{R}^2 \setminus \Gamma,
\]

\[
u = -u^{\text{inc}}, \quad \text{or} \quad Tu = -Tu^{\text{inc}}\quad \text{on} \quad \Gamma,
\]

with Kupradze radiation condition,

where \( \Delta^* := \mu \text{div} \text{grad} + (\lambda + \mu) \text{grad} \text{div}, \mu, \lambda \) being the Lamé parameters of the medium, \( \omega \) the angular frequency. The traction operator is \( T := 2\mu \partial_n + \lambda n \text{div} - \mu \tau \text{curl}, \) where \( n \) is the normal vector, \( \tau = (-n_2, n_1) \), and \( \text{curlu} = \partial_1 u_2 - \partial_2 u_1 \). We refer to [2] for the exact form of the radiation condition. Remark that this problem is relevant to many engineering applications such as non-destructive testing of materials or fractures characterization.

These volume problems are reduced to systems of first-kind boundary integral equations (BIEs) via appropriate indirect representations by means of layer potentials. These can be solved, for instance, by local polynomials defined on appropriate meshes of the arcs \( \Gamma \). Special care needs to be given to how the mesh is built as solutions may exhibit singular behaviors near the endpoints of each arc. Typically, this entails particular refinements near the endpoints are needed to recover the traditional algebraic convergence rate of local (low-order) approximation methods or super-algebraic convergence of the \( hp \)-methods. However, for large numbers of cracks and in the context of inverse problems or uncertain quantification (UQ), the number of degrees of freedom required by this technique becomes impractical.

Following [1], we avoid any meshing by defining global basis constructed as polynomials multiplied by a special singular function that captures the singular behavior of the real solution. By examining the polynomial expansion of the BIEs solutions, we can show that our error convergence rate is exponential in the polynomial degree, assuming that the incident wave and the geometry of each arc are given by analytic functions. This proof differs from traditional results for open arcs as we do not make use of the Mellin transform with localization of the singularities. Indeed, these proofs rely on the approximation of smooth window functions which are \( C^\infty \) but not analytic, thus preventing the obtention of exponential convergence rate.

Furthermore, and in contrast to [1], here we also extend the analysis to hyper-singular BIEs. The corresponding analysis was obtained using an adequate Maue’s representation formula (see [3]).
2 Boundary Integral Formulation and Discretization

For Dirichlet boundary conditions, the associated BIE is
\[ \sum_{j=1}^{M} \int_{\Gamma_j} E(x, y) \phi_j(y) ds_{by} = -u^{inc}|_{\Gamma}, \]
for every \( i \in \{1, \ldots, M\} \), and where \( E \) denotes the standard fundamental solution of the the Navier equation [2] and \( \phi_j \) are the unknown densities defined in \( \Gamma_j \) for each \( j \in \{1, \ldots, M\} \). For the Neumann problem the corresponding formulation is
\[ \sum_{j=1}^{M} T_{\Gamma_j} \int_{\Gamma_j} T_y E(x, y) \psi_j(y) ds_{by} = -T_{\Gamma}, u^{inc}, \]
where \( T_{\Gamma_j} \) is the traction operator on \( \Gamma_i \), and \( \psi_j \) are unknown densities defined in the corresponding arc \( \Gamma_j \). The solution of the associated volume problem is then obtained by taking the action of the appropriate layered potential over the densities \( \phi \), or \( \psi \) depending on the boundary condition.

Assuming that \( \Gamma_i \) is the image of an analytic function \( r_i : [-1,1] \rightarrow \mathbb{R}^2 \). We define \( \phi^N \circ r_i(t) = \sum_{p=1}^{2^N} \sum_{n=0}^{N} a_{n,p} T_n(t), \) and \( \psi^N \circ r_i(t) = \sum_{n=0}^{N} b_n U_n(t), \) where
\[ T_{n,p}(t) = (1 - t^2)^{\frac{1}{2}} \| r'_i(t) \|^{-1} T_n(t) e_p, \]
\[ U_{n,p}(t) = (1 - t^2)^{\frac{1}{2}} U_n(t) e_p, \]
with \( e_p \) denoting the \( p \)th canonical vector, and \( T_n \) and \( U_n \) are the \( n \)th Chebyshev polynomials of first and second kind, respectively. Then, we bound the convergence rates of \( \phi^N \) and \( \psi^N \) to \( \phi \) and \( \psi \), respectively, as a function of \( N \).

**Theorem 1** Assuming that \( u^{inc} \circ r_i \) and \( r_i \) have analytic extension to an open region of the complex plane containing \([-1,1]\), there exist \( \rho > 1 \), and \( g > 1 \), such that
\[ \| \phi - \phi^N \|_{L^1(\mathbb{R})} \leq C\rho^{-N}, \]
\[ \| \psi - \psi^N \|_{L^1(\mathbb{R})} \leq Cg^{-N}, \]
where \( C > 0 \) is a generic constant independent of \( N \).

3 Numerical Results

We consider a test case with 28 arcs, see Figure 1a, and the parameters \( \omega = 50, \lambda = 2, \mu = 1 \). Figure 1b illustrate the errors of the method as a function of the polynomial degree.

4 Conclusions and Future Work

We have developed a novel strategy to study the solution of first-kind boundary integral equations for open arcs and applied it to the analysis of a spectral Galerkin method, for which we proved the exponential convergence rate. Current work is on to prove the convergence rates for the Nyström discretization and the application of the method in UQ problems.

References


Computing singular and near-singular integrals in high-order boundary elements

Hadrien Montanelli$^{1,*}$, Matthieu Aussal$^2$, Houssem Haddar$^3$

$^1$Inria Saclay & ENSTA Paris
$^2$Ecole Polytechnique
$^3$Inria Saclay & ENSTA Paris

$^*$Email: hadrien.montanelli@gmail.com

Abstract

We present in this talk algorithms for computing singular and near-singular integrals arising when solving the 3D Helmholtz equation with high-order boundary elements. These are based on the computation of the preimage of the singularity on the reference element using Newton’s method, singularity subtraction with high-order Taylor-like asymptotic expansions, the continuation approach, and transplanted Gauss quadrature. We demonstrate the accuracy with several numerical experiments, including the scattering by two nearby half-spheres.

Keywords: Helmholtz equation, integral equations, boundary element method, singular integrals, continuation approach, Gauss quadrature

1 Introduction

The Helmholtz equation $\Delta u + k^2 u = 0$ in the presence of an obstacle may be rewritten as an integral equation on the obstacle’s boundary via layer potentials. For example, the radiating solution to the Dirichlet problem $\Delta u + k^2 u = 0$ in $\mathbb{R}^3 \setminus \Omega$ with $u = u_D$ on $\Gamma = \partial \Omega$, for some bounded $\Omega$ whose complement is connected, can be obtained via the equation

$$\int_{\Gamma} G(x, y) \varphi(y) d\Gamma(y) = u_D(x), \quad x \in \Gamma,$$  

(1)

based on the single-layer potential; the function $G$ is the Green’s function

$$G(x, y) = \frac{1}{4\pi} \frac{e^{ik|x-y|}}{|x-y|}.$$  

(2)

Once (1) is solved for $\varphi$, which is unique if $k^2$ is not an eigenvalue of $-\Delta$ in $\Omega$, the solution $u$ may be represented by the left-hand side of (1) for all $x \in \mathbb{R}^3 \setminus \Omega$.

From a numerical point of view, integral equations of the form of (1) are particularly challenging for several reasons. First, when $x$ approaches $y$, the integral becomes singular and standard quadrature schemes fail to be accurate—analytic integration or carefully-derived quadrature formulas are, hence, required. Second, the resulting linear systems after discretization are often dense. For large wavenumbers $k$, only iterative methods can be used to solve them (with the help of specialized techniques to accelerate the matrix-vector products, such as the Fast Multipole Method or hierarchical matrices). In this respect, the use of higher-order numerical discretization schemes may be helpful in enlarging the interval of feasible wavenumbers.

2 Computing singular integrals

When solving (1) with high-order boundary elements, one has to compute integrals of the form

$$I(x_0) = \int_{\mathcal{T}} \frac{\varphi(F^{-1}(x))}{|x - x_0|} dS(x),$$

where $\mathcal{T}$ is a curved triangular element defined by a polynomial transformation $F : \tilde{\mathcal{T}} \rightarrow \mathcal{T}$ of degree $q \geq 1$ from the flat reference triangle $\tilde{\mathcal{T}}$, $x_0$ is a point on or close to the element $\mathcal{T}$, and $\varphi : \tilde{\mathcal{T}} \rightarrow \mathbb{R}$ is of degree $p \geq 0$. Our method goes like this.

Step 1. We map $\mathcal{T}$ back to $\tilde{\mathcal{T}}$,

$$I(x_0) = \int_{\tilde{\mathcal{T}}} \frac{\psi(\tilde{x})}{|F(\tilde{x}) - x_0|} dS(\tilde{x}),$$

where $F : \tilde{\mathcal{T}} \rightarrow \mathcal{T}$, the transformation of degree $q$ from 2D flat $\tilde{\mathcal{T}}$ to 3D curved $\mathcal{T}$, has a $3 \times 2$ Jacobian matrix $J$ with columns $J_1$ and $J_2$, and $\psi(\tilde{x}) = \varphi(\tilde{x}) |J_1(\tilde{x}) \times J_2(\tilde{x})|$

Step 2. We write

$$x_0 = F(\tilde{x}_0) + x_0 - F(\tilde{x}_0)$$

for some $\tilde{x}_0 \in \tilde{\mathcal{T}}$ such that $F(\tilde{x}_0) \in \mathcal{T}$ is the closest point to $x_0$ on $\mathcal{T}$. We introduce here the parameter of singularity $h = |F(\tilde{x}_0) - x_0|$.

Step 3. We compute the singular term using the Taylor series of $F(\tilde{x}) - \tilde{x}_0$ at $\tilde{x}_0$.

$$T_{-1}(\tilde{x}, h) = \frac{\psi(\tilde{x}_0)}{\sqrt{|J(\tilde{x}_0)(\tilde{x} - \tilde{x}_0)|^2 + h^2}}.$$
and add it to/subtract it from $I(x_0)$, i.e.,

$$I(x_0) = I_{-1}(h) + \int_{\hat{T}} \left[ \frac{\psi(\hat{x})}{|F(\hat{x}) - x_0|} - T_{-1}(\hat{x}, h) \right] dS(\hat{x}).$$

The singular integral $I_{-1}(h)$ is given by

$$I_{-1}(h) = \int_{\hat{T}} T_{-1}(\hat{x}, h) dS(\hat{x}),$$

and will be computed in Steps 4–5. The other integral has a bounded integrand—it can be computed with standard Gauss quadrature.

**Step 4.** The integrand in $I_{-1}(h)$ is homogeneous in both $\hat{x}$ and $h$, and using the continuation approach, we reduce the 2D integral to a sum of three 1D integrals along the edges of the shifted triangle $\hat{T} - \hat{x}_0$,

$$I_{-1}(h) = \psi(\hat{x}_0) \sum_{j=1}^{3} \hat{s}_j \int_{\partial \hat{T}_j - \hat{x}_0} g_h(\hat{x}) ds(\hat{x}),$$

with 1D smooth functions

$$g_h(\hat{x}) = \frac{\sqrt{|J(\hat{x}_0)\hat{x}|^2 + h^2 - h}}{|J(\hat{x}_0)\hat{x}|^2}.$$

The $\hat{s}_j$’s are the distances from the origin to the edges of the shifted triangle.

**Step 5.** On the one hand, when the origin is far from all three edges, each integrand is analytic—convergence with Gauss quadrature is exponential. On the other, when the origin lies on an edge, the corresponding integrand is singular—however, the distance to that edge is 0, the product “$\hat{s}_j$ times integral” is also 0, and the integral does not need to be computed at all. Issues arise when the origin is close to one of the edges—the integrand is analytic but near-singular, convergence with Gauss quadrature is exponential but slow. We circumvent this issue by using transplanted Gauss quadrature.
Robust boundary integral equations of Helmholtz decomposition formulations of elastic scattering problems

Catalin Turc\textsuperscript{1, *}, Victor Domínguez\textsuperscript{2}

\textsuperscript{1}Department of Mathematics, NJIT, Newark, USA
\textsuperscript{2}Dep. Ingeniería Matemática e Informática, Universidad Pública de Navarra. Campus de Tudela
31500 - Tudela, Spain
\textsuperscript{*}Email: cct21@njit.edu

Abstract

We present a robust boundary integral equation formulation for elastodynamic scattering problems in two dimensions formulated via Helmholtz decompositions. The main advantage of this formulation is its reliance on Helmholtz layer potentials only, which are simpler than their counterparts that correspond to the fundamental solution of Navier equations.

Keywords: Navier equations, combined field integral equations

1 Introduction

Numerical solutions of elastic scattering problems based on boundary integral equation formulations are attractive alternatives over their volumetric counterparts \cite{4}. Following ideas introduced in [2], we introduce in this paper robust and well-conditioned boundary integral equation formulations of elastic scattering problems that are based on the Helmholtz decomposition of the elastic fields in two dimensions, which allows use to deal only with Helmholtz layer potentials.

2 Helmholtz decomposition formulation of Navier scattering problems

Considering a bounded domain $\Omega$ in $\mathbb{R}^2$ whose boundary $\Gamma$ is a closed Lipschitz curve, we are interested in solving the impenetrable elastic scattering problem in the exterior of $\Omega$, that is look for solutions of the time-harmonic Navier equation

\[
\nabla \cdot \sigma(u) + \omega^2 u = 0 \quad \text{in} \quad \Omega^+ := \mathbb{R}^2 \setminus \Omega \tag{1}
\]

that satisfy the Kupradze radiation condition at infinity, where $\sigma$ is the stress tensor associated with the field $u$ and the Lamé constants $\lambda$ and $\mu$. We assume that on the boundary $\Gamma$ the solution $u$ of (1) satisfies the Dirichlet boundary condition

\[
u = -u^{\text{inc}} \quad \text{on} \quad \Gamma.
\]

The scattered field can be expressed in the form of the Helmholtz decomposition $u = u_p + u_s$,

\[
u_p := -\frac{1}{k_p^2} \nabla \cdot u \quad \nu_s := \frac{1}{k_s^2} \nabla \times \nabla \times u \tag{2}
\]

where $\nabla \times u := \partial_1 u_2 - \partial_2 u_1$ and $\nabla \times \nu = [\partial_2 \nu - \partial_1 \nu]^T$. Hence, following the ideas in [2] we can look for the fields $u$ in the form

\[
u = \nabla \varphi_p + \nabla \times \varphi_s \tag{3}
\]

where the scalar functions $\varphi_p$ and $\varphi_s$ are radiative solutions of scalar Helmholtz equations in $\Omega^+$ with wavenumbers $k_p$ and $k_s$ respectively. It is straightforward to see that $\varphi_p$ and $\varphi_s$ satisfy the following coupled boundary conditions

\[
\partial_n \varphi_p + \partial_s \varphi_s = \frac{-u^{\text{inc}} \cdot n}{\nu} \quad \text{on} \quad \Gamma
\]

\[
-\partial_n \varphi_p + \partial_s \varphi_s = \frac{u^{\text{inc}} \cdot t}{\nu} \quad \text{on} \quad \Gamma \tag{4}
\]

where $\partial_n$ and $\partial_s$ denote the normal and respectively the tangential derivatives on $\Gamma$, whereas $n$ and $t$ denote the unit exterior normal and respectively the unit tangent on $\Gamma$. We look for $\varphi_p$ and $\varphi_s$ in the form of regularized combined field Helmholtz potentials with wavenumbers $k_p$ and respectively $k_s$

\[
\varphi_p := DL_{\Gamma,k_p}[Y_p g_p] - SL_{\Gamma,k_p}[g_p]
\]

\[
\varphi_s := DL_{\Gamma,k_s}[Y_s g_s] - SL_{\Gamma,k_s}[g_s] \quad \text{in} \quad \Omega^+,
\]

where $g_p$ and $g_s$ are unknown functional densities defined on $\Gamma$, and $Y_p$ and $Y_s$ are operators to be specified in what follows. We are led to the following system of BIE for the boundary densities $g_p$ and $g_s$

\[
A_{DH}^{11}[g_p] = -\left[ \begin{array}{c} u^{\text{inc}} \cdot n \\ -u^{\text{inc}} \cdot t \end{array} \right]
\]

\[
A_{DH}^{12}[g_p] := \frac{1}{2} I + N_p Y_p - K^T_p
\]

\[
A_{DH}^{21}[g_s] := \frac{1}{2} \partial_n Y_s - \partial_s V_s + k_s^2 t \cdot V_s[n] Y_s - K^T_s \partial_s Y_s
\]

\[
A_{DH}^{22}[g_s] := -\frac{1}{2} \partial_n Y_s + \partial_s V_s + k_s^2 t \cdot V_s[n] Y_s + K^T_p \partial_s Y_p
\]

\[
A_{DH}^{33}[g_s] := \frac{1}{2} I + N_s Y_s - K^T_s
\]

\[
\tag{5}
\]
<table>
<thead>
<tr>
<th>$\omega$</th>
<th>$N$</th>
<th>$\varepsilon_\infty$ Kite</th>
<th>$\varepsilon_\infty$ Starfish</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>64</td>
<td>$6.4 \times 10^{-4}$</td>
<td>$3.2 \times 10^{-4}$</td>
</tr>
<tr>
<td>16</td>
<td>128</td>
<td>$7.4 \times 10^{-7}$</td>
<td>$2.2 \times 10^{-7}$</td>
</tr>
<tr>
<td>16</td>
<td>256</td>
<td>$8.5 \times 10^{-16}$</td>
<td>$5.6 \times 10^{-16}$</td>
</tr>
<tr>
<td>32</td>
<td>128</td>
<td>$2.3 \times 10^{-9}$</td>
<td>$3.5 \times 10^{-8}$</td>
</tr>
<tr>
<td>32</td>
<td>256</td>
<td>$5.2 \times 10^{-9}$</td>
<td>$8.6 \times 10^{-9}$</td>
</tr>
<tr>
<td>32</td>
<td>512</td>
<td>$4.5 \times 10^{-15}$</td>
<td>$1.1 \times 10^{-14}$</td>
</tr>
</tbody>
</table>

Table 1: Errors in the method of manufactured solution using the Helmholtz decomposition BIE for the smooth kite and starfish geometries using the K-M Nyström discretization with different values of the frequency $\omega$ and material parameter values $\lambda = 1$, $\mu = 1$, at various levels of discretization.

In equation (5) the subscripts $p$ and $s$ refer to the wavenumbers $k_p$ and respectively $k_s$ in the definition of the corresponding boundary integral operators, $V$ is the Helmholtz single layer BIO, $K^T$ is the adjoint of the double layer BIO, and $N$ is the hypersingular operator. We establish the following:

**Theorem 1** Choosing $Y_p = -2V_{k_p+\varepsilon_p}$ and $Y_s = -2V_{k_s+\varepsilon_s}$, with $0 < \varepsilon_p$ and $0 < \varepsilon_s$, the operators $A_{DH}$ are invertible in $L^2(\Gamma) \times L^2(\Gamma)$ for all frequencies $\omega > 0$ when $\Gamma$ is a smooth closed curve.

### 3 Numerical results

The Nyström discretization of the BIE (5) is rather straightforward, and we present two such strategies, one based on the classical Kussmaul-Martensen (K-M) kernel singularity splitting [3], the other on QBX [1]. In the case of piece-smooth boundaries, we use sigmoid transforms (with polynomial degree $p$) in conjunction with K-M methods, and Chebyshev meshes together with Clenshaw-Curtis quadratures in connection with QBX Nyström discretizations. We present in Tables 1-2 far field errors achieved by the Nyström discretizations of the Helmholtz decomposition BIE (5) in the context of the method of manufactured solutions. Similar accuracy levels are observed in the case of plane wave incident fields. Furthermore, the BIE formulations (5) behave like integral equations of the second kind, and their numbers of GMRES iterations grow only logarithmically with the frequency in the high frequency regime.

<table>
<thead>
<tr>
<th>$\omega$</th>
<th>$N$</th>
<th>Teardrop</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>128</td>
<td>$8.6 \times 10^{-4}$</td>
</tr>
<tr>
<td>16</td>
<td>256</td>
<td>$1.0 \times 10^{-4}$</td>
</tr>
<tr>
<td>16</td>
<td>512</td>
<td>$1.2 \times 10^{-5}$</td>
</tr>
<tr>
<td>16</td>
<td>1024</td>
<td>$1.5 \times 10^{-6}$</td>
</tr>
<tr>
<td>32</td>
<td>256</td>
<td>$2.9 \times 10^{-3}$</td>
</tr>
<tr>
<td>32</td>
<td>512</td>
<td>$4.7 \times 10^{-4}$</td>
</tr>
<tr>
<td>32</td>
<td>1024</td>
<td>$6.0 \times 10^{-5}$</td>
</tr>
<tr>
<td>32</td>
<td>2048</td>
<td>$7.6 \times 10^{-6}$</td>
</tr>
</tbody>
</table>

Table 2: Far-field errors in the method of manufactured solution using the Helmholtz decomposition BIE for the singular teardrop geometry with different values of the frequency $\omega$ and material parameter values $\lambda = 1$, $\mu = 1$, at various levels of discretization.

### References


On the use of phased array data for the Linear Sampling Method in an elastic waveguide

Arnaud Recoquillay$^{1,*}$

$^1$Université Paris-Saclay, CEA, LIST, F-91120, Palaiseau, France

$^*$Email: arnaud.recoquillay@cea.fr

Abstract

We are interested here in using the Linear Sampling Method (LSM) [1] to image defects in an elastic waveguide [2] by using scattering data for sensors on the surface of the waveguide [3]. In particular, we use phase laws between sensors to emit more energy for each acquisition to improve the quality of the data and so the imaging results. However, the use of these phase laws has an impact on the condition number of the matrices used in the inversion, inducing that close attention must be paid to the acquisition parameters to improve the imaging.

Keywords: Linear Sampling Method, surface data, waveguide, elasticity, time domain

1 Setting of the problem

We consider a two dimensional waveguide $W = \Sigma \times \mathbb{R}$ of transverse section $\Sigma$ and boundary $\Gamma = \Gamma_0 \cup \Gamma_d$, $d$ being the height of the waveguide and $\Gamma_0$ and $\Gamma_d$ being respectively its lower and upper boundary. This waveguide is made of an isotropic material of density $\rho$ and Lamé constants $(\lambda, \mu)$. We want to retrieve the shape of a defect $D$, the support of which is supposed to be for axis coordinates bigger than $-R$, from data acquired with sources and measurements on the surface $\Gamma$. We consider a family of measurement points and sources $(g(x-x_i)\chi_i(t))_{1 \leq i \leq M}$ located on $\Gamma_d$ of compact support centered at $x_i = -R - i\delta$, $i = 1, \ldots, M$. The displacement $u$ solves the following problem for a given source $f$:

$$\begin{cases}
\rho \partial_\nu u - \text{div}(u) = 0 & \text{in} \quad (W \setminus D) \times (0, +\infty), \\
\sigma(u)\nu = f & \text{on} \quad \Gamma \times (0, +\infty), \\
u = 0 & \text{on} \quad \partial D \times (0, +\infty), \\
\mathbf{u} = 0 & \text{on} \quad (W \setminus D) \times \{0\},
\end{cases}$$

where $\sigma(u) = \lambda(\text{div} u) I + \mu(\nabla u + \nabla u^T)$ is the stress and $\nu$ is the exterior normal to $W$. A common acquisition setup is to use each emitting transducer successively, that is $f(x, t) = g(x-x_i)\chi_i(t)$, while all receivers record the field, which has already been used for the LSM [3]. However, this leads in general to poor signal to noise ratios in the data as the transducers emit limited unfocused energy in the waveguide.

That is why we consider here to emit simultaneously with all sources but with different delay laws for each acquisition, that is consider sources of expression

$$f(x, t) = \sum_{i=1}^{M} g(x-x_i)\chi(t-(M-i)\tau_k),$$

where $\tau_k$, $k = 1, \ldots, N$, are delays which must be chosen well to enable proper imaging results. We hereafter briefly describe the LSM in a modal formulation and its extension to surface data, which enables the choice of these delays. We hence consider in the following our problem in the frequency domain, the two problems being linked by the Fourier transform.

2 The Linear Sampling Method: a modal formulation

Decompose $u = (u_S, u_3)^T$, $\sigma_S = (t_S, -t_3)^T$, where the subscripts $S$ and $3$ denote the components of a vector along the transverse section and along the axis, respectively. We introduce the mixed variables $X$, $Y$ defined by $X = (t_S, u_3)^T$, $Y = (u_S, t_S)^T$. The guided modes are the solutions with separated variables to $\text{div}(u) + \rho \omega^2 u = 0$ in $W$ with boundary condition $\sigma(u)\nu = 0$ on $\Gamma$. They are given for $n \in \mathbb{N}$ by

$$(X_n^\pm(x), Y_n^\pm(x)) = (\pm\mathcal{X}_n(x_S), \mathcal{Y}_n(x_S)) e^{\pm i\beta_n x_3},$$

with $(\mathcal{X}_n, \mathcal{Y}_m)_\Sigma = \delta_{mn}$, where $(\cdot, \cdot)_\Sigma$ is a scalar product over $L^2(\Sigma)$ without complex conjugation. For a given frequency $\omega$, $\beta_n$ is real for only a finite number $P$ of guided modes, which are named propagating modes. The other ones are either inhomogeneous or evanescent and are not taken into account here. The assumption is then made that any elastic field, written in the
The scattered field \( u^s_n \) (and its \( Y \) extension \( Y^s_n \)) associated to the incident propagating mode \( u^i_n \) is solution of the following forward problem for a given frequency \( \omega \):
\[
\begin{aligned}
\text{div} \sigma(u^s_n) + \rho \omega^2 u^s_n &= 0 \quad \text{in} \quad W \setminus D, \\
\sigma(u^s_n) \nu &= g \quad \text{on} \quad \Gamma_d, \\
\sigma(u^s_n) \nu &= 0 \quad \text{on} \quad \Gamma_0, \\
u^s_n &= -u^i_n \quad \text{on} \quad \partial D, \\
\end{aligned}
\]
with (RC) a radiation condition. The data in this case are the components of one reflection block of the scattering matrix \( S \), namely the projections \( s^i_{mn} \) along the \( X_n \) on the section \( \Sigma - R \) of the scattered fields \( Y^s_n \), the number of lines and columns being limited to \( P \). The LSM consists in solving the following system for all sampling points \( z = (z_s, z_3) \):
\[
\sum_{n=0}^{P-1} U^f_{mn} h_n = e^{i\beta_n(R+z_3)} Y_{m}(z_3)p,
\]
with \( m = 0, \ldots, P - 1 \), where \( U = SK \), \( K \) is the \( P \times P \) diagonal matrix the components of which are \( e^{i\beta_n R/2i\beta_n} \). \( -R \) is the \( x_3 \) coordinate of the section \( \Sigma - R \) and \( p \) is a polarisation parameter. If, roughly speaking, a solution \( (h_0, \ldots, h_{P-1}) \), is found, then \( z \in D \) according to a classic result related to the LSM [2].

3 The case of surface sources and measurements

The method shown above needs data within the waveguide, which is not realistic in the context of Non Destructive Evaluation. We hence consider sources and measurements on \( \Gamma_d \), for which the diffraction problem satisfied by the total field \( u \) is, for a given source \( g \):
\[
\begin{aligned}
\text{div} \sigma(u) + \rho \omega^2 u &= 0 \quad \text{in} \quad W \setminus D, \\
\sigma(u) \nu &= g \quad \text{on} \quad \Gamma_d, \\
\sigma(u) \nu &= 0 \quad \text{on} \quad \Gamma_0, \\
u &= 0 \quad \text{on} \quad \partial D, \\
\end{aligned}
\]
The corresponding scattered field \( u^s \) is \( u - u^i \), where \( u^i \) solves the same problem (1) as \( u \) in \( W \) without the boundary condition \( u = 0 \) on \( \partial D \). The data are the components of a matrix \( M \) of general term defined by a single component of the scattered fields measured at points \( (d, x_j) \leq s \leq M \) for all considered sources. The measurement matrix \( M \) is related to the LSM matrix \( U \) by the relationship \( M = -RUE^T \), where \( R \) and \( E \) are some reception and emission matrices. Inverting this system enables to compute \( U \) and then to apply the modal LSM as in section 2.

The most straightforward acquisition setup is then to use individual sensors as sources, that is \( f(x) = g(x-x_i)\chi(\omega) \), leading to a poor insonification of the region of interest. The corresponding data are denoted \( \tilde{M} \). Another possibility as already mentioned is to use various time delays between all sources for each acquisition, that is \( f(x) = \sum_{n=1}^{M} g(x - x_n)\chi(\omega)e^{i(M-n)\tau_\omega} \).

The corresponding data are denoted \( \tilde{M} \). The two data are linked by \( \tilde{M} = MV \), where \( V \) is a Vandermonde Matrix of general coefficient \( e^{i(M-n)\tau_\omega} \). It is then possible to analyze the condition number of \( V \) as to ensure the best choice of delays \( \tau_\omega \).

![Figure 1: Imaging for simulated data corresponding to successive single sensor emissions (top) and for phased array data (bottom) with 64 sensors (log scale).]

References

Identification of a local perturbation in unknown periodic layers

Yosra BOUKARI1, Housssem HADDAR2, Nouha JENHANI1,*

1ENIT-LAMSIN, University of Tunis El Manar, Tunis, Tunisia
2INRIA, ENSTA Paris Tech (UMA), Institut Polytechnique de Paris, Palaiseau, France

*Email: nouha.jenhani@enit.utm.tn

Abstract

We revisit the differential sampling method introduced in [1] for the identification of a local perturbation in unknown periodic layers. We provide a theoretical justification of the method that avoids assuming that the local perturbation is also periodic. Our theoretical framework uses functional spaces with continuous dependence with respect to the Floquet-Bloch variable. The corner stone of the analysis is the justification of the Generalized Linear Sampling Method (GLSM) in this setting, which is the main topic presented here.

Keywords: inverse problem, Periodic layers, Floquet-Bloch Transform, domain reconstruction

1 Introduction

We consider in this work the inverse scattering problem for the reconstruction of a local perturbation in unknown periodic layers from near field measurements. This considered problem has connections with many practical applications, such as non-destructive testing of photonic structures, antenna arrays... It has motivated many research works over the recent years [1,2]. The presence of the perturbation does not allow us to reduce the problem to one-period cell, and this is what makes our problem more challenging since we are obliged to treat this problem in an unbounded band.

The GLSM Method was applied in similar setting of problem in [1] by adding a technical hypothesis on the distribution of the defect, they assumed that the defect is itself distributed periodically with a longer period, which allows them to reduce the problem to a larger and bounded domain. Then, in this work, and inspired by [2,3], we propose to get rid of this assumption and to work on the whole unbounded domain.

2 Setting of the direct problem

Let $U_0$ be the upper half-space $\mathbb{R} \times \mathbb{R}_+$. We denote by $D^p$ the periodic unbounded domain included in $\Omega^R := \mathbb{R} \times [0, R]$ delimited by $\Gamma^0 := \mathbb{R} \times \{0\}$ and $\Gamma^R := \mathbb{R} \times \{R\}$, with $R \geq R_0 > 0$ as shown in Figure 1. We consider $D := D^p \cup \tilde{D}$ where $\tilde{D}$ is a bounded domain included in $\Omega^R := [0, 2\pi] \times [0, R]$. We assume that the complement of $D$ is connected.

$$
\text{Figure 1: Sketch of the domain}
$$

Let $n \in L^\infty(U_0)$ be the refraction index verifying $n = n_p$ outside $\tilde{D}$, where $n_p \in L^\infty(U_0)$ with positive imaginary part, $2\pi$-periodic with respect to the first component $x_1$ such that $n_p = 1$ outside $D^p$. Consider an incident field $v \in L^2(D)$, the direct problem is to find the scattered field $w \in H^2_\text{loc}(U_0)$ verifying

$$
(\mathcal{P}) \left\{ \begin{array}{ll}
\Delta w + k^2 n w = k^2 (1 - n) v & \text{in } U_0 \\
 w = 0 & \text{on } \Gamma^0
\end{array} \right.
$$

and the angular spectrum representation

$$
w(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{i x_1 \xi + i \sqrt{k^2 - |\xi|^2} (x_2 - R)} \tilde{w}(|\xi|, R) d\xi
$$

for $x_2 > R$ as a radiation condition, where $\tilde{w}$ is the Fourier transform of the trace of $w$ on $\Gamma^R$.

For $s \in \mathbb{R}$, we denote by $H^s_\xi(\Omega^R)$ the Sobolev space of the $\xi$-quasi-periodic functions [1], and defining for $\phi \in C^0_\text{loc}(\Omega^R)$ the Horizontal Bloch-Floquet transform as the following for $\xi \in I = [0, 1]$

$$
\mathcal{J}_R \phi(\xi, x_1, x_2) = \sum_{j \in \mathbb{Z}} \phi(x_1 + 2\pi j, x_2) e^{-i 2\pi \xi j}
$$

which is an isomorphism between $H^s(\Omega^R)$ and $L^2(I, H^s_\xi(\Omega^R))$. We also define

$$
\tilde{H}^s(\Omega^R) := \{ u \in H^s(\Omega^R), \mathcal{J}_R u \in C^0_\text{loc}(I, H^s_\xi(\Omega^R)) \}
$$

and similarly for $H^s(\Gamma^R)$. For the sake of studying the inverse problem, for fixed $\xi_0 \in I$, we consider $v_{\xi_0} \in L^2_\text{loc}(D^p)$ and we rewrite the solution of $(\mathcal{P})$ seeking $w_{\xi_0} \in L^2_\text{loc}(U_0)$ solution of

$$
\Delta w_{\xi_0} + k^2 n w_{\xi_0} = k^2 (1 - n) v_{\xi_0} \text{ in } U_0,
$$
which is decomposed as \( w_{\xi_0} := w^p_{\xi_0} + \tilde{w}_{\xi_0} \), with \( w^p_{\xi_0} \in H^1_{\xi_0}(\Omega_R^0) \) verifying

\[
\Delta w^p_{\xi_0} + k^2 n_p w^p_{\xi_0} = k^2(1 - n_p)v_{\xi_0} \text{ in } \Omega_R^0
\]

and \( \tilde{w}_{\xi_0} \in \tilde{H}^1(\Omega_R) \) satisfying

\[
\Delta \tilde{w}_{\xi_0} + k^2 n \tilde{w}_{\xi_0} = k^2(n_p - n)(v_{\xi_0} + w^p_{\xi_0}) \text{ in } \Omega_R
\]

where both \( w^p_{\xi_0} \) and \( \tilde{w}_{\xi_0} \) satisfy homogeneous Dirichlet boundary conditions on \( \Gamma_0^R \) and some appropriate radiation conditions (for instance, condition (2) for \( \tilde{w}_{\xi_0} \)).

3 Setting of the inverse problem

Our inverse problem consists in reconstructing \( D \) having the measurements \( u^*(x, y) \) for all \( x, y \in \Gamma_R^0 \), where \( u^*(\cdot, \cdot) \) is the scattered field solution of \( (P) \) with \( v = \Phi(\cdot, y) \) the fundamental solution for the Dirichlet half space problem. We notice that for defining this solution, we need the imaginary part of \( n_p \) to be positive (at least in a subdomain of \( \Omega_R^0 \cap D^p \)). We introduce the near field operator \( N : \tilde{L}^2(\Gamma_R) \rightarrow \tilde{L}^2(\Gamma_R) \)

\[
Ng = \int_{\Gamma_R} u^*(x, y)g(y)ds(y)
\]

We shall explain how the positivity assumption on \( n_p \) allows us to define this operator. In fact the imaging procedure does not require all of \( N \) but only the Floquet-Bloch transform of \( N \) evaluated in few well chosen Floquet-Bloch variables. Let \( \xi_0 \in I \) be fixed and define \( u^p_{\xi_0}(\cdot, y) = w_{\xi_0} \) for \( v_{\xi_0} = \Phi_0(y, \xi) \) where \( \Phi_0(x, y) = J_{\xi_0}\Phi(\cdot, y)(\xi_0, x) \).

Using the decomposition \( w_{\xi_0} = w^p_{\xi_0} + \tilde{w}_{\xi_0} \) we decompose \( u^p_{\xi_0}(\cdot, y) = u^p_{\xi_0} + \tilde{u}_{\xi_0}(\cdot, y) \) and define two operators form \( \tilde{L}^2_{\xi_0}(\Gamma_R^0) \) into itself

\[
N^p_{\xi_0}g_{\xi_0} = \int_{\Gamma_R} u^p_{\xi_0}(x, y)g_{\xi_0}(y)ds(y)
\]

\[
\tilde{N}_{\xi_0}g_{\xi_0} = \int_{\Gamma_R} \tilde{u}_{\xi_0}^{\xi_0}(\xi, y)g_{\xi_0}(y)ds(y)
\]

These operators can be formally constructed using the operator \( N \) since one can prove that

\[
Ng = \int_I \int_{\Gamma_R} u^p_{\xi}(\cdot, \cdot)J_{\xi_0}g(\xi, y)ds(y)
\]

Using these operators we define the norm

\[
I_{\xi_0}(g_{\xi_0}) = ||N^p_{\xi_0}g_{\xi_0}|| + ||\tilde{N}_{\xi_0}g_{\xi_0}||
\]

We now explain how one can use the GLSM to identify \( D \) with either the operator \( N \) or its Floquet-Bloch transform. The simplest assumptions for which the following theorems hold are when \( D \cap D^p = \emptyset \), \((1 - n_p)\) and \((n_p - n)\) have fixed sign and definite real parts and negative imaginary parts on \( D^p \) and \( D \) respectively. We introduce the functional \( J_{\alpha_{\xi_0}}(\phi, \cdot) : \tilde{L}^2(\Gamma_R^0) \rightarrow \mathbb{R} \)

\[
J_{\alpha}(\phi, g) := \alpha I(g) + \|N_{\alpha}g - g\|^2,
\]

where \( I(g) := \sup_{g \in \Gamma} I_{\xi_0}(J_{\xi_0}g(\xi, \cdot)) \). We denote by \( J_{\alpha}(\cdot, \phi) = \inf_{g} J_{\alpha}(\phi, g) \).

**Theorem 1** Let \( c(\alpha) > 0 \) verifying \( \frac{c(\alpha)}{\alpha} \rightarrow 0 \) as \( \alpha \rightarrow 0 \) consider \( z \in \Omega_R^0 \), and let \( g^a \in \tilde{L}^2(\Gamma_R^0) \) such that

\[
J_{\alpha}(\Phi(\cdot, z), g^a(\cdot)) \leq J_{\alpha}(\Phi(\cdot, z) + c(\alpha))
\]

then \( z \in D \iff \lim_{\alpha \rightarrow 0} I(g^a(\cdot)) < \infty \).

The second theorem allows to reconstruct \( D \cap \Omega_R^0 \) using only one Floquet-Bloch mode by minimizing the functional \( J_{\alpha_0} : \tilde{L}^2_{\xi_0}(\Gamma_R^0) \rightarrow \mathbb{R} \)

\[
J_{\alpha_{\xi_0}}(\phi, g_{\xi_0}) = \alpha I_{\xi_0}(g_{\xi_0}) + \|\{N^p_{\xi_0}g_{\xi_0} + \tilde{N}_{\xi_0}g_{\xi_0} - \phi\|^2,
\]

We denote by \( J_{\alpha_{\xi_0}}(\phi) = \inf_{g_{\xi_0}} J_{\alpha_{\xi_0}}(\phi, g_{\xi_0}) \).

**Theorem 2** Let \( c(\alpha) > 0 \) verifying \( \frac{c(\alpha)}{\alpha} \rightarrow 0 \) as \( \alpha \rightarrow 0 \) consider \( z \in \Omega_R^0 \), and let \( g^a_{\xi_0} \in \tilde{L}^2_{\xi_0}(\Gamma_R^0) \) such that

\[
J_{\alpha}(\Phi_{0\xi}(\cdot, z), g^a_{\xi_0}(\cdot)) \leq J_{\alpha}(\Phi_{0\xi}(\cdot, z) + c(\alpha))
\]

then \( z \in D \cap \Omega_R^0 \iff \lim_{\alpha \rightarrow 0} I_{\xi_0}(g^a_{\xi_0}(\cdot)) < \infty \).

Based on Theorem 2 applied to integer multiples of \( \xi_0 \), we shall explain how one can design an indicator function that allows to directly reconstruct \( D \) using a similar differential indicator function as in [1].

**References**


The Time Domain Linear Sampling Method for Maxwell’s equations

Timo Lähivaara1, Peter Monk2,∗, Virginia Selgas3

1Department of Applied Physics, University of Eastern Finland, 70211 Kuopio, Finland
2Mathematical Sciences, University of Delaware, Newark DE 19716, USA
3Departamento de Matemáticas, Universidad de Oviedo, 33203 Gijón, Spain

∗Email: monk@udel.edu

Abstract

We investigate the use of the Time Domain Linear Sampling Method (TD-LSM) for determining the shape of a scatterer using electromagnetic waves. Assuming that the scatterer is impenetrable with an impedance boundary condition, we use the Fourier-Laplace transform approach to justify the TD-LSM. We provide numerical results for the impedance boundary condition, for a perfectly conducting obstacle, and for a penetrable body. The latter case cannot be analyzed by the Fourier-Laplace approach, yet still shows good reconstruction quality.

Keywords: Inverse problem, electromagnetism, impedance, linear sampling, time domain.

1 Introduction

The Time Domain Linear Sampling Method (TD-LSM) is an extension of the original frequency domain Linear Sampling Method to the time domain. Previous tests with the acoustic wave equation have shown that the method can be applied with the sound soft or impedance boundary conditions, as well as for penetrable objects. It can also be used with less source and measurement points than for a single frequency linear sampling method [2,3].

We shall describe an extension of the TD-LSM method to the time dependent Maxwell system governing scattering from an impenetrable scatterer with an impedance boundary condition [4]. We prove that the usual theorems underlying the TD-LSM hold in this case, and provide numerical examples of the method. It is interesting to note that current proofs based on the Fourier-Laplace transform cannot be used for the penetrable case [1], even though we shall give numerical results that show that the method does perform as expected in this case.

2 The forward problem

Given a bounded Lipschitz domain \( \Omega \subset \mathbb{R}^3 \) with unit outward normal \( \nu \) on \( \Gamma = \partial \Omega \), and setting \( \Omega^c = \mathbb{R} \setminus \overline{\Omega} \), the electromagnetic field \((\mathcal{E}, \mathcal{H})\) satisfies

\[
\begin{align*}
  c_0^{-1} \partial_t \mathcal{E} - \text{curl} \mathcal{H} &= 0 \quad \text{in } \Omega^c \quad \text{for } t > 0, \\
  c_0^{-1} \partial_t \mathcal{H} + \text{curl} \mathcal{E} &= 0 \quad \text{in } \Omega^c \quad \text{for } t > 0,
\end{align*}
\]

where \( c_0 \) is the speed of light. The field is subject to the initial conditions

\[
\mathcal{E} = \mathcal{E}_i = 0 \quad \text{for } t = 0 \quad \text{in } \Omega^c,
\]

and the impedance boundary condition

\[
\mathcal{H} \times \nu + \Lambda \mathcal{E}_T = - (\mathcal{H}^i \times \nu + \Lambda \mathcal{E}_T^i),
\]

on \( \Gamma \) for \( t > 0 \). Here the subscript \( T \) denotes the tangential trace here taken on \( \Gamma \), and \( \Lambda > 0 \) is the impedance constant. The incident field \( \mathcal{E}^i \) is given by a regularized magnetic dipole situated at \( y \in \mathbb{R}^3 \) with polarization \( p \in \mathbb{R}^3 \):

\[
\mathcal{E}^i(x, t; y, p) = -p \times \nabla_x \chi(t - c_0^{-1} |x - y|, t).
\]

Here

\[
\chi(t - c_0^{-1} |x|) = \frac{\chi(t - c_0^{-1} |x|)}{4\pi |x|}
\]

and \( \chi \in C^\infty_0((0, \infty)) \) is a smooth function of time. We prove that the above problem has a unique solution, \( \mathcal{E} := \mathcal{E}(x, t; y, p) \) for \( t > 0 \) and note that \( \mathcal{E} \) is linear in \( p \).

3 The inverse problem

We assume the existence of a surface \( \Sigma \) containing \( \Omega \) in its interior. Then the inverse problem we wish to solve is to reconstruct the boundary of the scatterer \( \Gamma \) from a knowledge of \( \mathcal{E}(x, t; y, p) \) for \( x, y \in \Sigma, t > 0 \) and \( p \in \mathbb{R}^3 \). To do this we define the near field operator applied to a suitable tangential space-time vector function \( f \) by

\[
(\mathcal{N}_\chi f)(x, t) = \int_{\mathbb{R}} \int_{\Sigma} \mathcal{E}_T(x, t - \tau; y, f(y, \tau)) dA_y d\tau
\]
for \((x, t) \in \Sigma \times \mathbb{R}\), where the subscript \(T\) refers to the tangential trace here taken on \(\Sigma\).

Using the near field operator, we seek an approximate solution \(g = g(\cdot, \cdot ; z, p_x, \tau_\kappa)\) in an appropriate weighted space-time Sobolev space of the near field equation

\[
(N_T g(\cdot, \cdot ; z, p_x, \tau_\kappa)) (x, t) = E_T^f(x, t - \tau; z, q)
\]

for \((x, t) \in \Sigma \times \mathbb{R}\). Here \(\tau\) is a fixed time translation parameter. This is an ill-posed problem, but we can prove that an approximate solution exists. We also show a usual version of the theorem of blowup of a suitable norm of \(g\) when \(z \in \Omega^c\) [4].

4 Numerical results

We choose a Ricker wavelet for \(\chi\):

\[
\chi(t) = -\left(1 + 2a(t - t_0)^2\right) \exp\left(a(t - t_0)^2\right),
\]

where \(a = -(\pi f_0)^2\), is used as the source modulation function for the incident field. Here \(f_0\) is the peak frequency of the source, and \(t_0 = 1.2/f_0\) is the time delay. For the example below, we choose \(f_0 = 1\), and use 96 measurements and 54 sources on this surface. The surface \(\Sigma\) is the boundary of the cube \([-4, 4]^3\) and we use 96 measurement points and 54 source points on this surface. Using a nodal discontinuous Galerkin scheme, we compute the solution of the forward problem and hence the near field operator.

By solving a discrete analogue of the near field equation using Tikhonov regularization for \(z\) in a \(41 \times 41 \times 41\) grid in the search domain \([-1.5, 1.5]^3\), we can graph isosurfaces of a suitable norm of \(g\) and hence visualize the scatterer. Preliminary results for two cubes are shown in Fig. 1. We show results for an impedance boundary condition with \(\Lambda = \sqrt{2}\), a perfectly electrically conducting boundary condition and a penetrable object (with \(\epsilon_r = 2\) in \(\Omega\)).

5 Conclusion

Our preliminary results show that the TD-LSM can be used to identify the shape of scatterers with a variety of boundary conditions. Future work will include a detailed study of the Maxwell TD-LSM with different source and measurement geometries, and more complex scatterers.

Acknowledgements

T. Lahiväara is supported by the Academy of Finland (the Finnish Centre of Excellence of Inverse Modeling and Imaging) and project 321761. P. Monk is partially supported by the US AFOSR under grant number FA9550-20-1-0024. V. Selgas is partially supported by the project MTM2017-87162-P of MINECO.

References


Wigner-Weyl description of radiative processes in correlated disordered semiconductor alloys

Jean-Philippe Banon$^{1,*}$, Pierre Pelletier$^{1}$, Claude Weisbuch$^{1}$, Svitlana Mayboroda$^{2}$, Marcel Filoche$^{1}$

$^{1}$Laboratoire de Physique de la Matière Condensée, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France
$^{2}$School of Mathematics, University of Minnesota, Minneapolis, Minnesota 55455, USA
$^*$Email: jean-philippe.banon@polytechnique.edu

Abstract

We present a model for light absorption and luminescence in correlated semiconductor alloys based on an approach in phase space combined with the localization landscape. The model was recently shown to give reliable results at low computational cost for uncorrelated disordered InGaN alloys when compared with a model based on the direct solution of the Schrödinger equation. We study the influence of compositional correlation on the absorption and spontaneous emission spectra.

Keywords: Disordered semiconductor alloys; phase space representation;

Introduction

Light absorption and emission measurements are commonly used to study the electronic and optoelectronic properties of semiconductor alloys, and to characterize devices made of heterostructures of such alloys such as LEDs. The absorption and luminescence spectra are in general affected by several processes: thermal processes, electric fields, Coulomb interaction, and alloy disorder. Alloy disorder corresponds to the random configuration of atoms of different species on the crystal lattice, and consequently, breaks the periodic symmetry of the ion lattice potential. In order to understand and predict the effect of alloy disorder on the optoelectronic properties of alloys and devices, we have developed a model of light absorption [1] and spontaneous emission based on a formulation in phase space (also called the Wigner-Weyl approach) for the electronic states and on results from the localization landscape theory [2,3]. The derived model is simple, computationally efficient and was shown to yield good approximations when compared with eigenstate-based computations. In this contribution, we apply the Wigner-Weyl-localization-landscape model to the case of light absorption and emission by correlated InGaN alloys.

1 Correlated alloys

The electronic properties of the disordered InGaN alloy are modeled in the framework of the effective mass approximation. The energy eigenstates of the electrons near the edges of the valence and conduction bands are sought as products of a Bloch-lattice-periodic cell function and of an envelope function satisfying an effective Schrödinger equation. The effective masses and potentials appearing in the conduction and valence effective Schrödinger equations are obtained via a continuous local indium concentration which is a regularization of the discrete atomic indium configuration on the InGaN wurtzite lattice. The indium ions are drawn randomly on the cation sites following a Bernoulli law either independently (uncorrelated alloy) or with some correlation by drawing them preferentially close to already present indium ions following the model proposed by Di Vito and co-workers [4] (a fraction $p_u$ of the In ions being drawn first without correlation).

2 Radiative processes in phase space

In Ref. [1] we have derived a model for the absorption coefficient which is based on a phase space approach and which draws inspiration from the modified Weyl law based on the localization landscape for the integrated density of states [3]. In the dipole approximation, the absorption coefficient was shown to be proportional to

$$\alpha(\omega) \propto \int \int \int D^{(c)}(r,k,\epsilon + \hbar\omega) \times D^{(v)}(r,k,\epsilon) \frac{d^3r \, d^3k}{(2\pi)^3},$$

(1)
where $D^{(c,v)}(r, k, E)$ are densities of states in phase space, whose definitions are given in Ref. [1]. A similar expression can be obtained for the spontaneous emission spectrum. Approximations for the densities of states in phase space can then be derived using the localization landscape, resulting in the following closed form expression for the absorption coefficient [1]

$$
\alpha(\omega) = K(\omega) \int_{\Omega} \left[ \frac{2m_r(r)}{\hbar^2} \right]^{3/2} \times \left( \hbar \omega - E_g^{(\text{eff})}(r) \right)^{1/2} \mathrm{d}^3r .
$$

(2)

Here $K(\omega)$ is a known material dependent function of the light angular frequency $\omega$, $m_r$ is the local reduced effective mass and $E_g^{(\text{eff})}$ is an effective band gap profile derived from the localization landscape theory. The effective band gap profile can be viewed as a smoothed version of the original disordered band gap profile. This smoothed version accounts for the typical length scale of the lowest energy eigenstates and their energy without having to resort to a diagonalization of the Hamiltonians. We can also derive an approximation of the absorbed power density which we show to be directly proportional to the integrand in Eq. (2). This allows for an intuitive physical interpretation. For a given value of $\hbar \omega$ the electromagnetic power is deposited in the volume defined by $\hbar \omega - E_g^{(\text{eff})} > 0$, and thus contributes to the absorption coefficient at frequency $\omega$. As $\hbar \omega$ increases the contributing volume increases to finally fill the whole space when $\hbar \omega > \text{max } E_g^{(\text{eff})}$.

3 Results

Figure 1 displays absorption coefficient spectra obtained with the Wigner-Weyl-localization-landscape model [Eq. (2)] for uncorrelated alloy, and correlated alloys. As the degree of correlation increases ($p_u$ decreases) the low energy absorption tail exhibits a broadening. The broadening of the absorption tail is attributed to the lowering of the conduction and valence potentials, and hence, of the energies of the eigenstates close to the band edges. This is captured by the effective band gap profile in our model. Figure 1 shows 3D maps of the absorbed power density for a fixed photon energy $\hbar \omega = 3$ eV and for the three values of $p_u$ studied in Fig. 1. We observe that as the correlation length increases, the volume contributing to the absorption increases and so does the absorbed power. The typical volumes in which the power density is localized correspond to In-rich regions in which the local band gap is lowered.

4 Acknowledgments

J.-P. B. P. and M. F. are supported by the Simons foundation grant 601944. S. M. is supported by the NSF RAISE-TAQS grant DMS-1839077 and the Simons foundation grant 563916. C. W. is supported by the Simons foundation grant 601944. S. M. is supported by the NSF RAISE-TAQS grant DMS-1839077.

References


Modelling and validating average waves in random particulate materials

Artur Gower1,∗, Gerhard Kristensson2, Stuart Hawkins3

1Department of Mechanical Engineering, University of Sheffield, Sheffield, UK
2Department of Electrical and Information Technology, Lund University, Lund, Sweden
3Department of Mathematics and Statistics, Macquarie University, New South Wales, Australia

*Email: arturgower@gmail.com

Abstract

When you measure the scattered field from a material filled with randomly placed particles, you will have to perform the measurement many times, and then take the average, to get a repeatable result. How then do you relate this average measurement to the particles? Here we show how to mathematical model this average scattering, and present results on validating these models against heavier Monte Carlo simulations. The recent breakthrough that has enabled us to achieve a broadband numerical validation of the theory is that we now have rigorous models for scattering from a sphere filled with particles. A sphere, in contrast to a plate or halfspace, filled with particles can be easily simulated with a Monte Carlo approach.

Keywords: multiple scattering, random media, particulate. pair correlation

1 Introduction

Detailed derivations are given in [1]. Below we give a brief overview. To define the average scattered wave from a random particulate, we first need to define the scattered wave from just one configuration of particles. Figure 1 illustrates a scattered wave from one configuration, and the average over all particle configurations.

For a point \( r \), outside of all particles, we can write the total field \( u(r) \) as a sum of the incident wave \( u_{in}(r) \) and all scattered waves:

\[
\begin{align*}
\text{u}(r) &= \text{u}_{in}(r) + \text{u}_{sc}(r), \\
\text{u}_{sc}(r) &= \sum_{i=1}^{J} \sum_{n} f_{n}^{i} u_{n}(kr - kr_{i}),
\end{align*}
\]

where \( r_{i} \) is a vector pointing to the centre of the \( i \)-th particle, we assumed \( |r - r_{i}| > a \) for \( i = 1, 2, \ldots, J \), with \( a \) being the particle radius, the \( u_{n} \) are the basis of outgoing spherical waves, and the coefficients \( f_{n}^{i} \) can be determined by applying the boundary conditions on all particles.

![Figure 1: Scattering of an incident plane-wave from a) a sample of \( J = 330 \) particles, and b) the ensemble average of the scattered field over all possible particle positions. Taken with permission from [1].](image)

where \( \mathcal{R} \) is the region where the particle centres are contained, \( p(r_{1}) \) is the probability of finding a particle centred at \( r_{1} \), when the position of all other particles is not known. The \( \langle f_{n} \rangle(r_{1}) \) are determined by ensemble averaging the boundary conditions (not shown above), which results in

\[
\langle u_{sc}(r) \rangle = J \sum_{n} \int_{\mathcal{R}} \langle f_{n}(r_{1}) \rangle u_{n}(kr - kr_{1}) p(r_{1}) \, dr_{1},
\]

where \( \langle f_{n}(r_{1}) \rangle = \sum_{n} \int_{\mathcal{R}} u_{n}(kr_{1} - kr_{2}) g(r_{1}, r_{2}) \, dr_{2}, \)

where \( U_{n}(kr_{1}) \) is a translation matrices, composed of known special functions, and \( G_{n}(r_{1}) \)

depends on the incident wave. The \( g(r_{1}, r_{2}) = \frac{p(r_{1}) p(r_{2})}{p(r_{1}) p(r_{2})} \) is the pair-correlation , and the \( T_{n} \) is the T-matrix which describes scattering from just one particle. If \( g(r_{1}, r_{2}) \) and \( T_{n} \) were known, then the aim is use the above to solve for \( \langle f_{n} \rangle \).

The above equation is exact, with no approximations. It is similar to Dyson’s equation, which is typically used by the physics community.
1.1 Statistical assumptions

To solve (3) it is typical to make some assumption about \( g(r_1, r_2) \), and how \( \langle f_{n'} \rangle(r_2, r_1) \) is related to \( \langle f_n \rangle(r_2) \). The simplest assumptions are

\[
g(r_2; r_1) \approx \begin{cases} 
1 & \text{for } |r_1 - r_2| \geq a_{12}, \\
0 & \text{for } |r_1 - r_2| < a_{12},
\end{cases}
\]

and \( \langle f_n \rangle(r_2, r_1) \approx \langle f_{n'} \rangle(r_2) \) for \( |r_1 - r_2| \geq a_{12} \), which are called hole correction and the Quasi Crystalline Approximation. There are many different models for \( g(r_2; r_1) \) that represent clumped materials, or even particles on a lattice. For particles distributed randomly, according to a uniform probability density, a more accurate modal is called the Percus-Yevick pair-correlation.

We will discuss validating these assumptions, and how these lead to analytic solutions below.

2 Effective waves

A key development has been to show that (3), together with the statistical assumptions above, leads to two simpler equations

\[
\langle f_n \rangle(r_1) = \sum_{n'} \int_{\partial B} W_{nn'}(r_2) \langle f_{n'} \rangle(r_2 + r_1) dr_2
\]

\[
G_n(r_1) = \sum_{n'} \int_{\partial \mathcal{R}} B_{nn'}(r_1 - r_2) \langle f_{n'} \rangle(r_2) dr_2
\]

where \( B \) is a small ball depending only on the particle geometry, and \( W_{nn'} \) and \( B_{nn'} \) are known special functions. The first equation we call the ensemble wave equation, as it does not depend on the incident wave, or the geometry of the whole material \( \mathcal{R} \), and can specify completely the modes of \( \langle f_n \rangle(r_1) \). The second equation we call the ensemble boundary conditions, as it depends on the incident wave and material geometry, and is needed to specify the amplitude of the modes of \( \langle f_n \rangle(r_1) \).

With the equations above we can calculate the average scattering from a material (filled with a random particulate) of any geometry. In particular, we choose a sphere filled with particles, as this allows us to achieve something that has long been a goal: a robust and broad numerical validation of typical statistical assumptions, see Section 1.1. A sphere filled with a finite number of particles is far easier to numerically simulate. We also make use recent developments in numerical techniques to perform Monte Carlo simulations [2, 3].

For most particle volume fractions, the results are similar to Figure 2. That is, the effective waves solution is equivalent to a direct numerical solution of (3), and the heavier Monte Carlo simulations agree well when using the Percus-Yevick approximation to calculate the pair-correlation. These results give confidence that the analytic methods shown here could form the basis for quantitative sensing of particulate materials.

![Figure 2](image-url)

Figure 2: Shows different methods to calculate the average scattering cross section from a sphere, filled a 15% particle volume fraction, for different incident wave lengths. Monte-Carlo simulates hundreds of different particle configurations explicitly. Eff. wave uses the Effective wave, and Integral uses a numerical method to solve equation (3). HC refers to using hole correction, shown in Section 1.1, where PY refers to the pair-correlation called Percus-Yevick.

References


Modeling scattering from a random thin coating: asymptotic model and numerical simulations

Amandine BOUCART\textsuperscript{1,*}, Sonia FLISS\textsuperscript{2}, Laure GIOVANGIGLIE\textsuperscript{1}, Bruno STUPFEL\textsuperscript{1}

\textsuperscript{1}CEA, CESTA, Le Barp, France
\textsuperscript{2}POEMS, UMA, ENSTA-Paris, Institut Polytechnique de Paris, Palaiseau, France
Email: amandine.boucart@ensta-paris.fr

Abstract
Using an asymptotic analysis, we propose an effective model for solving a time harmonic electromagnetic scattering problem of an object covered with a very thin coating of randomly distributed perfectly conductive particles. To obtain the coefficients of the model, we need to solve corrector problems set in a half space with a layer of randomly distributed rescaled particles. In this paper we explain how to compute the effective model and show numerical validations.

Keywords: Random media, asymptotic analysis, stochastic homogenization, Monte Carlo method.

1 Introduction
We consider a time harmonic electromagnetic scattering problem of an object covered with a very thin coating of randomly distributed perfectly conductive particles. We want to quantify the effect of this coating on the radar cross-section, i.e. the energy reflected in a specific direction. Since the particle size, distance and coating size are of the same order and all small compared with the incident wavelength \( \lambda \), the numerical solution of Maxwell’s equations becomes extremely costly in terms of memory size and computation time. In addition, we do not have access to the exact distribution particles a given object. To overcome these difficulties, we assume that the random particle distribution follows a given probability law. In this paper, we consider the 2D case where the structure is translationally invariant along the \( x_3 \) direction. Maxwell’s equations in TM or TE polarization are then reduced to the Helmholtz equation with Neumann or Dirichlet boundary condition on the particles. In this abstract, we focus on the first case.

2 Statement of the problem
We construct the thin layer as a collection of particles \( P^\varepsilon_n \) of size \( \varepsilon \ll \lambda \) distributed in the strip \( L^\varepsilon := \mathbb{R} \times [\varepsilon \delta, \varepsilon (\delta + h_L)] \), \( \delta > 0 \), \( h_L > 0 \), and spaced from each other by a minimal distance of \( \varepsilon \delta \). We consider that the particle distribution is stationary (the distribution law is the same at any point of \( L^\varepsilon \)), ergodic (spatially averaging on a large domain corresponds to averaging with respect to the randomness). Let us now consider the following problem

\[
\begin{align*}
- \Delta u^\varepsilon - k^2 u^\varepsilon &= 0 \text{ in } \mathbb{R} \times (\varepsilon H, +\infty) \\
\nabla u^\varepsilon \cdot \vec{n} + \gamma u^\varepsilon &= 0 \text{ on } \Sigma_0 := \{ x_2 = 0 \} \\
\nabla \cdot \vec{v}^\varepsilon &= 0 \text{ on } \Omega_0 \\
\vec{v}^\varepsilon - \vec{v}^1 &\text{ is outgoing}
\end{align*}
\]

with \( \vec{n} \) the outgoing unitary normal of \( \Omega^\varepsilon \), \( \mathcal{L} m(\gamma) > 0 \). Note that the impedance condition on \( \Sigma_0 \) models a multilayer object. By introducing an artificial surface \( \Sigma_{\varepsilon H} = \{ x_2 = \varepsilon H \} \) above the particles, we perform an asymptotic analysis of the solution \( u^\varepsilon \) and we derive the following effective model

\[
\begin{align*}
- \Delta v^\varepsilon - k^2 v^\varepsilon &= 0 \text{ in } \mathbb{R} \times (\varepsilon H, +\infty) \\
\nabla v^\varepsilon \cdot \vec{n} + \left( \gamma - \varepsilon a_0^{(2)} \right) v^\varepsilon &= 0 \text{ on } \Sigma_{\varepsilon H} \\
\nabla \cdot \vec{v}^\varepsilon &= 0 \text{ on } \Omega_{\varepsilon H} \\
\vec{v}^\varepsilon - \vec{v}^1 &\text{ is outgoing}
\end{align*}
\]

where the coefficients \( a_0^{(2)} \), \( a_1^{(2)} \) and \( a_2^{(2)} \) are deterministic and obtained from Laplace-type problems set in a half space with a layer of randomly distributed rescaled particles. Let us give an example of such a problem:

\[
\begin{align*}
- \Delta \phi^{(1)}_H &= 0 \text{ in } \Omega := \mathbb{R} \times \mathbb{R}_+ \setminus \cup_n \overline{P^1_n} \\
\nabla \phi^{(1)}_H \cdot \vec{n} &= 0 \text{ on } \Sigma_0 \\
\nabla \cdot \vec{\phi}^{(1)}_H &= -n_1 \text{ on } \Omega_0 \\

\end{align*}
\]
where $U_1^{(1)}$ is called a profile function and $a_2^{(2)}$ coefficient is given by
\[
a_2^{(2)} = \mathbb{E} \left[ 2 \int_{\Omega} \nabla_{y} U_1^{(1)} + \int_{\Omega} \chi_{\{y_2 \leq H\}} - \int_{\partial \Omega_1} U_1^{(1)} n_1 \right] =: \mathbb{E} \left[ F(U_1^{(1)}) \right]. \tag{4}
\]

### 3 Numerical method description

To simulate the random environment, we consider a Poisson point process for the center of the particles. We set a filling rate $\rho \in (0,1)$ and then the average density is given by $\nu = \rho \cdot \text{strip area}$. The number of particles in the strip follows the Poisson distribution with parameter $\nu$. Finally, we sample the centers uniformly in the strip. As in stochastic homogenization [1], we first penalize the profile problems by replacing, for example in (3), $-\Delta_y U_1^{(1)} = 0$ by $-\Delta_y U_1^{(1)} + \frac{1}{R} U_1^{(1)} = 0$ with $R > 0$. We then 1) truncate the domain in the $y_1$ direction ($y_1 \in (-T/2, T/2)$), 2) prescribe periodic conditions and 3) bound the domain in the $y_2$ direction by a DtN operator on a $\Sigma_L$ boundary
\[
\nabla_{y} U_1^{(1)} \cdot \vec{n} = -\frac{2\pi}{T} \sum_{m \in \mathbb{Z}} |m| \langle U_1^{(1)}, \phi_m \rangle_{L^2(\Sigma_L)} \phi_m(y_1), \tag{5}
\]

where $\phi_m(y_1) = \frac{1}{\sqrt{T}} e^{2\pi i m y_1}, \forall m \in \mathbb{Z}$. If $U_1^{(1)}_{T,R}(\omega)$ denotes such an approximated profile function, the coefficient given by (4) is then approximated by
\[
a_2^{(2)} \approx \lim_{T \to +\infty} \mathbb{E} \left[ F(U_1^{(1)}_{T,R}(\omega)) \right]. \tag{6}
\]

Figure 1(a) illustrates this convergence. We can also use the ergodicity and approximate the coefficient by
\[
a_2^{(2)} \approx \lim_{T \to +\infty} \mathbb{E} \left[ F(U_1^{(1)}_{T,R}(\omega)) \right]. \tag{7}
\]

To compute this $\mathbb{E} \left[ F(U_1^{(1)}_{T,R}(\omega)) \right]$, we use a Monte-Carlo method and consider $M$ independent and identically distributed samples:
\[
a_2^{(2)} \approx \lim_{T,M \to +\infty} \frac{1}{M} \sum_{m=1}^{M} F(U_1^{(1)}_{T,R}(\omega)). \tag{8}
\]

This technique is applied for $M = 100$ and $M = 500$ in Figure 1(b). Note that the convergence is achieved for smaller boxes $T$. As a consequence, it is interesting to play on the box size and the number of samples to accelerate the convergence.

To validate the method, we consider a scattering problem with an incident plane wave with angle $\theta = \pi/3$. Below are the real part of the reference solution and the effective solution, both obtained by a finite element discretization for $2\text{GHz}$, $\varepsilon = 10^{-4}$, $\gamma = k(1-i)$, $h_L = 10$ and $\rho = 0.4$.

![Figure 1: Convergence of $a_2^{(2)}$ w.r.t. $T$.](image1.png)

![Figure 2: Reference solution](image2.png)

![Figure 3: Effective solution](image3.png)

We plot below the difference between the reflection coefficient of those two solutions with respect to $\varepsilon$ for $\gamma = ik, T = 1500\varepsilon, \rho = 0.4$.

### References

Numerical Study on Spatial Evolution of Progressive Waves using Fully Nonlinear Numerical Wave Tank

Eun-Hong Min¹, WeonCheol Koo¹,*

¹Department of Naval Architecture and Ocean Engineering, Inha University, Incheon, Republic of Korea
*Email: wckoo@inha.ac.kr

Abstract

A spatial evolution by nonlinear wave-wave interaction was studied using the 2D FN-NWT technique which was based on boundary element method with Rankine panels. The present results were compared with previous experimental data for spatial evolution of Bi-chromatic waves, and the difference between fully nonlinear and linear calculation results was investigated. The nonlinear spatial evolution of traveling waves by wave-wave interaction was well realized through the fully nonlinear calculation, and it was in good agreement with the experimental results. The farther the wave propagated, the greater the difference between linear and nonlinear calculations. The spatial evolution of irregular waves was numerically analyzed.

Keywords: Bi-chromatic waves, Spatial evolution, Fully nonlinear numerical wave tank

1 Introduction

In general, a rogue wave is defined as a wave which height is greater than two times the significant wave height defined as the mean of the highest one third of waves occurring over a certain time period [1]. There are several reasons for the occurrence of sudden huge waves. One typical reason is that the extreme wave may occur by nonlinear interactions from various small waves as wave group. To simulate a spatial evolution of group waves, two-dimensional fully nonlinear potential flow numerical wave tank (2D-FN-NWT) technique was used, and this numerical model is based on boundary element method with constant Rankine panels. In addition, the mixed Eulerian-Lagrangian (MEL) method was applied for updating nonlinear free surface water particles in the time domain analysis. Bi-chromatic waves and irregular waves were numerically simulated, and linear and fully nonlinear calculation results of wave evolution by wave-wave interaction were compared.

2 Mathematical formulation

The computational domain is filled with incompressible, irrotational, and inviscid fluid in the 2D FN-NWT, so the governing equation can be Laplace equation using velocity potential(ϕ) and continuity equation satisfied in the fluid domain.

\[ \nabla^2 \phi = 0, \]  
\[ \alpha \phi_i = \iint_{\Omega} (G_{ij} \frac{\partial \phi_j}{\partial n} - \phi_j \frac{\partial G_{ij}}{\partial n}) ds \]  
\[ G_{ij} = -\frac{1}{2\pi} \ln R_{ij} \]  
\[ R_{ij} = \sqrt{(x_i - x_j)^2 + (z_i - z_j)^2} \]

where \( \alpha \) is a solid angle and it was set to 0.5 on the boundary of computational domain. \( \phi_i \) and \( \phi_j \) mean the velocity potential at the source \((x_j, z_j)\) and field \((x_i, z_i)\) points, respectively. For the free surface boundary condition, the full Lagrangian approach of MEL method, which expresses nodes that follow the motion of water particles on the free surface with velocity \( \vec{v} \) and \( \overrightarrow{\mathbf{v}} = \frac{\partial \phi}{\partial t} + \vec{\nabla} \cdot \vec{v} \), was applied (Eqs. (5) and (6)).

\[ \frac{\delta \eta}{\delta t} = \frac{\partial \phi}{\partial z}, \]  
\[ \frac{\delta \phi}{\delta t} = -g\eta + \frac{1}{2} |\nabla \phi|^2 \]

where \( g \) is gravitational acceleration, \( \rho \) is water density. An artificial damping zone was applied on the free surface near the end wall of fluid domain to prevent reflected waves due to the rigid end wall. The wave particle velocity profile was used as the incident wave boundary condition.

\[ \frac{\partial \phi}{\partial n} = \sum_{j=1}^{N} \left( -\frac{gA_j k_j \cosh[k_j(z + h)]}{\omega_j \cosh(k_j h)} \cos(k_j x - \omega_j t + \epsilon_j) \right) \]

where \( A_j, \omega_j, k, h \) and \( \epsilon_j \) denote wave amplitude, wave frequency, wave number, water depth, and random phase, respectively. Also, the impermeable boundary condition is applied to bottom and end wall.


3 Results and Discussion

Figure 1 compares the time series of traveling bi-chromatic wave elevations at two measurement points. Wave periods are set to \( T_1 = 1.9\text{s} \), \( T_2 = 2.1\text{s} \), and wave amplitude is \( A_1 = A_2 = 0.08\text{m} \). In the linear calculation, group waveforms generated from bi-chromatic waves were maintained and propagated. However, in the fully nonlinear calculation, the wave energy was concentrated within the group wave envelope as the generated group wave progresses. In addition, the difference between the phase angles of the linear result and the nonlinear result gradually increases as the wave propagates. The energy concentration and phase angle changes within the wave envelop, which can be seen in the nonlinear calculation results, were in good agreement with the previous experimental results [2].

\[
S(\omega) = \frac{5}{16} \omega^4 H_s^2 \frac{\omega^2}{\omega_p^2} \exp \left[ -\frac{5}{4} \left( \frac{\omega}{\omega_p} \right)^4 \right] \exp \left[ -\frac{(\omega - \omega_p)^2}{2\sigma^2} \right] 
\]

where the peak frequency was set to \( \omega_p = 3.14\text{rad/s} \), the significant wave height was set to \( H_s = 0.1336\text{m} \), the peak enhancement factor was set to \( \gamma = 3.3 \), \( \sigma = 0.07 \) for \( \omega \leq \omega_p \), and \( \sigma = 0.09 \) for \( \omega > \omega_p \), respectively. In the linear calculation, the shape of wave propagation was similar to the fully nonlinear result in the vicinity of the incident boundary (Fig. 2(a)). However, as the waves propagate, the linear results continue to maintain the initially formed waveform, but in the fully nonlinear calculation, wave energy was concentrated at a specific point similar to Figure 1, and the difference of phase angle between the two calculation results gradually increases.

4 Conclusions

The spatial evolution of wave groups by wave–wave interactions was simulated numerically using the 2D-FN-NWT technique. The fully nonlinear calculation results were in good agreement with the experimental data on the phase angle change and wave energy concentration within the wave envelope. The spatial evolution of irregular waves was numerically analyzed using the verified numerical model. As the wave propagated, the linear results kept the initially formed wave form, but in the fully nonlinear calculation, the wave energy was concentrated at a specific point and the phase angle difference between the two calculation results gradually increased.

Acknowledgment

This research is supported by the National Research Foundation of Korea, a basic research project in the field of science and engineering (NRF-2018R1D1A1B07040677)

References


Scattering of an Ostrovsky Wave Packet in a Delaminated Waveguide

Jagdeep Tamber1,∗, Matt Tranter1

1Department of Mathematical Sciences, Nottingham Trent University, NG11 8NS, United Kingdom
∗Email: N1039872@my.ntu.ac.uk

Abstract
Layered structures are highly dependant on the material and bonding between each solid waveguide. In this work we will analyse a two layered waveguide with a delamination in the centre and soft (imperfect) bonding either side of the centre. The lower layer of the waveguide is assumed to be significantly denser than the upper layer, leading to a system of Boussinesq-Klein-Gordon (BKG) and Boussinesq equations. Direct numerical modelling is difficult and so we will use a semi-analytical approach consisting of several matched asymptotic multiple-scale expansions, which leads to Ostrovsky equations in soft bonded regions and Korteweg-de Vries equations in the delaminated region. We will also discuss how the dispersion relation is used to determine the wave speed and hence classify the length of the delamination, in addition to changes in the amplitude of the wave packet. These results can provide a tool to control the integrity of layered structures.

Keywords: Boussinesq-Klein-Gordon equation; multiple-scales expansions; Ostrovsky wave packet.

1 Introduction
The discovery of solitons as localised stable structures [1] in combination with theoretical results of the propagation of long longitudinal bulk solitary waves in elastic waveguides [2] has provided a gateway to explore how the quality of bonding effects the integrity of a layered structure and recent experiment have confirmed the existence of solitons in layered waveguides [3].

In this work we will investigate a two layered bar with a initial delaminated region followed by delamination in the centre of soft bonding, where the material between the layers is distinctly different. The strain waves are described by Boussinesq-Klein-Gordon (BKG) equations in bonded regions and Boussinesq equations in the delaminated regions. A weakly nonlinear solution will be used to model the propagating waves in each section. Then we will compare a semi analytical solution, that makes use of the weakly-nonlinear solution, and a direct numerical solution.

Long waves propagate within these waveguides and the initial solitary wave undergoes a nonlinear steepening process, producing a wave packet consisting of a long wave envelope, through which shorter, faster solitary-like waves propagate [4]. This wave packet emerges as a solution of the Ostrovsky equation

\[ (u_t + \alpha uu_x + \beta u_{xxx})_x = \gamma u. \] (1)

The Ostrovsky equation was originally applied in the context of shallow internal and surface water waves as the effect of the Earth’s rotation was considered [5]. The envelope measures the amplitude, and the ratio of the carrier wavelength. The scattering of an Ostrovsky wave packet is present in the "soft" bonded region and generated from a solitary wave and the evolution of wave packets generated by an initial pulse has been thoroughly examined [6].

2 Weakly Nonlinear Solution
Consider the scattering of a long longitudinal strain solitary wave in a two layered bar with delamination in the centre as show in Figure 1.

Figure 1: Schematic of the bi-layer with initial small delaminated region followed by a delaminated region between two soft bonded regions.

The strain of the nonlinear wave propagating within the upper waveguide layer can be modelled by system of Boussinesq equations

\[ f_{tt}^{(i)} - f_{xx}^{(i)} = 2\varepsilon \left( -3 \left( f^{(i)} \right)_xx + f^{(i)}_{txx} \right), \] (2)
where \( i = 1, 3, \) and BKG equations
\[
\begin{align*}
    f_{tt}^{(j)} - f_{xx}^{(j)} &= 2\varepsilon \left( -3 \left( f^{(j)} \right)^2 \right)_{xx} + f_{tttt}^{(j)} - \gamma f^{(j)}, \\
    \end{align*}
\]
where \( j = 2, 4, \) with continuity conditions on the interface between the sections.

Substituting multiple-scale expansions into (3) and utilizing space averaging yields the following Ostrovsky equations
\[
\begin{align*}
    (T_X^{(j)} - 6T_{\xi}^{(j)} T^{(j)}_{\xi})_{\xi} &= \gamma T^{(j)}, \\
    (R_X^{(j)} - 6R_{\eta}^{(j)} R^{(j)}_{\eta})_{\eta} &= \gamma R^{(j)},
\end{align*}
\]
where \( T^{(j)}_X \) and \( R^{(j)}_X \) as the leading order transmitted and reflected waves respectively.

Similarly for (2) we get
\[
\begin{align*}
    T_X^{(i)} - 6T_{\xi}^{(i)} T^{(i)}_{\xi} &= 0, \\
    R_X^{(i)} - 6R_{\eta}^{(i)} R^{(i)}_{\eta} &= 0,
\end{align*}
\]
which are KdV equations, describing the leading order transmitted waves \( T_X^{(i)} \) and reflected waves \( R_X^{(i)} \).

3 Numerical Methods and Results

Numerically solving (2) - (3) directly using the finite difference method presented in [7] and comparing to the semi-analytical method gives the results outlined in Figure 2.

Figure 2: Longitudinal strain waves in a two layered waveguide with finite delamination for direct numerical simulations (blue, solid line) and semi-analytical solution (red, dashed line).

In Figure 2 initially, when the wave is in the delaminated region, the wave behaviour is soliton-like. Once the wave enters the first soft bonded region, the wave then evolves in an Ostrovsky wave. Once the wave re-enters the delaminated region for a sufficient duration, multiple solitons are generated behind a leading soliton. Then, when the wave re-enters a soft bonded region, we see at \( t = 2400 \) the leading wave evolves into an Ostrovsky wave packet.

The wave speed can be calculated from the simulations in Figure 2 as the waveguide length and time of propagation is known. The numerical wave speed can be compared to the wave speed obtained using the dispersion relation, which as suggested in [6] should output similar results for the speed. We see they are in good agreement.

Also, the delamination length can be varied to provide a further insight into the structure’s integrity by analysing the amplitude change and phase shift of the leading waves. Numerical results of this will be provided at the talk.

References


Higher Order Variational Time Discretizations for Nonlinear Dispersive Wave Equations

Nils Margenberg1,*, Franz X. Kärtner2, Markus Bause1

1 Helmut Schmidt University, Holstenhofweg 85, 22043 Hamburg, Germany
2 Center for Free Electron Laser Science (CFEL), Deutsches Elektronen-Synchrotron (DESY) & Department of Physics, University of Hamburg, Notkestraße 85, 22607 Hamburg, Germany

Abstract

We investigate the numerical simulation of complex nonlinear optical processes in dispersive media. A mathematical model and numerical discretization techniques are developed. In particular we study higher order variational time discretizations and the implementation of a perfectly matched layer within this framework. We use a scheme which combines finite element techniques with the concepts of collocation methods yielding discrete continuously differentiable in time solutions. We verify our techniques with convergence tests. As a practical example we investigate the generation of THz frequency radiation in periodically poled crystals.

Keywords: nonlinear optics, absorbing boundary conditions, variational time discretization

1 Introduction

Nonlinear optical phenomena form the basis of a wide range of applications such as novel optical sources and measurements or diagnostic techniques. With growing technical complexity, the reliability of models and algorithms, optimal numerical performance and minimization of costs and time in computer simulations remain key demands for investigations of nonlinear optical phenomena. We develop efficient and accurate methods for modelling complex phenomena in nonlinear optics. For the discretization we use variational space time methods. Within this framework we focus on higher order variational time discretizations. For these higher order time discretizations we implement absorbing boundary conditions based on perfectly matched layers.

2 Physical Model

Our model is motivated by the generation of THz radiation in periodically poled nonlinear crystals. THz radiation has a wide range of applications, e.g. medical imaging, biochemistry or free electron lasers. We address the arising physical problem with a dispersive and nonlinear model for the propagation of electromagnetic waves in the time domain. We transform the equations and quantities by applying a time transformation $\tilde{t} = c_0 t$ and omit the $\tilde{\cdot}$ from now on. We use a Lorentz model for the dispersion and include a second order instantaneous nonlinearity. In the Lorentz model the electric permittivity and refractive index can be modeled by the equation

$$\nu(\nu)^2 = n^2 + \frac{(n^2 - n^2_0)\nu^2}{\nu^2 + \Gamma_0^2}, \quad (1)$$

where $\Gamma_0$ is the damping coefficient and $\nu_t$ the phonon frequency. From this we derive the auxiliary differential equation (ADE) for Lorentz materials in the time domain $(2a)$. We couple $(2a)$ with the electromagnetic wave equation which leads to

$$\partial_t P + \Gamma_0 \partial_t P + \nu_0^2 P - (n_0^2 - n^2_0)\nu_0 P = 0, \quad (2a)$$

$$-\Delta E + n_0^2 \partial_t E + (n_0^2 - n^2_0)\nu_0 E - \nu^2_0 P - \Gamma_0 \partial_t P + \chi(2) \partial_t((E)E) = 0. \quad (2b)$$

In numerical simulations, wave propagation has to be truncated to bounded regions. To this end we apply the complex frequency shifted PML which allows us to derive ADEs similar to the Lorentz dispersion. This leads to a high level of flexibility regarding the applications of discretization techniques. We approximate $(2)$ by a finite element method in space and time, along the lines of $(3)$. We employ a higher order time discretization by extending $[1]$ to $(2)$. The method in $[1]$ has shown to be superior over standard continuous and discontinuous methods. It establishes a direct connection between the Galerkin method for the time discretization and the classical collocation methods, thereby achieving the
accuracy of the former with the reduced computational costs of the latter. The time discrete solutions are continuously differentiable by construction. The linearization is done by a damped version of Newton’s method, and the arising linear systems are solved by a preconditioned GMRES method.

3 Numerical investigations

We simulate THz generation in a periodically poled crystal by two Gaussian shaped pump pulses \( g(t) = \exp\left(-2\log\frac{1}{2} t^2 \right)(\cos(2\pi\omega_1 t) + \cos(2\pi\omega_2 t)) \) separated in center frequency by the THz frequency. We use a full width half maximum \( \tau = 200 \text{ ns} \) and frequencies \( \omega_1 = 291.56 \text{ THz}, \omega_2 = 291.26 \text{ THz} \). The pulse is applied at the left-hand side of the crystal by a Dirichlet boundary condition and then propagates through the domain until the PML is hit on the right-hand side. The problem setting is sketched in Fig. 1. For the implementation we use the finite element toolbox deal.II [2] along with the Trilinos library. The simulated results are presented in Fig. 2. We see, besides the THz radiation generated by difference frequency mixing in Fig 2(a), the harmonics in the optical domain in Fig. 2(b) simultaneously generated by second harmonic and sum-frequency generation.

4 Conclusion

We presented a mathematical model and finite element time domain framework for accurate and efficient simulation of phenomena in nonlinear optics. The approach employed has the advantage of a high flexibility with respect to physical models, simulation domains and order of approximation and accuracy. Although our implementation is highly efficient and the results are promising, a further reduction of computational costs is still needed.

Acknowledgements  N. Margenberg acknowledges support by the Helmholtz-Gesellschaft under grant number HIDSS-0002.

References


Friday, July 29, Morning Session
High frequency analysis of the Dirichlet to Neumann operator for the Helmholtz equation on a coated cylinder or elliptic cylinder

Olivier Lafitte\textsuperscript{1,*}

\textsuperscript{1}IRL-CNRS-CRM, University of Montréal, Québec, Canada and LAGA, Université Sorbonne Paris Nord, Villetaneuse France
\textsuperscript{*Email: lafitte@math.univ-paris13.fr}

Abstract

This paper studies the Dirichlet to Neumann operator for problems in $\Omega_0 \subset \mathbb{R}^3$, $\Omega = \Omega_0 \cup L$, where $\Omega_0$ is a perfectly conducting cylinder $S(0, R) \times \mathbb{R}$ or an elliptic cylinder $E \times \mathbb{R}$ coated with a layer $L$. Obtaining the exact expression of this operator leads to the high frequency behavior of this operator, in the elliptic and in the hyperbolic regions of the dual space (that we are able to characterize). The global high frequency behavior (extension of the classical microlocal expression of this operator) is given, the second term of the high frequency expansion is derived in a rigorous way.

Keywords: Helmholtz equation, Dirichlet to Neumann operator, high frequency expansion.

1 Introduction

This paper deals with a Helmholtz representation of the Maxwell equation in a dielectric material $L$. The dielectric constants $\epsilon, \mu$ satisfy $\epsilon \mu \notin \mathbb{R}_+$. As the problem for $u \in H^1(L)$, $u_0 \in H^{\frac{1}{2}}(\partial \Omega)$:

\[
\begin{cases}
(\Delta + \epsilon \mu \omega^2)u = 0, (x, y, z) \in L \\
\gamma_{n0} u = 0 \\
\gamma_{11} u = u_0
\end{cases}
\]

has a unique solution $U$ [2], the well defined operator $u_0 \to \partial_u U$ from $H^{\frac{1}{2}}(L)$ to $H^{-\frac{1}{2}}(L)$ is called the Dirichlet to Neumann operator (DTN).

In the classical case where $L$ is a layer $\mathbb{R}^2 \times (-l, 0)$, the solution of this problem is explicit and gives rise to the classical Dirichlet to Neumann operator for a plane layer as a Fourier multiplier on $S(\mathbb{R}^2)$ (including $k_1^2 + k_2^2 > R^2 \omega^2$):

\[DTN(\omega, \hat{\gamma}_{11}) = \frac{\sqrt{\epsilon \mu \omega^2 - k_2^2}}{\tan(\sqrt{\epsilon \mu \omega^2 - k_1^2 - k_2^2})} \hat{u}_0(\theta, k)\]

Its generalization to a curved layer [5] was derived with a local approximation of $\partial \Omega$, which gives rise to a representation of the Laplace operator as

\[
\frac{\partial^2}{\partial z^2} + g_{11}(x_1, x_2, n)\frac{\partial^2}{\partial x_1^2} + 2g_{12}(x_1, x_2, n)\frac{\partial^2}{\partial x_1 \partial x_2} + g_{22}(x_1, x_2, n)\frac{\partial^2}{\partial x_2^2} + l.o.t = \Delta
\]

in a semi-geodesic system of coordinates $(\partial \Omega \cap V(x^3) = \{r = 0\} \cap V(x^3) = \{M(x_1, x_2), (x_1, x_2) \in W(0, 0)\})$, and the DTN operator is equivalent locally to a pseudodifferential operator [4], of principal symbol $(\omega l)$ constant

\[\omega \frac{\nu(x, \eta)}{\tan(\nu(x, \eta) \omega)}\]

where $\nu(x, \eta), \exists \nu > 0$ is equal to

\[\sqrt{\epsilon \mu - (g_{11}^2 \eta_1^2 + 2g_{12}^2 \eta_1 \eta_2 + g_{22} \eta_2^2)(x_1, x_2, 0)}\].

Expressions of the other terms of this symbol are extremely tedious to obtain. Moreover this expression only gives a local analysis of the Dirichlet to Neumann operator which is a global operator on the boundary $\partial \Omega$. The aim of this Note is to give the global expression of the DTN in two particular cases and we derive the two first terms of its high frequency expansion.

2 Exact expression of the DTN in two cases

It is classical [3, 6] to obtain the DTN as a Fourier multiplier when $\Omega_0 = S(0, r_0) \times \mathbb{R}$ and $\Omega = S(0, R) \times \mathbb{R}$ thanks to the representation of the solutions of

\[(\Delta + \epsilon \mu \omega^2 - k^2)u = 0, \{r_0 \leq r \leq R, \theta \in [0, 2\pi]\}\]

in polar coordinates. Assuming

\[\hat{u}_0(\theta, k) = \sum_{n \in \mathbb{Z}} u(n, k)e^{in\theta}\]

one obtains, using $k_3 = \sqrt{\epsilon \mu \omega^2 - k^2}$

\[\mathcal{F}(DTN(u_0))(\theta, k) = \sum_{n \in \mathbb{Z}} D(k, n)u(n, k)e^{in\theta}\]

with $D(k, n) = \frac{j_n'(kr) \gamma_{11}(kr) - 2j_n(\omega l)Y_n'(kr)}{j_n(kR)\gamma_{11}(kr) - j_n'(kR)\gamma_{11}(kr)}$. Note that one can replace any pair of independent solutions of the Bessel equation by any
other pair.

The case \( \Omega_0 = \{(x, y, z), \frac{x^2}{\cosh^2 u_0} + \frac{y^2}{\sinh^2 u_0} \leq \rho^2 \} \) and \( \Omega = \{(x, y, z), \frac{x^2}{\cosh^2 u_1} + \frac{y^2}{\sinh^2 u_1} \leq \rho^2 \} \) (a layer between two ellipses with the same focal points) is less known. It is known from Floquet theory that the periodic Mathieu operator \( -\frac{d^2}{dx^2} + \cos 2\nu \) has Bloch eigenvalues \( a(n, k), b(n, k) \) associated with the normalized modes \( cn(v), sn(v) \) (generalization of the \( \cos n\theta, \sin n\theta \) modes for the operator \( \frac{d^2}{dx^2} \)). The set \( \{cn, sn\} \) is a basis of \( L^2([0, 2\pi]) \).

Denote by \( F_{n,k}^u, G_{n,k}^u \) a pair of independent solutions of the modified Mathieu equation
\[
\frac{d^2}{dx^2} \phi + \left( a(n, k) - \frac{1}{2} \rho^2 k^2 \cosh 2u \right) \phi = 0
\]
(a similar definition replacing \( a(n, k) \) by \( b(n, k) \)).

For \( \tilde{u}_0(n, k, v) = u(n, k)cn(v), \) the solution \( U \) of the Helmholtz equation satisfying the boundary conditions
\[
U(u_1, v) = cn(v) \quad \text{at} \quad u = u_1 \quad \text{and} \quad U(u_0, v) = cn(v) \quad \text{at} \quad u = u_0
\]
\[
F^n(n,k)(u)\tilde{u}_0(n,k,v) + G^n(n,k)(u)\tilde{u}_0(n,k,v)
\]
\[
F^n(n,k)(u)cn(v) \quad \text{in} \quad S'.
\]

It belongs to \( H^1(\Omega - \Omega_0) \) even if the function \( F^n(n, k)(u)cn(v) \) is not in \( S' \). Note that, as \( \eta = \frac{1}{\sqrt{\sin^2 v + \sinh^2 u_1}} \),
\[
\partial_n f = \frac{1}{\rho \sqrt{\sin^2 v + \sinh^2 u_1}} \partial_u f.
\]

3 High frequency estimate of the DTN operator

Using precise asymptotic expansions of the Bessel and modified Mathieu functions [1], we prove the two theorems:

**Theorem 1** Consider \( \omega \to +\infty \) and assume that \( \frac{n}{\omega} \in [c_1, c_2], c_1 > 0 \) (high frequency regime for the Fourier index). Denote by \( \eta = \frac{k}{\omega} \).

1. In the case \( k^2 + \frac{n^2}{\omega^2} < \Re \epsilon \mu \omega^2 \) (called the hyperbolic case), the symbol of the Dirichlet to Neumann operator is, up to \( O(\omega^{-1}) \)

\[
i \omega \sqrt{\epsilon \mu - \eta^2} - \frac{n^2}{\omega^2 R^2} - \frac{1}{2R} \frac{\epsilon \mu - \eta^2}{\omega^2 \Re \epsilon \mu - \eta^2 - \frac{n^2}{\omega^2 \Re} \omega^2}.
\]

2. In the case \( k^2 + \frac{n^2}{\omega^2} > \Re \epsilon \mu \omega^2 \) (called the elliptic case), the symbol of the Dirichlet to Neumann operator is, up to \( O(\omega^{-1}) \)

\[
\omega \sqrt{\epsilon \mu - \eta^2} - \frac{n^2}{\omega^2 R^2} - \frac{1}{2R} \frac{\epsilon \mu - \eta^2}{\omega^2 \Re \epsilon \mu - \eta^2 - \frac{n^2}{\omega^2 \Re} \omega^2}.
\]

One notices that the lower order term of the symbol does not change when we pass from the hyperbolic region to the elliptic region. The hyperbolic and elliptic region for the operator with respect to the boundary \( r = R \) are classically defined.

**Theorem 2** In the hyperbolic regime \( \Re \epsilon \mu \omega^2 - \frac{1}{2} (\Re \epsilon \mu \omega^2 - k^2) \cosh 2u_0 < 0 \), the asymptotics of \( \Re \epsilon \mu \omega^2 - \frac{1}{2} (\Re \epsilon \mu \omega^2 - k^2) \cosh 2u_0 \) read
\[
i \omega \sqrt{\epsilon \mu - \eta^2} \cosh 2u_1 - \frac{a(n, k)}{\rho \sqrt{\epsilon \mu}} (1 + O(\omega^{-2})).
\]

The contribution of the curvature of \( \partial \Omega \) appears through \( \frac{1}{\rho \sqrt{\sin^2 v + \sinh^2 u_1}} \), and through the Floquet modes. It is nonlocal in \( v \).

**References**

Handbook of mathematical functions 10th printing, 1972 (National Bureau of Standards)

[2] Cessenat, Michel

[3] David Colton and Peter Monk

[4] X. Antoine and H. Barucq:
Microlocal diagonalization of strictly hyperbolic pseudodifferential systems and application to the design of radiation conditions in electromagnetism. SIAM J. Appl. Math. 61 (2001), no. 6, 1877–1905

[5] O. Lafitte:
Diffractin in the high frequency regime by a thin layer of dielectric material I: the equivalent boundary condition SIAM J. Appl. Maths 59 (3) 1020-1052, 1999

[6] B. Stupfel:
Improved transmission conditions for a one-dimensional domain decomposition method applied to the solution of the Helmholtz equation Journal of Computational Physics 229 (2010) 851–874
Oscillatory RBF for Helmholtz problems with large wavenumber

Mauricio A. Londoño$^{1,∗}$, Francisco Rodríguez-Cortés$^2$

$^1$Department of Mathematics, Universidad de Antioquia, Medellín, Colombia
$^2$Department of Statistics, Universidad Nacional de Colombia, Medellín, Colombia

Abstract

In this paper, we deal with numerical solutions of the Helmholtz equation using interpolation techniques through oscillatory radial basis functions (RBF). We build a radial basis function-generated differences (RBF-FD) scheme by means of Bessel functions as RBF. By means of regularization with diagonal increments we solve the ill-conditioned local interpolation problem. Finally, we test the solver with absorbing boundary conditions (ABC) and find numerical evidence showing that pollution effects are mitigated.

Keywords: RBF-FD, Helmholtz equation, shape parameter, pollution effect, oscillatory RBF, wave scattering.

1 Introduction

In this paper we calculate approximated numerical solutions for Helmholtz problems given by

\[
\begin{cases}
-\Delta u(x) - \omega^2 c(x)^{-2} u(x) = f(x), \text{ in } \Omega \\
b \frac{\partial u}{\partial n}(x) + i \omega c(x)^{-1} B u(x) = g(x), \text{ on } \partial \Omega
\end{cases}
\]

where $\omega$ is the angular frequency, $c(x) > 0$ is the sound speed of a continuous media $\Omega \subset \mathbb{R}^d$, $f(x)$ is the source term, $n$ the is unitary normal vector field of the boundary $\partial \Omega$, $b$ takes values zero or one, $\mathcal{B}$ is a certain linear operator$^1$ and $g(x)$ is certain exact data on $\partial \Omega$. Here $i = \sqrt{-1}$.

Inspired by Trefethen methods [1], we use the class of oscillatory RBF given by

\[
\phi_k^{(d)}(r) = \frac{J_d(2k r)}{(k r)^{d/2 - 1}}, \quad d = 1, 2, \ldots,
\]

where $J_d$ is the Bessel function of the first kind. Since functions in (2) satisfy the homogeneous Helmholtz equation

\[
\Delta u + k^2 u = 0,
\]

any interpolant of the form

\[
s(x) = \sum_{j=1}^{n} \alpha_j \phi_k^{(d)}(|x - x_j|)
\]

will satisfy $\Delta s + k^2 s = 0$ as well. More details about this class of oscillatory functions can be consulted in [2].

2 Oscillatory RBF-FD for Helmholtz problems

We assume that $u$ is the solution of the problem (1). With $X = \{x_i\}_{i=1}^N \subset \Omega \cup \partial \Omega$ a set of nodes, we take stencils $S_i = \{x_j\}_{j=1}^n \subset X$ based on $x_i$, with $x_1 = x_i$. For $x \in \text{ConvexHull}(S_i)$ we define, with $k_i = \omega^2 c(x_i)^{-2}$, the interpolant

\[
\tilde{u}_i(x) = \sum_{j=1}^{n} \alpha_j \phi_k^{(d)}(|x - x_j|) \quad (3)
\]

From (3), evaluating in the set of nodes we have the local interpolation matrix$^2$ for $x_i$

\[
J_i = (\phi_k^{(d)}(|x_i - x_j|))_{1 \leq j \leq n_i},
\]

which is positive definite [2]. From (3) we have the linear equation $U_i = J_i \alpha_i$, where

\[
U_i = (\tilde{u}_i(x_1) \quad \tilde{u}_i(x_2) \ldots \quad \tilde{u}_i(x_{n_i}))^T
\]

and

\[
\alpha_i = (\alpha_1 \quad \alpha_2 \ldots \quad \alpha_{n_i})^T.
\]

Using the interpolant$^3$ (3) in (1), we obtain the system of linear equations$^4$

\[
\begin{cases}
\Gamma_i^T J_i^{-1} U_i = f(x_i), & \text{if } x_i \in \Omega \\
\Theta_i^T J_i^{-1} U_i = g(x_i), & \text{if } x_i \in \partial \Omega,
\end{cases}
\]

where

\[
\begin{align*}
\Gamma_i &= \left( F \phi_k^{(d)}(|x - x_1|)_{|x = x_i}, \ldots, \phi_k^{(d)}(|x - x_{n_i}|)_{|x = x_i} \right), \\
\Theta_i &= \left( G \phi_k^{(d)}(|x - x_1|)_{|x = x_i}, \ldots, G \phi_k^{(d)}(|x - x_{n_i}|)_{|x = x_i} \right), \\
F &= -\Delta - \omega^2 c(x)^{-2}, \text{ and } G = b \frac{\partial}{\partial n} + i \omega c(x)^{-1} \mathcal{B}.
\end{align*}
\]

---

$^1$The operator $\mathcal{B}$, joint the value $b = 0, 1$, is used to define absorbing boundary conditions (ABC) of several orders, even thought to define Dirichlet or Neumann boundary conditions.

$^2$Matrices $J_i$ are often ill-conditioned and is necessary to use some regularization technical [3].

$^3$Local interpolation is only used to calculate the weights to approximate the linear operators at each node, using the unknown values of the function $u$ (similar to the finite difference method), which are the final representation calculated from the sparse system of linear equations.

$^4$Which can be assembled in a sparse matrix equation.
$\begin{array}{|c|c|c|c|c|c|c|}
\hline
h & N & ||u - \overline{u}||_{\infty} \\
\hline
10 & 60 & 3721 & 1.79e-04 \\
20 & 120 & 14641 & 1.56e-04 \\
40 & 240 & 58081 & 1.10e-04 \\
80 & 480 & 231361 & 1.72e-04 \\
120 & 720 & 519841 & 1.21e-04 \\
\hline
\end{array}$

Table 1: Results for approximated solutions of (3). With a square uniform grid in $\Omega \cap \partial \Omega$. For inner nodes the stencil size is $n = 13$, at boundary nodes $n_b = 15$, and the number of nodes per wavelength is kept constant with $N_g = 6$, i.e., $h = 2\pi/6k$.  

3 Some examples and numerical results

In this section, we test the presented method with a couple of examples.

**Test 1** With $\Omega = (-0.5, 0.5) \times (-0.5, 0.5)$, $k = \omega c^{-1}$, constant wave speed $c \equiv 1$, and $u(x, y) = \sqrt{h}(-20, 20) + 2h(20, -20) + 0.5h(-20, 20) - h(20, -20))$ with $h(x_0, y_0) = H^1_0(k||x - (x_0, y_0)||)$, we solve

$$
\begin{align*}
\Delta u(x) - k^2 u(x) &= 0, & \text{in } \Omega \\
\frac{\partial}{\partial n} u(x) + iku(x) &= g(x), & \text{on } \partial \Omega.
\end{align*}
$$

Results in Table 1 show that with a fixed number of nodes per wavelength, the error keeps the same order as $k$ increases, which is evidence that pollution effect is mitigated.

**Test 2** We consider the acoustic scattering problem with a hard obstacle $\Omega_{obs} \subset \Omega$ and incident wave field given by $u_{inc}(x) = e^{ikx}$, see Figure 1. The total wave field is given by $u = u_{inc} + u_{sct}$. To compute the scattered wave field we use the follow approximation by ABC on the boundary $\partial \Omega$

$$
\begin{align*}
-\Delta u_{sct}(x) - \omega^2 u_{sct}(x) &= 0, & \text{in } \Omega/\Omega_{obs} \\
u_{sct} &= -u_{inc}, & \text{on } \partial \Omega_{obs} \\
\frac{\partial}{\partial n} u_{sct}(x) + i\omega B u_{sct}(x) &= 0, & \text{on } \partial \Omega
\end{align*}
$$

with $B = 1 + \frac{1}{2} \omega^{-2} \frac{\partial^2}{\partial r^2}$.

Acknowledgments

This work is supported by Minciencias-Colombia as a part of the research project grant No. 80740-735-2020.

References


---

$^5$We know empirically that it is desirable to keep the symmetry of the stencils at the inner nodes and a larger size at the boundary nodes to reduce the error. About it, there is something related in [4].
High-frequency estimates and error bounds on the $h$-BEM for the Helmholtz exterior Neumann problem

Jeffrey Galkowski$^1$, Pierre Marchand$^{2,*}$, Euan Spence$^3$

$^1$Department of Mathematics, University College London, 25 Gordon Street, London, WC1H 0AY, UK
$^2$POEMS, CNRS, INRIA, ENSTA Paris, Institut Polytechnique de Paris, 91120 Palaiseau, France
$^3$Department of Mathematical Sciences, University of Bath, Bath, BA2 7AY, UK

*Email: pierre.marchand@inria.fr

Abstract

In this talk, we consider solving the Helmholtz equation posed in the exterior of a smooth obstacle, with Neumann boundary conditions, and using second-kind boundary integral equations (BIEs). We study the $h$-version of the Galerkin boundary element method, and its accuracy at high-frequency.

The study of the behaviour of Galerkin error when the frequency increases requires, in particular, high-frequency estimates for the considered boundary integral operators. In the case of Dirichlet boundary condition, results are well-known in the literature for the standard second-kind BIE, but in the case of Neumann boundary condition, where regularisation techniques are commonly used, such estimates are rare.

Our contribution is twofold: we first present high-frequency estimates for a particular regularised formulation in the case of Neumann boundary conditions, and then, we present a frequency-explicit bound for its discretisation error.

Keywords: boundary integral equations, high-frequency, Helmholtz, Neumann boundary condition

1 Introduction

We are interested in scattering problems with a smooth obstacle, and we consider solving the Helmholtz equation $\Delta u + k^2 u = 0$ using second-kind BIEs posed in $L^2(\Gamma)$, where $\Gamma$ is the boundary of the obstacle. We consider the $h$-version of the Galerkin boundary element method, i.e., we consider a sequence of piecewise-polynomial approximation spaces with fixed polynomial degree $p$ and decreasing $h$.

The focus of our work is to understand how quickly $h$ needs to decrease with $k$ to maintain accuracy of the Galerkin solution as $k \to \infty$. For the finite element method, numerous works have been published since the seminal work of [1], and it is still the subject of ongoing research. In the context of the boundary element method, there has been fewer investigations of this question, and they all focused on the Dirichlet problem.

A standard approach for solving scattering problems is to use “combined-field” BIEs, which have the advantage to be well-posed for every $k > 0$. Then, an intrinsic difficulty of the Neumann problem is the presence of the hypersingular operator, which is an operator of order 1, so that the associated boundary integral operator is not bounded from $L^2(\Gamma) \to L^2(\Gamma)$.

A classical solution is to use regularised versions of the combined formulation, composing the hypersingular operator with an operator of order -1, in other words, we precondition the hypersingular operator within the combined formulation. Several regularisers have been introduced, using approximation of pseudodifferential operators (see the recent review [4]), or integral operators and Calderón relations. We focused on the latter approach, where the regulariser is a single-layer operator associated with the complex frequency $i k$. This strategy was introduced in [2], and studied in [3]. In our work, we first derived new high-frequency estimates for these regularised formulations (see our preprint [5]), and then, frequency-explicit error bounds when using $h$-BEM to solve Neumann problems with these operators.

2 High-frequency estimates

We studied the integral operators

$$B_{k,\eta} := i \eta \left( \frac{1}{2} I - K_k \right) + S_k H_k,$$

$$B'_{k,\eta} := i \eta \left( \frac{1}{2} I - K'_k \right) + H_k S_{ik},$$

Suggested members of the Scientific Committee:

Oscar Bruno, Simon Chandler-Wilde
where \( \eta \in \mathbb{C} \setminus \{0\} \) and \( S_k, K_k, K_k' \) and \( H_k \) are the standard single-, double-, adjoint-double-layer and hypersingular operators defined for \( k \in \mathbb{C} \). They both can be used to solve scattering problems with Neumann condition, \( B^s_{k,\eta} \) in the context of an indirect formulation, and \( B_{k,\eta} \) for a direct formulation.

We proved new upper bounds on the norm of these operators. For example, when \( \Gamma \) is \( C^\infty \), we obtained

\[
\|B_{k,\eta}\|_{L^2(\Gamma)\to L^2(\Gamma)} + \|B'_{k,\eta}\|_{L^2(\Gamma)\to L^2(\Gamma)} \lesssim |\eta|(1 + k^{1/4} \log(k + 2)) + \log(k + 2),
\]

where \( \lesssim \) means lower or equal up to a multiplicative constant independent of \( k \) and \( h \). We also proved invertibility of these operators on \( L^2(\Gamma) \), and upper bounds on the norm of the inverse, which is obtained expressing the inverse of these operators using the Dirichlet-to-Neumann map and the Impedance-to-Dirichlet map. The usual approach to derive bounds on the inverse of the integral operators is to use bounds on such maps. In the case of regularised formulations, the major difficulty stems from the fact that the Impedance-to-Dirichlet map is associated with the following non-standard problem:

\[
\begin{align*}
\Delta u + k^2 u &= 0 \quad \text{in } \Omega \\
S_k \partial_n^i u - i \eta \gamma \partial_n^i u &= g \quad \text{on } \Gamma.
\end{align*}
\]

It led us to study this problem to finally obtain, for example when \( \Gamma \) is \( C^\infty \) and nontrapping:

\[
\| (B_{k,\eta})^{-1} \|_{L^2(\Gamma)\to L^2(\Gamma)} + \| (B'_{k,\eta})^{-1} \|_{L^2(\Gamma)\to L^2(\Gamma)} \lesssim k^{2/3},
\]

where \( \eta \) is fixed.

### 3 Frequency-explicit error bounds

Equipped with the previous estimates, the next step was to find sufficient conditions on \( h \) under which we can obtain a frequency-explicit error bound. Note that, while results of this type have been derived for the combined-field formulation with Dirichlet boundary conditions, there was, to our knowledge, no such result for the Neumann problem.

Denoting \( V_h \) the approximation space, we assume the following approximation property

\[
\min_{v_h \in V_h} \| u - v_h \|_{L^2(\Gamma)} \lesssim h^{p+1} \| u \|_{H^{p+1}(\Gamma)}. \]

We first proved sufficient conditions for quasioptimality: for \( k \) large enough, if

\[
(hk)^{p+1} \text{cond}(B_{k,\eta}) \lesssim 1,
\]

then the Galerkin solution \( u_h \) exists, is unique, and satisfies the quasioptimality property \( \| u - u_h \|_{L^2(\Gamma)} \lesssim \min_{v_h \in V_h} \| u - v_h \|_{L^2(\Gamma)} \). Then, using properties of the solution, we deduced that under the previous sufficient condition, we have the following error bound:

\[
\frac{\| u - u_h \|_{L^2(\Gamma)}}{\| u \|_{L^2(\Gamma)}} \lesssim (\text{cond}(B_{k,\eta}))^{-1},
\]

with similar results holding for \( B'_{k,\eta} \). This last result associated with the previous estimates gives a precise answer on how fast \( h \) needs to decrease to guarantee a frequency-explicit bound on the relative error.

### References


Effective wave motion in periodic origami structures

Othman Oudghiri-Idrissi1,∗, Bojan B. Guzina1

1Department of Civil, Environmental & Geo-Engineering, University of Minnesota, Twin Cities, Minneapolis, MN 55405, USA.
∗Email: oudgh001@umn.edu

Abstract
We establish a dynamic homogenization framework for describing linear elastic wave motion in periodic origami structures by adopting a “bar-and-hinge” modeling paradigm. In this setting, we conduct a finite wavenumber – finite frequency homogenization in the spectral neighborhood of simple, repeated, and nearby eigenfrequencies at an arbitrary wavenumber within the first Brillouin zone. For completeness, the source term representing the nodal forces is expanded in Bloch waves and included in the analysis. We express the leading-order (system of) effective equation(s) in a given spectral neighborhood, and we approximate asymptotically the corresponding Bloch dispersion relationship. We illustrate the proposed framework by (i) comparing numerically the Bloch dispersion relationship to its asymptotic approximation for a 2D-periodic Miura-ori structure and (ii) computing the effective motion near an isolated eigenfrequency.

Keywords: Dynamic homogenization, periodic origami structures, tunable metamaterials

1 Origami structures

Origami, the ancient Japanese art of paper folding, has become a source of technologic inspiration and a keen subject of studies for its unique scalability, programability, deployability and configurability properties. This class of structures have rapidly found applications ranging from nano to large scales in science and engineering with examples including medical stents, energy absorbing structures, vibration control instruments, emergency shelters, inflatable structures, and large spacecraft structures. Origami-like engineered structures have also been found to exhibit the so-called metamaterials that are not observed in conventional structures and natural materials, such as auxeticity, infinite shear stiffness, negative bending stiffness, unidirectional flexibility or strain reversal (in origami tubes).

The existing literature on the homogenization of periodic origami-like structures can be classified chiefly by (i) the dynamic regime of study, and (ii) the mechanistic framework adopted to model the origami panels. In the static regime, Lebee and Sab [4] pursued a homogenization analysis of periodic thick plates using the bending-gradient plate theory. On the other hand, when an origami structure is modeled using a bar-and-hinge paradigm [2], the existing literature on trusses can be deployed to study its dynamic properties. In this framework, Craster et al. [1] extended the homogenization theory of discrete periodic lattices to high frequency and small wavelengths regimes. A generic finite wavelength-finite frequency (FW-FF) homogenization framework was proposed by Guzina et al. [3] to describe the effective wave motion in periodic media with rectangular Bravais lattices in the spectral neighborhood of simple, repeated, and nearby eigenfrequencies located at the origin or vertices of the first Brillouin zone (BZ). More recently, Oudghiri-Idrissi et al. [5] extended the FW-FF homogenization framework to “perforated” periodic continua supported on general Bravais lattices by considering the spectral neighborhood of an arbitrary wavenumber within the first BZ and eigenfrequency clusters of arbitrary size.

By building upon the FW-FF homogenization approach [3, 5], we aim to better understand the wave motion in origami structures by providing an origami-specific, dynamic homogenization framework that leverages the bar-and-hinge paradigm [2]. Such formulation specifically aims to: (i) capture the essential dynamics of the problem, (ii) analytically illuminate the origami behavior near spectral singularities (e.g. Dirac points), (iii) reduce the computational cost, and (iv) aid the design of programable and tunable (periodic) origami structures.

2 Effective wave motion

We model periodic origami structures using a “bar-and-hinge” paradigm where: (i) the folding
of the structure and bending of the origami panels are modeled via elastic hinges, and (ii) the in-plane deformation of each panel is modeled with elastic bars [2]. Using the Bloch-wave expansion of the source term acting on the nodes of the discretized structure, the analysis is reduced, thanks to the linearity of the system and periodicity of the material properties, to that of a “unit cell” of the origami structure. The homogenous part of the unit cell system constitutes an eigenvalue problem that defines the “origamons”, i.e. the Bloch waves that can propagate freely in the discrete periodic origami structure (DPOS) at a given eigenfrequency, and which form a local basis that describes the leading-order response of the DPOS. By pursuing an asymptotic analysis in the neighborhood of isolated, repeated, and nearby eigenfrequencies at the wavenumber of interest, we express the leading-order approximation of the total and effective motion in those spectral neighborhoods. In this way, we formulate the (system of) effective equation(s) that includes the homogenized source term and forms the basis from which the leading-order asymptotic approximation of the corresponding dispersion relationship is obtained. Fig. 1 illustrates a discretized unit cell of the 2D-periodic Miura-ori structure. Fig. 2 examines the performance of the homogenization framework by plotting the numerically-evaluated dispersion relationship together with its asymptotic approximation computed at different wavenumber-eigenfrequency pairs. Fig. 3 illustrates the effective wave motion in a 2D-periodic Miura-ori structure for an excitation frequency (b) inside a band gap, and (c) inside a pass band.

Figure 1: (a) Truncated 2D periodic Miura-ori sheet (b) unit cell of periodicity, (c) discretized unit cell, and (d) first BZ of the lattice.

Figure 2: Approximation of the first twelve dispersion branches for the Miura-ori periodic structure.

Figure 3: (a) Amplitude of the driving force and corresponding leading-order approximation of the induced effective motion within: (b) band gap, and (c) pass band near the origin of the first BZ.

References


Abstract
We consider the propagation of Transverse Electric (TE) waves in a 2D photonic crystal made of an homogeneous bulk containing high permittivity identical inclusions localized at the vertices of a honeycomb lattice [1, 2]. In this high contrast regime, we analyse the band structure of the underlying elliptic operator. We prove global results on the evolution of the band structure with respect to the contrast as well as detailed local information such as the existence of Dirac points, which are conical crossings between consecutive dispersion surfaces. Our study is illustrated by numerical simulations. Moreover, essential differences between this electromagnetic setting and the quantum model of graphene [3] will be discussed during the talk.

Keywords: Honeycomb photonic crystals, high contrast regime, band structure, Dirac points

1 Introduction and mathematical model
Honeycomb media such as graphene have been recently intensively studied for the new physical properties. These properties such as the existence of topological protected edge states rely on the existence of Dirac points, conical crossings of dispersion surfaces. The existence of such points has been demonstrated for Schrödinger equations in the strong binding (high contrast) regime model of graphene [3]. In this work, we study (see [1, 2]) a similar configuration for photonic crystals and show many differences with the quantum case analysed in [3].

We consider a 2D honeycomb photonic crystal (cf. figure 1) with constant permeability $\mu_0$ made of a two phase dielectric material: an homogeneous bulk of permittivity $\varepsilon_0$ that contains identical inclusions with high permittivity $\varepsilon_{0g}$. The inclusions centers are localized on the vertices of a honeycomb lattice $(\mathbf{v}_A + \Lambda) \cup (\mathbf{v}_B + \Lambda)$, where $\Lambda := \mathbb{Z} v_1 \oplus \mathbb{Z} v_2$. The crystal is partitioned into diamond-shaped periodic cells that contains two inclusions: a $A$-site (in red) and a $B$-site (in blue). The fundamental cell $\Omega$ encloses two inclusions centered at $\mathbf{v}_A$ and $\mathbf{v}_B$ whose shape is assumed invariant by a rotation of $\pi/6$ with respect to $\mathbf{v}_A$ or $\mathbf{v}_B$.

Figure 1: Honeycomb media in the case of disk shaped inclusions (left). Dual lattice $\Lambda^*$, hexagonal Brillouin zone $\mathcal{B}$, dual basis $(\mathbf{k}_1, \mathbf{k}_2)$ and high symmetry quasimomenta $\mathbf{K}$ and $\mathbf{K}'$ (right).

In this structure, we analyse the propagation of (TE) modes $(E_x, E_y, H_z)$. For such modes and a circular frequency $\omega \neq 0$, the magnetic component $H_z$ is solution of $-\nabla \cdot \varepsilon_{0g}^{-1} \nabla H_z = \omega^2 \mu_0 H_z$ where the permittivity function $\varepsilon_{0g}$ takes two values: $\varepsilon_{0g}$ within the inclusions and $\varepsilon_0$ in the bulk. The transverse field $(E_x, E_y)$ is then computed explicitly from $H_z$. After of multiplication of the $H_z$ equation by $\varepsilon_{0g}$, we obtain an equivalent spectral problem for the self-adjoint elliptic unbounded operator $\mathcal{H}_g = -\nabla \cdot \sigma_g \nabla$:

$$\mathcal{H}_g H_z = \lambda H_z$$

where $\lambda = g \left( \frac{\omega}{c} \right)^2$, $c = (\mu_0 \varepsilon_0)^{-\frac{1}{2}}$, and the function $\sigma_g$ takes two values: 1 in the inclusions and $g$ in the bulk.

As $\mathcal{H}_g$ commutes with lattice ($\Lambda$) translations, its spectrum is obtained via a family of Floquet-Bloch eigenvalue problems. More precisely, for each $\mathbf{k} \in \mathcal{B}$, the hexagonal Brillouin zone (cf. figure 1), we denote by $\lambda_1(\mathbf{k}; g) \leq \cdots \leq \lambda_n(\mathbf{k}; g) \leq \cdots$ the sequence of eigenvalues (listed with multiplicity) of $\mathcal{H}_g$ subject to $\mathbf{k}$-quasiperiodic boundary conditions. The graphs of the Lipschitz continuous maps $\mathbf{k} \mapsto \lambda_n(\mathbf{k}; g)$, $n \geq 1$, are called dispersion surfaces. The $L^2(\mathbb{R}^2)$ spectrum of $\mathcal{H}_g$ is the union of closed real intervals, that are
swept out by its dispersion maps as \( k \) varies over \( B \). The collection of all Floquet-Bloch eigenpairs is referred to as the band structure of \( h_g \).

2 Summary of our main results

We analyse the band structure of \( h_g \) in the high contrast regime: \( g \gg 1 \). We summarize our results for the two first dispersion maps. However, we point out that they hold in some configurations for dispersion surfaces arbitrary high in the spectrum, see [1].

a) High contrast global behavior. We show that:
- The first dispersion map \( \lambda_1(\cdot; g) \) converges uniformly as \( g \to +\infty \) on any compact set of \( B \setminus \{0\} \) to the constant function \( \delta_1 > 0 \) equal to the first Dirichlet eigenvalue on a single inclusion. The uniform convergence on all \( B \) fails since \( \lambda_1(0; g) = 0 \) for all \( g > 0 \). Unlike, \( \lambda_1(\cdot; g) \) and \( \lambda_2(\cdot; g) \) converges uniformly to \( \delta_1 \) on all \( B \).
- For \( g \) large enough, there exists a gap between the second and third dispersion surfaces.

b) Existence of Dirac point for \( g \gg 1 \). A Dirac points is as an energy / quasimomentum pair \((\lambda_D, k_D) \in \mathbb{R}^+ \times B\) where \( \lambda_D = \lambda_-(k_D; g) = \lambda_+(k_D; g) \) is of multiplicity two and the consecutive dispersion maps \( \lambda_-(\cdot; g) \leq \lambda_+(\cdot; g) \) touch conically. Namely, there exists a constant \( v_D(g) > 0 \), referred to as the Dirac velocity, such that:

\[
\lambda_\pm(k; g) = \lambda_D \pm v_D(g) |k - k_D| + o(|k - k_D|).
\]

In [1], we establish (for \( g > 0 \) fixed) sufficient conditions for the existence of Dirac points at any of the six vertices \( K_\pm \) of \( B \). In addition, we show that \( v_D(g) \) in (1) is explicitly given in terms of a basis of the two dimensional eigenspace \( \mathcal{V}_{k_D} \) of Floquet-Bloch modes at \( k_D = K_\pm \). Furthermore, we show (under the hypothesis \( v_D(g) \neq 0 \), satisfied numerically) that these conditions hold for large contrast for the two first dispersion maps. Thus, there exists a Dirac point \((\lambda_D, k_D) \) between \( \lambda_-(\cdot; g) = \lambda_1(\cdot; g) \) and \( \lambda_+(\cdot; g) = \lambda_2(\cdot; g) \) at the six vertices \( K_\pm \) of \( B \). We refer to the figure 2 for a numerical illustration of the results described in a) and b) at \( g = 50 \) and \( K_\pm = K \).

c) Asymptotic expansions of Floquet-Bloch eigenvalues at the Dirac point. We obtain at \( k_D = K_\pm \) asymptotic expansions at any order in powers of \( g^{-1} \) of the Dirac energy \( \lambda_D(g) \) and a basis \( \{\Phi_1, \Phi_2\} \) of the two-dimensional space \( \mathcal{V}_{k_D} \) of Floquet-Bloch modes. At leading order \( \lambda_D(g) = \delta_1 + O(g^{-1}) \) and \( \{\Phi_1, \Phi_2\} \) satisfies \( \Phi_1(\cdot; g) = P_{k_D,A} + O(g^{-1}) \) and \( \Phi_2(\cdot; g) = P_{k_D,B} + O(g^{-1}) \).

Here, \( P_{k_D,A} \) and \( P_{k_D,B} \) are \( k_D \)-quasiperiodic superpositions of single inclusion Dirichlet states; supported respectively on the \( A \)-inclusions and on the \( B \)-inclusions. They play the role of atomic orbitals in the strong-binding Schrödinger regime; see [3]. Unlike ground state quantum atomic orbitals, they are compactly and disjointly supported, rather than exponentially localized in the well-depth parameter. The disjointness of the supports of \( \Phi_-(\cdot; g) \) at leading order (cf. figure 3 for disks inclusions with \( R = 0.2 \)) implies that \( v_D(g) = v_D(1) g^{-1} + O(g^{-2}) \), where we have verified that \( v_D(1) > 0 \) numerically. It explains why the “Dirac cones” flatten as \( g \) becomes large (see figure 2 for \( g = 50 \)).

Figure 2: \( k \mapsto \lambda_1(k; 50), \lambda_2(k; 50), \lambda_3(k; 50) \) plotted along the (yellow) contour: \( \text{M-O-K-M} \) of \( B \) for disks inclusions of radius \( R = 0.2 \).

Figure 3: \( |\Phi_1(\cdot; 50)| \) and \( |\Phi_1(\cdot; 50)| \) on \( \Omega \) at \( K \).

References


Dislocation model for hexagonal periodic graphs perturbed along the Zig Zag direction

Sonia Fliss$^1$, Bérangère Delourme$^2$

$^1$POEMS (INRIA-ENSTA-CNRS), Palaiseau, France
$^2$LAGA, Université Sorbonne Paris Nord, Villetaneuse, France

Abstract

We consider a periodic graph having the honeycomb symmetry that we cut along the Zig Zag direction, the exact location of the cut depending on a dislocation parameter $t$. For any $t$, we prove the existence of guided waves traveling along the cut. For some particular frequencies, those modes exist independently of the quasi-momentum $\beta$.

Keywords: periodic media, spectral theory, guided modes.

1 Setting

We consider the hexagonal infinite graph $G$ of Figure 1 with $L = \frac{1}{\sqrt{3}}$. For a parameter $t \in [0, 2L]$ (see figure 1), we consider the truncated graph $G_t$ obtained by truncating the infinite graph $G$ at $s = t$ parallelly to the direction $e_y$ (see Figure 2 for two illustrations of $G_t$ at $t = L/2$ and $t = 3L/2$).

Figure 1: infinite graph $G$

Figure 2: $G_t$ at $t = L/2$ and $t = 3L/2$

We are interested in guided waves, namely solutions to the wave equation of the form $u(x) = w(x,y)e^{i\beta y + \omega t}$, where $w$ is periodic with respect to $y$. To be more specific, we denote by $\mathcal{E}$ the set of edges of $G$ in the yellow region of Figure 1, and by $\mathcal{E}_t$ the restriction of $\mathcal{E}$ to $G_t$. For any $\beta \in [0,\pi]$ (the case $\beta \in [-\pi,0]$ resulting from a time symmetry argument), we define the sets $L^{2,\beta}(G_t)$ and $H^{2,\beta}(G_t)$ of $\beta$ quasi-periodic functions

$$L^{2,\beta}(G_t) = \{ v \text{ s.t. } v \in L^2(e), \forall e \in \mathcal{E}_t; \left\| u \right\|^2_{L^2(G_t)} = \sum_{e \in \mathcal{E}_t} \left\| u \right\|^2_{L^2(e)} < \infty, \quad v(x_1,x_2 + 1) = e^{i\beta}v(x_1,x_2) \}, \quad (1)$$

$$H^{2,\beta}(G_t) = \{ u \in L^{2,\beta}(G_t) / u \in C(G_t); \quad u \in H^2(e), \forall e \in \mathcal{E}_t; \left\| u \right\|^2_{H^2(G_t)} = \sum_{e \in \mathcal{E}} \left\| u \right\|^2_{H^2(e)} < \infty \}, \quad (2)$$

where $C(G_t)$ stands for the set of functions that are continuous on $G_t$. We then consider the self-adjoint operator $A_t^\beta$ defined by

$$(A_t^\beta u)_e = -u'_e, \quad \forall e \in \mathcal{E}_t, \quad (3)$$

on the domain

$$D(A_t^\beta) = \{ u \in H^2(G_t) / \sum_{e \in \mathcal{E}(M)} u'_e(M) = 0, \quad \forall M \in \mathcal{M}_t \},$$

In the previous definition, $\mathcal{M}_t$ denotes the set of vertices of $G_t$, $u_e$ stands for the restriction of $u$ to the edge $e$, and $u'_e(M)$ is the outward derivative of $u_e$ at the vertex $M$. In that setting, we can see that guided waves correspond to eigenvectors of the operator $A_t^\beta$. We therefore investigate the discrete spectrum of $A_t^\beta$.

2 Main result

The essential spectrum of $A_t^\beta$ is independent of $t$, and is periodic of period $\pi/L$ (with respect to $\omega = \sqrt{\lambda}$). Moreover, for any $\beta \neq \frac{\pi}{L}$ and for non negative integer $n$, $\sigma_{ess}(A_t^\beta)$ has a gap $\lambda_n = |a_n(\beta)|^2, |b_n(\beta)|^2$ around the critical value

$$\lambda_n = (\omega_n)^2, \quad \omega_n = \frac{\pi}{2L} + n\frac{\pi}{L}$$
Remark 1 The frequency $\lambda_n$ corresponds to a frequency of a Dirac point of the dispersion surfaces associated with the operator $A^G_n$ defined on the full graph $G$ (having the honeycomb symmetry).

Our main results, illustrated by the Figure 3 states that there is a spectral flow made of $2n+1$ eigenvalues of $A^G_n$ inside the gap $G_n$.

Theorem 2 For any $\beta \in [0, \frac{2\pi}{3}] \cup \left(\frac{2\pi}{3}, \pi\right]$, the operator $A^G_n$ has exactly $2n+1$ eigenvalues in $G_n$. Moreover, the dispersion curves $t \mapsto \omega(t)$ are strictly increasing.

The proof of the previous result follows the next three points:

1. We first prove that the number of eigenvalues remains constant in the intervals $G_n^+ = ]\lambda_n(\beta)^2, \lambda_n[ \text{ and } G_n^- = ]\lambda_n, \lambda_n(\beta)^2[.$

2. We investigate the particular case $\lambda = \lambda_n$ where explicite computations can be made.

3. A standard differentiable argument gives that $t \mapsto \omega(t)$ are strictly increasing, which therefore ends the proof.

We point out that our result can be seen as an extension of the ones of [3], obtained for the one dimensional Schrödinger equation (with smooth periodic potential) dislocation models. More specifically, the first and third points of the demonstrations rely on the same arguments. As in [3], the presence of eigenmodes is equivalent to the existence of zeros of a particular function depending only of the ‘bulk’. However, the lack of continuity of our model at $t = L$ prevents us to link that to any topological index (defined as winding number of a continuous function living on the unit circle) and to refer to it as bulk edge correspondence (see [4, 5]).

Remark 3 By proving Theorem 2, we also demonstrate that, for any $n \geq 0$, there are $2n+1$ particular values $t_{n,k}$ ($k \in \{0, 2n+1]\}$ of $t$ such that the corresponding eigenvectors are independent of the quasi-momentum $\beta$. For instance, in the case $\beta < \frac{2\pi}{3}$,

$$t_{n,k} = \begin{cases} L - \frac{2L(n-k)}{1+2n} & 0 \leq k \leq n \\ L + \frac{2L(k-n)}{1+2n} & n+1 \leq k \leq 2n \end{cases}$$

This property is well-known in the case of Zig Zag tight-binding models [6] (corresponding to $t = 0$ or $t = L$).

Figure 3: Representation of the function $t \mapsto \omega(t)$ in the gaps $G_0, G_1$ and $G_2$ for $\beta = \frac{\pi}{3}$. The blue points correspond to eigenvalues independent of $\beta$.

References


Acoustoelasticity of soft viscoelastic solids and phononic crystals

Harold Benjamin\textsuperscript{1,∗}, Riccardo De Pascalis\textsuperscript{2}

\textsuperscript{1}School of Mathematical and Statistical Sciences, NUI Galway, Galway, Republic of Ireland
\textsuperscript{2}Dipartimento di Matematica e Fisica ‘E. De Giorgi’, Università del Salento, Lecce, Italy

∗Email: harold.berjamin@nuigalway.ie

Abstract
The effective dynamic properties of specific periodic structures involving rubber-like materials can be adjusted by pre-strain, thus facilitating the design of custom acoustic filters. While nonlinear viscoelastic behaviour is one of the main features of soft solids, it has been rarely incorporated in the study of such phononic media. Here, we study the dynamic response of nonlinear viscoelastic solids within a ‘small-on-large’ acoustoelasticity framework. Incompressible soft solids whose behaviour is described by the Fung–Simo quasi-linear viscoelasticity theory (QLV) are considered. Generalised Maxwell-type wave dispersion is obtained, where the coefficients depend on the large static pre-strain. The acoustoelasticity theory is then applied to phononic crystals involving a lattice of hollow cylinders. Results highlight the effect of viscoelastic dissipation on the first band gap. In particular, we show that dissipation increases the band gap width.

Keywords: viscoelasticity, phononic crystal, finite strain

1 Introduction
Rubber-like solids are very soft. Due to their high strength, they can support very large elastic deformations. For specific phononic crystals, the effective wave filtering properties can be adjusted by imposing a large static pre-deformation. Known as the acoustoelastic effect, the influence of static pre-deformation on wave dispersion results from nonlinear constitutive behaviour. Such a system is presented in Barnwell et al. [1] within the framework of incompressible finite elasticity, where vertical pre-stretch is applied to a lattice of hollow cylinders embedded in a soft matrix (Fig. 1).

In addition to their nonlinear elastic response, soft solids can exhibit large hysteresis loops in loading-unloading experiments, as well as creep and relaxation phenomena. These observations suggest that dedicated large strain viscoelasticity theories should be used to study the deformation and motion of real elastomers, as well as related soft phononic crystals.

In the present study [2], we consider soft solids governed by the Fung–Simo quasi-linear viscoelasticity theory (QLV). We derive the incremental equations using stress-like memory variables governed by linear evolution equations. Then, we apply the acoustoelasticity theory to the periodic structure of Fig. 1 by means of Bloch wave analysis and perturbation theory. Results are relevant to practical applications of soft viscoelastic solids subject to static pre-stress.

2 Governing equations
Let us introduce the deformation gradient tensor $F = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$ describing a finite motion from the initial position $\mathbf{X}$ in the reference configuration to the current position $\mathbf{x}$. The incompressible QLV theory involves stress-like memory variables $S_{\ell}$ arising naturally in the expression of the second Piola–Kirchhoff stress [2]

$$S = -pC^{-1} + \text{Dev}(S^0) - \sum_{\ell=1}^{N} S_{\ell}^0. \quad (1)$$

Here, $pC^{-1}$ is a hydrostatic stress due to incompressibility, $\text{Dev}(\bullet) = (\bullet) - \frac{1}{3}\text{tr}(\bullet C) C^{-1}$ is the Lagrangian deviatoric operator, and $C = F^T F$ is the right Cauchy–Green strain tensor. The elastic response is assumed of Mooney–Rivlin

...
Figure 2: Acoustoelasticity. Incremental motion superimposed on a large static deformation.

\[ S' = (2c_1 + 2c_2 \text{tr} C) I - 2c_3 C. \tag{2} \]

The memory variables are governed by linear evolution equations of the form

\[ \tau_1 \dot{S'} = g_1 \text{Dev}(S') - S' \tag{3} \]

where the overdot denotes the material time derivative. Finally, the motion is governed by the equation of motion \( \rho \ddot{u} = \text{Div}(FS) \) where \( u = x - X \) is the displacement field, \( \rho \) is the mass density, and the divergence is computed with respect to the Lagrangian coordinate \( X \). Typical values of the parameters \( c_1, c_2, \tau_c, g_1, \tau_1, \rho \) for rubber are given in Ref. [2] where \( N = 1 \) relaxation mechanism (3) is considered.

3 Incremental motion of a pre-stressed phononic crystal

Let us consider an infinitesimal vertical displacement \( u \) superimposed on a large static pre-deformation \( F \) (Fig. 2), here a vertical pre-stretch of the cylinders. The cylindrical coordinate system \( r, \theta \) of a cylinder is used. The effective radial and angular shear moduli take the form [2]

\[ \mu_\alpha = (1 - g_1) [T^\alpha_2]_{\alpha\alpha} + \left(1 - \frac{g_1}{1 + i\omega \tau_1}\right) \bar{\mu'}_\alpha, \tag{4} \]

where the real coefficients \( [T^\alpha_2]_{\alpha\alpha}, \bar{\mu'}_\alpha \) with \( \alpha \in \{r, \theta\} \) depend on the static pre-stretch, \( \omega \) is the angular frequency, and \( i \) is the imaginary unit — here, we have set \( N = 1 \) in Eq. (1). Thus, the dispersion of antiplane shear waves is governed by a generalised Maxwell relation whose coefficients depend on \( F \).

These expressions are then used to perform Bloch wave analysis. The dispersion of plane shear waves propagating in the periodic structures is governed by an eigenvalue problem of the form

\[ (K - \omega^2 M) w = 0, \tag{5} \]

with complex-valued and \( \omega \)-dependent matrices \( K, M \) in the viscoelastic case \( g_1 \neq 0 \).

In practice, the angular frequency \( \omega \) in Eq. (5) is computed by implementing a perturbation method with respect to the small parameter \( g_1 \). For sake of simplicity, we assume that the viscoelastic parameters \( g_1, \tau_1 \) are identical in the cylinders and in the matrix, contrary to the elastic parameters \( c_1, \rho \). The dispersion diagrams include a band gap, i.e. a frequency range for which waves cannot propagate.

Results show that the band gap width increases monotonously with \( g_1 \) for constant \( \tau_1 \). Moreover, we demonstrate that the evolution of the band gap width with respect to \( \tau_1 \) at constant \( g_1 \) is not monotonous.

4 Concluding remarks

Viscoelastic behaviour does not modify dramatically the dynamic response of the phononic crystal. Nevertheless, dissipation definitively influences the band gap width, a property to keep in mind for practical applications.

Acknowledgements. HB was supported by the Irish Research Council [project ID GOIPD/2019/328]. RDP was supported by Regione Puglia (Italy) through the research programme ‘Research for Innovation’ (REFIN) [project number UNISAL023 - protocol code 2BDDFA20] and partially supported by Italian National Group for Mathematical Physics (GNFM-INdAM).

References


These matrices are real-valued and constant in the elastic case \( g_1 = 0 \) [1].
The Half-space Matching method and the Perfectly Matched Layers for scattering problem in anisotropic elastic media

E. Bécache¹, A.-S. Bonnet-Ben Dhia¹, S. Fliss¹, A. Tonnoir²,
¹POEMS(UMR 7231 CNRS-ENSTA-INRIA, Palaiseau, France)
²LMI (EA 3226 - FR CNRS 3335), Rouen, France
*Email: antoine.tonnoir@insa-rouen.fr

Abstract
In this work, we are interested in solving scattering problems in anisotropic elastic unbounded domains. We propose an extension of a new method called the Half-Space Matching (HSM) method which enables to consider any anisotropy. Also, we compare HSM results with Perfectly Matched Layers (PMLs) results for several anisotropic media to emphasize the robustness of the HSM method.

Keywords: Anisotropic elastodynamics, unbounded domains, Domain decomposition methods.

1 Introduction
Elastodynamics scattering problems occur for instance in the context of geophysical surveys or non destructive testing simulations. Classically, the difficulty is to reformulate the problem in a bounded domain to solve it numerically. Several approaches exist in the literature, such as absorbing layers, absorbing or transparent boundary conditions or integral equation methods, but they usually cannot handle every anisotropy. In particular, it is well-known for time-domain regime [1] that the PMLs method suffers from instabilities for some anisotropic materials. For frequency-domain, to the best of our knowledge, fewer results exist and the equivalent of the instabilities is less clear.

To consider general anisotropic materials, we propose an extension of the HSM method, first introduced for anisotropic scalar equations [2], to the elastodynamic case. Also, we believe that the HSM formulation can help to understand some curious results observed using PMLs in the frequency-domain for elastic media. A comparison study between the HSM and the PMLs methods for various anisotropic materials will also be shown.

2 The HSM formulation
We consider the scattering problem:

\[-\text{div}(\sigma(u)) - \rho \omega^2 u = 0 \quad \text{in} \quad \Omega = \mathbb{R}^2 \setminus \mathcal{O},
\]

\[\sigma(u)\nu = g \quad \text{on} \quad \partial\Omega,\]

(1)

where u is the diffracted field, O is a bounded obstacle, \(\nu\) is the unit outward normal and the stress tensor \(\sigma(\cdot)\) is linked to the strain tensor \(\varepsilon(\cdot)\) via the general anisotropic Hooke’s law (using Voigt’s notations):

\[
\begin{bmatrix}
\sigma_{xx}(u) \\
\sigma_{yy}(u) \\
\sigma_{xy}(u)
\end{bmatrix} =
\begin{bmatrix}
C_{11} & C_{12} & C_{13} \\
C_{12} & C_{22} & C_{23} \\
C_{13} & C_{23} & C_{33}
\end{bmatrix}
\begin{bmatrix}
\varepsilon_{xx}(u) \\
\varepsilon_{yy}(u) \\
2\varepsilon_{xy}(u)
\end{bmatrix}.
\]

The coefficients \(C_{ij}\) are supposed to be local perturbation of constant coefficients as well as the density \(\rho\).

Figure 1: Schema and notations.

To get the HSM formulation of this problem, the idea is to split the domain into five parts, see Figure 1:

- a square \(\Omega_b = [-b, b]^2 \setminus \mathcal{O}, \ b > 0\), containing all the heterogeneities and in which we use a finite elements representation of the solution denoted by \(u^b\);
- and four half-spaces \(\Omega_j\) in which we use Fourier-integral representations of the solution denoted by \(u^j\).

More precisely, taking advantage of the homogeneity of the medium in the half-spaces, we can...
use the Fourier transform in the transverse direction to express the solution $u_j$ in $\Omega^j$ as a function of its trace $\Phi_j$ on $\Sigma_j := \partial \Omega^j$. For instance, in $\Omega^j = \{x \geq a\} \times \mathbb{R}, 0 < a < b$, we get an expression of the form:

$$u^0(x, y) = \int_{\mathbb{R}} Q(\xi)e^{iK(\xi)(x-a)+i\xi y}Q^{-1}(\xi)\hat{\Phi}^0(\xi)d\xi$$

(2)

where $Q(\xi)$ is a $2 \times 2$ matrix and $K(\xi)$ is a $2 \times 2$ diagonal matrix that will be precisely defined in the talk. As we can notice, this representation is similar to plane waves representation, with the difference that it also takes into account evanescent plane waves (when $\text{Re}(K(\xi)) \neq 0$). Let us simply add that to get these expressions in each half-space, we need to properly select outgoing waves based on the direction of their group velocity.

Then, to ensure the matching between these different representations in the different subdomains, we must impose compatibility conditions on the boundaries of each subdomain. This leads to a formulation where the new unknowns are $u^b$ in the $\Omega_b$ and the traces $\Phi^j$ on $\Sigma^j$ which are coupled via integral operators. This HSM formulation is suitable for discretization and has been validated in the isotropic case by comparison with an analytical reference solution. As already mentioned, it is also suitable for anisotropic media, as illustrated on Figure 2, and we can make an a posteriori reconstruction of the solution in the four half-spaces discretizing formula (2).

Figure 2: On the left, slowness diagram of the anisotropic material. On the right, modulus of the diffracted field in $\Omega_b$ and reconstruction in $\Omega^j$.

3 The PMLs method

In the time-harmonic regime, the PMLs formulation is obtained by using a complex scaling in the exterior of the domain of interest. In particular, we can consider the simple change of variables $t = \alpha(t)(t-b) + b$, $t \in \{x,y\}$, where $\alpha(t) = 1$ if $|t| \leq b$ and $\alpha(t) = me^{\theta}$ if $|t| > b$ with $m > 0$ and $\theta \in [0, \frac{\pi}{2}]$. Then, we expect the PML solution to exponentially decay in the layers, so that we can truncate them at a finite distance.

Now, using the half-space representation (2), we easily show that the PML solution in $\Omega^j$ (considering only stretching in direction $x$) is exponentially decaying if $\text{Im}(e^{\theta}K(\xi)) > 0$, $\forall \xi \in \mathbb{R}$. One interesting feature is the fact that this condition concerns both propagative and evanescent plane waves. In particular, in presence of backward waves, which corresponds to the case where $\text{Im}(K(\xi)) = 0$ and $\text{Re}(K(\xi)) < 0$ for $\xi$ in an interval, this condition can never be satisfied (let us mention that this case leads to instabilities in time-domain). Also, for evanescent waves when $\text{Im}(K(\xi)) > 0$, if $\text{Re}(K(\xi)) \neq 0$ (corresponding to inhomogeneous waves) this condition imposes that $\theta \leq \theta^*$ with $\theta^* < \frac{\pi}{2}$. Numerically, if this condition for evanescent waves is not satisfied, even in absence of backward waves, we can observe a strange behavior of the solution in the PMLs as illustrated in Figure 3. We therefore guess that these inhomogeneous plane waves are important to understand the behavior of the PML solution. In the talk, several numerical tests will be shown to study this question.

Figure 3: On the left, slowness diagram of the orthotropic material. On the right, modulus of the diffracted field in the physical domain and in the PMLs.

References


Radial complex scaling/PML for anisotropic scalar resonance problems

Martin Halla$^{1,*}$

$^1$Georg-August Universität Göttingen, Germany
$^*\text{Email: m.halla@math.uni-goettingen.de}$

Abstract

We consider radial complex scaling/perfectly matched layer (PML) methods for scalar resonance problems. First we focus on isotropic problems and prove the convergence of approximations. In particular, the analysis covers the simultaneous approximation due to domain truncation and discretization, and a broad range of scaling profile functions. In addition, we obtain convergence of eigenfunctions, convergence rates and correct algebraic multiplicities of eigenvalues. Core ingredients of the analysis are the framework of T-compatible approximations of weakly T-coercive operators, and the interpretation of the domain truncation as Galerkin approximation.

In a second part we show how to extend the former results to anisotropic materials, whereat some restrictions on the choice of parameters have to be respected. To this end it is necessary to take a close look at the complex transformation of the fundamental solution, and to obtain an estimate on the numerical range of certain nonhermitian matrices.

Keywords: complex scaling, perfectly matched layer, resonances, eigenvalues, anisotropic materials, convergence analysis

1 The resonance problem

Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain such that $\Omega^c$ is nonempty and bounded. Let $B_r := \{x \in \mathbb{R}^3: |x| < r\}$ and $r_0 > 0$ be such that $\Omega^c \subset B_{r_0}$. We consider the resonance problem to find nontrivial solutions $(\omega, u)$ to

$$-\Delta - \omega^2 u = 0 \quad \text{in } \Omega,$$

$$u = 0 \quad \text{on } \partial \Omega,$$

$$u(x) = \frac{\i \omega}{4\pi} \int_{\partial B_{r_0}} u(y) \nabla_y G_\omega(x, y) \cdot \nu(y)$$

$$- G_\omega(x, y) \nabla_y u(y) \cdot \nu(y) \, dy, \quad x \in B_{r_0}^c,$$

where the fundamental solution of the Helmholtz equation.

2 Radial complex scaling

Let $r_1 > r_0, \gamma \in \{z \in \mathbb{C}: \Re(z) \geq 0, \Im(z) > 0\}$ and $\alpha$ be such that $\alpha(r) = 0$ for $r \leq r_1$, $\alpha$ is continuous, $\alpha(r) > 0$ for $r > r_1$, $\alpha$ is nondecreasing, $\alpha$ is twice continuously differentiable in $[r_1, +\infty)$ with continuous extensions of $\partial_r \alpha$ and $\partial_r^2 \alpha$ to $[r_1, +\infty)$, and $\alpha$ and $\beta$ are bounded.

We define the auxiliary functions

$$\tilde{d}(r) := 1 + \gamma \alpha(r), \quad \tilde{r}(r) := \tilde{d}(r)r,$$

$$\alpha(r) := r \partial_r \tilde{d}(r) + \alpha(r), \quad d(r) := 1 + \gamma \alpha(r),$$

and $d_0 := \lim_{r \to +\infty} (\tilde{d}(r)/\tilde{d}(r))$. Then for any resonance function we define formula in spherical coordinates $\tilde{u}(x) := u(\tilde{r}(r)x)$. This definition can indeed be justified rigorously, and if $\Re(\omega d_0) < 0$, then $\tilde{u} \in H^1_0(\Omega)$ solves $a_\Omega(\omega; \tilde{u}, u') = 0$ for all $u' \in H_0^1(\Omega)$, where $P_x(x) := |x|^{-1}xx^\top$ and

$$a_D(\omega; u, u') := -\omega^2 \langle \tilde{d}^2 du, u' \rangle_{L^2(D)}$$

$$+ \langle (\tilde{d}^2 d^{-1} P_x + d(I - P_x)) \nabla u, \nabla u' \rangle_{L^2(D)}.$$
First we follow [4] and identify $H^1_0(\Omega_n)$ with $\{u \in H^1_0(\Omega) : u|_{\Omega^c_n} = 0\}$, and thus $X_n \subset H^1_0(\Omega)$. This way we can interpret the domain truncation as conform Galerkin approximation. Second we employ the abstract framework [3] for the Galerkin approximation of eigenvalue problems for holomorphic operator functions. To this end for each $\omega \in \Lambda_{d\omega}$ we need to find an invertible operator $T \in L(H^1_0(\Omega))$ and a compact operator $K \in L(H^1_0(\Omega))$ such that $T^*A + K$ is coercive, whereat $A$ is the operator associated to $a(\omega; \cdot, \cdot)$. Let $d(r) := \lim_{\rho \to r_1^+} d(\rho)$ for $r < r_1$ and $\tilde{d}(r) := d(r)$ for $r \geq r_1$. Then we achieve the goal with the multiplication operator $Tu := d^{-1}u$ for $\arg(-\omega^2d_0^2) \in [-\pi, 0)$ and $Tu := \tilde{d}^{-2}u$ for $\arg(-\omega^2d_0^2) \in [0, \pi)$. The second main assumption of [3] is that we construct operators $T_n \in L(X_n)$ such that $\lim_{n \to \infty} \|T - T_n\|_{L(X_n, H^1_0(\Omega))} = 0$. Let $\Pi_n$ be the Scott-Zhang interpolant. Then we achieve the latter assumption with $T_n := \Pi_nT|_{X_n}$ by means of a suitable adaptation of the discrete commutator property. Finally we construct an appropriate function to estimate the best approximation error by the discretization error plus the truncation error, whereat the latter decreases exponentially with the layer size.

4 Anisotropic materials

A widespread observation is that PMLs for anisotropic elastodynamics can be unstable. However, this might not be true for radial PMLs. As a step in this direction we generalize the former convergence results to anisotropic scalar materials under some mild additional assumptions on the parameters. The recipe from the isotropic case can be reused in the main for the anisotropic case, and we focus on the points which require some additional care. At first we note that the we require a minimal distance $r_1 > c(\varsigma)r_0$ from the scattering object to the complex scaled layer, whereat $c_1(\varsigma)$ is a constant which depends on the material $\varsigma$. For scattering problems also all source terms must be supported in $B_{r_0}$. This assumption is necessary to guarantee that the complex scaled fundamental solution $\tilde{G}_{\omega, \varsigma}(x, y)$ is well-defined and holomorphic. Secondly we need to assume $\sup_{r \geq r_1} \arg(d(r)/\tilde{d}(r)) < c_2(\varsigma)$ with a certain constant $c_2(\varsigma) > 0$. For the simplest possible scaling $\tilde{r}(r) = (1 + \gamma)(r - r_1) + r_1$, $r > r_1$ this condition can be interpreted as a restriction on the damping strength. In Fig. 1 we show the geometries and meshes for an anisotropic and two isotropic examples which admit the same resonances. In Fig. 2 we present the computed spectrum with a radial PML method. We recognize a good correspondence between the computations and the reference values. The quality of the computed resonances from the anisotropic example is intermediate between the quality of the isotropic examples.

4 Anisotropic materials

A widespread observation is that PMLs for anisotropic elastodynamics can be unstable. However, this might not be true for radial PMLs. As a step in this direction we generalize the former convergence results to anisotropic scalar materials under some mild additional assumptions on the parameters. The recipe from the isotropic case can be reused in the main for the anisotropic case, and we focus on the points which require some additional care. At first we note that the we require a minimal distance $r_1 > c(\varsigma)r_0$ from the scattering object to the complex scaled layer, whereat $c_1(\varsigma)$ is a constant which depends on the material $\varsigma$. For scattering problems also all source terms must be supported in $B_{r_0}$. This assumption is necessary to guarantee that the complex scaled fundamental solution $\tilde{G}_{\omega, \varsigma}(x, y)$ is well-defined and holomorphic. Secondly we need to assume $\sup_{r \geq r_1} \arg(d(r)/\tilde{d}(r)) < c_2(\varsigma)$ with a certain constant $c_2(\varsigma) > 0$. For the simplest possible scaling $\tilde{r}(r) = (1 + \gamma)(r - r_1) + r_1$, $r > r_1$ this condition can be interpreted as a restriction on the damping strength. In Fig. 1 we show the geometries and meshes for an anisotropic and two isotropic examples which admit the same resonances. In Fig. 2 we present the computed spectrum with a radial PML method. We recognize a good correspondence between the computations and the reference values. The quality of the computed resonances from the anisotropic example is intermediate between the quality of the isotropic examples.
A PML implementation for convex domains of general shape in time-harmonic acoustics

Hadrien Bériot¹, Axel Modave²,*

¹Siemens Industry Software N.V., Leuven (Belgium)
²POEMS, CNRS, Inria, ENSTA Paris, Institut Polytechnique de Paris (France)
*Email: axel.modave@ensta-paris.fr

Abstract

We address the efficient finite element solution of exterior acoustic problems with convex truncated computational domains of general shape surrounded by perfectly matched layers (PMLs). In this contribution, we will present a PML implementation that is versatile and automatic for the end-user. It relies on a mesh extrusion, a modification of the Jacobian matrix in the element-wise integrals and a parameter-free absorbing function. Only the PML thickness must be chosen. It will be validated and compared to other implementations using 2D and 3D cases.

Keywords: Finite elements, Helmholtz equation, Non-reflecting boundary condition, PML

1 Introduction

The PML is a popular absorbing boundary technique that combines accuracy, geometric flexibility and computational efficiency. In order to reduce the computational cost, it can be advantageous to minimize the size of the domain, leading to regions with general shapes.

Conformal PML formulations can address convex domains of general shape with smooth boundaries [3,5]. However, they depend on geometric parameters (e.g. principal curvatures and principal directions of the border), which may not be explicitly known if the geometry is complicated or if only the mesh is available.

In this short paper, we present a comprehensive implementation strategy, recently studied in [2] and based on [1], for Helmholtz problems. It is a specific implementation of the conformal PML for cases with smooth borders, but it can also be applied to cases with non-regular borders in an empirical way. After a presentation of the conformal PML, we present key aspects of our implementation and a numerical illustration.

2 Conformal PML

Let us consider a convex computational domain \( \Omega_{\text{dom}} \) with a regular exterior border \( \Gamma \). The layer \( \Omega_{\text{pml}} \) is generated by extruding \( \Gamma \) in the normal direction \( \mathbf{n} \) with a constant thickness.

To derive the PML equation, the Helmholtz equation is written in a local curvilinear coordinate system \((\xi_1, \xi_2, \xi_3)\) associated to \( \Gamma \). For each point \( \mathbf{x} \) of the layer, the coordinate \( \xi_1 \) is the distance to the closest point \( \mathbf{p} \) belonging to \( \Gamma \), and the coordinates \((\xi_2, \xi_3)\) are provided by a local parametrization of \( \Gamma \) at \( \mathbf{p} \). After, the coordinate \( \xi_1 \) is replaced with the complex coordinate \( \xi_1(\xi_1) := \xi_1 - f(\xi_1)/(\iota k) \), with \( f(\xi_1) := \int_0^{\xi_1} \sigma(\zeta) \, d\zeta \), where \( \sigma(\zeta) \) is the so-called absorbing function. See e.g. [3,5].

By using standard techniques, we get the following variational formulation of the problem:

\[
\begin{aligned}
\text{Find } u \in H^1(\Omega) \text{ such that, for all } v \in H^1(\Omega), \\
\int_{\Omega_{\text{dom}}} \left( (\mathbf{J}_{\text{pml}}^{-1} \nabla_x u) \cdot (\mathbf{J}_{\text{pml}}^{-1} \nabla_x v) - k^2 uv \right) \, d\Omega + \int_{\Gamma} \nabla_x u \cdot \nabla_x v - k^2 uv \, d\Omega = \int_{\Omega_{\text{dom}}} f v \, d\Omega,
\end{aligned}
\]

with \( \alpha_{\text{pml}} := \det(\mathbf{J}_{\text{pml}}) \) and the Jacobian matrix associated to the complex stretch,

\[
\mathbf{J}_{\text{pml}} := 1 - \frac{1}{\iota k} \left( \sigma(\xi_1) \mathbf{n} \mathbf{n}^\top + \sum_{j=2,3} \frac{\kappa_j f(\xi_1)}{\iota + \kappa_j f(\xi_1)} \mathbf{t}_j \mathbf{t}_j^\top \right),
\]

where \( \{\kappa_j\}_{j=2,3} \) are the principal curvatures and \( \{\mathbf{t}_j\}_{j=2,3} \) are the principal directions of \( \Gamma \).

3 PML implementation

The direct finite element implementation of the conformal PML requires the knowledge of the coordinate \( \xi_1 \) (which is a distance function) and the principal curvatures/directions of \( \Gamma \) at every point of the layer. We propose an implementation that provides all the required data.

Mesh extrusion and interpolation

The mesh of the layer is generated by extruding the mesh of the surface, \( \Gamma_h \), along a direction \( \mathbf{n}_h \) corresponding to the exterior normal. An empirical rule is proposed in [2] to deal with
polyhedral surfaces. During this step, the distance function $r_h$, the direction $n_h$ and the position of the closest point $p_h$ are recorded at the nodes of the extruded mesh. Then, these nodal values are interpolated on every element of the layer by using polynomial basis functions. The interpolated fields verify $x_h = p_h + r_h n_h$ everywhere, not only at the nodes.

**Computation of element-wise integrals**

The second key aspect of our approach is related to the computation of the element-wise integrals in the finite element matrix. For a given element $D_e$ of $\Omega_{\text{pml}}$, a typical integral reads

$$\int_{D_e} (J_{\text{pml},h}^{-\top} \nabla x_A) \cdot (J_{\text{pml},h}^{-\top} \nabla x_B) \alpha_{\text{pml},h} \, dD_e,$$

where $\Psi_A$ and $\Psi_B$ are global basis functions. Using the mapping between the physical element $D_e$ and the reference element $D_{\text{ref}}$, this integral can be rewritten as

$$\int_{D_{\text{ref}}} (J^{-\top} \nabla x_A) \cdot (J^{-\top} \nabla x_B) \left( \det J \right) \, dD_{\text{ref}},$$

where $\psi_a$ and $\psi_b$ are local basis functions that depend on the reference coordinates $(u_1, u_2, u_3)$. The Jacobian matrix $J := J_{\text{pml}} J_{\text{ref}}$ contains both the reference mapping and the complex stretch. The expression of $J$ can be simplified by considering that the stretched coordinate actually is the interpolated distance function $r_h$. Then, the matrix $J$ can be written explicitly as

$$J = J_{\text{ref}} - \frac{1}{ik} \left[ \left( \partial_{u_1} r_h \right) \sigma(r_h) n_h ; \right.$$

$$\left. f(r_h) \partial_{u_2} n_h ; f(r_h) \partial_{u_3} n_h \right].$$

This specific representation of the Jacobian matrix is the main novelty of this work.

**Remarks**

If the border of the domain is smooth, this approach is a specific implementation of the conformal PML with $\xi_1 \approx r_h$. Otherwise, it is an empirical approach that is rather good for edges and corners with obtuse angles.

A simple alternative [4] corresponds to using $J := \left[ \partial_{u_1} \tilde{x}_h ; \partial_{u_2} \tilde{x}_h ; \partial_{u_3} \tilde{x}_h \right]$, where $\tilde{x}_h$ corresponds to the stretched interpolated position vector. However, with this alternative, the function $\sigma$ and $f$ are interpolated, which introduce spurious errors if they are not polynomial.

We use a hyperbolic absorbing coefficient, $\sigma(r_h) = 1/(\delta - r_h)$, with the layer thickness $\delta$. It provides good accuracy without requiring the tuning of free parameters, by contrast with polynomial functions.

**4 Numerical illustration**

We consider the scattering of a plane wave by a submarine. The border of the domain has been generated automatically with a convex hull algorithm. Simulations have been performed with P2 elements and PML thicknesses with 1, 5 and 10 mesh cells. The results are very close. More details and validation results are proposed in [2].

![Mesh of the computational domain](image1)

Figure 1: Mesh of the computational domain

![Directivity pattern of the scattered field](image2)

Figure 2: Directivity pattern of the scattered field for several PML thicknesses

**References**


Learned Infinite Elements

Thorsten Hohage¹,², Christoph Lehrenfeld¹, Janosch Preuß¹,²

¹Institute of Numerical and Applied Mathematics, University of Göttingen, Germany
²Max-Planck-Institute for Solar Systems Research, Göttingen, Germany

Abstract

We propose a new type of transparent boundary conditions which shares the algebraic boundary conditions with standard transparent boundary conditions, while the matrix entries are not derived analytically from the exterior PDE, but optimized or “learned” from a given Dirichlet-to-Neumann (DtN) operator. We study scalar time-harmonic second-order wave equations, which are separable in the exterior domain such that DtN can be written as a functional calculus of (typically) the Laplace-Beltrami operator on the coupling boundary. The optimization problem reduces to a rational approximation problem for the symbol of DtN. Convergence rates are determined by the singularities of the holomorphic extension of the symbol, and they are typically exponential. Learned Infinite Elements outperform classical methods such as Perfectly Matched Layers for the Helmholtz equation and also work seamlessly for strongly inhomogeneous layered media such as the atmosphere of the Sun.

Keywords: transparent boundary conditions, rational approximation, stratified media, exponential convergence

1 Introduction

We consider a linear second-order elliptic PDE

\[ Lu = f \quad \text{in} \quad \Omega + \quad \text{radiation condition}, \quad (1) \]

on some unbounded domain \( \Omega \subset \mathbb{R}^d \) which is the disjoint union of a bounded interior domain \( \Omega_{\text{int}} \) with \( \text{supp} f \subset \Omega_{\text{int}} \), an unbounded exterior domain \( \Omega_{\text{ext}} \) where \( \Delta \) is separable and a smooth coupling boundary \( \Gamma = \partial \Omega_{\text{int}} \cap \partial \Omega_{\text{ext}} \). For computing accurate approximations of the solution \( u \) in \( \Omega_{\text{ext}} \) with as little as possible computational effort for the treatment of \( \Omega_{\text{ext}} \) a number of different methods have been proposed and analyzed including Perfectly Matched Layers, different type of infinite elements, local transparent boundary conditions, and others.

\[ \Delta u = dtn(\lambda)u \quad \text{in} \quad \Omega_{\text{ext}} \]

Figure 1: Learned Infinite Elements can be seen as classical finite elements on some artificial domain, the violet are indicates one such element. System matrices are learned within the algebraic structure of finite element discretizations to approximate a given DtN operator.

2 Reduction to a rational approximation problem

By separability we mean that there exists a diffeomorphism \( \Psi : (a, \infty) \times \Gamma \rightarrow \overline{\Omega}_{\text{ext}} \) such that \( \Psi((a) \times \Gamma) = \Gamma, |\partial_x \psi(a, x)| = 1, x \in \Gamma \) and

\[ (Lu) \circ \Psi = [A \otimes \text{Id}_{\Gamma} + B \otimes (-\Delta_{\Gamma})](u \circ \Psi) \quad (2) \]

Here \( A \) is a second-order differential operator in \( r \), \( B \) is a multiplication operator on \( L^2((a, \infty)) \), \( \Delta_{\Gamma} \) is the Laplace-Beltrami operator on \( \Gamma \), and \( \text{Id}_{\Gamma} \) the identity operator on \( L^2(\Gamma) \). Then the exterior PDE separates into a sequence of ordinary differential equations \( (A + \lambda \partial_x B)\varphi_{\ell} \) indexed by the eigenvalues \( \lambda \) of \( -\Delta_{\Gamma} \). If \( \{\varphi_{\ell} : \ell \in \mathbb{N}\} \) is a corresponding orthonormal \( L^2 \) basis of eigenvectors of \( \Delta_{\Gamma} \), the Dirichlet-to-Neumann map DtN on \( \Gamma \) can be written as a functional calculus

\[ \text{DtN} u_0 = dtn(-\Delta_{\Gamma})u_0 = \sum_{\ell=1}^{\infty} dtn(\lambda_{\ell}) \langle u_0, \varphi_{\ell} \rangle \varphi_{\ell} \]

with a function \( dtn(\lambda_{\ell}) = \varphi'_{\ell}(a)/\varphi_{\ell}(a) \) that we will refer to as symbol of DtN.
It turns out that for tensor product discretizations of Perfectly Matched Layers, infinite elements and other methods, the discrete analog $\text{DtN}$ of DtN has a similar form,

$$\text{DtN} = \text{dtN}(\Delta_{\Gamma})$$

with a discrete approximation $\Delta_{\Gamma}$ of $\Delta_{\Gamma}$. Here $\text{dtN}_N$ is a rational function which is given explicitly in terms of the matrix representations $\mathbf{A}, \mathbf{B} \in \mathbb{C}^{(N+1) \times (N+1)}$ of the operators $\mathbf{A}$ and $\mathbf{B}$ in (2) (or transformations of these operators), more precisely $\text{dtN}_N = r/q$ with polynomial $r, q$ of degrees $\deg(r) = N + 1$ and $\deg(q) = N$ (see Fig. 1).

In Learned Infinite Elements the matrices $\mathbf{A}$ and $\mathbf{B}$ are not derived analytically, but “learned” from the symbol $\text{dtN}$ of DtN by solving a rational approximation problem in a preprocessing step. If $\text{dtN}_N$ has only simple poles (and such rational functions are dense in the set of rational functions of the given degree), then the right lower $N \times N$ blocks of $\mathbf{A}$ and $\mathbf{B}$ can be chosen diagonal such that Learned Infinite Elements lead to sparser system matrices than most other methods.

3 holomorphic extensions of the symbol and convergence rates

The error of the DtN approximation can be bounded in terms of a weighted error of the rational $\text{dtN}$ approximation. It is known that the approximation rate of the latter is usually exponential in $N$ if $\text{dtN}$ has a holomorphic extension, and it is determined by the position of singularities of this holomorphic extension. E.g., for the Helmholtz equation, $L = \Delta + k^2$ in the exterior of a disk with radius $a$, the symbol $\text{dtN}^\text{hom}(\lambda) = \frac{kH(1)}{a\sqrt{\lambda}}(ka)/H(1)(ka)$ has simple poles tending to infinity along an implicitly defined curve (see Fig. 2a and [2]). We get exponential convergence, which is considerably faster than for competing methods (see Fig. 3). For a homogeneous waveguide, rational approximations to $\text{dtN}^\text{guide}(\lambda) = -i\sqrt{k^2 - \lambda}$ are also known to converge of order $O(\exp(-\sqrt{N}))$ as $N \to \infty$.

For stratified media exhibiting internal reflections where $\text{dtN}$ is usually not explicitly known, in particular the solar atmosphere, we observed poles close to the real axis, but only very few. This is in line with the observed very rapid convergence of Learned Infinite Elements in our numerical experiments.

References


Transient, global-in-time, convergent iterative coupling of acoustic BEM and elastic FEM

Alice Nassor\textsuperscript{1,*}, Marc Bonnet\textsuperscript{1}, Stéphanie Chaillat\textsuperscript{1}
\textsuperscript{1}POEMS, ENSTA Paris, Institut Polytechnique de Paris, 828 boulevard des Maréchaux, 91120 Palaiseau, France
\textsuperscript{*}Email: alice.nassor@ensta-paris.fr

Abstract. Motivated by ongoing studies in naval engineering, we address a domain decomposition approach for the numerical solution of transient problems involving submerged elastic structures subjected to pressure waves. The fluid region is treated with boundary elements (BEM), formulated in discrete time by the Convolution Quadrature method (CQM), a classical finite element method (FEM) is used for the solid, and the two media are coupled globally in time via iteratively solving Robin problems in each domain. We prove the convergence of this iterative algorithm, and demonstrate it on 2D numerical examples.

Keywords: Acoustic-elastic coupling, iterative methods, convolution quadrature

Introduction Motivated by an ongoing applied study in naval engineering, this work addresses a domain decomposition approach for the numerical solution of large-scale transient problems involving submerged structures subjected to pressure shock waves caused by remote underwater explosions and travelling in the surrounding fluid at short time scales.

Treating such situations as transient acoustic scattering by elastic obstacles is valid from an industry standpoint. The fluid response is formulated in the discrete-time domain, using a Z-BEM approach that combines a fast boundary element method (BEM) implemented in the in-house fast multipole solver COFFEE in the Laplace domain [2] with the convolution quadrature method (CQM), see details in [6]. Efficiency requires the Z-BEM formulation to be applied for the entire time interval at once. The structure response is modelled using standard finite element and time-stepping methods.

Earlier attempts at iteratively solving the resulting BEM-FEM coupling by alternating Neumann solutions in each domain have failed due to non-convergence. We hence focus in this work on an iterative algorithm based on Robin boundary conditions for the coupled elastodynamic-acoustic problem.

Acoustic-elastic scattering problem The fluid-structure interaction (FSI) problem is:

\begin{equation}
-\Delta \phi(t, x) + \frac{1}{c^2} \partial_t \phi(t, x) = 0 \quad \text{in } \Omega \times [0, T],
\end{equation}

\begin{equation}
-\text{div}[\mathbf{u}] + \rho_g \partial_t \mathbf{u} = \mathbf{0} \quad \text{in } \Omega_g \times [0, T],
\end{equation}

\begin{equation}
\mathbf{t} = \rho_i \partial_t \phi + \rho_f \partial_t \phi^{\text{inc}} \mathbf{n} \quad \text{in } \Gamma \times [0, T],
\end{equation}

\begin{equation}
v = \partial_t \mathbf{u} - \partial_n \phi^{\text{inc}} \quad \text{in } \Gamma \times [0, T]
\end{equation}

and initial-rest conditions, where \( \Omega_s \) is an elastic solid surrounded by the acoustic fluid domain \( \Omega_f := \mathbb{R}^3 \setminus \Omega_s \) and \( \Gamma = \partial \Omega_s \). The fluid velocity potential is decomposed into a given incident field \( \phi^{\text{inc}} \) and an unknown scattered field \( \phi \) (with velocity \( v = \nabla \phi \) and pressure \( p = -\rho \partial_t \phi \)). The total solid displacement is \( \mathbf{u} \), and \( \mathbf{t} := \sigma \mathbf{n} \) is the stress vector. Problem (1) is well-posed [5], and so is its frequency-domain counterpart [1].

Robin-Robin iterations Inspired by the convergent iterative domain decomposition (DD) approach of [3] for frequency-domain Helmholtz problems, based on Robin solutions in each domain, we propose for solving the problem (1) an iterative DD method based on a sequence of Robin initial-boundary value problems, iteration \( i + 1 \) being defined by boundary conditions of the form

\begin{equation}
-\rho \partial_t \phi^{i+1} + k_t \partial_n \phi^{i+1} = g^{i+1} \quad \text{in } \Gamma \times [0, T]
\end{equation}

\begin{equation}
\mathbf{t}^{i+1} + k_s \partial_t \mathbf{u}^{i+1} = \mathbf{g}^{i+1} \quad \text{in } \Gamma \times [0, T]
\end{equation}

where \( k_t, k_s > 0 \) are adjustable parameters and the Robin data \( g^{i+1} \) (for the fluid) and \( \mathbf{g}^{i+1} \) (for the solid) are defined in terms of the solution traces from iteration \( i - 1 \) by

\begin{equation}
g^{i+1} = \mathbf{n} \cdot (-\mathbf{t} + k_s \partial_n \mathbf{u}) + \rho \partial_t \phi^{\text{inc}} + k_s \partial_n \phi^{\text{inc}}
\end{equation}

\begin{equation}\mathbf{g}^{i+1} = (\mathbf{n} \otimes \mathbf{n} - \mathbf{I}) \cdot (\mathbf{t} - k_s \partial_n \mathbf{u}) + \mathbf{n} (\rho \partial_t \phi + k_s \partial_n \phi)^{\text{inc}}
\end{equation}

for the simplest case \( k_t = k_s \) (corresponding formulas for \( k_t \neq k_s \) being also available). The RR iterations (2a,b) are started by setting \( \phi^0 = \)
\( u^0 = 0 \). With the terminology used in [3], the incoming traces of iterate \( i+1 \) are related by (2a,b) to the outgoing traces of iterate \( i \).

**Convergence** We prove that the RR iterations defined by (2a,b) converge; more precisely, we show that:

(a) If \( \partial \phi^{\text{inc}}, \partial_n \phi^{\text{inc}} \in L^2(\Gamma \times [0, T]) \), the incoming and outgoing traces of each iterate generated by (2a,b) also are in \( L^2(\Gamma \times [0, T]) \), by a classical energy estimate argument [4].

(b) the \( C^0([0, T], H^1(\Omega_i) \cap C^1([0, T], L^2(\Gamma_i)) \) norm of the error field \( \phi' - \phi \) vanishes in the limit \( i \to \infty \), and similarly for the error field \( u' - u \). This is proved by showing that the norms of all error iterates have a sum bounded by a positive constant.

In addition, transient BEM-FEM coupling based instead on Neumann-Neumann iterations would be problematic as energy estimates indicate that each iteration degrades the regularity of boundary traces (unlike in the elliptic case).

We are also currently working on obtaining data-to-solution solvability mappings for problem (1) that supplement the result of [5] and show that the FSI solution has all (co)normal derivatives and velocity traces in \( L^2(\Gamma \times [0, T]) \) if \( \partial_n \phi^{\text{inc}}, \partial_n \phi^{\text{inc}} \in H^1([0, T], L^2(\Gamma)) \), in which case the FSI solution is attainable by RR iterates.

**Numerical results** Numerical examples for the FSI problem (1) for 2D geometries solved using FEM-BEM iterative coupling will be presented, demonstrating convergence as well as enhancements such as a relaxed version of (2a,b) and Aitken-type convergence acceleration.

Consider for example the case of an elastic ring subjected to an internal radially-symmetric transient pressure and immersed in an acoustic fluid. This problem, which can be put in the format (1) upon splitting the solid (rather than the fluid) response, is useful for validation purposes as it has a radially-symmetric analytical solution against which to compare the response computed using the 2D BEM-FEM iterative coupling method (Figure 1). Figure 2 shows the convergence of the relative solution error (in space-time \( L^2 \) norm) as iterations progress.

**Acknowledgement.** The thesis of A. Nassor is funded by DGA (Direction Générale de l’Armement) and Naval Group. We thank G. Barras, O. Grosset (DGA) and B. Leblé (NG) for their support and input.

References


Dirichlet-to-Neumann Coupling for 2D-1D Time-Dependent Wave Problems

Dan Givoli\(^1,\star\), Daniel Rabinovich\(^1\)

\(^1\)Dept. of Aerospace Engineering, Technion, Haifa, Israel\(^{\star}\)

Email: givolid@technion.ac.il

Abstract

The coupling of two-dimensional (2D) and one-dimensional (1D) models to form a single hybrid 2D-1D model is considered, for the time-dependent linear scalar wave equation. The 1D model is an approximation of a part of the original 2D model where the solution behaves approximately in a 1D way. This hybrid model, if designed properly, is a more efficient way to solve the problem compared to the full 2D model. The 2D-1D coupling is done using the Dirichlet-to-Neumann (DtN) map associated with the 1D part of the problem. We shall discuss two ways in which the DtN coupling can be done: in one of them the 2D and 1D problems exchange information in each time step, whereas in the other the two problems are solved independently. The well-posedness of the hybrid problem as well as the coupling error are discussed, and numerical examples are presented.

Keywords: coupling, mixed-dimensional, 2D-1D, Dirichlet-to-Neumann, DtN

1 Introduction

A reoccurring theme in computational mechanics in recent years is the need to reduce the size of large discrete models. One type of such a reduction is spatial dimensional reduction, which one may perform in cases where the solution in some region of a high-dimensional (highD) computational domain, say two-dimensional (2D), behaves in a low-dimensional (lowD) way, say one-dimensional (1D). There are several scenarios where this could be the case. Most significant is the scenario where the solution in a certain region behaves in a way that is weakly (or hardly) dependent on a certain coordinate, relative to the other coordinates. Another possible scenario is when we are interested in the solution within a geometrically slender region. In this case we might be interested in the lateral average of the solution within this region rather than in its lateral distribution. Alternatively we might already know the nature of the lateral distribution of the solution within this region and wish to know the axial distribution. In these cases, the lateral dimension is the dimension we would eliminate, resulting in a mixed-dimensional model. Fig. 1 describes the typical characteristics of the highD and lowD sub-models.

The motivation in constructing a mixed-dimensional model comes from the fact that solving the problem in its highD form everywhere may require a very large computational effort. The idea is thus to partly reduce the spatial dimension of the problem in order to obtain a hybrid model which is much more efficient. Fields of application where mixed-dimensional coupling is of special interest include, among others, the following:

- **Blood-flow analysis.** Typically the HighD model corresponds to a specific blood vessel in the human body and the LowD model corresponds to the rest of the blood system. An example can be found in [1].

- **Hydrological and geophysical flow models.** Here the LowD region represents a collection of channel-like entities (rivers, flood streams, etc.) and the HighD region is that of a large water body (a river delta, a lake, etc.).

- **Elastic structures.** Typically the LowD model consists of the slender parts of the structure that have rod- or beam- or plate- or shell-like behavior, and which constitute most of the structure volume, while the HighD parts are the regions that have to be modeled as 3D elastic bodies. Panasenko et al. have developed an asymptotic-variational approach for such structural problems, under static conditions. See, e.g., [2].

Our focus in this work is the latter application, although the coupling methods developed are general and may be useful for other applications as well. In this talk, we apply 2D-1D cou-
Two regions: highD (e.g., 2D) and lowD (e.g., 1D)

<table>
<thead>
<tr>
<th>highD</th>
<th>lowD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Region of interest</td>
<td>‘Outer region’ – less of interest in itself, but affects the behavior in the highD region significantly</td>
</tr>
<tr>
<td>General geometry</td>
<td>Typically a slender region</td>
</tr>
<tr>
<td>highD behavior of the solution</td>
<td>lowD behavior of the solution (e.g., the solution varies only slightly in the lateral direction, or only the average in that direction is of importance)</td>
</tr>
<tr>
<td>PDE, BCs, ICs: faithful to the highD physics</td>
<td>PDE, BCs, ICs are lowD approximations of their highD counterparts (reduced model)</td>
</tr>
</tbody>
</table>

Figure 1: The characteristics of the highD and lowD sub-models

After splitting the given problem into a 2D part and a 1D part, thus creating a hybrid 2D-1D model, we need to consider the interface conditions imposed at the continuous level (i.e., before any discretization takes place). There are two interface conditions: on the wave function $u$ (the acoustic pressure) and on its “flux” (the normal derivative $\partial u/\partial n$). We discuss the well-posedness of the hybrid problem using these two continuity conditions.

3 DtN mixed-dimensional coupling

As mentioned above, the 2D-1D coupling is done using the Dirichlet-to-Neumann (DtN) map associated with the 1D part of the problem. The DtN map relates the primary variable to the “flux” on an interface. In the mixed-dimensional context, the DtN method couples the highD and lowD models by enforcing the continuity of the DtN map across the highD-lowD interface. The rationale is that rather than insisting that both the primary variable and the flux be continuous across the interface, it makes sense to have the mapping between them continuous. The DtN method was used in [3] for the Helmholtz equation, for the case where the 2D behavior is persistent in the 1D region. In the time-harmonic case (the frequency domain), the DtN method has been found to be especially effective [3, 4]. Here we use the DtN map coupling in the time domain, which is a major extension.

We shall discuss two ways in which the DtN coupling can be done: in one of them the 2D and 1D problems exchange information in each time step [5], whereas in the other the two problems are solved independently.

By experimenting with various numerical examples, we shall investigate the performance of these methods and estimate the errors that each of them generates.

References


One-equation coupling of Curvilinear Virtual Element and Boundary Element methods for the wave equation in unbounded domains

Matteo Ferrari\textsuperscript{1,\ast}, Luca Desiderio\textsuperscript{2}, Silvia Falletta\textsuperscript{1}, Letizia Scuderi\textsuperscript{1}
\textsuperscript{1}DISMA, Department of Mathematical Sciences “Giuseppe Luigi Lagrange”, Politecnico di Torino, Corso Duca degli Abruzzi, 24, 1029 Torino, Italy
\textsuperscript{2}Department of Mathematical, Physical and Computer Sciences, University of Parma, Parco Area delle Scienze, 53/A, 43124 Parma, Italy
\ast Email: matteo.ferrari@polito.it

Abstract

We consider here wave propagation problems in bi-dimensional unbounded domains and, for their numerical solution, we propose the one-equation coupling of a Curvilinear Virtual Element Method (CVEM) with a Boundary Element Method (BEM). In particular, for the approximation in space, we consider decoupled approximation orders for the interior CVEM and the collocation BEM. For the approximation in time, we apply a time marching Crank-Nicolson scheme in the interior domain with the Lubich time convolution quadrature (CQ) formulas on the boundary. Exploiting the high order flexibility of the CVEM, the overall method allows us to use a low order BEM to retrieve accurate discrete solutions. Numerical tests show the effectiveness of the proposed approach.

Keywords: CVEM-BEM, one-equation coupling, convolution quadrature formula

1 Introduction

Let $\Omega_0 \subset \mathbb{R}^2$ a bounded domain with Lipschitz boundary $\Gamma_0$. We consider the damped wave equation in the unbounded domain $\Omega_e := \mathbb{R}^2 \setminus \overline{\Omega}_0$

$$\frac{1}{c^2} \ddot{u}_e(x; t) + \alpha \dot{u}_e(x; t) - \Delta u_e(x; t) = f(x; t) \ (1)$$

with proper initial data and a Dirichlet boundary condition prescribed on $\Gamma_0$. $c$ and $\alpha$ being the speed propagation and the damping parameter. Among the most commonly used approaches to solve (1), the Boundary Element Method turns out to be an appealing one, since it reduces the problem dimension by one, requiring only the discretization of the obstacle boundary. Once the boundary density is retrieved, the solution of the original problem at each point of the exterior domain is obtained by a post-processing procedure, based on an accurate computation of boundary integrals. However, this procedure may result not efficient, especially when the solution has to be evaluated in a wide region surrounding the obstacle. As an alternative approach, we define a finite computational domain, and we apply a coupling of an interior domain method with a boundary one. In literature, various coupling strategies have been proposed and extensively studied, among which we mention the Costabel-Han and the Johnson-Nédélec. Here we choose the latter, known also as the one-equation coupling, that, not involving a boundary integral operator of hypersingular type, is cheaper and easier to implement.

2 The one-equation coupling

Aiming at determining the solution $u_e$ of (1) in a bounded subregion of $\Omega_e$, we introduce an artificial boundary $\Gamma$ which defines a finite computational domain $\Omega$, bounded internally by $\Gamma$ and externally by $\Gamma$. Reformulating the PDE in the unbounded residual domain, in terms of a boundary integral equation (BIE) on $\Gamma$, and taking into account compatibility and equilibrium conditions, we reformulate the original problem as the coupling of the variational formulation of the wave equation in the interior domain, with the BIE on $\Gamma$. This latter involves both $u$, restriction of $u_e$ to $\Omega$, and its external normal derivative $\lambda := \nabla u \cdot n$, and reads

$$\frac{1}{2} u(x; t) + V \lambda(x; t) + K u(x; t) = 0$$

for $(x; t) \in \Gamma \times [0, T]$, $V$ and $K$ being the single- and double-layer integral operators associated to the wave equation, respectively. The BIE is discretized by means of a collocation BEM in space and the BDF2 Lubich CQ formula in time.

3 Curvilinear Virtual Element Method

We discretize the weak formulation of (1), in the interior domain, by applying a CVEM which, in
the spirit of the Virtual Element Method, consists in choosing conforming finite dimensional subspaces of $H^1(\Omega)$, whose “virtual” basis functions are not explicitly known. However, using only appropriate degrees of freedom, it is possible to compute an approximate version of the bilinear forms associated with the weak formulation. To avoid the approximation of the geometry in case of curvilinear obstacles, we consider a curvilinear VEM to guarantee the optimal convergence rate of the numerical method.

4 Decoupled approximation orders

We denote by $k_\circ$ and $k_\partial$ the approximation orders of the CVEM and the BEM, respectively, associated with the mesh diameters $h_\circ$ in $\Omega$ and $h_\partial$ on $\Gamma$. Based on the analysis performed in [2, 3] for the Helmholtz and Poisson problems, we may conjecture that at each fixed time, the error in the $L^2(\Omega)$-norm is bounded by

$$\|u - u_h\|_{L^2(\Omega)} = O(h_\circ^{k_\circ+1}) + O(h_\partial^{k_\partial+2}) + O(\Delta t^2),$$

$\Delta t$ being the time discretization parameter. The numerical tests confirm the expected error bound. We remark that the possibility of decoupling the approximation orders allows us to use a high order CVEM and a low order BEM. This turns out to be a great advantage for the global scheme, the accurate computation of the boundary integrals being a well-known bottleneck of the BEM, especially when the associated approximation order increases.

5 Numerical results

We consider equation (1) with null initial conditions and source term, $c = 1$, $\alpha = 0$, and Dirichlet datum

$$g(x; t) = t^2 e^{-t^2} \cos(x_1^2 + 2x_2^2), \quad (2)$$

in the region outside the unitary disk centered at the origin and, as artificial boundary, we choose the circle of radius 2. In Figure 1 we show the numerical solution obtained with orders $k_\circ = 2$, $k_\partial = 1$ in a mesh with 332,288 degrees of freedom, at the final time $T = 1$, with $\Delta t = 2.5\cdot10^{-3}$. In Figure 2 we report the convergence rate of the $L^2$-norm error for a fixed $\Delta t$ with respect to space refinements. The optimal expected rate is reached for both choices of the discretization parameters.

![Figure 1: Solution of problem (1)-(2) at $T = 1$.](image1)

![Figure 2: $L^2$-norm at $T = 1$, with fixed $\Delta t$.](image2)

References


Discontinuous Galerkin-based domain decomposition method for boundary integral equations in electromagnetism

Francis Collino\textsuperscript{1}, Justine Labat\textsuperscript{1,}\textsuperscript{*}, Agnès Pujols\textsuperscript{1}

\textsuperscript{1}CEA-CESTA, Le Barp, France
\textsuperscript{*}Email: justine.labat@cea.fr

Abstract

We propose a domain decomposition method to solve boundary integral equations applied to the time-harmonic electromagnetic wave scattering problem by perfectly conducting objects. Our entirely surface-based approach is derived from the formalism of volume interior penalty discontinuous Galerkin methods. The numerical solution is part of a preconditioned Krylov subspace method, all in the context of a massively parallel industrial code. Accuracy and efficiency of this method are illustrated with numerical simulations.

Keywords: Boundary integral equations, electromagnetism, domain decomposition methods, discontinuous Galerkin methods.

1 Introduction

The time-harmonic electromagnetic wave scattering problem by a perfectly conducting object $\Omega$ consists in finding the scattered electromagnetic fields $E$ and $H$ satisfying

\begin{align*}
\nabla \times E + i\kappa Z_0 H &= 0 \quad \text{in} \; \mathbb{R}^3 \setminus \Omega, \\
\nabla \times H - i\kappa Z_0^{-1} E &= 0 \quad \text{in} \; \mathbb{R}^3 \setminus \Omega, \\
n \times E &= -n \times E^{\text{inc}} \quad \text{on} \; \Gamma = \partial \Omega,
\end{align*}

where $\kappa$ is the wave-number, $Z_0$ is the impedance in vacuum, $n$ is the outward-pointing normal vector to $\Omega$ and $E^{\text{inc}}$ is the incident electric field. Uniqueness of the solution is guaranteed by a Silver-Müller radiation condition at infinity,

$$
\lim_{|x| \to \infty} |x| (Z_0 H \times \hat{x} - E) = 0, \quad \text{unif. in} \; \hat{x} = \frac{x}{|x|}.
$$

The scattered electromagnetic fields can be obtained using the Stratton-Chu formulas,

\begin{align*}
E &= -i\kappa T J \quad \text{and} \quad H = \frac{1}{Z_0} \kappa J \quad \text{in} \; \mathbb{R}^3 \setminus \Omega,
\end{align*}

where $T$ and $K$ denote respectively the electric and magnetic potential operators defined from the single-layer vector and scalar potential $S$ by

\begin{align*}
TJ &= \frac{1}{\kappa^2} \nabla (\nabla \cdot J) + SJ \quad \text{and} \quad KJ = \nabla \times SJ, \\
\mathcal{S} \lambda &= \frac{1}{\kappa^2} \int_{\Gamma} G(|x-y|) \lambda(y) \, ds_y, \quad G(r) = \exp(-i\kappa r)\frac{1}{4\pi r}.
\end{align*}

The electric current $J = Z_0 n \times (H + H^{\text{inc}})$, where $H^{\text{inc}}$ is the incident magnetic field, can then be obtained by solving one of the following boundary integral equations

\begin{align*}
i\kappa TJ &= (n \times E^{\text{inc}}) \times n \quad \text{on} \; \Gamma, \quad (\text{EFIE}) \\
\frac{1}{2} J - KJ &= Z_0(n \times H^{\text{inc}}) \quad \text{on} \; \Gamma, \quad (\text{MFIE}) \\
\alpha(\text{EFIE}) + (1 - \alpha)(\text{MFIE}) \quad \text{on} \; \Gamma, \quad (\text{CFIE})
\end{align*}

where $T$ is the tangential trace of $T$, $K$ is the principal value of twisted tangential trace of $K$ and $\alpha \in (0,1)$.

2 Discontinuous surface formulation

We consider a non-overlapping partitioning $\Gamma_n$ for $n = 1, \ldots, N$ of the surface $\Gamma$ and we denote $\gamma_{nm} = \Gamma_n \cap \Gamma_m$ the interfaces between two adjacent subdomains. The derivation of the variational weak formulation for the discontinuous EFIE requires to enrich the Sobolev functional space associated with the current $J$. After restricting the EFIE to each subdomain, testing it with an appropriate test-function, integrating on each subdomain and integrating by parts, we sum over all the subdomains and finally obtain: Find $J \in \bigoplus_{n=1}^{N} L^2_{\Gamma_n}(\nabla \Gamma_n, \Gamma_n)$ such that

\begin{align*}
ar_T(J, v) &= a_T^J(J, v) + p_e^s(J, v) \\
&= \sum_{n=1}^{N} \langle (n \times E^{\text{inc}}) \times n, v_n \rangle\gamma_n,
\end{align*}

for any $v \in \bigoplus_{n=1}^{N} L^2_{\Gamma_n}(\nabla \Gamma_n, \Gamma_n)$. The bilinear form $a_T$ comes from the classical EFIE formulation and is given by

\begin{align*}
ar_T(J, v) &= \sum_{n=1}^{N} \sum_{m=1}^{N} \frac{1}{i\kappa} \langle S nm(\nabla \Gamma_n J_m, \nabla \Gamma_n v_n)\gamma_n \\
&\quad + i\kappa \langle S nm J_m, v_n \rangle\gamma_n,
\end{align*}
where $S_{nm} : \Gamma_m \rightarrow \Gamma_n$ is the restriction of the single-layer operator $S$. The bilinear form $a_{\gamma}^{\pm} (J, v) = -\frac{1}{\kappa} \sum_{m=1}^{N} \sum_{\gamma_{nm}} \left[ S_{nm} \text{div}_{\Gamma_m} J_m, [v]_{\gamma_{nm}} \right]_{\gamma_{nm}}$

$$\pm \frac{1}{\kappa} \sum_{m=1}^{N} \sum_{\gamma_{nm}} \left[ S_{nm} \text{div}_{\Gamma_m} v_m, [J]_{\gamma_{nm}} \right]_{\gamma_{nm}},$$

where $[\cdot]_{\gamma}$ denotes the normal jump operator at contour $\gamma$. The choice of a non-local or an anti-symmetric formulation can have an impact on the convergence of the iterative solver depending on the choice of the boundary integral equation. Finally, the bilinear form $p_{\gamma}^\pm$, generally known as penalization term in discontinuous Galerkin volume methods, can take as value one of the two following expressions

$$p_{\gamma}^\pm (J, v) = \frac{\beta_h}{\kappa} \sum_{\gamma_{nm}} ([J]_{\gamma_{nm}}, [v]_{\gamma_{nm}})_{\gamma_{nm}},$$

$$\left( p_{\gamma}^{-\frac{1}{2}} (J, v) = \beta \sum_{\gamma_{nm}} (S_{\gamma_{nm}} [J]_{\gamma_{nm}}, [v]_{\gamma_{nm}})_{\gamma_{nm}} \right),$$

where $\beta_h$ and $\beta$ are two positive real numbers and $S_{\gamma} \lambda = \frac{1}{2\pi} \int_{\gamma} K_0(|x| - y) \lambda(y) \, d\sigma_y$ is the two-dimensional single-layer potential defined on a contour $\gamma$. In comparison with [1], the novelty is the introduction of a non-local penalization term $p_{\gamma}^{-\frac{1}{2}}$ which defines a $H^{-\frac{1}{2}}(\gamma)$ inner product and allows to make sense at continuous level when $J \in \bigoplus_{m=1}^{N} L^2(\text{div}_{\Gamma_m}, \Gamma_m)$. While the interior penalty parameter $\beta_h$ depends on the mesh size $h$ in $p_{\gamma}^\pm_h$ as for instance $\beta_h = c |\log \kappa h|$ with $c > 0$, the parameter $\beta$ in $p_{\gamma}^{-\frac{1}{2}}$ is independent on the mesh size because it is taken into account intrinsically into the single-layer operator $S_{\gamma}$. Moreover, that involves more robustness in the convergence of the iterative solver when the mesh size tends to zero. The variational formulation for the discontinuous MFIE is not subtle because no integration by parts is required.

### 3 Discretization and iterative solution

On each subdomain $\Gamma_n$, we introduce a boundary element space composed of restrictions of Raviart-Thomas boundary element of lowest degree. We end up with a linear system to solve $Ax = b$, where $A$ corresponds to the matrix coming from the chosen boundary integral formulation, $x$ is the unknown vector and $b$ the right hand-side composed of incident data. The matrix equation is then solved using a GMRes solver, for which we propose a block-diagonal Jacobi preconditioner where the diagonal blocks are associated with individual subdomains.

### 4 Numerical results

Numerical simulations show the accuracy of the approximation method compared to a classical boundary element solution. Figure 1 depicts the surface total electric current on a perfectly conducting cube of side 1m, at frequency 1GHz, using the EFIE formulation. The global mesh is partitioned into ten subdomains using Metis and admits non-conformities in the top face. The approximate solution is computed from a symmetric discontinuous Galerkin formulation using penalization $p_{\gamma}^{-\frac{1}{2}}$ where $\beta = 1$. Table 1 shows $L^2$-errors on jump at interfaces between subdomains and on radar cross-sections.

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Jump error</th>
<th>RCS error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Refined</td>
<td>$1.19 \cdot 10^{-3}$</td>
<td>$1.79 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>Coarse</td>
<td>$3.30 \cdot 10^{-3}$</td>
<td>$3.27 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>Non-conformal</td>
<td>$3.42 \cdot 10^{-3}$</td>
<td>$3.26 \cdot 10^{-3}$</td>
</tr>
</tbody>
</table>

Table 1: Comparison of $L^2$ errors between conformal and non-conformal meshes.

### References

Reduction of Leading-Edge Noise by Tailored Turbulence Anisotropy

Alistair D. G. Hales¹, Lorna J. Ayton²

¹DAMTP, University of Cambridge, Cambridge, United Kingdom
²DAMTP, University of Cambridge, Cambridge, United Kingdom

*Email: adgh3@cam.ac.uk

Abstract

This paper investigates the effect of anisotropic turbulence on the generation of turbulence-aerofoil interaction noise, also known as leading-edge noise, for a rigid plate. Thin aerofoil theory is used to model an aerofoil as a semi-infinite plate and the scattering of incoming turbulence is solved via application of the Wiener-Hopf technique. This theoretical solution encapsulates the diffraction problem for gust-aerofoil interaction, and is integrated over a wavenumber-frequency spectrum to account for general incoming turbulence. The specific wavenumber-frequency spectrum in the anisotropic case can be obtained using the method of Gaussian decomposition, in which the generalized spectrum is approximated through the weighted sum of individual Gaussian eddy models.

Keywords: Leading Edge Noise, Noise Control, Aeroacoustics, Turbulence Modelling

1 Introduction

Leading-edge noise, also known as turbulence-aerofoil interaction noise, is produced by the scattering of surface pressure fluctuations that are due to turbulent velocity fluctuations of a given incoming flow by the leading edge of a blade. It is known to be a dominant noise mechanism for many applications, such as in wind turbines, helicopter rotors, and turbofan engines. In this latter case, for engines with multi-row rotor systems, we find that the wake from turbulence interacting with rotor blades impinges on the downstream blade and is a dominant source of noise [1]. Regarding wind turbines, we find that the interaction of the blades with atmospheric turbulence causes unwanted noise particularly at low frequencies. Thus, there are industrial and social reasons to focus on reducing leading-edge noise, particularly to counteract harmful noise pollution.

2 Body of the paper

In this paper we calculate the power spectral density denoted $\Psi(\omega)$ for the rigid leading edge diffraction problem, given by

$$\Psi(\omega) = \int_{-\pi}^{\pi} \int_{-\infty}^{\infty} P(k, \theta) \Phi_{22}(k) \delta \left( k_1 - \frac{\omega}{U_\infty} \right) dk d\theta,$$

which will be given in SPL as a measure of the total observed far-field noise.

We discuss the two terms in the integrand separately, since they require different mathematical tools to model and solve them accurately and efficiently. This inherent duality in the problem provides scope in noise reduction by targeting both the scattering via the plate modelling, and by targeting how the spectrum modelling distributes energy.

First, $P(k, \theta)$ is the far-field pressure perturbation found by solving a convected Helmholtz equation for the scattered velocity perturbation $\phi_s$ and then applying Taylor’s frozen turbulence hypothesis to relate this to the pressure via $p = -\rho_0 \frac{D\phi_s}{Dt}$.

Having set up our governing equations, which include a pressure jump upstream and Neumann boundary conditions along the plate, we apply the Wiener-Hopf technique and the method of steepest descent to find the far-field scattered pressure.

$\Phi_{22}$ is the energy density spectrum, describing how the turbulent kinetic energy is distributed over wavenumbers. We model this using the method of Gaussian decomposition derived in [3] and applied to leading edge noise in [4].

We extend this approach to the case of axisymmetric turbulence via the model given in [2], however, unlike [4], we take a more mathematical approach. We derive a model that sums axisymmetric Gaussian filter kernels in order to approximate a generalized von Kármán type model (which differs by generalizing the inertial subrange scaling of the turbulence via the exponent.
p in the denominator) of the form

\[ \Phi_{22}^a(k) = \frac{2k_T(L^*\Lambda_a)^5\Lambda_4^4\Gamma(p)}{(1 + 2u_2^2)^{5/2}T(p - \frac{1}{2})} \times \frac{k_1^2 + \gamma k_3^2}{[1 + L^2\Lambda_2^2(k_1^2 + \Lambda_2^2 + k_3^2)]^p}. \]

Here we define the kinetic turbulence energy \( k_T \), \( L^* \) is a lengthscale parameter that ensures \( \Lambda_2 = \int_{0}^{\infty} R_{11}(x, 0, 0) dx \).

where \( R_{11} \) is the 1,1 velocity autocorrelation, or in the context of our work the spatial Fourier transform of the wavenumber spectrum \( \Phi_{11}(k) \). The subscripts \( a \) and \( t \) refer to quantities in either the axial or transverse direction with respect to the oncoming mean flow, and \( r \) denotes that it is a ratio of transverse to axial. Moreover, we use the parameter \( \gamma = 2u_2^2 - \Lambda_2^2 \) from [2]. The ratios of root mean velocity and integral length-scales in the transverse and axial direction satisfy the important constraint \( 2u_2^2 \geq \Lambda_2^2 \) in [2], which ensures that the power-spectral density remains non-negative.

Then, by finding a suitable weighting function \( f \) we get a good approximation to this axisymmetric model. The primary benefit of this turbulence model is that we can sum individual kernels with different \( p \) values or different length-scale ratios, which effectively allows us to adapt our modelling to the behaviour of the turbulence itself.

In figure 1, in which we have fitted our model to experimental data for a rigid plate in slightly anisotropic turbulence from our collaborators at UNSW Sydney. Different ratios of anisotropy were obtained by placing the leading edge at different distances from the wake of a cylinder.

In figure two we further test the trends observed from the experimental data using our model which was verified as accurate over a wide range of frequencies. We first test fully isotropic data, and then reverse the anisotropy ratio to favour the streamwise direction. Both cases show good noise reduction.

When matching to data, we find that \( p = \frac{11}{3} \) (the constant found for the Rapid Distortion Theory description of turbulence) gave excellent agreement to high frequency cut-off, verifying that cylinder turbulence has different scalings in the inertial subrange than standard grid generated turbulence that is usually modelled with either Liepmann (\( p = 3 \)) or von Kármán (\( p = \frac{17}{6} \)) turbulence models. The benefit of the Gaussian decomposition model is that the turbulence can be studied without considering scattering, and the behaviour can be modelled beforehand thanks to its versatility.

3 References

References


One-Way methods for wave propagation in complex flows

Maëlys Ruello1,∗, Clément Rudel1, Sébastien Pernet1, Jean-Philippe Brazier1

1ONERA The French Aerospace Lab, Toulouse, France
∗Email: Maelys.Ruello@onera.fr

Abstract
We propose a numerical factorization of the propagation operator in a privileged direction for linearized Navier-Stokes equations. From the latter, One-Way models such as the True Amplitude formalism and the Bremmer series can be derived.

Keywords: Wave propagation, Hydrodynamic waves, One-Way methods.

1 Introduction
The One-Way (OW) approach is an effective tool to compute wave propagation in a direction of interest. For example, such a method could be used to study the laminar-turbulent transition zone in boundary layers. However, the construction of this type of method in this context remains a challenge due to complex operators involved.

Towne & Colonius [1] have overcome this difficulty for slowly varying flows by proposing a purely numerical OW method based on a non-reflecting boundary condition applied to the Euler and Navier-Stokes equations.

We extend these works by proposing a new factorization of the propagation operator which allows a sorting of the modes according to their direction and accessing to a refraction/reflection operator. We can then derive OW models with broader validity, such as True Amplitude OW (TAOW) or Bremmer series.

2 Linearized Navier-Stokes equations
We are interested in computing with a low numerical cost the time-harmonic wave propagation in a complex flow, and considering a preferred direction: the \( x \)-axis in this presentation. To do so, we start with a 2D linearized model of the Navier-Stokes equations around a mean flow where the unknown fluctuation vector is \( \vec{q} = (\vec{v}, \vec{u}, \vec{v}, \vec{p})^T \) with \( \vec{v}, \vec{u}, \vec{v} \) and \( \vec{p} \) being the specific volume, velocity and pressure perturbations, respectively. Using standard hypothesis in wave propagation, the second derivatives in \( x \) are neglected. We next process as in [1] by isolating the term \( \frac{\partial}{\partial x} \) and by performing a first discretization in the transverse direction \( y \) (a compact high-order finite difference scheme in our case). So, we get the following matrix ODE in \( x \)-variable:

\[
A \frac{d\vec{q}}{dx} = \left( i\omega I - B_y D_y - B_{yy} D_{yy} - C \right) \vec{q}
\]

with \( D_y \) and \( D_{yy} \) the first and second order discrete derivative operators in \( y \)-variable. All the matrices are of size \((4N_y) \times (4N_y)\) with \( N_y \) the number of discretization points in the transverse direction \( y \). The matrix \( A \) is assumed to be diagonalizable, i.e. \( A = T \tilde{A} T^{-1} \) and invertible. If it contains singularities, they can be treated by extraction.

The equation (1) can be rewritten in terms of characteristic variables \( \phi = T^{-1} \vec{q} \):

\[
\frac{d\phi}{dx} = M(x)\phi
\]

where the propagation operator \( M \) is defined by:

\[
M = \tilde{A}^{-1} T^{-1} BT - T^{-1} \frac{dT}{dx}.
\]

3 New factorization of \( M \)
The construction of OW methods to solve (2) requires identifying the left and right-going modes contained in the propagation operator. A natural way is to perform a diagonalization of \( M \) and to analyze the behavior of the eigenvalues to find the different sets of modes (Briggs’ criterion). Unfortunately, this approach is generally costly in terms of computational resources, especially because \( M \) is \( x \)-dependent. To bypass this problem, we propose to construct a new decomposition of \( M \) based on the concept of high-order non-reflecting boundary conditions. The starting point is this remark: a strict diagonalization of \( M \) is not needed to realize a OW decoupling.
More precisely, by using this type of matrices
\[ Z^{r,N} := \prod_{j=0}^{N-1} (M - i\beta_j^r I)^{-1} (M - i\beta_j^l I) \]
\[ Z^{l,N} := \prod_{j=0}^{N-1} (M - i\beta_j^l I)^{-1} (M - i\beta_j^r I) \]
with \((\beta_j^r, \beta_j^l)_{j=0,\ldots,N-1}\) a set of parameters, the following theorem can be proven.

**Theorem 1** Let \( VDU \) be a diagonalization of \( M \) where \( D \) contains the \( N_\pm \) eigenvalues \( \alpha_\pm \) corresponding to the \( \pm x \) direction. The parameters \((\beta_j^r, \beta_j^l)_{j\in\mathbb{N}}\) satisfy the condition (C):
\[
\lim_{N \to +\infty} R^N(\alpha_+) = 0 \quad \text{and} \quad \lim_{N \to +\infty} R^N(\alpha_-) = +\infty
\]
with \( R^N(\alpha) := \prod_{j=0}^{N-1} \left| \frac{\alpha - \beta_j^r}{\alpha - \beta_j^l} \right| \).

We introduce the matrix
\[
\tilde{U}^N := \begin{pmatrix} I_{++} & (Z_{++}^{l,N})^{-1} Z_{++}^{r,N} \\ (Z_{--}^{r,N})^{-1} Z_{--}^{l,N} & I_{--} \end{pmatrix}
\]
where the subscripts denote the number of rows and columns (\( N_+ \) or \( N_- \)) of each block.

The following decoupling result holds: for \( \tilde{D}^N := \tilde{U}^N M (\tilde{U}^N)^{-1} \), let \( \tilde{D} := \lim_{N \to +\infty} \tilde{D}^N \),
\[
\tilde{D} = \begin{pmatrix} U_{++}^{-1} D_{++} U_{++} & U_{++}^{-1} D_{+-} U_{--} \\ 0 & U_{--}^{-1} D_{-+} U_{+-} \end{pmatrix}
\]
This theorem implies that by choosing a finite number of parameters \( \beta_j^r \), we can construct
\[
\tilde{D}^N = \tilde{U}^N M (\tilde{U}^N)^{-1} = \begin{pmatrix} \tilde{D}_{++}^{N} & \varepsilon \\ \varepsilon & \tilde{D}_{--}^{N} \end{pmatrix}
\]
where \( \tilde{D}_{++}^{N} \) and \( \tilde{D}_{--}^{N} \) are two block matrices containing the information about the right-going and left-going eigenvalues of \( M \), respectively and \( \varepsilon \) represents the residuals of the approximations, which will be neglected.

This choice is guided by (C). It is easy to find such kind of family, for example, \( \beta_{ij}^{r,l} = \pm (j + ij) \) for \( j \in \mathbb{N}^* \) but the convergence of the method can be greatly improved by using parameters nearer to the spectrum of \( M \). In practice, we use some *a priori* information on the spectrum of \( M \) such as the branch position of evanescent modes, the range of the convective modes branch etc., which are deduced from analytical results for simple mean flows [1] or from a numerical local stability analysis (see example below).

By using the factorization (3), the equation (2) can be written in terms of OW variables \( \psi = U^N \phi \):
\[
\frac{d\psi}{dx} = \tilde{D}^N \psi + W^N \psi
\]
with \( W^N := -\tilde{U}^N \frac{d\tilde{U}^N}{dx} \) the refraction/reflection matrix. Finally, we construct several OW propagation models: for example, right-going OW equations are derived as follows
\[
\frac{d\psi_+}{dx} = \tilde{D}_+^N \psi_+ + \delta W_+^N \psi_+ \quad \text{and} \quad \psi_- = 0
\]
with \( \delta = 0 \) for the standard OW and \( \delta = 1 \) for the TAOW. In the case of Bremmer series, we need to solve right and left OW equations iteratively until convergence.

### 4 Numerical example

![Figure 1](image.png)

**Figure 1:** Convergence on the spectrum: \( N = 7 \)

We consider a duct of height \( h \) and a mean flow verifying \((\overline{\varphi}, \overline{\varphi})\) constant and the velocity is:
\[
\overline{\varphi}(y) = 4V_{\max} \frac{y}{h} (1 - \frac{y}{h}) \quad \text{and} \quad \varphi = 0
\]
where \( V_{\max} \) is the maximum axial velocity.

In Fig. 1, \( \alpha \) corresponds to the exact operator spectrum, \( \lambda_+ \) and \( \lambda_- \) to the spectra of the operators \( D_{++}^N \) and \( D_{--}^N \), respectively. We see a good restitution of the spectrum from few \( \beta_\pm \) coefficients. During the congress, we will present numerical results obtained by some OW methods based on this new factorization.

### References

Instability and over-reflection of acoustic waves in compressible boundary layer flows

Felician Putz$^{1, *}$, Yi Zhang$^1$, Martin Oberlack$^1$

$^1$Chair of Fluid Dynamics, TU Darmstadt, Darmstadt, Germany

*Email: putz@fdy.tu-darmstadt.de

Abstract

2D direct numerical simulations of acoustic waves in supersonic compressible boundary layer flows were conducted using the high order discontinuous Galerkin method. The purpose was to verify both theoretically predicted instabilities and to show two mode doubling effects caused by a doubling in frequency and wave number, respectively. Secondly, simulated over-reflection coefficients show good agreements to theoretical results, and, most important, resonant over-reflection is verified in a narrow frequency band.

Keywords: PBE, over-reflection, DNS, stability, boundary layer acoustics

1 Introduction

Acoustic waves play a key role in numerous engineering applications. When these waves interact with a mean shear flow, e.g. in a boundary layer, the propagation is significantly affected and effects such as instabilities can arise so that the amplitude of an unstable wave increases with time. This may lead to a transition to turbulence and hence must be well understood.

Another acoustic effect in boundary layers is the reflection at the surface. During this process an incident wave traveling through the large velocity gradients in the shear layer deforms in amplitude and shape. Therefore over-reflection may occur which is when the amplitude of the reflected wave is larger than the amplitude of the incident wave. In this case, the acoustic wave absorbs energy from the main flow. The strength of this effects varies with wave number and frequency of the incident wave and in particular resonant over-reflection may occur in the vicinity of unstable modes, which is accompanied by a strong exaggeration of the amplitude.

2 Boundary layer acoustics

This study is confined to compressible, inviscid, homentropic boundary layer flows with an exponential velocity profile as a model problem. Based on these assumptions, the Euler equations can be linearized in terms of small acoustic perturbations. Combined into one equation and non-dimensionalized with the boundary layer thickness, the free-stream velocity and the density of the free-stream, this yields the Pridmore-Brown equation

$$
\frac{d^2 \rho}{d y^2} + \frac{2 \alpha e^{-y}}{\omega - \alpha + \alpha e^{-y}} \frac{d \rho}{d y} + \left[M^2 (\omega - \alpha + \alpha e^{-y})^2 - \alpha^2 \right] \rho = 0. \tag{1}
$$

This second order ODE for the density amplitude $\rho$ defines both the propagation and stability of the acoustic wave. Zhang & Oberlack [1] derived an exact solution to eq. (1) in terms of confluent Heun functions denoted by $He \left( \frac{\alpha}{\alpha - \omega} \right)$, in which “$\ast$” is an abbreviation for parameters depending on the dimensionless wave number $\alpha$, dimensionless frequency $\omega$ and Mach number $M$ [1]. The solution contains two Heun functions $He$ and $He'$ with different parameters that represent the incident and the outgoing wave. Based on this, the over-reflection coefficient is defined by

$$
R = \frac{(i M \alpha + \sqrt{\theta}) He \left( \frac{\alpha}{\alpha - \omega} \right) + \frac{\alpha}{\alpha - \omega} He' \left( \frac{\alpha}{\alpha - \omega} \right)}{(-i M \alpha + \sqrt{\theta}) He \left( \frac{\alpha}{\alpha - \omega} \right) - \frac{\alpha}{\alpha - \omega} He' \left( \frac{\alpha}{\alpha - \omega} \right)} \tag{2}
$$

with the parameter $\theta$ depending on $\alpha$, $\omega$ and $M$. $R$ is the ratio between the amplitude of the reflected to the incident wave. It is calculated from the solution to eq. (1) using the boundary conditions of an unit amplitude incident wave and vanishing normal velocity at the wall.

Stability is investigated by only considering a vanishing amplitude $\rho$ as $y \rightarrow \infty$. This is equivalent to the special case of $R = 0$ in which the numerator of eq. (2) defines an eigenvalue equation for the eigenvalue $\omega$ [1].
The frequency given by the eigenvalue problem is $\omega_{EV} = 1.028 + 11.0770 \cdot 10^{-2}$.

3 Temporal instability

The above mentioned eigenvalue equation has at least one solution for each Mach and wave number. The eigenvalue is written as $\omega_{EV} = \omega(M, \alpha)$ and is temporarily unstable for $\text{Im}(\omega_{EV}) > 0$. Having this in mind, a DNS is conducted with the non-linear Euler equations using the dG method of order 6. The initial condition is the incident wave of the linearized solution of eq. (1). Comparison of DNS and theory shows good agreement between the simulation as long as the amplitude of the pressure perturbation is less than 3% of the base flow pressure [2].

A deeper analysis reveals that the error caused by the linearization are due to two different mode doubling effects. A mode with twice the eigenvalue frequency $\omega_1 = 2\omega_{EV}$ and a mode, whose frequency $\omega_2 = \omega(M, 2\alpha)$ is the solution to the eigenvalue problem with a doubling of the wave number, are present. The two mode doubling frequencies are shown in figure 1 at $\omega_1 \approx 2$ and $\omega_2 \approx 1.5$. Additional modes for $n > 2$ are present but their amplitude is negligible compared to $n = 1$. The growth rates differ for each mode and for long times the amplitude at the original eigenvalue is dominant and the mode doubling effects become negligible.

4 Over-reflection

Simulations of over-reflection are conducted by placing an incident wave packet in the unsheared region of the domain. As $R$ is sensitive towards variations of wave number or frequency, particular attention was paid to the generation of the wave packet so that the wave is not distorted. The wave packet is then reflected at the wall and the ratio of the amplitude of the reflected wave to the incident wave is the over-reflection coefficient $R$, see eq. (2). The coefficient is extracted from the simulation by comparing the amplitude of incident and reflected waves over a section outside of the boundary layer. The result in comparison with the analytical values for $R$ computed by Zhang et. al (2022) are shown in figure 2 for $M = 5$, $\alpha = 4$ and varying frequencies [3]. Over-reflection occurs for all frequencies and a sharp peak, the resonant over-reflection, is located at $\omega \approx 1.85$. This is the frequency of the eigenvalue solution (numerator of eq. (2)) for the Mach and wave number. The simulation shows good agreements with the theoretical values of $R$. In particular, the resonant over-reflection is captured well.

References

[1] Zhang, Y. & Oberlack, M. Inviscid instability of compressible exponential boundary layer flows. AIP Advances. 11, 105308 (2021,10)
Accounting for viscothermal boundary losses in time-domain acoustics

Linus Hägg\textsuperscript{1,*}, Martin Berggren\textsuperscript{1}

\textsuperscript{1}Department of Computing Science, Umeå University, Umeå, Sweden
Email: linush@cs.umu.se

Abstract
It has recently been shown that viscothermal boundary losses may be accurately and efficiently captured by altering the boundary condition at solid walls in standard frequency-domain simulations of the acoustic pressure Helmholtz equation. Here, we investigate the corresponding time-domain boundary condition involving fractional differintegral operators. We analyze an initial-boundary-value problem with thermal boundary losses and report numerical experiments.

Keywords: acoustics, viscothermal boundary losses, Riemann–Liouville fractional integral

1 Introduction
Viscothermal boundary losses may have a significant impact on sound propagation in narrow geometries. In these situations sound propagation may be modeled by the linearized compressible Navier–Stokes equations. Unfortunately, it is computationally expensive to obtain numerical solutions to the linearized Navier–Stokes equations due to the high resolution needed to resolve the thermal and viscous boundary layers. Starting with the work of Cremer [2], simplified models that are appropriate close to the walls of the domain have been derived based on acoustic boundary layer theory. A notable contribution in this respect is the approximate boundary condition derived by Pierce [6] for single-frequency sound propagation. Recently, Berggren et al. [1] proposed a computationally effective procedure by rederiving and implementing Pierce’s boundary condition to account for viscothermal boundary losses in standard quiescent, linear frequency-domain acoustics, that is, as a boundary condition for the pressure Helmholtz equation.

The frequency-domain boundary condition (phase convention $\exp(i \omega t)$, $\omega > 0$) may be expressed in the (complex) acoustic pressure $\hat{p}$ and velocity $\hat{u}$, satisfying $i \omega \rho_0 \hat{u} = -\nabla \hat{p}$, as

\begin{equation}
\mathbf{n} \cdot \hat{u} = -\frac{c_{\gamma \tau}}{\sqrt{i \omega \gamma \tau}} \nabla \hat{u} + \sqrt{i \omega \tau} \frac{\hat{p}}{\rho_0 c^2}, \quad (1)
\end{equation}

where $\mathbf{n}$ denotes the exterior unit normal, $\sqrt{i} = (1 + i)/\sqrt{2}$, $\nabla \hat{u} \cdot \hat{u}$ the tangential divergence, $\rho_0$ the ambient mass density, $c$ the speed of sound, and $\tau_\gamma$ and $\tau_T$ the viscous and thermal timescales

\begin{equation}
\tau_\gamma = \frac{\nu}{c^2} \quad \text{and} \quad \tau_T = \frac{(\gamma - 1)^2 \kappa}{\rho_0 c^2 c_p}, \quad (2)
\end{equation}

where $\nu$ denotes the kinematic viscosity, $\kappa$ the thermal conductivity, $\gamma$ the heat capacity ratio, and $c_p$ the specific heat capacity at constant pressure. The boundary condition may be interpreted as a generalized impedance boundary condition, and the appearance of $\sqrt{i \omega}$ is characteristic of diffusion processes [5]. When appropriate, boundary condition (1) is a small perturbation to the regular wall condition $\mathbf{n} \cdot \hat{u} = 0$; in air $\tau_\gamma \sim 10^{-10}$ s and $\tau_T \sim 10^{-11}$ s at atmospheric conditions. Here, we investigate the corresponding boundary condition in time domain.

There is a plethora of versatile time-domain impedance boundary conditions for acoustic simulations; however, these typically require parameter tuning [5]. Moreover, specialized models, such as the Webster–Lokshin equation [3], have been developed for lossy sound propagation in special geometries. However, the boundary condition introduced here is applicable to general geometries and requires no parameter tuning.

2 Viscothermal BC in time domain
It is possible to derive the time-domain analogue of boundary condition (1) from the linearized Navier–Stokes equations by repeating, in time domain, the frequency-domain procedure outlined by Berggren et al. [1]. However, the same expression may also be obtained using Fourier transforms [7, expressions (7.1) and (7.4)],

\begin{equation}
\mathbf{n} \cdot \mathbf{u} = -c \nabla \cdot \left( \sqrt{\tau_T} \mathbf{D}_t^{-1/2} \mathbf{u} \right) + \sqrt{\tau_T} \mathbf{D}_t^{-1/2} \frac{\mathbf{p}}{\rho_0 c}, \quad (3)
\end{equation}

where $\mathbf{D}_t^{-1/2}$ and $-\mathbf{D}_t^{-1/2}$ denote the causal Riemann–Liouville fractional integral and derivative of order 1/2 starting at $-\infty$. Typically, specialized discretizations of the nonlocal differintegrals are required to achieve sufficient computational efficiency [4].
3 Energy balance including thermal losses

To derive an energy balance that accounts for thermal boundary layer effects using boundary condition (3), we consider an initial–boundary-value problem for the acoustic pressure and scaled velocity $u_p = \rho_0 c u$,

\[
\begin{align*}
\partial_t p + \nabla \cdot (c u_p) &= 0, \; Q = (0,T) \times \Omega, \\
\partial_t u_p + c \nabla p &= 0, \; Q = (0,T) \times \Omega, \\
p &= 0, \; u_p = 0, \; Q_0 = \{0\} \times \Omega, \\
n \cdot u_p - \sqrt{\tau_T} D_1^{1/2} p &= 0, \; \Sigma_w = (0,T) \times \Gamma_w, \\
p - n \cdot u_p - 2g &= 0, \; \Sigma_{io} = (0,T) \times \Gamma_{io},
\end{align*}
\]

where $T > 0$ is an arbitrary end time, and $g$ is a finite duration source acting at the in/out-boundary part $\Gamma_{io}$, which is complementary to the solid wall $\Gamma_w$. We have assumed that $p \equiv 0$ for $t \leq 0$, so that $-\infty D_1^{1/2} p = q D_1^{1/2} p$ in boundary condition (4d). Assuming that $p$ and $u_p$ are sufficiently regular, applying $\int_\Omega p \, dq$ to equation (4a), $\int_\Gamma u_p \, dt$ to equation (4b), summing, and integrating by parts either of the spatial derivatives, rearranging the terms, and invoking the boundary conditions, we obtain

\[
\begin{align*}
\frac{1}{\Omega} \int_{t_0}^{t_1} \left( \int_{\Gamma_w} (p^2 + |u_p|^2) \, d\Sigma \right) &= -\int_{\Gamma_w} c p n \cdot u_p \\
&= \int_{\Gamma_{io}} \left( c(g - p)^2 - \int_{\Gamma_w} \sqrt{\tau_T} D_1^{1/2} p \right). \\
\end{align*}
\]

Multiplying equation (5) by $1/(\rho_0 c^2)$, we find that the rate of change of the acoustic energy is determined by the net influx power, represented by the first two terms in the right side, and the exchange of energy in the thermal boundary layer, represented by the last term. Integrating balance (5) in time, we obtain the energy estimate

\[
\int_{t_0}^{t_1} \left( \int_\Omega (p^2 + |u_p|^2) \right) \leq 2 \int_{\Sigma_{io}} c g^2,
\]

provided that the term $\int_{\Sigma_{io}} c \sqrt{\tau_T} D_1^{1/2} p \geq 0$, that is, the term represents a thermal boundary loss. Indeed, we may prove the required positivity using a diffusive representation of the half-derivative [3].

In case the viscous contribution to boundary condition (3) is included, we have not succeeded to derive an energy estimate. In fact, if viscous effects are included, we may demonstrate that an infinite duct subject to boundary condition (3) supports arbitrarily fast growing modes, which indicates ill-posedness of the formulation.

4 Numerical experiments

Figure 1 displays two snapshots of a wave packet traveling from left to right in a straight duct with thermal boundary losses. The duct has been simulated in planar symmetry; the upper boundary is a solid wall and the lower a symmetry line.

Figure 1: Two snapshots of a wave packet traveling from left to right in a straight duct with thermal boundary losses. The duct has been simulated in planar symmetry; the upper boundary is a solid wall and the lower a symmetry line.

References

# Index of Authors

<table>
<thead>
<tr>
<th>Author</th>
<th>Page Numbers</th>
</tr>
</thead>
<tbody>
<tr>
<td>Abboud Toufic</td>
<td>302</td>
</tr>
<tr>
<td>Aimi Alessandra</td>
<td>214</td>
</tr>
<tr>
<td>Allouko Amond</td>
<td>226</td>
</tr>
<tr>
<td>Almqvist Martin</td>
<td>326</td>
</tr>
<tr>
<td>Amenoagbadji Pierre</td>
<td>292, 294</td>
</tr>
<tr>
<td>Anderson Thomas G.</td>
<td>126</td>
</tr>
<tr>
<td>Anne Alexis</td>
<td>352</td>
</tr>
<tr>
<td>Appelö Daniel</td>
<td>148, 174, 200, 234</td>
</tr>
<tr>
<td>Aquino Wilkins</td>
<td>134</td>
</tr>
<tr>
<td>Arens Tilo</td>
<td>238</td>
</tr>
<tr>
<td>Arnold Anton</td>
<td>210</td>
</tr>
<tr>
<td>Arrieta Rodrigo</td>
<td>158</td>
</tr>
<tr>
<td>Asensio Paul</td>
<td>110, 240</td>
</tr>
<tr>
<td>Assier Raphael</td>
<td>180, 270, 272</td>
</tr>
<tr>
<td>Aussal Matthieu</td>
<td>364</td>
</tr>
<tr>
<td>Aytton Lorna</td>
<td>230, 418</td>
</tr>
<tr>
<td>Badier Jean-Michel</td>
<td>110</td>
</tr>
<tr>
<td>Baek Youngsoo</td>
<td>134</td>
</tr>
<tr>
<td>Baffet Daniel H.</td>
<td>308</td>
</tr>
<tr>
<td>Bagur Laura</td>
<td>154</td>
</tr>
<tr>
<td>Baker Katherine</td>
<td>76</td>
</tr>
<tr>
<td>Baldassari Lorenzo</td>
<td>138</td>
</tr>
<tr>
<td>Banjai Lehel</td>
<td>76</td>
</tr>
<tr>
<td>Bannister Joshua</td>
<td>264</td>
</tr>
<tr>
<td>Banon Jean-Philip</td>
<td>374</td>
</tr>
<tr>
<td>Baratchart Laurent</td>
<td>106, 240</td>
</tr>
<tr>
<td>Baronian Vahan</td>
<td>226</td>
</tr>
<tr>
<td>Barucq Hélène</td>
<td>188, 318, 350</td>
</tr>
<tr>
<td>Bauinger Christoph</td>
<td>306</td>
</tr>
<tr>
<td>Bause Markus</td>
<td>384</td>
</tr>
<tr>
<td>Beck Geoffrey</td>
<td>340</td>
</tr>
<tr>
<td>Bellam Muralidhar Nanda Kishore</td>
<td>136</td>
</tr>
<tr>
<td>Bellassoued Mourad</td>
<td>342</td>
</tr>
<tr>
<td>Bellis Cédric</td>
<td>270, 272</td>
</tr>
<tr>
<td>Beni Hamad Akram</td>
<td>198</td>
</tr>
<tr>
<td>Berggren Martin</td>
<td>252, 424</td>
</tr>
<tr>
<td>Benjamin Harold</td>
<td>400</td>
</tr>
<tr>
<td>Bernkopf Maximilian</td>
<td>44, 122</td>
</tr>
<tr>
<td>Betcke Timo</td>
<td>132</td>
</tr>
<tr>
<td>Bignardini Paolo</td>
<td>220</td>
</tr>
<tr>
<td>Bianchi Biondo</td>
<td>32</td>
</tr>
<tr>
<td>Bongarti Marcelo</td>
<td>70</td>
</tr>
<tr>
<td>Bonizzoni Francesca</td>
<td>120</td>
</tr>
<tr>
<td>Bonnet Marc</td>
<td>160, 410</td>
</tr>
<tr>
<td>Bonnet-Ben Dhia Anne-Sophie</td>
<td>226, 276, 352, 358, 360, 402</td>
</tr>
<tr>
<td>Bonnetier Éric</td>
<td>186</td>
</tr>
<tr>
<td>Boccamandine</td>
<td>266, 378</td>
</tr>
<tr>
<td>Boukari Yosra</td>
<td>370</td>
</tr>
<tr>
<td>Bourgeois Laurent</td>
<td>182, 184</td>
</tr>
<tr>
<td>Boutin Henri</td>
<td>254</td>
</tr>
<tr>
<td>Boyaval Sébastien</td>
<td>244</td>
</tr>
<tr>
<td>Brazier Jean-Philip</td>
<td>420</td>
</tr>
<tr>
<td>Briet Philippe</td>
<td>278</td>
</tr>
<tr>
<td>Bruno Oscar P.</td>
<td>126, 258, 306</td>
</tr>
<tr>
<td>Burkhard Selina</td>
<td>212</td>
</tr>
<tr>
<td>Bécache Eliane</td>
<td>192, 402</td>
</tr>
<tr>
<td>Bériot Hadrien</td>
<td>406</td>
</tr>
<tr>
<td>Caetano Antonio</td>
<td>100</td>
</tr>
<tr>
<td>Calandra Henri</td>
<td>188</td>
</tr>
<tr>
<td>Cantin Pierre</td>
<td>282</td>
</tr>
<tr>
<td>Carvalho Camille</td>
<td>156, 208, 260, 336</td>
</tr>
<tr>
<td>Cassier Maxence</td>
<td>128, 396</td>
</tr>
<tr>
<td>Castera Guillaume</td>
<td>328</td>
</tr>
<tr>
<td>Cessenat Olivia</td>
<td>164</td>
</tr>
<tr>
<td>Chabassier Juliette</td>
<td>254, 328</td>
</tr>
<tr>
<td>Chaigne Benoît</td>
<td>302</td>
</tr>
<tr>
<td>Chaillet Stéphanie</td>
<td>154, 410</td>
</tr>
<tr>
<td>Chandler-Wilde Simon</td>
<td>100, 224</td>
</tr>
<tr>
<td>Chaumont-Frelet Theophile</td>
<td>44, 150</td>
</tr>
<tr>
<td>Chesnel Lucas</td>
<td>274, 346, 358, 360</td>
</tr>
<tr>
<td>Chollet Igor</td>
<td>304</td>
</tr>
<tr>
<td>Claeyns Xavier</td>
<td>56, 304</td>
</tr>
<tr>
<td>Colbrook Matthew</td>
<td>86</td>
</tr>
<tr>
<td>Collino Francis</td>
<td>56, 416</td>
</tr>
<tr>
<td>Cornaggia Rémi</td>
<td>232</td>
</tr>
<tr>
<td>Cortes Elsie</td>
<td>260</td>
</tr>
<tr>
<td>Cotterill Philip</td>
<td>272</td>
</tr>
<tr>
<td>Cousin Theau</td>
<td>194</td>
</tr>
<tr>
<td>Name</td>
<td>Page(s)</td>
</tr>
<tr>
<td>----------------------</td>
<td>-------------</td>
</tr>
<tr>
<td>Darbas Marion</td>
<td>38</td>
</tr>
<tr>
<td>De Pascalis Riccardo</td>
<td>400</td>
</tr>
<tr>
<td>Dekkers Adrien</td>
<td>64</td>
</tr>
<tr>
<td>Delaunay Tiphaine</td>
<td>284, 312</td>
</tr>
<tr>
<td>Delourme Bérangère</td>
<td>398</td>
</tr>
<tr>
<td>Demaldent Edouard</td>
<td>160</td>
</tr>
<tr>
<td>Desiderio Luca</td>
<td>214, 414</td>
</tr>
<tr>
<td>Després Bruno</td>
<td>112</td>
</tr>
<tr>
<td>Di Credico Giulia</td>
<td>214</td>
</tr>
<tr>
<td>Dias Frederic</td>
<td>166</td>
</tr>
<tr>
<td>Diaz Julien</td>
<td>188</td>
</tr>
<tr>
<td>Direkx Simon</td>
<td>300</td>
</tr>
<tr>
<td>Dohnal Tomáš</td>
<td>338</td>
</tr>
<tr>
<td>Dominguez Victor</td>
<td>114</td>
</tr>
<tr>
<td>Dubois Juliette</td>
<td>242</td>
</tr>
<tr>
<td>Duchemin Ivan</td>
<td>88</td>
</tr>
<tr>
<td>Dupuy Mi-Song</td>
<td>82</td>
</tr>
<tr>
<td>Duruflé Marc</td>
<td>318</td>
</tr>
<tr>
<td>Dörich Benjamin</td>
<td>212, 324</td>
</tr>
<tr>
<td>Engquist Björn</td>
<td>310</td>
</tr>
<tr>
<td>Erath Christoph</td>
<td>118</td>
</tr>
<tr>
<td>Eriksson Gustav</td>
<td>176</td>
</tr>
<tr>
<td>Escapil-Inchauspé Paul</td>
<td>130</td>
</tr>
<tr>
<td>Falletta Silvia</td>
<td>414</td>
</tr>
<tr>
<td>Faria Luiz</td>
<td>158, 352</td>
</tr>
<tr>
<td>Fauchard Cyrille</td>
<td>194</td>
</tr>
<tr>
<td>Feliśoci Marek</td>
<td>302</td>
</tr>
<tr>
<td>Ferrari Matteo</td>
<td>414</td>
</tr>
<tr>
<td>Ferrières Xavier</td>
<td>282</td>
</tr>
<tr>
<td>Fierro-Piccardo Ignacia</td>
<td>132</td>
</tr>
<tr>
<td>Filoche Marcel</td>
<td>166, 374</td>
</tr>
<tr>
<td>Fliss Sonia</td>
<td>182, 226, 266, 292, 294, 378, 398, 402</td>
</tr>
<tr>
<td>Florian Francesco</td>
<td>104</td>
</tr>
<tr>
<td>Fornerod Jean</td>
<td>348</td>
</tr>
<tr>
<td>Fortin Pierre</td>
<td>304</td>
</tr>
<tr>
<td>Fournier Damien</td>
<td>314</td>
</tr>
<tr>
<td>Fraschini Sara</td>
<td>286</td>
</tr>
<tr>
<td>Fritsch Jean-François</td>
<td>182, 184</td>
</tr>
<tr>
<td>Galkowski Jeffrey</td>
<td>392</td>
</tr>
<tr>
<td>Ganesh Mahadevan</td>
<td>114</td>
</tr>
<tr>
<td>Garcke Harald</td>
<td>66</td>
</tr>
<tr>
<td>Garnier Josselin</td>
<td>170</td>
</tr>
<tr>
<td>Gaskell Philip</td>
<td>74</td>
</tr>
<tr>
<td>Gaucher Samuel</td>
<td>164</td>
</tr>
<tr>
<td>Geever Sjoerd</td>
<td>210</td>
</tr>
<tr>
<td>Genovese Luigi</td>
<td>88</td>
</tr>
<tr>
<td>Gerber-Roth Anthony</td>
<td>108</td>
</tr>
<tr>
<td>Gibbs Andrew</td>
<td>100, 102, 264</td>
</tr>
<tr>
<td>Gillman Adrianna</td>
<td>116</td>
</tr>
<tr>
<td>Gimperlein Heiko</td>
<td>218</td>
</tr>
<tr>
<td>Giovangigli Laure</td>
<td>170, 266, 378</td>
</tr>
<tr>
<td>Givoli Dan</td>
<td>412</td>
</tr>
<tr>
<td>Gizon Laurent</td>
<td>314</td>
</tr>
<tr>
<td>Gleichmann Yannik G.</td>
<td>308</td>
</tr>
<tr>
<td>Goepfert Quentin</td>
<td>170</td>
</tr>
<tr>
<td>Gomez Sergio</td>
<td>172</td>
</tr>
<tr>
<td>Gout Christian</td>
<td>194, 318</td>
</tr>
<tr>
<td>Gower Artur L.</td>
<td>168, 376</td>
</tr>
<tr>
<td>Grigori Laura</td>
<td>304</td>
</tr>
<tr>
<td>Grote Marcus J.</td>
<td>150, 308</td>
</tr>
<tr>
<td>Grubišić Luka</td>
<td>320</td>
</tr>
<tr>
<td>Guardasoni Chiara</td>
<td>214</td>
</tr>
<tr>
<td>Guifaut Christophe</td>
<td>164</td>
</tr>
<tr>
<td>Guillaume Puigt</td>
<td>282</td>
</tr>
<tr>
<td>Guzina Bojan B.</td>
<td>296, 394</td>
</tr>
<tr>
<td>Haddar Houssem</td>
<td>106, 342, 364, 370</td>
</tr>
<tr>
<td>Hagemann Felix</td>
<td>238</td>
</tr>
<tr>
<td>Haider Anita</td>
<td>216</td>
</tr>
<tr>
<td>Hale Jonathan</td>
<td>334</td>
</tr>
<tr>
<td>Hales Alistair</td>
<td>418</td>
</tr>
<tr>
<td>Halla Martin</td>
<td>206, 404</td>
</tr>
<tr>
<td>Hassaourp Guilvaiiee Hamideh</td>
<td>330</td>
</tr>
<tr>
<td>Hawkins Stuart C.</td>
<td>114, 376</td>
</tr>
<tr>
<td>Hazard Christophe</td>
<td>182, 276</td>
</tr>
<tr>
<td>Heleine Jérémy</td>
<td>274, 346</td>
</tr>
<tr>
<td>Hettlich Frank</td>
<td>238</td>
</tr>
<tr>
<td>Hewett David</td>
<td>100, 102, 228, 264</td>
</tr>
<tr>
<td>Hinz Michael</td>
<td>64</td>
</tr>
<tr>
<td>Hiptmair Ralf</td>
<td>104, 262</td>
</tr>
<tr>
<td>Hochbrucker Marlis</td>
<td>196, 212</td>
</tr>
<tr>
<td>Holage Thorsten</td>
<td>314, 408</td>
</tr>
<tr>
<td>Horning Andrew</td>
<td>86</td>
</tr>
<tr>
<td>Hu Guanghui</td>
<td>142</td>
</tr>
<tr>
<td>Hu Yuxi</td>
<td>72</td>
</tr>
<tr>
<td>Huybrechs Daan</td>
<td>98, 300</td>
</tr>
<tr>
<td>Hägg Linus</td>
<td>424</td>
</tr>
<tr>
<td>Hélie Thomas</td>
<td>254</td>
</tr>
<tr>
<td>Ilan Boaz</td>
<td>344</td>
</tr>
<tr>
<td>Imbert-Gérard Lise-Marie</td>
<td>94, 202</td>
</tr>
<tr>
<td>Imperiale Sébastien</td>
<td>198, 242, 284, 312</td>
</tr>
<tr>
<td>Ionescu-Tira Mathias</td>
<td>338</td>
</tr>
<tr>
<td>Ismail-Sutton Sara</td>
<td>74</td>
</tr>
<tr>
<td>Ivanyshyn Yaman Olha</td>
<td>236</td>
</tr>
<tr>
<td>J</td>
<td>M</td>
</tr>
<tr>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>Jaiswal Monu</td>
<td>Maier Bernhard</td>
</tr>
<tr>
<td>Jenhani Nouha</td>
<td>Mandel Rainer</td>
</tr>
<tr>
<td>Jerez-Hanckes Carlos</td>
<td>Marchand Pierre</td>
</tr>
<tr>
<td>Joly Patrick</td>
<td>Marcia Roumel</td>
</tr>
<tr>
<td>Jorkowski Philipp</td>
<td>Margenbarg Nils</td>
</tr>
<tr>
<td>Joubert-Doriol Loïc</td>
<td>Marmorat Jean Paul</td>
</tr>
<tr>
<td>Kachanovska Maryna</td>
<td>Martin Paul</td>
</tr>
<tr>
<td>Kaltenbacher Barbara</td>
<td>Mascotto Lorenzo</td>
</tr>
<tr>
<td>Kaltenbacher Manfred</td>
<td>Masthay Tyler</td>
</tr>
<tr>
<td>Karnezis Aristeidis</td>
<td>Matignon Denis</td>
</tr>
<tr>
<td>Khajah Tahsin</td>
<td>Matt Tranter</td>
</tr>
<tr>
<td>Kim Arnold</td>
<td>Mattsson Ken</td>
</tr>
<tr>
<td>Kirsch Andreas</td>
<td>Mayboroda Svitlana</td>
</tr>
<tr>
<td>Knöller Marvin</td>
<td>Mayerhofer Dominik</td>
</tr>
<tr>
<td>Koo Weon Cheol</td>
<td>Mccullough Cory</td>
</tr>
<tr>
<td>Kreiss Gunilla</td>
<td>Meerbergen Karl</td>
</tr>
<tr>
<td>Krejcirik David</td>
<td>Melenk Markus</td>
</tr>
<tr>
<td>Kristensson Gerhard</td>
<td>Meliani Mostafa</td>
</tr>
<tr>
<td>Kumbar Pratik</td>
<td>Meng Shixu</td>
</tr>
<tr>
<td>Körten Franz</td>
<td>Mikhaylenko Andrey</td>
</tr>
<tr>
<td>Köhler Jonas</td>
<td>Millien Pierre</td>
</tr>
<tr>
<td>Labarca Ignacio</td>
<td>Min Eun-Hong</td>
</tr>
<tr>
<td>Labat Justine</td>
<td>Mitra Sourav</td>
</tr>
<tr>
<td>Labidi Amal</td>
<td>Modave Axel</td>
</tr>
<tr>
<td>Lafitte Olivier</td>
<td>Moiola Andrea</td>
</tr>
<tr>
<td>Lammering Rolf</td>
<td>Moireau Philippe</td>
</tr>
<tr>
<td>Langdon Stephen</td>
<td>Moitier Zoë</td>
</tr>
<tr>
<td>Lannes David</td>
<td>Monk Peter</td>
</tr>
<tr>
<td>Lanteri Stéphane</td>
<td>Montanelli Hadrien</td>
</tr>
<tr>
<td>Lasiecka Irena</td>
<td>Moufid Ilyes</td>
</tr>
<tr>
<td>Latham Benjamin</td>
<td>Mousavi Abbas</td>
</tr>
<tr>
<td>Law Yann-Meijing</td>
<td>Mukherjee Sayan</td>
</tr>
<tr>
<td>Le Louër Frédérique</td>
<td>Munnier Alexandre</td>
</tr>
<tr>
<td>Leblond Juliette</td>
<td>Müller Björn</td>
</tr>
<tr>
<td>Leclerc Augustin</td>
<td>(^{136})</td>
</tr>
<tr>
<td>Lee Spencer</td>
<td>(^{280})</td>
</tr>
<tr>
<td>Lehrenfeld Christoph</td>
<td>(^{230})</td>
</tr>
<tr>
<td>Leibold Jan</td>
<td>(^{410})</td>
</tr>
<tr>
<td>Letourneu Eloïse</td>
<td>(^{134})</td>
</tr>
<tr>
<td>Levitt Antoine</td>
<td>(^{112})</td>
</tr>
<tr>
<td>Li Jichun</td>
<td>(^{176})</td>
</tr>
<tr>
<td>Lombard Bruno</td>
<td>(^{22})</td>
</tr>
<tr>
<td>Londoño Mauricio</td>
<td>(^{272})</td>
</tr>
<tr>
<td>Lorenz Dirk A.</td>
<td>(^{272})</td>
</tr>
<tr>
<td>Lucero Lorca Jose Pablo</td>
<td>(^{116})</td>
</tr>
<tr>
<td>Lükens Vladimir</td>
<td>(^{268})</td>
</tr>
<tr>
<td>Lähivaara Timo</td>
<td>(^{372})</td>
</tr>
<tr>
<td>Lukeš Vladimír</td>
<td>(^{280})</td>
</tr>
<tr>
<td></td>
<td>Oberlack Martin</td>
</tr>
<tr>
<td>Name</td>
<td>Page(s)</td>
</tr>
<tr>
<td>-----------------------------</td>
<td>-----------------</td>
</tr>
<tr>
<td>Oudghiri-Idrissi Othman</td>
<td>296, 394</td>
</tr>
<tr>
<td>Pankrashkin Konstantin</td>
<td>280</td>
</tr>
<tr>
<td>Parnell William</td>
<td>180, 272</td>
</tr>
<tr>
<td>Parolin Emile</td>
<td>56, 98</td>
</tr>
<tr>
<td>Pelletier Pierre</td>
<td>374</td>
</tr>
<tr>
<td>Peng Zhichao</td>
<td>148</td>
</tr>
<tr>
<td>Perez Arancibia Carlos</td>
<td>158</td>
</tr>
<tr>
<td>Pernet Sébastien</td>
<td>96, 282, 420</td>
</tr>
<tr>
<td>Perrussel Ronan</td>
<td>316</td>
</tr>
<tr>
<td>Perugia Ilaria</td>
<td>118, 210</td>
</tr>
<tr>
<td>Phillips Oliver</td>
<td>224</td>
</tr>
<tr>
<td>Piche Alexandre</td>
<td>302</td>
</tr>
<tr>
<td>Pinto Jose</td>
<td>362</td>
</tr>
<tr>
<td>Piot Estelle</td>
<td>246, 256</td>
</tr>
<tr>
<td>Poirier Jean-René</td>
<td>316</td>
</tr>
<tr>
<td>Ponomarev Dmitry</td>
<td>210</td>
</tr>
<tr>
<td>Pradovera Davide</td>
<td>120</td>
</tr>
<tr>
<td>Preuß Janosch</td>
<td>408</td>
</tr>
<tr>
<td>Ptashnyk Mariya</td>
<td>76</td>
</tr>
<tr>
<td>Pujois Agnès</td>
<td>416</td>
</tr>
<tr>
<td>Putz Felician</td>
<td>422</td>
</tr>
<tr>
<td>Quaine Kieran</td>
<td>218</td>
</tr>
<tr>
<td>Rabinovich Daniel</td>
<td>412</td>
</tr>
<tr>
<td>Racke Reinhard</td>
<td>72</td>
</tr>
<tr>
<td>Ramdani Karim</td>
<td>108</td>
</tr>
<tr>
<td>Rauscher Teresa</td>
<td>78</td>
</tr>
<tr>
<td>Rauter Natalie</td>
<td>136</td>
</tr>
<tr>
<td>Recqueillay Arnaud</td>
<td>182, 184, 368</td>
</tr>
<tr>
<td>Reineix Alain</td>
<td>164</td>
</tr>
<tr>
<td>Riedel Alexander</td>
<td>118</td>
</tr>
<tr>
<td>Rihani Mahran</td>
<td>358, 360</td>
</tr>
<tr>
<td>Ritzenhaller Valentin</td>
<td>282</td>
</tr>
<tr>
<td>Rodríguez-Cortés Francisco</td>
<td>390</td>
</tr>
<tr>
<td>Rohan Eduard</td>
<td>268</td>
</tr>
<tr>
<td>Roncen Rémi</td>
<td>246, 256</td>
</tr>
<tr>
<td>Rosas Alejandro</td>
<td>128</td>
</tr>
<tr>
<td>Rotem Amit</td>
<td>234</td>
</tr>
<tr>
<td>Rouxelin Nathan</td>
<td>350</td>
</tr>
<tr>
<td>Rozanova-Pierrat Anna</td>
<td>64</td>
</tr>
<tr>
<td>Rudel Clément</td>
<td>420</td>
</tr>
<tr>
<td>Ruello Maëlys</td>
<td>420</td>
</tr>
<tr>
<td>Ruget Simon</td>
<td>88</td>
</tr>
<tr>
<td>Ruggeri Michele</td>
<td>120</td>
</tr>
<tr>
<td>Ruiz Matias</td>
<td>276</td>
</tr>
<tr>
<td>Runborg Olof</td>
<td>17, 234</td>
</tr>
<tr>
<td>Rösler Frank</td>
<td>322</td>
</tr>
<tr>
<td>S</td>
<td></td>
</tr>
<tr>
<td>Sainte-Marie Jacques</td>
<td>242</td>
</tr>
<tr>
<td>Sangalli Giancarlo</td>
<td>286</td>
</tr>
<tr>
<td>Sauter Stefan</td>
<td>104, 122</td>
</tr>
<tr>
<td>Schanz Martin</td>
<td>216</td>
</tr>
<tr>
<td>Schenker Carla</td>
<td>320</td>
</tr>
<tr>
<td>Schmidt Kersten</td>
<td>320</td>
</tr>
<tr>
<td>Scholle Markus</td>
<td>74</td>
</tr>
<tr>
<td>Schumann Rolf</td>
<td>320</td>
</tr>
<tr>
<td>Schweizer Ben</td>
<td>144</td>
</tr>
<tr>
<td>Scuderri Letizia</td>
<td>414</td>
</tr>
<tr>
<td>Selgas Virginia</td>
<td>372</td>
</tr>
<tr>
<td>Semblat Jean-François</td>
<td>154</td>
</tr>
<tr>
<td>Seppecher Laurent</td>
<td>186</td>
</tr>
<tr>
<td>Seyfert Fabien</td>
<td>240</td>
</tr>
<tr>
<td>Shafieeaboyaneh Nasim</td>
<td>298</td>
</tr>
<tr>
<td>Sirdey Margot</td>
<td>96</td>
</tr>
<tr>
<td>Skvortsoy Alex</td>
<td>250</td>
</tr>
<tr>
<td>Smyshlyaev Valery</td>
<td>228</td>
</tr>
<tr>
<td>Spence Euan</td>
<td>392</td>
</tr>
<tr>
<td>Stefanou Ioannis</td>
<td>154</td>
</tr>
<tr>
<td>Stellin Filippo</td>
<td>166</td>
</tr>
<tr>
<td>Stepanenko Alexei</td>
<td>322</td>
</tr>
<tr>
<td>Stiernström Vidar</td>
<td>326</td>
</tr>
<tr>
<td>Stocker Paul</td>
<td>202, 206</td>
</tr>
<tr>
<td>Stolk Chris</td>
<td>152</td>
</tr>
<tr>
<td>Stupfel Bruno</td>
<td>378</td>
</tr>
<tr>
<td>Sylvand Guillaume</td>
<td>94, 302</td>
</tr>
<tr>
<td>T</td>
<td></td>
</tr>
<tr>
<td>Tamber Jagdeep</td>
<td>382</td>
</tr>
<tr>
<td>Tang Jet H.</td>
<td>150</td>
</tr>
<tr>
<td>Teplyaev Alexander</td>
<td>64</td>
</tr>
<tr>
<td>Thibault Alexis</td>
<td>254</td>
</tr>
<tr>
<td>Thicke Kyle</td>
<td>86</td>
</tr>
<tr>
<td>Thierry Bertrand</td>
<td>112</td>
</tr>
<tr>
<td>Tomnoir Antoine</td>
<td>194, 318, 402</td>
</tr>
<tr>
<td>Tordeux Sébastien</td>
<td>96, 350</td>
</tr>
<tr>
<td>Torres Céline</td>
<td>122</td>
</tr>
<tr>
<td>Toth Florian</td>
<td>330</td>
</tr>
<tr>
<td>Touboul Marie</td>
<td>270, 272</td>
</tr>
<tr>
<td>Tsogka Chryssoul</td>
<td>260</td>
</tr>
<tr>
<td>Turc Catalin</td>
<td>158, 366</td>
</tr>
<tr>
<td>V</td>
<td></td>
</tr>
<tr>
<td>Vanel Alice</td>
<td>138</td>
</tr>
<tr>
<td>Vasanthan Vinduja</td>
<td>188</td>
</tr>
<tr>
<td>Veit Alexander</td>
<td>122</td>
</tr>
<tr>
<td>Verfürth Barbara</td>
<td>356</td>
</tr>
<tr>
<td>Vial Grégory</td>
<td>186</td>
</tr>
<tr>
<td>Villalobos Guillen Cristóbal</td>
<td>106</td>
</tr>
<tr>
<td>Villamizar Vianey</td>
<td>334</td>
</tr>
<tr>
<td>Name</td>
<td>Page</td>
</tr>
<tr>
<td>--------------------</td>
<td>------</td>
</tr>
<tr>
<td>Wadbro Eddie</td>
<td>252</td>
</tr>
<tr>
<td>Wakeling James</td>
<td>22</td>
</tr>
<tr>
<td>Wang Na</td>
<td>72</td>
</tr>
<tr>
<td>Watson Alex</td>
<td>86</td>
</tr>
<tr>
<td>Waurick Marcus</td>
<td>338</td>
</tr>
<tr>
<td>Weber Ivy</td>
<td>288</td>
</tr>
<tr>
<td>Weinstein Michael I</td>
<td>396</td>
</tr>
<tr>
<td>Weisbuch Claude</td>
<td>374</td>
</tr>
<tr>
<td>Werpers Jonatan</td>
<td>176</td>
</tr>
<tr>
<td>Wess Markus</td>
<td>192</td>
</tr>
<tr>
<td>Weynans Lisl</td>
<td>340</td>
</tr>
<tr>
<td>White Tom</td>
<td>180</td>
</tr>
<tr>
<td>Wik Niklas</td>
<td>176</td>
</tr>
<tr>
<td>Wright Kyle</td>
<td>344</td>
</tr>
<tr>
<td>Yin Tao</td>
<td>362</td>
</tr>
<tr>
<td>Zethrin Valter</td>
<td>176</td>
</tr>
<tr>
<td>Zhang Ruming</td>
<td>298</td>
</tr>
<tr>
<td>Zhang Yi</td>
<td>422</td>
</tr>
</tbody>
</table>