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North Carolina State University
2701 Sullivan Drive
Admin Srvcs III, Box 7514
Raleigh, NC 27695 -7514

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RPPR Final Report
as of 27-Aug-2021

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INVESTIGATOR(S):

Name: Semyon Victor Tsynkov
Email: stsynkov@ncsu.edu
Phone Number: 9195151877
Principal: Y

Organization: **North Carolina State University**
Address: 2701 Sullivan Drive, Raleigh, NC 276957514
Country: USA
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Submitted By: Semyon Tsynkov Email: stsynkov@ncsu.edu
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Major Goals: The wave (d'Alembert) equation is an established model for a broad range of problems in acoustics and electromagnetism. The overall objective of our effort is to build a numerical methodology for solving this equation over long times and on large and generally shaped spatial regions with high fidelity and robustness.

Finite difference (FD) methods are known to yield inexpensive and efficient algorithms for computing smooth solutions to partial differential equations on regular domains/grids. Their primary disadvantage is in dealing with more complicated geometries and solutions with low regularity. Finite element methods (FEM) may help alleviate these two constraints. Yet in practical problems of wave propagation, especially in 3D, both FD and FEM have serious limitations because of the numerical pollution, i.e., dispersion (or phase) error.

This drawback can be (partially) overcome by high-order FD schemes. They, however, usually need a wider stencil, which complicates the boundary conditions. A class of schemes aimed at reducing the phase error are the dispersion relation preserving schemes. Yet they need an even wider stencil than conventional schemes of the same order of accuracy.

The high-order schemes that do not require a wider stencil rely on a targeted approximation of the class of solutions rather than generic sufficiently smooth functions. The equation-based compact schemes that we have developed for the Helmholtz equation are in this category. A key goal of the current project is to extend these schemes from the frequency domain to time domain in both 2D and 3D. Such schemes reduce pollution while keeping the treatment of the boundary conditions simple. However, geometry still remains a hurdle.

In FEM, a high-order accurate approximation can be built for arbitrary boundaries with the help of isoparametric elements. However, grid generation can be nontrivial for complex geometries and interfaces. In generalized FEM, high-order accuracy also requires additional degrees of freedom. For linear problems with smooth solutions, this implies substantial redundancy, which entails additional computational costs.

Boundary element methods (BEM) provide broad flexibility from the standpoint of geometry. They typically apply to steady-state or time-harmonic problems (elliptic PDEs). In these methods, linear boundary value problems are reduced to boundary integral equations (BIE) with respect to equivalent boundary sources. BEM automatically account for the correct far field behavior of the solution. However, these methods rely on the explicit knowledge of the fundamental solution. Moreover, the treatment of the boundary conditions requires care in choosing the boundary sources so as to maintain the equivalence of the reduction from the domain to the boundary and well-posedness of the resulting boundary formulation.

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Standard BEM cannot be used directly for unsteady problems of wave propagation (hyperbolic PDEs). A special class of BIEs called the retarded potential boundary integral equations (RPBIE), provide a venue toward extending the BEM from elliptic to hyperbolic PDEs. However, the corresponding time domain numerical methods are not nearly as popular as their frequency domain counterparts. One difficulty is that the time domain discretizations of RPBIEs may be prone to instabilities, even if the RPBIE per se is well-posed. Another reason is that, as the time elapses the boundary extends, and the computation of convolutions involved in RPBIEs becomes progressively more expensive.

In our earlier work on the Helmholtz equation, we employed the method of difference potentials (MDP) developed by Ryaben'kii. The MDP can be viewed as a discrete analog of Calderon's potentials and Calderon's boundary equations with projections. Its capacity of handling the boundaries of general shape is comparable to that of BIEs. Yet the MDP does not need a fundamental solution and automatically guarantees the equivalence of the reduced boundary problem to the original one. It uses discretizations on regular structured grids and can maintain high-order accuracy for non-conforming boundaries. Difference potentials for the Helmholtz equation have been built using compact equation-based schemes that enable high-order accuracy while avoiding the extensive redundancy inherent in high-order FEM methods.

The current effort focuses on extending the MDP-based approach to genuinely time-dependent formulations. Our goal is to achieve the same geometric flexibility and high-order accuracy as we have obtained for the Helmholtz equation. There are two ways of pursuing this goal. One can build an MDP algorithm in the 3+1-dimensional space-time. In doing so, computing the operators may turn out increasingly costly as the time elapses. To eliminate the cost increase, one can employ the strong Huygens' principle and lacunae in the solutions of the 3D wave equation. Previously, we used a similar idea for building the lacunae-based artificial boundary conditions for the numerical simulation of unsteady waves.

Alternatively, one can first discretize the wave equation in time by means of an implicit scheme. This discretization yields an elliptic equation to be solved on the upper time level at every time step. This can be done using the MDP similarly to how the Helmholtz equation is solved.

Additional goals of the project include various extensions of our previous ARO-supported work on the Helmholtz equation (time-harmonic waves), specifically, computation of solutions with singularities, multiple scattering problems, and domain decomposition.

Conventional numerical methods lose consistency near the singularity, which causes a deterioration of their performance. Earlier, we have developed a special approach based on regularization near the singularity and numerical solution of the regularized problem by high order difference potentials. It has shown no loss of accuracy for the case of a smooth boundary and discontinuous data, as well as for the case of a non-smooth boundary with a re-entrant corner. The regularization is rendered by subtracting several leading terms of an asymptotic expansion of the solution near the singularity. Eventually, the problem is reduced to a discrete variational formulation at the boundary that is solved in the sense of l_2, i.e., least squares. Given that discontinuities are common in defense and industrial applications, one of our current objectives is to investigate the efficiency of applying alternative variational formulations, in particular, l_1-type methods, to computing singular solutions of the Helmholtz equation.

Multiple scattering problems appear in various physical applications, including electrodynamics, photonics, and others. They involve scattering about multiple bodies so that the signal scattered off one obstacle impinges on the others and scatters again, etc. Previously, we have developed an MDP-based approach for computing multiple scattering solutions in 2D. A current objective is to be able to solve 3D multiple scattering problems with high order accuracy.

Many wave propagation problems involve discontinuous material properties. Our goal is to solve time-harmonic problems with material discontinuities by non-overlapping domain decomposition (DD) combined with the MDP. The MDP reduces the Helmholtz equation on each subdomain to a Calderon's boundary equation with projection on the boundary. The unknowns for the Calderon's equation are the Dirichlet and Neumann data. Then, coupling between neighboring subdomains is rendered by applying their respective Calderon's equations to the same data at the common interface. Solutions on individual subdomains are computed concurrently using a direct solver. The method is insensitive to large jumps in the wavenumber, as well as interior cross-points and mixed boundary conditions, which may be a challenge to many other DD methods.

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Accomplishments: By the time the project terminated, all its research objectives have been successfully met. Most of the results have also been published in peer reviewed journals and presented at scientific conferences. The most recent results are still awaiting publication.

We built a new finite difference scheme for the 3D time-dependent wave equation that is fourth order accurate in both space and time while retaining a small compact stencil. The scheme is implicit and conditionally stable, yet it is much more efficient than lower order schemes. The equation to solve on the upper time level is the modified Helmholtz equation, which is elliptic and positive definite. We use FFT in the case of constant coefficients and multigrid in the case of variable coefficients. Due to the large amount of positivity, multigrid iterations converge very fast. Computations corroborate the design accuracy for the inhomogeneous, variable coefficient wave equation and also confirm the pollution effect for these time-dependent problems.

We then combined this compact scheme with the method of difference potentials (MDP) to solve initial boundary value problems (IBVPs) for the unsteady wave equation with high order accuracy. The resulting numerical methodology is cost-effective and capable of handling boundaries and interfaces that are not aligned with the grid with no accuracy loss.

The MDP can be thought of as a discrete counterpart of the method of Calderon’s operators. The first strategy of its time-dependent implementation is to do that directly in the 3+1-dimensional space-time. Then, the operators are computed on a (3+1)-D computational domain with a (2+1)-D boundary. The discretization grid is also four-dimensional, and all the necessary constructs of difference potentials are built in 4D.

To compute the difference potentials and projections, one needs an auxiliary problem (AP). The AP is driven by a specially constructed near-boundary source terms. We take the AP as a pure initial value problem (IVP). Although its spatial domain is unbounded, this formulation has a crucial advantage as it satisfies the Huygens’ principle. The Huygens’ principle allows us to solve the AP numerically for arbitrarily long times on an auxiliary domain that has a finite and non-increasing size. Moreover, instead of having to integrate the IVP continuously from the initial to the current moment of time, the Huygens’ principle enables a sliding window of a fixed and non-increasing duration. As a very important implication, it completely eliminates the need for any treatment of the artificial outer boundary (such as an ABC or PML), because during this finite time window the outgoing wave can travel only a finite distance away, beyond which the computational domain can be truncated. Altogether, this yields an efficient procedure for computing the difference potentials and projections. For long simulation times, it shows sub-linear computational complexity.

Our MDP/Huygens' solver for the 3D unsteady wave equation handles various boundary conditions, including Dirichlet, Neumann, and Robin. Its performance has been corroborated by numerical simulations. For exterior problems, the method requires no ABCs of PML.

We have also reformulated the MDP to streamline its discrete implementation. The reformulation replaces the framework that involves the finite difference counterparts to Calderon's operators with a simpler and more intuitive computational algorithm that fully relies on solving a series of simple auxiliary problems. Yet it remains fully equivalent to the original MDP and inherits all its advantageous properties, such as the geometric flexibility and universal handling of the boundary conditions.

Our algorithm based on the MDP and Huygens’ principle yields a major breakthrough in the area of numerical solution of unsteady hyperbolic PDEs in three space dimensions. It can be considered a time-dependent counterpart of BIEs/BEM that have proven superior in the elliptic case. The algorithm has full geometric flexibility and enables high order accuracy. For long simulation times, its computational cost increases as N^3, as opposed to N^4 that characterizes the standard explicit time marching, where N is the dimension of the discretization grid in one space direction. In practice, we have observed two orders of magnitude performance gains per unit time. The algorithm also allows one to share the computational cost among multiple similar problems. On the flip side, our algorithm has a one-time initiation cost that can be substantial in terms of sheer numbers. However, this part is fully (and effortlessly) parallelizable — one can think of an effective parallelization in time. Parallelization has been successfully demonstrated on a small-scale system. On a modern large-scale HPC platform, the initiation cost is going to be negligible.

Another strategy for solving the time-dependent wave equation by means of the MDP is to first use the compact implicit scheme to discretize the equation in time and then apply the MDP to the resulting 3D steady-state elliptic equation on the upper time level (modified Helmholtz equation). This agenda has been successfully implemented for 2D interior problems at an earlier stage of the project. Its extension to 3D is complete by now, but the results have not been published yet. Compared to the 3+1-D implementation based on the Huygens' principle, it does not offer a sub-linear computational complexity. On the other hand, since it does not rely on the Huygens' principle, it allows for the variable propagation speed, which is a key advantage. For exterior problems, it requires a closure at the artificial outer boundary. We use an extension to the time domain of the previously developed MDP-based implementation of high order local artificial boundary conditions.

In the frequency domain, we developed an algorithm for the numerical solution of 3D multiple scattering problems. The Helmholtz equation is approximated with 6th order accuracy on a Cartesian grid by means of a compact finite difference scheme. The shape of the scatterers does not have to conform to the discretization grid, yet the MDP enables the approximation with no loss of accuracy. At the artificial outer boundary, the computational domain is terminated by a 6th order Bayliss-Gunzburger-Turkel radiation boundary condition. The method enables efficient solution of a series of similar problems, for example, when the incident field changes while everything else stays the same, or when the type of the scattering changes (e.g., sound-soft vs. sound-hard) while the shape of the scatterer remains the same. A paper has been accepted for publication in Wave Motion.

Another frequency domain development is domain decomposition. We designed a methodology where the MDP enables a very efficient matching of partial solutions at the interfaces between subdomains. The finite difference approximation is fourth order accurate; the boundary conditions are arbitrary; and the propagation speed (i.e., wavenumber) can vary from one subdomain to the next, including jumps across interfaces. The method proves completely insensitive to even strong material discontinuities, as well as interior cross-points. A paper has been submitted to Applied Numerical Mathematics. The next step of this development will be the simulation of photonic crystal ring resonators.

We have also looked into possibly improving the previously developed capability of computing the solutions with singularities. There is evidence in the literature, albeit for other problems, that computing the weak solutions in the sense of l_1, as opposed to least squares (l_2), may offer certain benefits. For the variational formulation of the MDP, however, we have not been able to identify any noticeable advantages of l_1 over l_2.

Training Opportunities: Two graduate students, Mr Fouche Smith and Mr Evan North, have received training and conducted their PhD work in the framework of the project. Both are expected to graduate during the 2021-2022 Academic Year. The subject of Mr Smith's work is MDP for unsteady problems via solving the elliptic equation on the upper time level of an implicit scheme. The subject of Mr North's work is domain decomposition for the Helmholtz equation.

A former PhD student is Dr Steven Britt who graduated in 2015, before this project has started. Dr Britt's work was supported by a previous ARO grant received by the PI. For his PhD, Dr Britt had worked on the solution of the 2D Helmholtz equation by difference potentials. Upon graduation, Dr Britt took a postdoctoral position with Prof Turkel, who is a close collaborator of the PI. Between 2016 and 2018, Dr Britt worked on the time-dependent implementation of the MDP for the two-dimensional wave equation.

Two post-PhD researchers, Dr Sergey Petropavlovsky and Dr Michael Medvinsky, have receive guidance and training from the PI and worked on the project in the capacity of Research Assistant Professors. The subject of Dr Petropavlovsky's work is full-fledged unsteady MDP in (3+1)-D formulation with the Huygens' principle. The subject of Dr Medvinsky's work is the 3D Helmholtz equation, including multiple scattering.

Results Dissemination: The results have been published in top scholarly journals (Journal of Computational Physics, Journal of Scientific Computing, SIAM Journal on Scientific Computing, and others), and presented at high profile national and international research conferences (International Conference on Spectral and High Order Methods series, International Conference on Mathematical and Numerical Aspects of Wave Propagation series, international conference Mathematics and its Applications, 14th World Congress in Computational Mechanics and ECCOMAS Congress, Advanced Computational Electromagnetics Society Conference, and others).

Honors and Awards: Nothing to Report

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PARTICIPANTS:

Participant Type: Faculty
Participant: Eli Turkel
Person Months Worked: 1.00 **Funding Support:**
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Participant Type: Graduate Student (research assistant)
Participant: Evan North
Person Months Worked: 6.00 **Funding Support:**
Project Contribution:
National Academy Member: N

Participant Type: Graduate Student (research assistant)
Participant: Fouche Smith
Person Months Worked: 6.00 **Funding Support:**
Project Contribution:
National Academy Member: N

Participant Type: PD/PI
Participant: Semyon Tsynkov
Person Months Worked: 2.00 **Funding Support:**
Project Contribution:
National Academy Member: N

Participant Type: Staff Scientist (doctoral level)
Participant: Michael Medvinsky
Person Months Worked: 4.00 **Funding Support:**
Project Contribution:
National Academy Member: N

Participant Type: Staff Scientist (doctoral level)
Participant: Sergey Petropavlovsky
Person Months Worked: 3.00 **Funding Support:**
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Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)
Participant: Steven Britt
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Article Title: A high order compact time/space finite difference scheme for the wave equation with variable speed of sound
Authors: Steven Britt, Eli Turkel, Semyon Tsynkov
Keywords: compact finite differences, wave equation, variable coefficients, high order accuracy
Abstract: We consider fourth order accurate compact schemes, in both space and time, for the second order wave equation with a variable speed of sound. We demonstrate that usually this is much more efficient than lower order schemes despite being implicit and only conditionally stable. Fast time marching of the implicit scheme is accomplished by iterative methods such as conjugate gradient and multigrid. For conjugate gradient, an upper bound on the convergence rate of the iterations is obtained by eigenvalue analysis of the scheme. The implicit discretization technique is such that the spatial and temporal convergence orders can be adjusted independently of each other. In special cases, the spatial error dominates the problem, and then an unconditionally stable second order accurate scheme in time with fourth order accuracy in space is more efficient. Computations confirm the design convergence rate for the inhomogeneous, variable wave speed equation and also confirm the pollution effect.
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Article Title: Non-deteriorating time domain numerical algorithms for Maxwell's electrodynamics
Authors: Sergei Petropavlovsky, Semyon Tsynkov
Keywords: Unsteady electromagnetic waves; Maxwell's equations; unbounded regions; grid truncation; artificial outer boundaries; artificial boundary conditions (ABCs); non-reflecting boundaries; perfectly matched layer (PML); long time deterioration; loss of accuracy, loss of stability, error build-up; the Huygens' principle; aft fronts of the waves; lacunae of the solutions; quasi-lacunae; accumulation of charge; guaranteed accuracy; temporally uniform error bounds.
Abstract: In this paper, we develop and test a new algorithm that can furnish an exact artificial boundary condition (ABC) for the numerical simulation of electromagnetic waves propagating over unbounded regions, and can also stabilize any existing ABC or PML (perfectly matched layer) on arbitrarily long time intervals. The algorithm applies to a broad range of 3D problems that may involve some sophisticated physical phenomena in the near field (generation, absorption, reflection, scattering, etc.\ of waves inside a bounded region) yet reduce to the propagation of electromagnetic waves in vacuum in the far field. In practice, only the near-field solution is actually computed, while the far field is truncated off and replaced by an ABC or a PML at the artificial outer boundary. The overall original problem must be uniquely solvable and well-posed.
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Article Title: High-order numerical solution of the Helmholtz equation for domains with reentrant corners

Authors: S. Magura, S. Petropavlovsky, S. Tsynkov, E. Turkel

Keywords: singularity subtraction, regularization, asymptotic expansion near singularity, difference potentials, curvilinear boundaries, compact differencing

Abstract: Standard numerical methods often fail to solve the Helmholtz equation accurately near reentrant corners, since the solution may become singular. The singularity has an inhomogeneous contribution from the boundary data near the corner and a homogeneous contribution that is determined by boundary conditions far from the corner. We present a regularization algorithm that uses a combination of analytical and numerical tools to distinguish between these two contributions and ultimately subtract the singularity. We then employ the method of difference potentials to numerically solve the regularized problem with high-order accuracy over a domain with a curvilinear boundary. Our numerical experiments show that the regularization successfully restores the design rate of convergence.

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Article Title: Numerical solution of the wave equation with variable wave speed on nonconforming domains by high-order difference potentials

Authors: S. Britt, S. Tsynkov, E. Turkel

Keywords: method of difference potentials (MDP); compact finite difference scheme; implicit scheme; regular structured grid; nonconforming boundary; high-order accuracy; high-order MDP

Abstract: We solve the wave equation with variable wave speed on nonconforming domains with fourth order accuracy in both space and time. This is accomplished using an implicit finite difference (FD) scheme for the wave equation and solving an elliptic (modified Helmholtz) equation at each time step with fourth order spatial accuracy by the method of difference potentials (MDP). High-order MDP utilizes compact FD schemes on regular structured grids to efficiently solve problems on nonconforming domains while maintaining the design convergence rate of the underlying FD scheme. Asymptotically, the computational complexity of high-order MDP scales the same as that for FD.

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Article Title: A method of boundary equations for unsteady hyperbolic problems in 3D
Authors: S. Petropavlovsky, S. Tsynkov, E. Turkel
Keywords: Time-dependent wave equation; Calderon's boundary equation; The Huygens' principle; Method of difference potentials (MDP); Sub-linear complexity; Parallelization in time.
Abstract: We consider interior and exterior initial boundary value problems for the three-dimensional wave equation. First, we reduce a given problem to an equivalent operator equation with respect to unknown sources defined at the boundary of the original domain. The Huygens' principle enables us to obtain the operator equation in a form that involves only finite and non-increasing pre-history of the solution in time. Next, we discretize the resulting boundary equation and solve it efficiently by the method of difference potentials. The overall numerical algorithm handles boundaries of general shape using regular structured grids with no deterioration of accuracy. For long simulation times it offers sub-linear complexity with respect to the grid dimension. In addition, our algorithm allows one to share the computational cost between multiple similar problems. On multi-processor platforms, it benefits from what can be considered an effective parallelization in time.
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Article Title: Direct implementation of high order BGT artificial boundary conditions
Authors: Michael Medvinsky, Semyon Tsynkov, Eli Turkel
Keywords: Propagation of waves over unbounded regions; Helmholtz equation; Spherical artificial boundary; Expansion with respect to continuous basis; Method of difference potentials (MDP); Beltrami operator.
Abstract: Local artificial boundary conditions for the numerical simulation of waves are well known. The basic idea is to cancel several leading terms in the far-field expansion of the solution. The larger the number of terms canceled, the higher the order of the boundary condition and the smaller the reflection error. In practice, however, the use of local ABCs has been limited to low orders, because higher order derivatives in the ABCs may harm well-posedness and cause numerical instabilities. In the current paper, we implement high order ABCs directly --- with no auxiliary variables and no discrete approximation of the high order derivatives. We represent the solution at the boundary as an expansion with respect to a basis that consists of eigenfunctions of the Beltrami operator. This enables replacing the high order derivatives with powers of the eigenvalues. Continuous representation at the boundary is coupled to higher order finite differences by the method of difference potentials.
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Authors: Steven Britt, Sergei Petropavlovsky, Semyon Tsynkov, Eli Turkel
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Authors: Sergey Petropavlovsky, Semyon Tsynkov, Eli Turkel
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Authors: S. V. Petropavlovsky, S. V. Tsynkov, and E. Turkel
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Authors: S. V. Petropavlovsky, S. V. Tsynkov, and E. Turkel
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Authors: Sergey Petropavlovsky ,Semyon Tsynkov, Eli Turkel
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Authors: Sergey Petropavlovsky, Semyon Tsynkov, Eli Turkel
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Paper Title: A Fourth Order Compact Scheme with Difference Potentials for the 3D Wave Equation
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Paper Title: Numerical Solution of 3D Unsteady Scattering Problems with Sub-linear Complexity
Authors: Sergey Petropavlovsky, Semyon Tsynkov, Eli Turkel
Acknowledged Federal Support: **Y**

Partners

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I certify that the information in the report is complete and accurate:
Signature: Semyon Tsynkov
Signature Date: 8/27/21 1:34PM

Numerical Solution of 3D Unsteady Scattering Problems with Sub-linear Complexity

Semyon Tsynkov[1]

[1] Department of Mathematics
North Carolina State University, Raleigh, NC, USA

https://stsynkov.math.ncsu.edu
tsynkov@math.ncsu.edu

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Virtual Delivery, 1–5 August, 2021

Collaborators and support

- Collaborators:
  - Sergey Petropavlovsky
    - ★ National Research University Higher School of Economics, Moscow, Russia
    - ★ North Carolina State University, Raleigh, NC, USA
  - Eli Turkel
    - ★ Tel Aviv University, Tel Aviv, Israel
- Support:
  - US ARO (W911NF-16-1-0115 and W911NF-14-C-0161)
  - US-Israel BSF (2014048 and 2020128)

Retrospect and objectives

- Develop an efficient time-dependent counterpart to BIEs/BEM.
- The Huygens' principle enables a very accurate treatment of artificial outer boundaries in numerical simulation of waves:
  - Partition the time domain into segments and stop the simulation for each segment once the domain falls into the lacuna;
  - [Ryaben'kii, Turchaninov, Tsynkov, et al., 1990, 2000, 2001, ...]
- Also stabilizes ABCs and PMLs over long simulation times.
  - [Petropavlovsky, Tsynkov, Turkel, et al., 2008, 2012, 2017, ...]
- Current objective: use it to treat other types of boundaries:
  - Extend the methodology to general unsteady hyperbolic IBVPs;
  - Allow for a variety of boundary shapes and boundary conditions;
  - Include both interior and exterior formulations;
  - Allow for high order accuracy;
  - Allow for arbitrarily long time intervals.

Motivation and overview

- BIEs reduce the dimension of the problem:
  - Typically used for elliptic equations;
  - Offer substantial flexibility from the standpoint of geometry;
  - Cenefits for unsteady problems include the reduced complexity and automatic treatment of outer boundaries.
- RPBIEs generalize BIEs to hyperbolic case [Ha-Duong, 2003], [Michielssen, et. al., 2005, 2006], [Abboud, 2011], [Sayas, 2016] :
  - Discretization may be unstable [Epstein, Greengard, Hagstrom, 2016]
  - Quadratures are increasingly costly at longer times [Lubich, 1994].
- The Huygens' principle removes the main limitation of RPBIEs:
  - Yields an equivalent boundary operator equation with finite and non-increasing backward dependence on time.
- Solved by Ryaben'kii's method of difference potentials:
  - Renders parallelization in time on multi-processor systems.

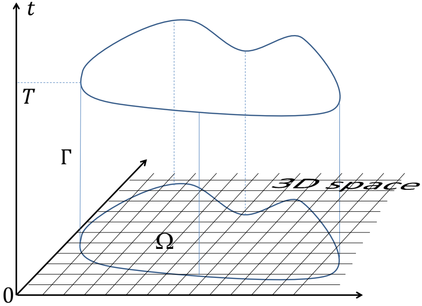
Exterior problem for the d'Alembert equation

An exterior IBVP for the 3D wave equation on $\tilde{\Omega} \overset{\text{def}}{=} \mathbb{R}^3 \backslash \bar{\Omega}$:

$$\Box_c u(\boldsymbol{x}, t) \equiv \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} - \Delta u = 0, \quad (\boldsymbol{x}, t) \in \tilde{\Omega} \times (0, T],$$

$$u\Big|_{t=0} = 0, \quad \frac{\partial u}{\partial t}\Big|_{t=0} = 0, \quad \boldsymbol{x} \in \tilde{\Omega},$$

$$\boldsymbol{l}_\Gamma u = \phi, \quad (\boldsymbol{x}, t) \in \Gamma \equiv \partial\tilde{\Omega} \times (0, T].$$



- Exterior scattering problem — relevant for many applications.
- Inhomogeneous ICs are allowed (compactly supported).
- Boundary conditions may be of any type and may depend on time.
- Time T may be arbitrarily long.
- Equations beyond d'Alembert can be considered (e.g., Maxwell's).

Calderon's operators

- $\Omega \subset \mathbb{R}^3$ — bounded; $\tilde{\Omega} = \mathbb{R}^3 \backslash \bar{\Omega}$. Calderon's potential for $\boldsymbol{x} \in \tilde{\Omega}$:

$$\boldsymbol{P}_{\tilde{\Omega}} \boldsymbol{\xi}_{\Gamma_t}(\boldsymbol{x}, t) = \int\limits_{\Gamma_t} \left\{ \xi_1(\boldsymbol{y}, t') G(\boldsymbol{x} - \boldsymbol{y}, t - t') - \xi_0(\boldsymbol{y}, t') \frac{\partial G}{\partial \boldsymbol{n}}(\boldsymbol{x} - \boldsymbol{y}, t - t') \right\} dt' dS_{\boldsymbol{y}},$$

  where $G(\boldsymbol{x}, t) = \frac{c}{2\pi} \theta(t) \delta(c^2 t^2 - |\boldsymbol{x}|^2)$ is the fundamental solution.
- The density $\boldsymbol{\xi}_{\Gamma_t} = (\xi_0, \xi_1)$ is defined on the space-time boundary Γ_t.
- Vector trace of the potential is Calderon's projection:

$$\boldsymbol{P}_{\Gamma_t} \overset{\text{def}}{=} \boldsymbol{Tr}_{\Gamma_t} \boldsymbol{P}_{\tilde{\Omega}}, \quad \text{where} \quad \boldsymbol{Tr}_{\Gamma_t} w \overset{\text{def}}{=} \left(w, \frac{\partial w}{\partial \boldsymbol{n}} \right) \Bigg|_{\Gamma_t}.$$

- Calderon's boundary equation with projection (BEP):

$$\boldsymbol{P}_{\Gamma_t} \boldsymbol{\xi}_{\Gamma_t} = \boldsymbol{\xi}_{\Gamma_t}$$

  holds if and only if $\boldsymbol{\xi}_{\Gamma_t} = \boldsymbol{Tr}_{\Gamma_t} u$, where $\Box_c u = 0$ on $\tilde{\Omega}$.
- Advantages: physical sources and independence of the BCs.
- The BC $\boldsymbol{l}_{\Gamma_t} u = \phi$ is added to the BEP to form a combined system.

Partition in time

- As the time elapses, the boundary Γ_t extends — unlike elliptic!
- Let $0 \leqslant t \leqslant K \cdot T_0 \equiv T$. Partition the boundary Γ_T into K equal parts:

$$\Gamma_T = \Gamma_1 \cup \Gamma_2 \cup \ldots \cup \Gamma_K, \quad \text{where} \quad \Gamma_k = \partial\Omega \times ((k-1)T_0, kT_0].$$

- The partial densities $\boldsymbol{\xi}_{\Gamma_k}$ can be determined consecutively:

$$\begin{gathered} \boldsymbol{P}_{\Gamma_{T_0}} \boldsymbol{\xi}_{\Gamma_K} + \textstyle\sum_{k=1}^{K-1} \boldsymbol{Tr}_{\Gamma_K} \boldsymbol{P}_{\tilde{\Omega}} \boldsymbol{\xi}_{\Gamma_k} = \boldsymbol{\xi}_{\Gamma_K}, \\ \boldsymbol{l}_{\Gamma_K} \boldsymbol{\xi}_{\Gamma_K} = \phi. \end{gathered}$$

- System of equations to obtain $\boldsymbol{\xi}_{\Gamma_K}$ given the previous $\boldsymbol{\xi}_{\Gamma_k}$, $k \leqslant K-1$.
- T and K arbitrary. Can continue consecutive updates $K \mapsto K+1$.
- Still full backward dependence on time: $\boldsymbol{\xi}_{\Gamma_K} = \boldsymbol{\xi}_{\Gamma_K}(\boldsymbol{\xi}_{\Gamma_{K-1}}, \ldots, \boldsymbol{\xi}_{\Gamma_1})$.

Huygens' principle and lacunae

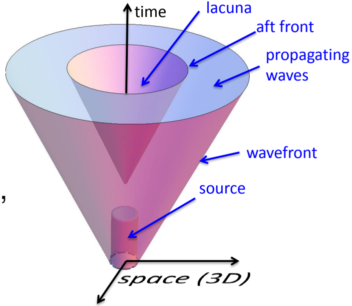
- The fundamental solution $G(\boldsymbol{x},t)=\frac{c}{2\pi}\theta(t)\delta(c^2t^2-|\boldsymbol{x}|^2)$ is an expanding spherical layer with "empty" interior — lacuna.
- 3D wave equation with a compactly supported RHS, $\Box_c u = f$, $\operatorname{supp} f \subseteq Q$, has a secondary lacuna of the solution:

$$u(\boldsymbol{x},t)\equiv 0 \quad \forall(\boldsymbol{x},t)\in \bigcap_{(\boldsymbol{\xi},\tau)\in Q}\left\{(\boldsymbol{x},t)\big|\,|\boldsymbol{x}-\boldsymbol{\xi}|<c(t-\tau),\ t>\tau\right\} \overset{\text{def}}{=} \Lambda.$$

- Implication of the Kirchhoff integral:

$$u(\boldsymbol{x},t)=\frac{1}{4\pi}\iiint\limits_{|\boldsymbol{x}-\boldsymbol{\xi}|\leqslant ct}\frac{f(\boldsymbol{\xi},t-|\boldsymbol{x}-\boldsymbol{\xi}|/c)}{|\boldsymbol{x}-\boldsymbol{\xi}|}d\boldsymbol{\xi}.$$

- Overall, a rare phenomenon. Its opposite, the diffusion of waves, is more common.
- Important applications are Huygens': electromagnetic and elastic waves.



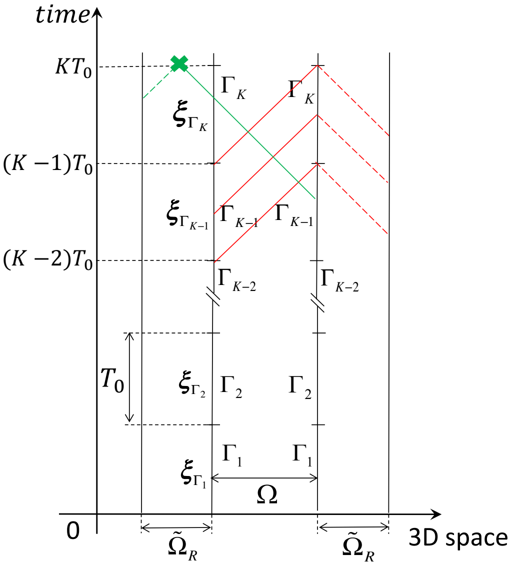
Application of lacunae to IBVPs

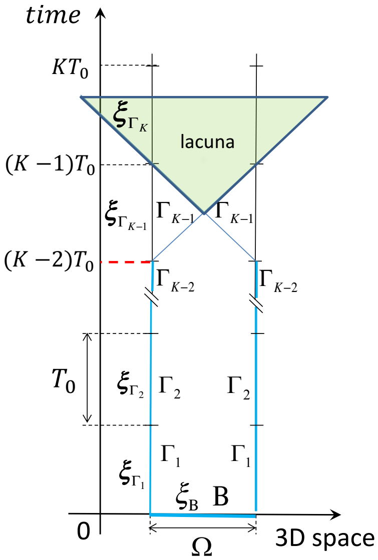
- Choose $T_0 \geqslant \frac{1}{c}\,\mathrm{diam}\,\Omega$. As $\boldsymbol{P}_{\tilde{\Omega}}$ is convolution with G, there will be no contribution from any of $\boldsymbol{\xi}_{\Gamma_k}$, $k = K-2, \ldots, 1$. Therefore,

$$\boldsymbol{P}_{\Gamma_{T_0}} \boldsymbol{\xi}_{\Gamma_K} + \underbrace{\boldsymbol{Tr}_{\Gamma_K} \boldsymbol{P}_{\tilde{\Omega}}}_{\boldsymbol{R}_{\Gamma_{T_0}}} \boldsymbol{\xi}_{\Gamma_{K-1}} = \boldsymbol{\xi}_{\Gamma_K}.$$

  Thus, $\boldsymbol{\xi}_{\Gamma_K}$ depends only on the immediately preceding $\boldsymbol{\xi}_{\Gamma_{K-1}}$.
- To determine $\boldsymbol{\xi}_{\Gamma_K}$, one needs the BC: $\boldsymbol{l}_{\Gamma_K} \boldsymbol{\xi}_{\Gamma_K} = \phi$.
- Effective time marching with respect to K, $\boldsymbol{\xi}_{\Gamma_{K-1}} \mapsto \boldsymbol{\xi}_{\Gamma_K}$:
  - Performed along a $(2+1)$-dimensional lateral boundary.
- The limited backward dependence on time is a direct implication of the Huygens' principle:
  - Calderon's operators take advantage of the lacuna of G;
  - This enables the two-step time-marching algorithm: $K-1 \mapsto K$.

Application of lacunae to IBVPs (schematic)





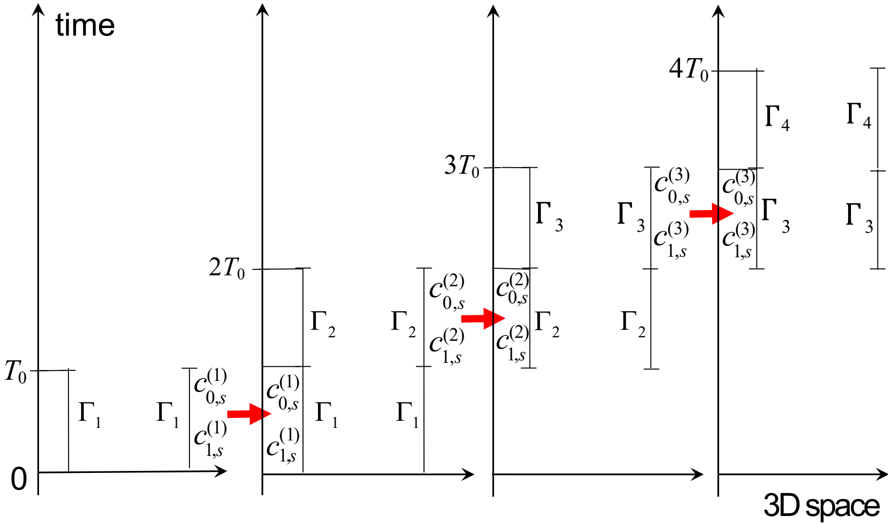
Time marching with respect to K

- Basis on Γ_{K-1} and Γ_K, $\{\boldsymbol{\psi}_{0,s} = (\psi_s, 0),\ \boldsymbol{\psi}_{1,s} = (0, \psi_s)\}$:

$$\boldsymbol{\xi}_{\Gamma_{K-1}} = \sum_s c_{0,s}^{(K-1)} \boldsymbol{\psi}_{0,s} + c_{1,s}^{(K-1)} \boldsymbol{\psi}_{1,s}, \qquad \boldsymbol{\xi}_{\Gamma_K} = \sum_s c_{0,s}^{(K)} \boldsymbol{\psi}_{0,s} + c_{1,s}^{(K)} \boldsymbol{\psi}_{1,s}.$$

- The operators $\boldsymbol{P}_{\Gamma_{T_0}}$ and $\boldsymbol{R}_{\Gamma_{T_0}}$ do not depend on K.
- The basis functions $\boldsymbol{\psi}_{0,s}$ and $\boldsymbol{\psi}_{1,s}$ are also the same for all K.
- Operators $\boldsymbol{P}_{\Gamma_{T_0}}$ and $\boldsymbol{R}_{\Gamma_{T_0}}$ are precomputed in the basis $\{\boldsymbol{\psi}_{0,s}, \boldsymbol{\psi}_{1,s}\}$.
- In time marching w.r.t. K, $c_{0,s}^{(K)}$, $c_{1,s}^{(K)}$ are the unknowns, and $c_{0,s}^{(K-1)}$, $c_{1,s}^{(K-1)}$ are the data. Solve for $c_{0,s}^{(K)}$, $c_{1,s}^{(K)}$ by least squares.
- After the coefficients $c_{0,s}^{(K)}$, $c_{1,s}^{(K)}$ have been determined, perform one time step: solve for $c_{0,s}^{(K+1)}$, $c_{1,s}^{(K+1)}$ given $c_{0,s}^{(K)}$, $c_{1,s}^{(K)}$.
- We solve only for the coefficients of an expansion at the boundary.

Time marching with respect to K (schematic)

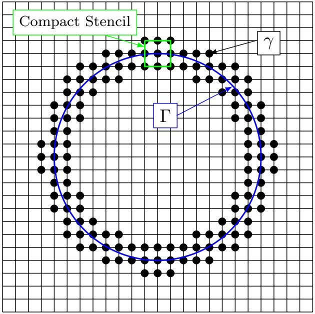


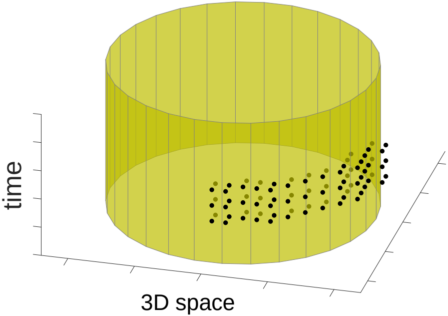
Full discretization by difference potentials

- Surface integrals are replaced with a special auxiliary problem (AP).
  - Solved by finite differences on a regular structured grid (Cartesian);
  - The shape of the boundary can be non-conforming.
- Solution of the difference AP yields discrete counterparts of Calderon's operators:
  - Discrete Calderon's operators are not tied to any BCs;
  - Specific boundary conditions are later added to the overall system;
  - No approximation of the boundary conditions on the grid is required.
- The boundary is coupled to the grid via extension operators:
  - Constructed by means of equation-based Taylor formulae;
  - Enable approximation of continuous potentials by difference potentials.

Discrete Calderon's operators

- The grid boundary γ_t straddles the continuous boundary Γ_t. γ_t depends on the scheme stencil.



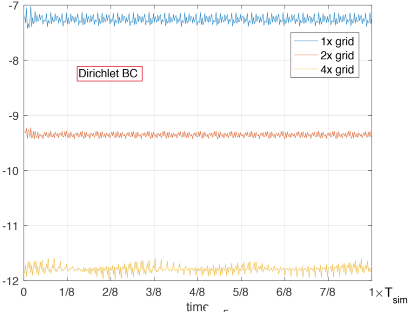


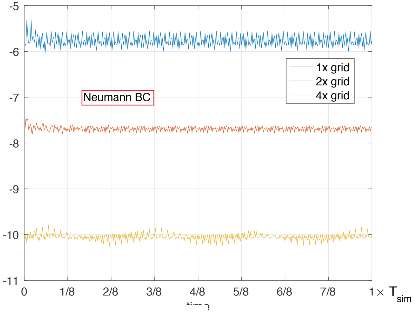
- Difference boundary projection $\boldsymbol{P}_{\gamma_t}$ is an operator in the space of grid functions defined on γ_t — obtained by solving the discrete AP.
- The discrete BEP $\boldsymbol{P}_{\gamma_t}\xi_{\gamma_t} = \xi_{\gamma_t}$ holds iff there is a solution $u^{(h)}$ of the discrete wave equation such that $u^{(h)}\big|_{\gamma_t} = \xi_{\gamma_t}$.

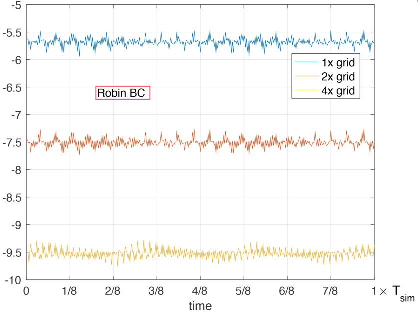
Summary of key features

- High order accuracy for general (non-conforming) shapes with no limitations on stability due to cut cells.
- Numerical efficiency via reduced complexity (sub-linear) and low cost solution of similar problems.
- Compact discretizations in space and time to attain high order accuracy inexpensively.
- Efficient and universal treatment of a broad range of boundary conditions.
- Non-deteriorating performance over long simulation times.
- Efficient implementation on parallel platforms, including parallelization in time.

Second order scheme: Grid convergence







Second order scheme: Error and complexity

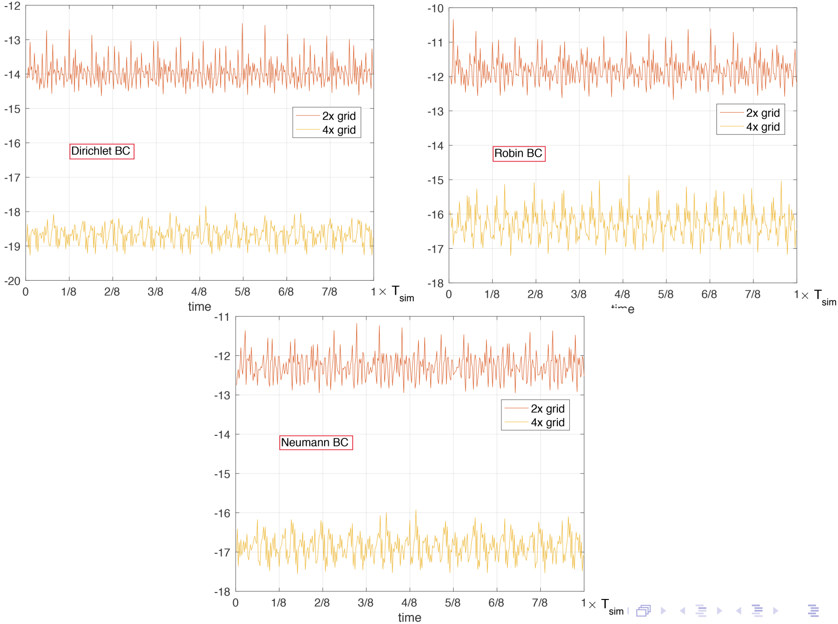
Grid	Dirichlet		Neumann		Robin	
	Mean error	Rate	Mean error	Rate	Mean error	Rate
1x	6.55×10^{-3}	-	1.84×10^{-2}	-	2.02×10^{-2}	-
2x	1.52×10^{-3}	4.27	4.84×10^{-3}	3.81	5.74×10^{-3}	3.52
4x	2.91×10^{-4}	5.25	9.69×10^{-4}	4.99	1.41×10^{-3}	4.06

Actual values of the error and convergence rates.

Grid	volumetric method+PML		MDP+lacunae	
	CPU time, sec	scaling rate	CPU time, sec	scaling rate
1x	1.26	-	0.0614	-
2x	19.8	15.7	0.516	8.44
4x	322	16.3	4.44	8.61

Cost comparison against volumetric method: sub-linear complexity.

Fourth order scheme: Grid convergence



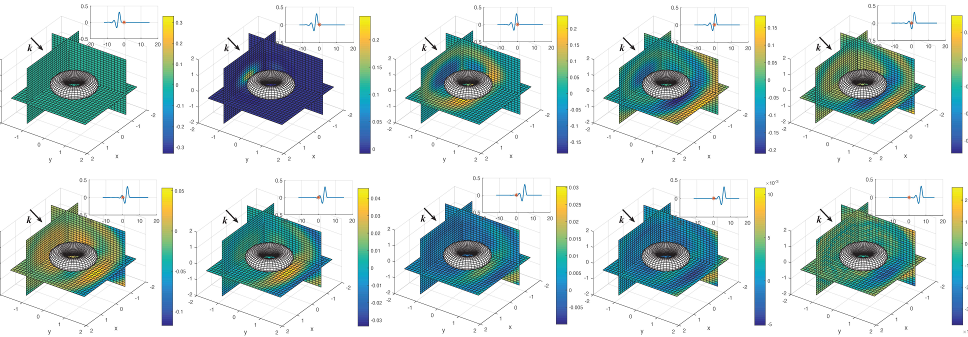
Fourth order scheme: Error

Grid	Dirichlet		Neumann		Mixed	
	Mean error	Rate	Mean error	Rate	Mean error	Rate
2x	6.52×10^{-5}	-	2.09×10^{-4}	-	2.86×10^{-4}	-
4x	2.44×10^{-6}	26	8.60×10^{-6}	24	1.31×10^{-5}	21

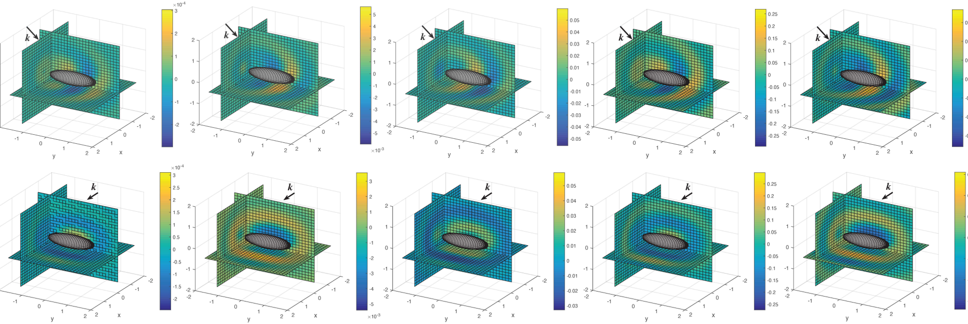
Actual values of the error and convergence rates.

- Compared to the second order scheme:
  - Convergence rates are higher (expected);
  - Specific values of the error are lower on respective grids.

Scattering of a chirp about a torus

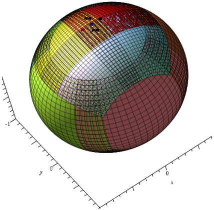


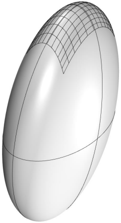
Scattering about a prolate spheroid at two incident directions

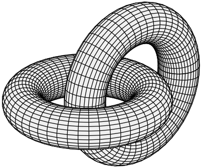


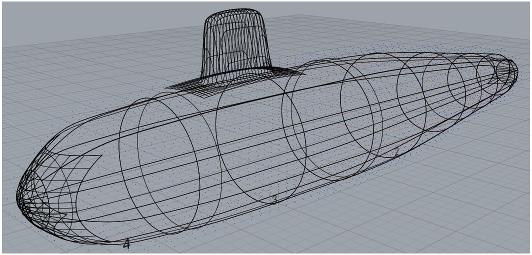
Future work

- More sophisticated geometries/shapes; Multiple scattering; Interfaces, transmission/scattering problems; Systems (Maxwell's).









Difference potentials for 3D time-dependent wave propagation

Semyon Tsynkov[1]

[1] Department of Mathematics
North Carolina State University, Raleigh, NC, USA

https://stsynkov.math.ncsu.edu
tsynkov@math.ncsu.edu

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12th - 16th July 2021 | Vienna, Austria
(virtual delivery)

Collaborators and support

- Collaborators:
  - Sergey Petropavlovsky (Higher School of Economics, Moscow, Russia and NC State University, Raleigh, NC, USA)
  - Fouche Smith (NC State University, Raleigh, NC, USA)
  - Eli Turkel (Tel Aviv University, Tel Aviv, Israel)

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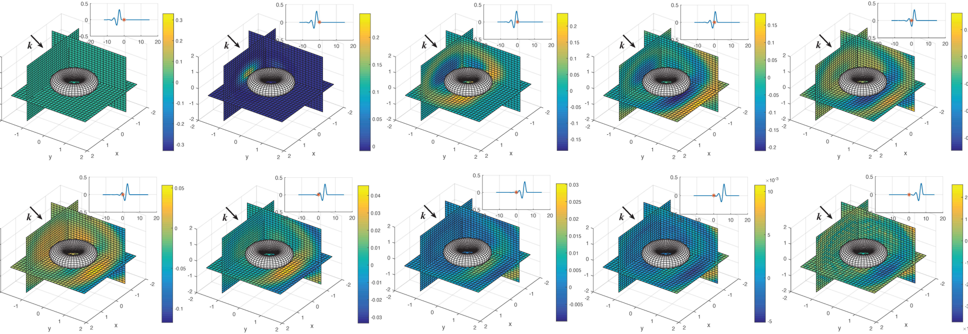
  - US-Israel BSF (2014048 and 2020128)

Difference potentials

- Discrete counterparts to Calderon's operators.
- Originally developed for elliptic problems (Poisson, Helmholtz, ...).
- Provide equivalent reduction from the domain to the boundary.
- High order accuracy (regular grids & non-conforming boundaries).
- Universal treatment of the boundary conditions:
  - Boundary conditions do not need to be approximated on the grid.
- Efficient solution of multiple similar problems.
- Two ways of implementation for time-dependent problems.
- Direct application to full (3+1)D equation/system:
  - The use of the Huygens' principle enables sub-linear complexity
  - and automatic treatment of artificial outer boundaries.
  - Guaranteed non-deteriorating performance over long times.
- Application on the upper time level of an implicit scheme (elliptic):
  - Allows for a variable speed of propagation.

Scattering of a chirp about a torus



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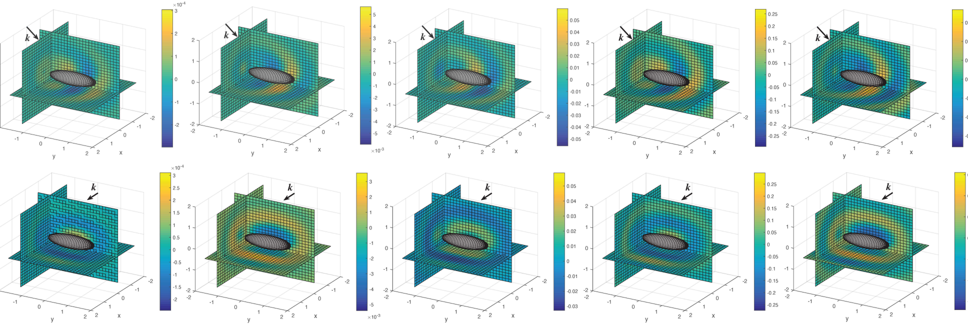

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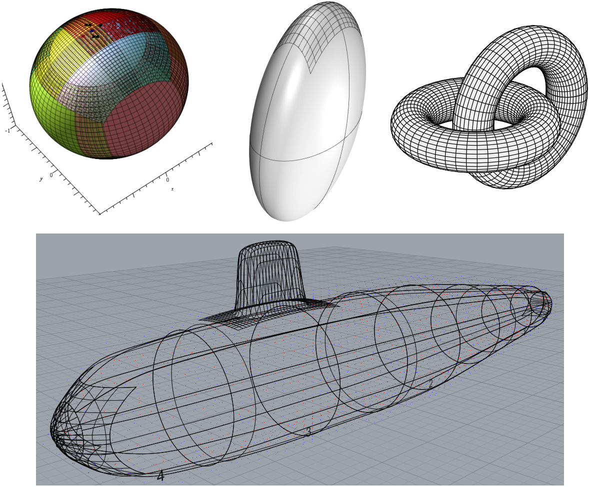

A Fourth Order Compact Scheme with Difference Potentials for the 3D Wave Equation

Fouche Smith[1], Semyon Tsynkov [1], and Eli Turkel[2]

[1]North Carolina State University, Raleigh, NC, USA

[2]Tel Aviv University, Tel Aviv, Israel

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Problem Statement

Consider the interior or exterior problem

$$\begin{cases} \frac{\partial^2 u}{\partial t^2} - c^2(\boldsymbol{x})\Delta u & = F(\boldsymbol{x}, t), \quad (\boldsymbol{x}, t) \in \Omega \times (0, \infty) \\ u(\boldsymbol{x}, 0) & = u_0(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega \\ \frac{\partial u}{\partial t}(\boldsymbol{x}, 0) & = v_0(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega \\ \boldsymbol{l}(u) & = \psi(\boldsymbol{x}, t), \qquad \boldsymbol{x} \in \Gamma = \partial\Omega \end{cases} \tag{1}$$

where $\Omega = B_R(\mathbf{0})$ or $\Omega = \mathbb{R}^3 \setminus B_R(\mathbf{0})$. If $\Omega = \mathbb{R}^3 \setminus B_R(\mathbf{0})$ the initial data and source term are compactly supported in space.
GOAL: Solve the interior/exterior problem with fourth order accuracy in space and time efficiently.
Keywords: Compact Finite Differences, Method of Difference Potential (MDP), artificial boundary conditions (ABCs), efficient implicit time marching scheme, multigrid methods

Outline of Approach

- Discretize the wave equation in t with the θ-scheme. The resulting implicit semi-discrete approximation in time is an elliptic BVP (Chabassier 2013).
- Embed the elliptic BVP in a cube (via MDP).
- Discretize in space using a compact finite difference scheme.
- Use geometric multigrid to solve the embedded elliptic BVP.
- Advance the time marching scheme.

Boundary Equations of Calderón-Seely Type

The following is the continuous counterpart to the MDP

- Construct an auxiliary problem (AP)
  1. Choose a simple set Ω^0 such that $\bar{\Omega} \subset \Omega^0$.
  2. Choose a BC so the the AP on Ω^0 is well posed.
  3. The PDE of the AP must coincide w/ the PDE on Ω.
- The Calderón potential, $P_{\bar{\Omega}\Gamma}\boldsymbol{v}_\Gamma$, with vector density $\boldsymbol{v}_\Gamma$ is a solution to the AP driven by the source term that depends on $\boldsymbol{v}_\Gamma$.
- The Calderón projection is the vector trace of the potential: $P_\Gamma \boldsymbol{v}_\Gamma = \left(P_{\bar{\Omega}\Gamma}\boldsymbol{v}_\Gamma|_\Gamma, \frac{\partial}{\partial n} P_{\bar{\Omega}\Gamma}\boldsymbol{v}_\Gamma|_\Gamma\right)$.
- The PDE on Ω is equivalent to the boundary equation with projection (BEP) on Γ: $\quad P_\Gamma \boldsymbol{u}_\Gamma = \boldsymbol{u}_\Gamma$.
- In other words, u is a solution on Ω if and only if its vector trace $\boldsymbol{u}_\Gamma = (u|_\Gamma, \frac{\partial u}{\partial n}|_\Gamma)$ satisfies the BEP.
- The MDP solves the PDE on Ω by replacing the above with discrete counterparts.
- See "Method of Difference Potentials and Its Applications" by Ryaben'kii for the definitive guide on MDP.

Multigrid Cycle (MGCYC)

- Family of fast iterative methods for solving discrete elliptic PDEs.
- Based on the smoothing and coarse grid principles.

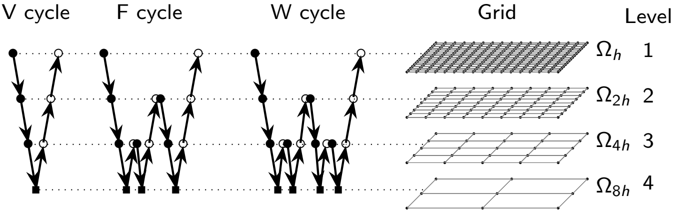


Figure: Schematic of three common MGCYC. The symbols (●) denote pre-smoothing steps, (○) — post-smoothing steps, (■) — direct solver, (↘) — restriction, and (↗) — prolongation + coarse grid correction.

- Gauss-Seidel, Full Weighting, and Tri-Cubic Interpolation are our smoother, restriction operator, and prolongation operator respectively.
- See "A Multigrid Tutorial" by Briggs or "Multigrid" by Trottenburg and Schuller for a complete look into multigrid methods.

Approximating the Wave Equation in Time

- Applying the θ-scheme to the wave equation yields $\delta_t^2 u^n = F^n + c^2(\boldsymbol{x})\Delta u^n + \theta\tau^2(\delta_t^2 F^n + c^2(\boldsymbol{x})\delta_t^2 \Delta u^n),\ \theta \in \mathbb{R}$
- After rearranging (assuming $\theta \neq 0$) $(\Delta - \kappa^2(\boldsymbol{x}))u^{n+1} = 2(\Delta - \kappa^2(\boldsymbol{x}))u^n - (\Delta - \kappa^2(\boldsymbol{x}))u^{n-1} - \frac{1}{\theta}\Delta u^n + \tilde{F}^{n+1}$ where the "wavenumber" $\kappa^2(\boldsymbol{x}) = \frac{1}{\theta\tau^2 c^2(\boldsymbol{x})}$ and $\tilde{F}^{n+1} = -\frac{1}{c^2(\boldsymbol{x})}\left(F^{n+1} + (1/\theta - 2)F^n + F^{n-1}\right)$
- If $f^n \triangleq (\Delta - \kappa^2(\boldsymbol{x}))u^n$, the above satisfies the modified Helmholtz equation

$$(\Delta - \kappa^2(\boldsymbol{x}))u^{n+1} \triangleq f^{n+1} = (2 - 1/\theta)f^n - f^{n-1} - \frac{\kappa^2(\boldsymbol{x})}{\theta}u^n + \tilde{F}^{n+1}, \quad \boldsymbol{x} \in \Omega$$

$$\boldsymbol{I}(u) = \psi(x, t^{n+1}), \quad \boldsymbol{x} \in \Gamma$$

- $\theta = 1/12$ is the only 4^{th} order scheme which uses three levels in time.

Discrete Modified Helmholtz Equation

- In (Smith 2019), we derived the fourth order compact (FOC) discretization of the modified Helmholtz equation $\boldsymbol{L}_h[\kappa^2]u = h^2\boldsymbol{R}_h f$ where the LHS/RHS operators are given by

$$\boldsymbol{L}_h[\kappa^2]u = -4u_{i,j,k} + \frac{u_{ss}}{3} + \frac{u_{sc}}{6} - h^2\left(\frac{2}{3}(\kappa^2 u)_{i,j,k} + \frac{(\kappa^2 u)_{ss}}{36} + \frac{(\kappa^2 u)_{sc}}{72}\right)$$

$$\boldsymbol{R}_h f = \frac{2}{3}f_{i,j,k} + \frac{f_{ss}}{36} + \frac{f_{sc}}{72}$$

and the sums

$$\begin{aligned} u_{ss} &= u_{i+1,j,k} + u_{i-1,j,k} + u_{i,j+1,k} + u_{i,j-1,k} + u_{i,j,k+1} + u_{i,j,k-1} \\ u_{sc} &= u_{i+1,j,k+1} + u_{i-1,j,k+1} + u_{i,j+1,k+1} + u_{i,j-1,k+1} + u_{i+1,j+1,k} + u_{i+1,j-1,k} \\ &\quad + u_{i+1,j,k-1} + u_{i-1,j,k-1} + u_{i,j+1,k-1} + u_{i,j-1,k-1} + u_{i-1,j+1,k} + u_{i-1,j-1,k}. \end{aligned}$$

- Combining the θ-scheme with the FOC Modified Helmholtz Equation yields the time marching scheme.
- The CFL number $\lambda(\boldsymbol{x}) = \frac{c(\boldsymbol{x})\tau}{h} \leq \sqrt{\frac{5}{8}}$ where τ, h are the uniform steps in time and space. This ONLY applies when Ω is a cube and has constant periodic boundary conditions.
- Empirically, choose the CFL number $\varepsilon\lambda(\boldsymbol{x})$ where $0 < \varepsilon < 1$.

Auxiliary Problem (AP)

- Consider the generic Modified Helmholtz equation on the upper time level:

$$(\Delta - \kappa^2(\boldsymbol{x}))w^{n+1} = g^{n+1}, \quad \boldsymbol{x} \in \Omega$$
$$\boldsymbol{l}(w^{n+1}) = \psi(\boldsymbol{x}, t^{n+1}), \quad \boldsymbol{x} \in \Gamma$$

- The AP for the Modified Helmholtz equation is

$$(\Delta - \kappa^2(\boldsymbol{x}))w^{n+1} = g^{n+1}, \quad \boldsymbol{x} \in \Omega^0$$
$$w^{n+1}|_{\partial\Omega^0} = 0$$

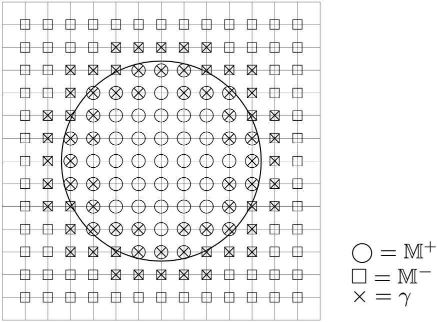
  where Ω^0 is a cube containing Ω.
- Choose Ω^0 large enough so the discrete counter part of Γ won't overlap with $\partial\Omega^0$.
- The discrete AP (DAP) satisfies

$$\boldsymbol{L}_h[\kappa^2]w^{n+1} = g^{n+1}, \quad \boldsymbol{x}_h \in \Omega^0_h$$
$$w^{n+1}|_{\partial\Omega^0_h} = 0$$

- Let $\boldsymbol{G}_h$ denote the solution operator of the DAP: $w^{n+1} = \boldsymbol{G}_h g^{n+1}$.
- $\boldsymbol{G}_h$ produces a unique solution for ANY given RHS.

Grid Sets Discrete Auxiliary Problem

- $\mathbb{M}^+/\mathbb{M}^-$: $\boldsymbol{x}_h$ which belong to $\bar{\Omega}/(\Omega^0 \setminus \bar{\Omega})$.
- $\mathbb{N}^+/\mathbb{N}^-$: union of all nodes contained in the $3 \times 3 \times 3$ stencil centered at $\boldsymbol{x}_h$ which belongs to $\mathbb{M}^+/\mathbb{M}^-$.
- γ : The discrete boundary $\gamma = \mathbb{N}^+ \cap \mathbb{N}^-$.



Boundary Equation with Projection (BEP)

Definition

The difference potential with density v_γ is $\boldsymbol{P}_{\mathbb{N}^+} v_\gamma = w - \boldsymbol{G}_h[\boldsymbol{L}_h[\kappa^2]w\big|_{\mathbb{M}^+}]$, for any w such that $w|_\gamma = v_\gamma$. The difference projection is the trace of the potential: $\boldsymbol{P}_\gamma v_\gamma = \boldsymbol{P}_{\mathbb{N}^+} v_\gamma|_\gamma$

Theorem (Boundary Equation with Projection)

Consider the discrete Modified Helmholtz equation

$$\boldsymbol{L}_h[\kappa^2]u^{n+1}_{\mathbb{N}^+} = \tilde{f}^{n+1}_R = \begin{cases} 0, \boldsymbol{x}_h \in \mathbb{M}^- \\ h^2 \boldsymbol{R}_h f^{n+1}, \boldsymbol{x}_h \in \mathbb{M}^+. \end{cases}$$

Then, the density $v^{n+1}_\gamma = u^{n+1}_{\mathbb{N}^+}|_\gamma$ iff it satisfies the inhomogeneous BEP

$$v^{n+1}_\gamma = \boldsymbol{P}_\gamma v^{n+1}_\gamma + \boldsymbol{G}_h \tilde{f}^{n+1}_R|_\gamma.$$

If the above holds, the solution $u^{n+1}_{\mathbb{N}^+}$ can be reconstructed using the generalized Green's formula:

$$u^{n+1}_{\mathbb{N}^+} = \boldsymbol{P}_{\mathbb{N}^+} v^{n+1}_\gamma + \boldsymbol{G}_h \tilde{f}^{n+1}_R|_{\mathbb{N}^+}$$

Extension Operator I

- The extension operator approximates the density u_γ^{n+1} on the discrete boundary, γ, using the continuous boundary, Γ.
- Assume that $\Omega = B_R(\mathbf{0})$.
- By Taylor's Theorem $u_\gamma^{n+1} = \sum_{j=0}^{J-1} \frac{\rho^j}{j!} \frac{\partial^j u^{n+1}}{\partial r^j}|_\Gamma + O(\rho^J)$, $J = 4, 5$ where ρ is the signed distance from $\boldsymbol{x}_h \in \gamma$ to the orthogonal projection onto Γ.
- Differentiate the wave equation (in spherical coordinates)

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r} + \frac{\Delta_{\theta,\varphi} u}{r^2} + \frac{1}{c^2} F$$

  to replace $\frac{\partial^j}{\partial r^j}$ for $j = 2, \cdots, J-1$ where $\Delta_{\theta,\varphi}$ is the Laplace-Beltrami operator.
- Replace $\frac{\partial^2}{\partial t^2}$ with one sided difference formulas.
- Consequently the extension operator has the form

$$u_\gamma^{n+1} = \boldsymbol{Ex}(u^{n+1}|_\Gamma, \frac{\partial u}{\partial r}|_\Gamma) = \sum_{i=0}^{2} \alpha_J^{(i)}(\rho)\Delta_{\theta,\varphi}^i u^{n+1}|_\Gamma + \beta_J^{(i)}(\rho)\Delta_{\theta,\varphi}^i \frac{\partial u^{n+1}}{\partial r}|_\Gamma + \boldsymbol{Ex}_I^{n+1}$$

where $\boldsymbol{Ex}_I^{n+1}$ contains known quantities.

Extension Operator II

- We will represent the trace $\left(u^{n+1}|_\Gamma, \frac{\partial u^{n+1}}{\partial r}|_\Gamma\right)$ in terms of the spherical harmonics.
- The spherical harmonics have several desirable properties
  - An orthonormal basis on the ball
  - Converge rapidly for smooth functions.
  - Eigenfunctions of the Laplace-Beltrami operator i.e. $\Delta_{\theta,\varphi} Y_l^m(\theta,\varphi) = -l(l+1)Y_l^m(\theta,\varphi)$.
- Consider the expansions

$$(\xi_0,\xi_1) = \sum_{l=0}^{L}\sum_{m=-l}^{l}\left(\langle u^{n+1}, Y_l^m\rangle Y_l^m, \langle \frac{\partial u^{n+1}}{\partial r}, Y_l^m\rangle Y_l^m\right) \approx (u^{n+1}|\Gamma, \frac{\partial u^{n+1}}{\partial r}|_\Gamma)$$

where the weighted inner product

$$\langle f, Y_l^m\rangle = \int_0^{2\pi}\int_0^{\pi} f(R\cos\varphi\sin\theta, R\sin\varphi\sin\theta, R\cos\theta)Y_l^m(\theta,\varphi)d\theta d\varphi.$$

- Substituting the spectral representations into the extension operator produces

$$u_\gamma^{n+1} = \mathbf{Ex}(\xi_0,\xi_1) + \boldsymbol{Ex}_l^{n+1} = \boldsymbol{A}_\Gamma^{\text{Dir}}\boldsymbol{c}_{DIR}^{n+1} + \boldsymbol{A}_\Gamma^{\text{Neu}}\boldsymbol{c}_{NEU}^{n+1} + \boldsymbol{Ex}_l^{n+1}$$

where $\boldsymbol{c}_{DIR}^{n+1}$ and $\boldsymbol{c}_{NEU}^{n+1}$ are vectors for Fourier coefficients for $u^{n+1}|_\Gamma$ and $\frac{\partial u^{n+1}}{\partial r}|_\Gamma$ respectively.

Solving Boundary Equation with Projection

- Substituting the extension operator into the inhomogeneous BEP

$$\boldsymbol{Q}_\Gamma^{\text{Dir}}\boldsymbol{c}_{DIR}^{n+1} + \boldsymbol{Q}_\Gamma^{\text{Neu}}\boldsymbol{c}_{NEU}^{n+1} = -\left(\boldsymbol{G}_h\tilde{\boldsymbol{f}}_R^{n+1}\right)|_\gamma - (\boldsymbol{P}_\gamma - \boldsymbol{I}_\gamma)\boldsymbol{Ex}_I^{n+1}$$

  where $\boldsymbol{Q}_\Gamma^{\text{Dir}}$ and $\boldsymbol{Q}_\Gamma^{\text{Neu}}$ are the result of applying $(\boldsymbol{P}_\gamma - \boldsymbol{I}_\gamma)$ to each of the columns of and $\boldsymbol{A}_\Gamma^{\text{Dir}}$ and $\boldsymbol{A}_\Gamma^{\text{Neu}}$. Compute these ONCE !!!
- In spectral form the boundary condition $\boldsymbol{l}(u) = \psi(\boldsymbol{x}, t^{n+1})$ satisfy

$$\begin{cases} \boldsymbol{c}_{DIR}^{n+1} & = \boldsymbol{c}_\Psi^{n+1}, \text{Dirichlet BC} \\ \boldsymbol{c}_{NEU}^{n+1} & = \boldsymbol{c}_\Psi^{n+1}, \text{Neumann BC} \\ a\boldsymbol{c}_{DIR}^{n+1} + b\boldsymbol{c}_{NEU}^{n+1} & = \boldsymbol{c}_\Psi^{n+1}, \text{Robin BC} \end{cases}$$

- $\#(\text{ spherical harmonics}) = (1+L)^2 \ll |\gamma|$. Solve the overdetermined least squares problem with QR factorization.
- Substitute $\boldsymbol{c}_{DIR}^{n+1}$ and $\boldsymbol{c}_{NEU}^{n+1}$ into the extension operator to compute u_γ^{n+1}.
- Use the generalized Green's formula to compute $u_{\mathbb{N}^+}^{n+1}$.
- Advancing the time marching scheme requires three calls to $\boldsymbol{G}_h$.

Interior Problem

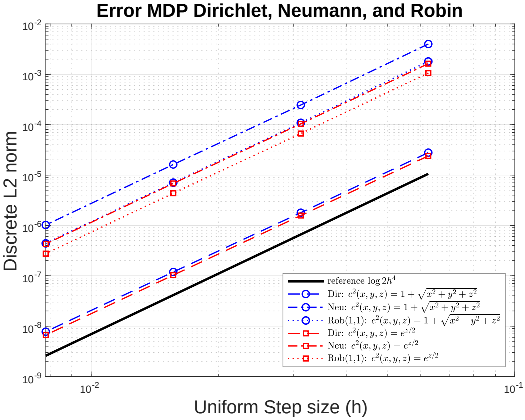


Figure: Problem generated by $u = |\mathbf{x}|^{3/2}\sin(\pi|\mathbf{x}|)e^{t/2}$, with $J = 5$, $L = 15$, $t_F = 1$ where $\Omega = B_{.85}(\mathbf{0})$, $\Omega^0 = [-1,1]^3$ and 90 % of max CFL for various speeds.

How To Set Up the Exterior Problem

- We need to truncate the domain of the exterior problem $\Omega = \mathbb{R}^3 \setminus B_R(\mathbf{0})$.
- Choose $\bar{R} > R$ where $\Omega = B_{\bar{R}}(\mathbf{0}) \setminus B_R(\mathbf{0})$ is the computational domain of the exterior problem.
- The boundary $\Gamma = \Gamma_1 \cup \Gamma_2$ where $\Gamma_1 = \partial B_R(\mathbf{0})$ has BC $\boldsymbol{l}(u) = \psi(\boldsymbol{x}, t)$ and $\Gamma_2 = \partial B_{\bar{R}}(\mathbf{0})$ has a high order ABC enforced to attenuate any outgoing waves.
- The density u_γ can be split into two parts u_{γ_1} and u_{γ_2}.
- Substituting the extension operator into the inhomogeneous BEP yields the block system

$$\boldsymbol{Q}^{\text{Dir}}_{\Gamma_1}\boldsymbol{c}^{n+1}_{DIR,1} + \boldsymbol{Q}^{\text{Neu}}_{\Gamma_1}\boldsymbol{c}^{n+1}_{NEU,1} = -\left(\boldsymbol{G}_h\tilde{f}^{n+1}_R\right)|_{\gamma_1} - (\boldsymbol{P}_{\gamma_1} - \boldsymbol{I}_{\gamma_1})\boldsymbol{Ex}^{n+1}_{I,\Gamma_1}$$

$$\boldsymbol{Q}^{\text{Dir}}_{\Gamma_2}\boldsymbol{c}^{n+1}_{DIR,2} + \boldsymbol{Q}^{\text{Neu}}_{\Gamma_2}\boldsymbol{c}^{n+1}_{NEU,2} = -\left(\boldsymbol{G}_h\tilde{f}^{n+1}_R\right)|_{\gamma_2} - (\boldsymbol{P}_{\gamma_2} - \boldsymbol{I}_{\gamma_2})\boldsymbol{Ex}^{n+1}_{I,\Gamma_2}$$

- There are two sources of error for the exterior problem
  - Discretization error - due to approximating the continuous variables on a grid.
  - Reflection error - the spurious reflections from the ABC.

“Convergence” of Artificial Boundary Condition

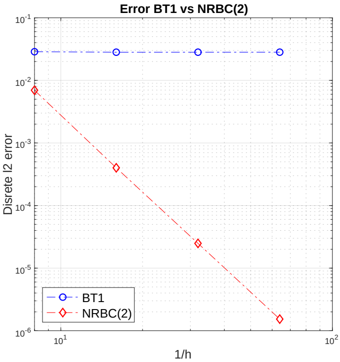


Figure: Test solution u_x, where $u = \frac{\phi_\varepsilon^n(r)}{4\pi r}\left(\sin^9(t) + \frac{1}{2}\sin^9\left(\frac{t}{\sqrt{2}}\right)\right)\chi_{(0,\infty)}$, ϕ_ε^n is the smooth step function, $c = 1$, $t_F = 5$, $\Omega^0 = [-2,2]^3$, and $\Omega = B_{1.5}(\mathbf{0})$.

- Grid refinement analysis is only possible if the reflection error is relatively small.
- ↓ h only improves the discretization error.
- ↑ order ABC or ↑ size of domain decreases reflection error.
- BT1: reflection error $\gg$ discretization error.
- NRBC(2): reflection error $\ll$ discretization error.

Future Work

- Were having issues with the long run stability for Neumann and Robin BC. The ABC resembles a Robin BC when discretized in time.

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High order Algorithm for 3D Multiple Scattering Problem

Michael Medvinsky[1], Semyon Tsynkov[1], and Eli Turkel[2]

[1]North Carolina State University, Raleigh, NC, USA
[2]Tel Aviv University, Tel Aviv, Israel

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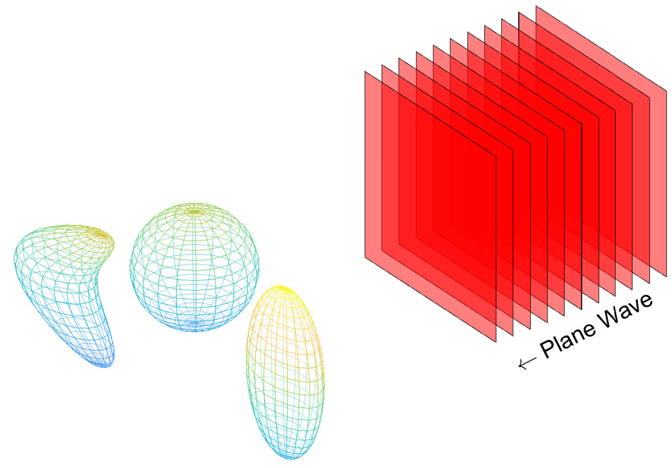
Physical Problem

- Let $\{\Omega_q\}_{q=1}^N$ be a set of smooth disjoint objects in an open space.
    - Denote $\Gamma_q = \partial\Omega_q$ and let $S_N = \bigcup_{q=1}^N \Omega_q$.
- Consider the Helmholtz equation in an unbounded domain driven by an incident field specified by a wavenumber $\boldsymbol{k}$ with $\|\boldsymbol{k}\| = k$, e.g. plane wave $u^{(inc)}(\boldsymbol{x}) = e^{i\boldsymbol{k}\cdot\boldsymbol{x}}$:

$$\begin{cases} \Delta u + k^2 u = f & \boldsymbol{x} \in \mathbb{R}^3 \setminus S_N \\ u\big|_{\Gamma_q} = -u^{(inc)} & \Omega_q \text{ is a soft scatterer} \\ \frac{\partial u}{\partial n}\Big|_{\Gamma_q} = -\frac{\partial u^{(inc)}}{\partial n} & \Omega_q \text{ is a hard scatterer} \\ \left(\frac{\partial}{\partial\|\boldsymbol{x}\|} - ik\right) u \to \frac{1}{\|\boldsymbol{x}\|} & \|\boldsymbol{x}\| \to \infty, \end{cases}$$

Schematic



Computational Problem

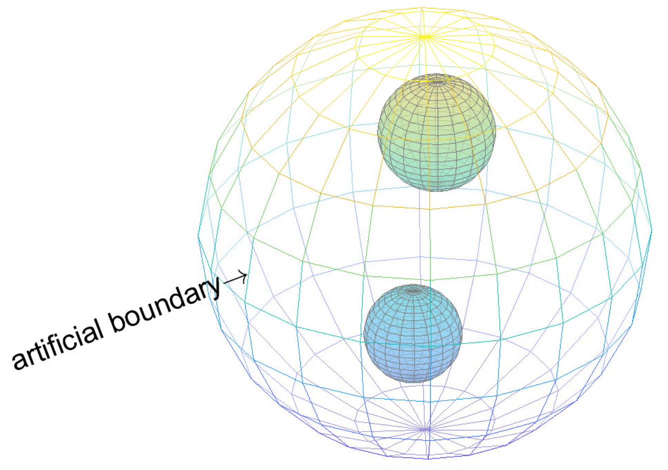
- Truncation by an artificial sphere $\Omega_0 = \{r \leq R\}$ and ABCs:

$$\begin{cases} \frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r} + \frac{\Delta_{\theta,\varphi} u}{r^2} + k^2 u = f & \Omega \equiv \Omega_0 \setminus S_N \\ u\big|_{\Gamma_q} = -u^{(inc)} & \Omega_q \text{ is a soft scatterer} \\ \frac{\partial u}{\partial n}\Big|_{\Gamma_q} = -\frac{\partial u^{(inc)}}{\partial n} & \Omega_q \text{ is a hard scatterer} \\ B_m u = 0 & \partial\Omega_0 = \{r = R\} \end{cases}$$

  - $\Delta_{\theta,\varphi}$ is the Beltrami operator: $\Delta_{\theta,\varphi} u = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial u}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 u}{\partial\varphi^2}$,
  - B_m is the m'th Bayliss, Gunzburger, Turkel (BGT) ABC:

$$B_0 u = I, \quad B_m u = \left(\tfrac{\partial}{\partial r} - ik + \tfrac{2m-1}{r}\right) B_{m-1} u, \quad m = 1, 2, 3, \ldots$$

Schematic



Method of difference potentials

- Employs discrete counterparts of Calderon’s operators:
  - Easily computed on regular structured grids;
  - The shape of the boundary can be non-conforming.
- Equivalently reduces the PDE to the boundary:
  - Regardless of specific boundary conditions;
  - Representation of solution at the boundary is also spectral.
- The boundary is coupled to the grid via extension operators:
  - Constructed by high order Taylor formulae.

Calderon's potentials and projections

- $\boldsymbol{L}u = 0$ on Ω, $\Gamma = \bigcup\limits_q \Gamma_q$, G — fundamental solution, and $\boldsymbol{G} = L^{-1}$.
- Calderon's potential:

$$P_\Omega \xi_\Gamma(\boldsymbol{x}) = \int_\Gamma \xi_0(\boldsymbol{y}) \frac{\partial G}{\partial \boldsymbol{n}}(\boldsymbol{x} - \boldsymbol{y}) - \xi_1(\boldsymbol{y}) G(\boldsymbol{x} - \boldsymbol{y})\, ds_{\boldsymbol{y}},\ x \in \Omega$$

  - Yields the classical Green's formula if $\xi_\Gamma \equiv (\xi_0, \xi_1)|_\Gamma = \boldsymbol{Tr}\, u \equiv \left(u, \frac{\partial u}{\partial \boldsymbol{n}}\right)\Big|_\Gamma$.
- Calderon's boundary projection: $P_\Gamma \xi_\Gamma = \boldsymbol{Tr}\, P_\Omega \xi_\Gamma$.
  - Key property: $P_\Gamma \xi_\Gamma = \xi_\Gamma$ iff $\exists u$, $\boldsymbol{L}u = 0$ and $\boldsymbol{Tr}u = \xi_\Gamma$.

  Similarly: $P_\Gamma \xi_\Gamma + \boldsymbol{Tr}\,\boldsymbol{G}f = \xi_\Gamma$ iff $\exists u$, $\boldsymbol{L}u = f$ and $\boldsymbol{Tr}u = \xi_\Gamma$.
- Calderon's operators can be constructed using other inverses $\boldsymbol{G}$ — especially important for discretization.

Boundary conditions

- A boundary value problem reduces to Calderon's boundary equation with projection (BEP) w.r.t. $\boldsymbol{Tr}u = \xi_\Gamma$ supplemented by the given boundary condition:

$$\begin{cases} \boldsymbol{L}u = f & \boldsymbol{x} \in \Omega \\ \ell_\Gamma u = \phi & \boldsymbol{x} \in \Gamma \end{cases} \iff \begin{cases} \boldsymbol{P}_\Gamma \xi_\Gamma + \boldsymbol{Tr}\,\boldsymbol{G}f = \xi_\Gamma \\ \ell_\Gamma \xi_\Gamma = \phi \end{cases} \iff \quad u = \boldsymbol{P}_\Omega \xi_\Gamma + \boldsymbol{G}f$$

- *Note*: In this work

$$\ell_\Gamma = \begin{cases} \text{Dircihlet or Neumann} & \text{on } \Gamma_q, q \geq 1 \\ B_m u = \alpha_m \frac{\partial u}{\partial r} + \sum_{n=1}^{\lfloor \frac{m}{2} \rfloor} \beta_{m,n} \Delta^n_{\theta,\varphi} u + \sum_{n=1}^{\lfloor \frac{m-1}{2} \rfloor} \gamma_{m,n} \Delta^n_{\theta,\varphi} \frac{\partial u}{\partial r} + \left(\frac{1}{r} - ik \right) \alpha_m u & \text{on } \Gamma_0 \end{cases},$$

where $\alpha_m, \beta_{m,n}, \gamma_{m,n}$ with $(m = 6)$ are precomputed by recursive formulae - a spectral BGT implementation, Medvinsky, Tsynkov, Turkel (2019).

Discretization of the Helmholtz equation

- One can choose any scheme deemed convenient and appropriate for a given task.
- The scheme can be built on a regular structured grid:
  - We used a 6th order compact finite difference scheme on a uniform Cartesian grid.
  - The boundary Γ does not have to conform to the grid,
    - No approximation of the boundary conditions on the grid.
    - The BCs are done using spectral representation on Γ, e. g. Spherical Harmonics :

$$\frac{\partial^d}{\partial r^d} u(r,\theta,\varphi)\Big|_{\Gamma_q} = \sum_{l=0}^{\infty}\sum_{s=-l}^{l} c_{ls}^{(d,q)} Y_l^s(\theta,\varphi), \quad d \in \{0,1\},\ Y_l^s(\theta,\varphi) = \mathcal{P}_l^{|s|}(\cos\theta)e^{is\varphi}$$

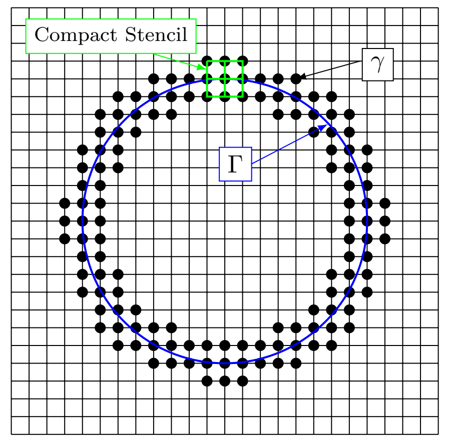
Furthermore: no high order derivatives on Γ_0 ($\Delta_{\theta,\phi} Y_l^s = \lambda_l Y_l^s = -l(l+1)Y_l^s$):

$$0 = c_{ls}^{(1,0)}\alpha_m + c_{ls}^{(0,0)}\sum_{n=1}\beta_{m,n}\lambda_l^n + c_{ls}^{(1,0)}\sum_{n=1}\gamma_{m,n}\lambda_l^n + c_{ls}^{(0,0)}\left(\frac{1}{r} - ik\right)\alpha_m.$$

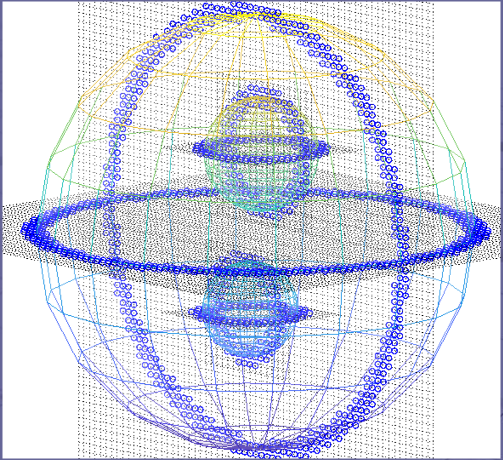
Similarly, on soft (hard) scatterer, $q \geq 1$, the problem reduces to a linear system for $c_{ls}^{(1,q)}$ ($c_{ls}^{(0,q)}$).

Discrete Calderon's operators

- The grid boundary γ straddles the continuous boundary Γ. γ depends on the scheme stencil.



Grid boundary γ in 2D.



Cross-sections of the γ in 3D.

Discrete Calderon's operators

- Difference boundary projection $\boldsymbol{P}_\gamma$ is an operator in the space of grid functions defined on γ.
  - $\boldsymbol{P}_\gamma$ is computed by applying a specially chosen inverse $\boldsymbol{G}^{(h)}$ - auxiliary problem.
- The discrete BEP: $\boldsymbol{P}_\gamma \xi_\gamma + \boldsymbol{Tr}_\gamma^{(h)} \boldsymbol{G}^{(h)} f = \xi_\gamma$ holds iff $\exists u$, $\boldsymbol{L}^{(h)} u = f$ and $\boldsymbol{Tr}^{(h)} u = \xi_\gamma$.
- Equation-based extension $\xi_\gamma = \boldsymbol{Ex} \boldsymbol{\xi}_\Gamma$:
  - Consider $\Gamma = \bigcup_{q=0}^{N} \Gamma_q$, denote $\boldsymbol{\xi}_\Gamma = (\boldsymbol{\xi}_{\Gamma_0}, \boldsymbol{\xi}_{\Gamma_1}, \dots, \boldsymbol{\xi}_{\Gamma_N})$, and define

$$\boldsymbol{\xi}_{\Gamma_q} = (\xi_0^q, \xi_1^q) = \sum_{\ell=0}^{L_q} \sum_{s=-\ell}^{\ell} c_{ls}^{(0,q)} (Y_\ell^s, 0) + \sum_{\ell=0}^{L_q} \sum_{s=-\ell}^{\ell} c_{ls}^{(1,q)} (0, Y_\ell^s),$$

  - Discrete density : $\xi_\gamma = \left(\xi_{\gamma_0}, \xi_{\gamma_1}, \dots, \xi_{\gamma_N}\right)$, $\xi_{\gamma_q} = \boldsymbol{Ex}_q \boldsymbol{\xi}_{\Gamma_q} = v(\boldsymbol{x}) = v(\boldsymbol{x}_0) + \sum_{j=1}^{J} \frac{h^j}{j!} \frac{\partial^j v(\boldsymbol{x}_0)}{\partial \boldsymbol{n}^j}$, $v(\boldsymbol{x}_0) = \xi_0^q$, $v_{\boldsymbol{n}}(\boldsymbol{x}_0) = \xi_1^q$, $\frac{\partial^j v(\boldsymbol{x}_0)}{\partial \boldsymbol{n}^j}, j > 1$ obtained by differentiating the Helmholtz equation.
  - *Note*: $\boldsymbol{Ex}_q(Y_l^s, Y_{l'}^{s'}) = \alpha Y_l^s + \beta Y_{l'}^{s'} + \widetilde{\boldsymbol{Ex}}_q f$, where $\widetilde{\boldsymbol{Ex}}_q f$ - extension of f.

Numerical algorithm

- The extension $\boldsymbol{Ex}$ couples continuous functions at the boundary Γ with grid functions on γ:
  - Discrete Calderon's operators approximate the continuous ones as long as the order of the extension is sufficiently high.
- The unknowns are $c_{ls}^{(0,q)}$ and $c_{ls}^{(1,q)}$ — coefficients of the expansion of ξ_{Γ_q} with respect to spherical harmonics on Γ_q.
- Yet the equation to be solved is the discrete BEP

$$\boldsymbol{P}_{\gamma}\xi_{\gamma} + \boldsymbol{Tr}_{\gamma}^{(h)}\boldsymbol{G}^{(h)}f = \xi_{\gamma}.$$

- Once we substitute $\xi_{\gamma} = \boldsymbol{Ex}\xi_{\Gamma}$, the discrete BEP and the BCs becomes a system of linear algebraic equations with respect to $c_{ls}^{(0,q)}$, $c_{ls}^{(1,q)}$.

Efficiency

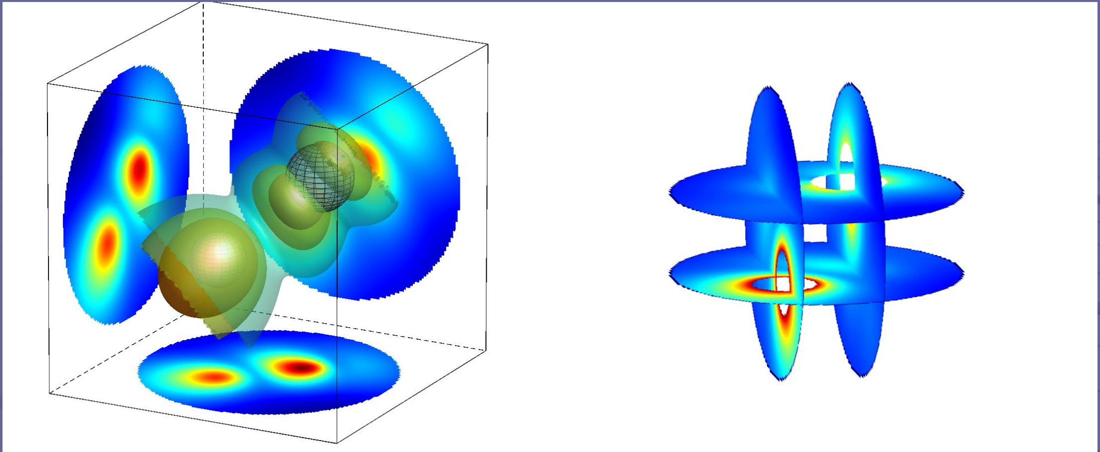
- Denote the system to be solved is $\boldsymbol{A}_{|\gamma|\times L^{(0)}}\,\boldsymbol{c}=\boldsymbol{f}=\boldsymbol{B}_{|\gamma|\times L^{(1)}}\,\tilde{\boldsymbol{c}}$
- $L^{(p)}=\sum_{q=p}^{N}(1+L_q)^2$, $p\in\{0,1\}$
- $\boldsymbol{c}$ are all unknown coefficients $c_{ls}^{(0,q)}$ and $c_{ls}^{(1,q)}$
- $\tilde{\boldsymbol{c}}$ are known coefficients $c_{ls}^{(0,q)}$ and $c_{ls}^{(1,q)}$ - obtained from Dirichlet and/or Neumann data.
- The columns of $\boldsymbol{A}$ and $\boldsymbol{B}$ are $(\boldsymbol{P}_\gamma-\boldsymbol{I}_\gamma)\boldsymbol{Ex}'_q\psi_{ls}^{(q)}$, $\psi_{ls}^{(q)}\in\{(0,Y_\ell^s),(Y_\ell^s,0)\}$, where

$$\boldsymbol{Ex}'_q\psi_{ls}^{(q)}=\begin{cases}\boldsymbol{Ex}_q\psi_{ls}^{(q)}, & \text{on } \gamma_q,\\ 0, & \text{on } \gamma\backslash\gamma_q,\end{cases}.$$

  Note: The columns are independent — straightforward parallelization.
- The system is solved by least squares by means of QR factorization: $c=R^{-1}Q^*B\tilde{c}\equiv D_{L^0\times L^1}\tilde{c}$
- D remains unchanged with the change in incident field.
- Change in BCs, say soft to hard, will swap the respective $c_{ls}^{(0,q)}$ and $c_{ls}^{(1,q)}$ as well as the corresponding columns of $\boldsymbol{A}$ and $\boldsymbol{B}$.

Results

- Scatterers and BCs
  - An artificial sphere, $R = 2.3$ at $(0, 0, 0)$ terminated by BGT6.
  - A sound-hard sphere of radius 0.6 at $(0.65, 0.65, 0.65)$.
  - A sound-soft sphere of radius 0.5 at $(-0.65, -0.65, -0.65)$.
- We study the grid convergence, $\|u^{(h)} - u^{(h/2)}\|$, on subsequent grids $2^d \times 2^d \times 2^d$ with $d = 6,\ 7,\ 8$, and 9.
- The number of basis functions is limited by $L = 31$ and the Dirichlet/Neumann data so that known coeffs satisfies $|c_{ls}^{(0,q)}|, |c_{ls}^{(1,q)}| > 1E - 11$.
  The specific values are stated in the tables as $L = (L_0, L_1, L_2)$.



(a) Isosurface of the solution (b) Slices of the solution

Planewave scattering, $\theta_{inc} = 45^\circ$, $\phi_{inc} = 55^\circ$

Grid	h	$k = 5, L = (31, 19, 18)$		$k = 10, L = (31, 24, 22)$	
		$\|\|u^{(h)} - u^{(2h)}\|\|_\infty$	rate	$\|\|u^{(h)} - u^{(2h)}\|\|_\infty$	rate
64	0.088	104.2970663	–	2.211100776	–
128	0.044	0.001532719	16.05	0.007001168	8.30
256	0.022	$1.0832e-05$	7.14	$6.4567e-05$	6.76
512	0.011	$7.0310e-08$	7.26	$4.9136e-07$	7.03

Planewave scattering, $\theta_{inc} = 0$, $\phi_{inc} = 0$

Grid	h	$k=5$, $L=(31,19,17)$ $\|\|u^{(h)}-u^{(2h)}\|\|_\infty$	$k=5$, $L=(31,19,17)$ rate	$k=10$, $L=(31,24,22)$ $\|\|u^{(h)}-u^{(2h)}\|\|_\infty$	$k=10$, $L=(31,24,22)$ rate
64	0.088	107.3527362	–	2.201265058	–
128	0.044	0.001710109	15.93	0.006842025	8.32
256	0.022	$9.6635e-06$	7.46	$5.7465e-05$	6.89
512	0.011	$6.3080e-08$	7.25	$4.4879e-07$	7.00

Planewave scattering, $\theta_{inc} = 5^\circ$, $\phi_{inc} = 5^\circ$

		$k = 5, L = (31, 19, 18)$		$k = 10, L = (31, 24, 22)$			
Grid	h	$\|\|u^{(h)} - u^{(2h)}\|\|_\infty$	rate	$\|\|u^{(h)} - u^{(2h)}\|\|_\infty$	rate		
64	0.088	0.01113527	–	104.2970663	–	2.2111007760	–
128	0.044	0.00010730	6.69	0.001532719	16.05	0.0070011686	8.30
256	0.022	$7.8706e-07$	7.09	$1.0832e-05$	7.14	$6.45675e-05$	6.76
512	0.011	$6.7534e-09$	6.86	$7.0310e-08$	7.26	$4.91365e-07$	7.03

Planewave scattering, $\theta_{inc} = 10^\circ$, $\phi_{inc} = 10^\circ$

Grid	h	$k=5$, $L=(31,19,18)$		$k=10$, $L=(31,24,22)$	
		$\|\|u^{(h)}-u^{(2h)}\|\|_\infty$	rate	$\|\|u^{(h)}-u^{(2h)}\|\|_\infty$	rate
64	0.088	110.8849260	–	2.301299822	–
128	0.044	0.001901825	15.83	0.007401438	8.28
256	0.022	$9.4656e-06$	7.65	$5.7444e-05$	7.00
512	0.011	$6.3881e-08$	7.21	$4.2852e-07$	7.06

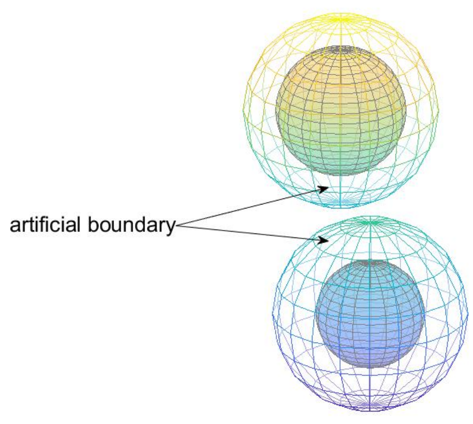
Planewave scattering, $\theta_{inc}=10^\circ$, $\phi_{inc}=0^\circ$

Summary

- The Method of Difference Potentials described.
- The method is naturally parallelizable and extremely efficient for the multiple data/input problems (multiple incident fields).
- A thorough study of performance is presented.
- Two independent sources of error: interior discretization and reflections from artificial outer boundary.

Future work

- Even more efficient solution to the constant wavenumber Multiple Scattering problem - as depicted.
- General and a non-smooth shapes (requires compatible extension Ex and basis).
- Time dependent problems (wave equation).
- Applications to ring resonator filters (2D).



The end

Thank you for your attention!

Non-Iterative Domain Decomposition for the Helmholtz Equation Using the Method of Difference Potentials

Evan North, Semyon Tsynkov, and Eli Turkel

North Carolina State University

August 26, 2021

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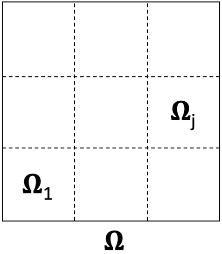
Motivating Problem

Goal: Solve the Helmholtz equation over a tiled domain, where material properties can differ from subdomain to subdomain.

$$\begin{cases} \Delta u + k^2 u = f, & \Omega \\ \alpha u + \beta \frac{\partial u}{\partial n} = \phi, & \partial\Omega \end{cases}$$



- $k = k(j)$ is piecewise constant across Ω, split at each Ω_j
- α and β are piecewise constant along $\partial\Omega$
- Interfaces couple the subdomains, requiring special interface matching conditions (e.g. $u_i = u_j$, $\frac{\partial u_i}{\partial n_i} = \frac{\partial u_j}{\partial n_i}$)

These domains naturally arise in problems with layered, heterogeneous media, as well as problems with large domains that need to be broken down for computational purposes.

Domain Decomposition Methods

The primary approach is a class of iterative solvers. These DDMs often alternate between updating the boundaries of the subdomains, and solving the resulting interior problems. Some desirable characteristics of DDMs are:

- \+ Cheap boundary updates when high-accuracy is not necessary.
- \+ Parallelization of subproblem solutions.
- \+ Greatly benefit from careful implementation of pre-conditioners.

Of course, DDMs have drawbacks to consider in implementation:

- Cross-points and jumps in wavenumber require special care.
- More subdomains $\implies$ More iterations $\implies$ More subproblem solutions (expensive at fine grid refinement).

Approach Based on Difference Potentials

- Originally introduced by Ryaben'kii in 1969; a comprehensive account available in monograph [Ryaben'kii, 2002].
- Reduces the PDE from its domain to its boundary
  - Efficient and flexible in handling boundary conditions
  - Interface conditions are able to be enforced directly
- The method is non-iterative
  - Decouples subproblems with one global solve, then performs a collection of independent local solves
- Can utilize high-order FDM to combat pollution effect
- Inherently insensitive to interior cross-points and wavenumber jumps

A detailed account of our implementation can be found in our manuscript [E. North, S. Tsynkov, and E. Turkel, 2021]

Difference Potential Operator

- Difference Potentials are a discrete analogue of Calderon's operators
- Truncation to the discrete boundary gives its Projection operator and the corresponding discrete Boundary Equation with Projection (BEP), with the following key property:

A grid function ξ_γ satisfies the BEP if and only if ξ_γ is the trace of a solution to the discrete Helmholtz equation.

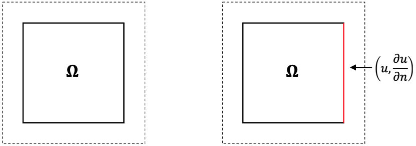
Given such a ξ_γ the solution on the domain can be recovered with an application of the difference potential.

Base Subdomain Construction (Building Block)

- An auxiliary domain (dotted line) establishes the computational domain, permitting flexibility in geometry and boundary conditions.
- Construct a series representation (our choice of orthogonal basis) of the Dirichlet and Neumann data along each side.

$$u = \sum_{i=1}^{M} c_i^{(0)} \psi_i^{(0)}, \quad \frac{\partial u}{\partial n} = \sum_{i=1}^{M} c_i^{(1)} \psi_i^{(1)}$$

- MDP constructs a linear system (Boundary Eq. with Projection) with unknowns $c^{(0)}$ and $c^{(1)}$, which is completed with the boundary conditions. Solution is recovered with an application of the difference potential.



Multiple Subdomains

- Each subdomain has an independent auxiliary domain and BEP.
- BEPs are underdetermined, and completing them requires coupling along the matching subdomain interfaces.
- When completing the linear system, there are two cases of sides:
  1. Exterior: Use BCs as before, independent of extra subdomains.
  2. Interior (interface): Enforce chosen transmission conditions
     - e.g. $u_1 = u_2$, $\frac{\partial u_1}{\partial n_1} = -\frac{\partial u_2}{\partial n_2} \implies c_1^{(0)} = c_2^{(0)}$, $c_1^{(1)} = -c_2^{(1)}$
- Solving the system now provides the series representation of the solution to each subproblem along the corresponding boundaries.
  - Interior solutions are recovered from boundary representations by the difference potential.
  - Local solutions are pieced together to assemble the global solution.

Implementation Remarks

Parallelization:

- ✓ Initialization Steps
  - Definition of grid sets
  - Source term contributions.
- ✓ Resolution of boundary conditions
- ✓ Recovery of subproblem solutions on each subdomain
  - Via difference potential.
- × QR factorization

Precomputation:

- Core matrix of the BEP is precomputed once for a given geometry and wavenumber, leading to the use of “building blocks”.
- QR-factorization remains valid when source/boundary data are changed.

Numerical Results - Duct

n	QR Time	Ratio	$\mathcal{G}^{(h)}$ time	Ratio	Error	Rate
64	3.23	-	0.0064	-	3.89e-02	-
128	6.58	2.00	0.0083	1.30	8.08e-04	5.59
256	13.50	2.05	0.042	5.07	4.85e-05	4.06
512	28.91	2.14	0.186	4.44	3.01e-06	4.01
1024	60.13	2.08	0.824	4.44	1.89e-07	4.00
2048	108.77	1.81	3.430	4.17	1.39e-08	3.77

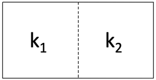
- Test solution: $e^{i\frac{k}{\sqrt{2}}(x+y)}$
- $k = 13,\ M = 40,$ $\alpha = \beta = 1$

- Horizontal duct of $N = 24$ subdomains
- QR (global) and $\mathcal{G}^{(h)}$ (local, parallel) scale as expected

Numerical Results - Transmission

	$k_1 = 5$ $k_2 = 20$ $M = 50$		$k_1 = 5$ $k_2 = 40$ $M = 60$	
n	Error	Rate	Error	Rate
64	8.81e-02*	-	1.27e+01*	-
128	5.13e-03	4.10	1.08e-01	6.88
256	3.13e-04	4.03	6.51e-03	4.06
512	1.96e-05	4.00	4.03e-04	4.01
1024	1.22e-06	4.01	2.52e-05	4.00
2048	7.78e-08	3.97	1.57e-06	4.01

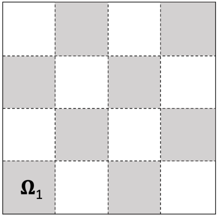
- Two subdomains, Dirichlet boundary conditions
- Incident wave $u_{inc} = e^{ik_1 x}$
- Error is comparable to classical pollution effect



Numerical Results - Checkerboard Square

	$N = 16$		$N = 36$	
n	$\|u_n^{(h)} - u_{\frac{n}{2}}^{(h)}\|_\infty$	Rate	$\|u_n^{(h)} - u_{\frac{n}{2}}^{(h)}\|_\infty$	Rate
256	8.54e-04	-	4.31e-04	-
512	6.90e-05	3.63	1.76e-05	4.61
1024	4.36e-06	3.98	1.09e-06	4.01
2048	2.73e-07	4.00	6.79e-08	4.01

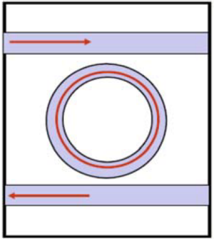
- Homogeneous Dirichlet boundary conditions
- Switched to different metric for convergence
- $M = 60$, $k_1 = 5$ (gray), $k_2 = 40$ (white)
- Cross-points, wavenumber mismatch at every interface

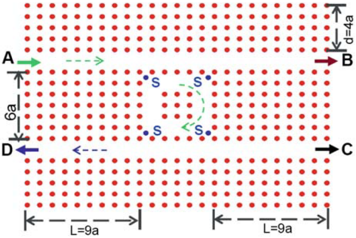


Photonic Crystal Ring Resonator (PCRR)

Ring resonators consist of a straight waveguide (bus) coupled with a ring-shaped waveguide to create a filter for resonant frequencies. In a PCRR, this shape is implied by removing specific scattering rods from the lattice.

- Ring resonators have important applications in fiber-optic cables and biosensing
- PCRR is better suited for nano-scale photonics (compared to traditional RR)



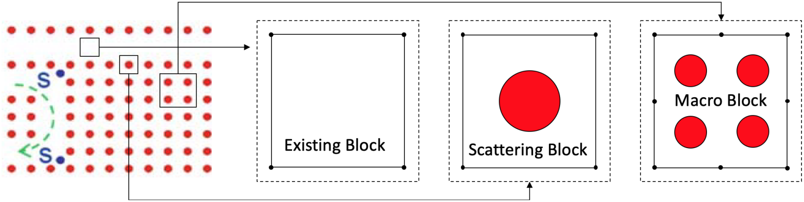


This domain has a natural tiling decomposition around each scatterer.

Composite Subdomains

To build on the idea of breaking a domain down into mostly identical "building blocks", we want to incorporate the following possibilities into the methodology:

- ✓ Inclusion of interior, circular subdomains (scattering rods)
- Implementation of (local) absorbing boundary conditions
- Computational scaling with respect to the number of subdomains
- Cost-benefit of utilizing macro-blocks in the pre-computation steps for large sections
  - Does splitting one edge of a square affect performance?



Thank You!
Any questions?