Computational and Numerical Analysis of Transient Problems in Acoustics, Elasticity, and Electromagnetism (16w5071)

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1 Overview of the Field

Wave propagation underlies several important technologies that are at the center of our world. For example, communications like WiFi and cell-phones use electromagnetic waves to transmit information. Acoustic, elastic or electromagnetic waves are used in seismic prospecting and medical imaging to probe inaccessible regions. The control of acoustic and elastic waves is also important for noise abatement. These areas, and others, rely on computational modeling tools to predict performance and optimize design.

Although acoustic, electromagnetic or elastic wave propagation has been studied for many years, there is still no single strategy that can solve all problems. Constraints imposed by the need to approximate oscillatory solutions and difficulties with numerical dispersion (which causes waves to move at slightly the wrong velocity in different directions) still impose limits on all types of solvers (and particularly on solvers that are based on discretizing the appropriate equations in a computational volume). Higher order methods can mitigate but not remove these problems. In addition solving the large linear system resulting from the discretization of these wave equations also requires special techniques. Furthermore complex media (for example dispersive, heterogeneous or multi-scaled) requires further elaboration of standard algorithms. Indeed in April 2014 the 'Fast Track Action Committee on Optics and Photonics', sanctioned by the US Committee on Science of the National Science and Technology Council, noted that 'theoretical and computational methods for analyzing, understanding, and optimizing light propagation and imaging in heterogeneous media' is a key area for support in the study of imaging through heterogeneous media [3].

Broadly speaking there are two regimes in which computational wave propagation is performed. These are the frequency and time domain. To understand the difference between the two domains, let us consider the scattering of s-polarized electromagnetic waves, first in the time domain. Given a bounded domain $D \subset \mathbb{R}^2$ occupied by a perfectly conducting scatterer, let $\epsilon_r := \epsilon_r(x)$ denote the relative permittivity of the medium surrounding D, and c denote the speed of light in air. Typically we assume $\epsilon_r = 1$ far enough from the scatterer (i.e. the scatterer is surrounded by air). If $x \in \mathbb{R}^2$ denotes position and t denotes time, the s-polarized total electric field $u := u(x,t)$ satisfies

$$\frac{\epsilon_r}{c^2}\frac{\partial^2 u}{\partial t^2} = \Delta u \text{ in } \Omega := \mathbb{R}^2 \setminus \overline{D}, \text{ for } t > 0. \tag{1}$$

We suppose the field u is due to a known incident field u^i that solves the wave equation with $\epsilon_r = 1$ in the neighborhood of the scatterer and the region where $\epsilon_r \neq 1$. The incident field may be due to a remote source such as an antenna and is such that $u^i = 0$ for $t < 0$ in this neighborhood (i.e. the incident field reaches the scatterer at some time $t > 0$). In that case

$$u = u^i + u^s \text{ in } \mathbb{R}^2 \setminus D,\ t \geq 0$$

where u^s is called the scattered field, together with the initial conditions

$$u^s = 0 \text{ and } \frac{\partial u^s}{\partial t} = 0 \text{ in } \Omega \text{ at } t = 0.$$

The assumption that D is perfectly conducting implies the boundary condition

$$u = 0 \text{ on } \partial D,\ t > 0. \tag{2}$$

Under suitable conditions on the domain and data, equations (1)-(2) uniquely define the scattered field (and hence the total field). There is no need for a condition at infinity because the finite speed of propagation of the wave implies u vanishes outside an ever increasing sphere.

In the time domain, the main computational tool in current use is the finite difference time domain (FDTD) (for example, in electrodynamics, the method of Yee dates back to the mid 1960s [13]), usually coupled to the Perfectly Matched Layer (PML) absorbing layer [2]. There is a wealth of experience tuning FDTD to practical problems but it is generally only second order accurate and curved boundaries need to be approximated by stairsteps. A less commonly used alternative is to use finite elements [11], often employing discontinuous Galerkin formulations [4]. These can handle curved boundaries but are more complex than FDTD. A major advantage of the volume based approach, particularly finite element variants, is that the methods can handle spatially varying ϵ_r easily.

To discretize this equation using FDTD or finite elements directly, we first choose a bounded domain Ω_R containing the scatterer (and the region where $\epsilon_r \neq 1$) in its interior and use finite differences or finite elements to discretize the solution in space. Then a suitable time stepping method (often leap-frog) is used to discretize in time. One serious issue remains: on the surface of the unbounded complement of Ω_R we need an algorithm for closing the system that mimics wave propagation in the external region. This is often provided by a transparent absorbing PML layer, an absorbing boundary condition [5], or, as was discussed in detail by several speakers at the conference, a system of time domain integral equations. The latter method can be applied on a non-convex outer boundary and can match the interior time stepping scheme, but may have stability issues that force rather complex coupling procedures.

Two further issues bedevil the discretization of the wave equation. First the solution is typically oscillatory in space and time so a small enough time step and spatial mesh size needs to be taken to approximate such solutions. Worse, dispersion error can ruin the solution by the so called "pollution effect". Suppose (1) holds in all space with $\epsilon_r = 1$ then the plane wave

$$u = \exp(i(k \cdot x - \omega t))$$

where $k \in \mathbb{R}^2$ is a solution provided ω and k satisfy the dispersion relation

$$\omega^2 = c^2 |k|^2.$$

This gives the phase velocity $\omega/|k| = c$. When the equation is discretized, even if we use a uniform grid for FDTD we only have a discrete approximation

$$\omega_h^2 = c|k|^2 + O(\Delta t^\alpha + h^\beta)$$

where h is the spatial mesh size, Δt is the time step and α and β depend on the details of the method used. In this case the discrete phase velocity $\omega_h/|k|$ is not exactly c and may vary in different directions. To control this error may require a much finer mesh than the mesh for simple approximation of the wave. For example, roughly speaking, for piecewise linear finite elements (without considering time discretization), best approximation error requires $h\omega/c$ to be small enough (where h is the diameter of the largest element in the mesh), but control of the dispersion error requires that $(\omega/c)^3 h^2$ be small so that as the angular frequency ω increases the mesh must become smaller moe quickly than expected on the basis of best approximation [8]. One way to handle this is to use high order finite element methods in which the order of approximation increases with $\ln(\omega)$ (and the mesh is refined to control best approximation error) [10].

When $\epsilon_r = 1$, an alternative approach is to use time domain integral equations. Typically the scattered field is represented by a single layer potential

$$u^s(x,t) = \int_{\partial D} \int_{-\infty}^{t} \Phi(x, y, t-\tau)\psi(y,\tau)\, d\tau\, ds(y), \text{ for } x \in \Omega, \tag{3}$$

where Φ is the fundamental solution of the wave equation which $\epsilon_r = 1$ in the time domain, and ψ is an unknown density. For a suitable class of densities, u^s satisfies the wave equation and initial conditions. Only the boundary condition remains to be satisfied. By allowing x to approach ∂D it is then possible to derive a boundary integral equation for ξ:

$$\int_{\partial D}\int_{-\infty}^{t} \Phi(x,y,t-\tau)\psi(y,\tau)\,d\tau\,ds(y) = -u^i(x,t) \text{ for } x\in\partial D, t>0, \tag{4}$$

and on solving this equation for the density ψ we can compute u^s by (3). For a thorough introduction to boundary integral equations, see [12].

Historically the solution of this time domain boundary integral equation (TDBIE) has suffered from stability problems. However, pioneering work by Nedelec's group in France has lead to the understanding that space-time Galerkin type schemes require very accurate quadrature backwards in time in order to preserve stability. More recently Michielssen's group in Michigan has developed very impressive electromagnetic simulations using fast multipole like solvers and special preconditioners. Nevertheless time domain boundary integral equations remain comparatively underutilized, in part because implementation of the Galerkin type algorithms requires very complicated integration rules that practically rule out high order methods or curved boundary patches.

By contrast, the frequency domain problem, which was not the focus of this conference, proceeds by taking (formally) the time Fourier transform of u^s denoted $\hat{u}^s$. We then see that $\hat{u}^s$ satisfies

$$\Delta\hat{u}^s + \frac{\omega^2}{c^2}\epsilon_r\hat{u}^s = 0 \text{ in } \Omega$$

subject to the boundary condition

$$\hat{u}^s = -\hat{u}^i \text{ on } \partial D.$$

Now it is necessary to select outgoing waves and this is done using the Sommerfeld radiation condition

$$r^{1/2}\left(\frac{\partial\hat{u}^s}{\partial r} - i\frac{\omega}{c}\hat{u}^s\right) = o\left(1\right) \text{ as } r\to\infty.$$

In the frequency domain, a single frequency solution is computed and both finite element and integral equation techniques are regularly used. These are comparatively well developed [7], although significant difficulties still remain in developing an optimal linear system solver for volume methods. Generally volume based methods (for example the finite element method) handle heterogeneous media more efficiently than integral equations. On the other hand integral equations can efficiently model free space or large homogeneous regions.

2 Recent Developments and Open Problems

Recently, following Lubich's work on Convolution Quadrature [9], there has been renewed interest in the numerical analysis community in understanding and implementing time domain integral equations for acoustics, electromagnetism and elasticity applications [12]. Using modern solution techniques for linear systems including H-matrices, AIM and fast-multipole methods it is possible to construct relatively simple boundary integral techniques with well established stability and convergence criteria. This is at the expense of more dense linear systems and dispersive solutions.

Compared to the space-time Galerkin method, convolution quadrature is more stable but because it is based on an underlying solution of the semi-discrete wave equation (discrete in time not space) it suffers from dispersion error. This can be controlled by using a higher order time stepping scheme or smaller time step. By contrast the space-time Galerkin method must be carefully implemented to preserve stability, but likely has less dispersion error and a more efficient matrix implementation.

Important advances have also recently been made in improving time domain volume based solvers on general domains. These include discontinuous Galerkin methods that build on the work of Warburton and Hesthaven [6], as well as Bruno's Fourier based schemes [1]. In addition local time stepping can be applied to improve efficiency of explicit time integrators on general grids. At the same time improved iterative solution techniques (often involving domain decomposition) allow the use of implicit solvers that may be useful in the presence of highly refined meshes or when complex material laws govern dispersive waves.

A third strand of development has been the improvement of mesh truncation techniques. These are important because wave propagation problems are often posed on infinite domains, and efficient truncation allows a volume scheme to approximate the infinite domain. Of course time domain boundary integral equations can be used to provide boundary conditions on truncated meshes.

A synergetic connection also exists with work on proving wave number dependent estimates for frequency domain algorithms.

It was thus timely to bring together experts on time domain integral equations, experts on volume based methods, and experts on absorbing boundary conditions (or Perfectly Matched Layers), in order to explore the strengths and weaknesses of the various approaches in a collaborative environment. Researchers from these groups are very rarely together in one venue. The goal was to build connections between the various techniques.

As discussed above, there has been much exciting progress recently in each of the different areas of wave propagation covered by this workshop. This raises fundamentally important questions about the "best" strategy for solving different types of problems. In particular, about the relative merits of the BIE and PDE approaches for time domain problems. For example, should time domain problems be solved by means of Fourier transforming frequency domain solutions, or are time domain strategies always better (i.e. more accurate, efficient, reliable)? Do time domain boundary integral methods have other advantages that allow them to compete with timed domain differential equation formulations that use sophisticated absorbing boundary conditions and overlapping grid techniques? Are there situations when a combination of these approaches is most suitable (for example when dealing with scattering from large bodies with attached wires)?

We aimed to exploit better connections between time domain integral equations and volume techniques. Other specific problems discussed include fast solvers for time domain boundary integral equations, and the stabilization of time domain integral equations for Maxwell's equations (instability, likely due to low frequency degeneration of the integral equations, is sometimes observed for Maxwell's equations).

3 Presentation Highlights

3.1 Time Domain Integral Equations

These presentations focused on aspects of solving the TDBIE either by space-time Galerkin methods or convolution quadrature. A clear message is that more needs to be done to develop solution techniques for the solution of discrete TDBIE. In his presentation entitled *A Wavelet-Based PWTD Algorithm-Accelerated Time Domain Surface Integral Equation Solver*, **Eric Michielssen** discussed techniques for accelerating space-time Galerkin based TDBIE solvers using a new local cosine wave basis. Such methods can solve transient problems involving ten million spatial unknowns.

The difficulties of developing a general library for solving boundary element methods was further discussed by **Eric Darrigrand** in his talk on *A generic fast method library*. This library is based on the fast multipole method and aims to facilitate implementation of various kernels by the user.

Concerning time domain integral equations themselves, **Francisco-Javier Sayas** talked on *New and improved analysis of time domain boundary integral equation*. Rather than using analysis in the Laplace transform domain, he advocated to analyze such equations in the time domain directly thereby obtaining improved theorems on the existence and regularity of solutions.

3.1.1 Space-Time Galerkin Methods

Probably the most commonly used approach to solving TDBIEs is the space-time Galerkin approach already mentioned in the context of Eric Michielssen's talk. Because the standard analogue of the single layer equation (4) for Maxwell's equations becomes ill-conditioned at low frequency, long time instability can manifest itself. The use of the Helmholtz decomposition and appropriate trial and test function was shown to stabilize the problem by **Kristof Cools** in his talk on *Late Time Stable Space-Time Galerkin Discretisations of Retarded Potential Boundary Integral Equations*.

TDBIEs can be used to couple to finite element methods and provide an absorbing boundary condition. In his talk on *Mathematical aspects of variational boundary integral equations for time dependent wave propagation*, **Jerónimo Rodríguez** provided a mathematical analysis of convergence of a FEM-BEM coupling due to himself and coworkers in a simplified setting.

Development of alternative space-time Galerkin methods is still an important research direction according to **Penny Davies** who spoke about *Time approximation of transient boundary integral equations* via collocation and compactly supported spline basis functions. These methods give fourth order convergence in time. The connection between these spline based methods and lower order Galerkin methods was the subject of **Dugald Duncan**'s talk *Connections between collocation and Galerkin methods*

3.1.2 Convolution Quadrature

Convolution quadrature applied to TDBIE has proved to be a mathematically and computationally fruitful way to discretize such equations in time. But there is still much need to improve computational approaches, particularly for long-time integration. In her talk on *Fast and oblivious algorithms for dissipative and 2D wave equations*, **Maria Lopez Fernandez** discussed how to use ideas initially developed for parabolic equations to speed the calculation of the tail of the convolution, often the most time consuming part of the algorithm.

The z-transform is intimately linked to convolution quadrature and one way to perform time domain calculations is to calculate several z-transform domain solutions and then compute an inverse z-transform. **Nicolas Salles** discussed the *Influence of several parameters on the accuracy of a Convolution Quadrature method* during his talk which culminated in presenting numerical results using multistep and Runge-Kutta CQ.

The application of convolution quadrature to compute the acoustic and elastodynamic waves was considered by **Martin Schanz** in his talk *Generalized Convolution Quadrature for an Elastodynamic BEM*. He presented results using Lopez-Fernandez & Sauter's variable time step convolution quadrature approach. Using collocation in space, he presented numerical studies showing the behavior of this formulation with respect to temporal discretization, and investigated stability issues arising from the use of collocation.

A central difference between space-time Galerkin and convolution quadrature discretization is that the latter suffers from dispersion and dissipation. Speaking on *Numerical dispersion mitigation for convolution quadrature approaches to electromagnetic scattering simulation*, **Daniel Weile** presented a hybrid approach. By allowing the standard CQ numerical dispersion inside a small sphere, the method preserves basic accuracy and stability of CQ methods. By halting the evolution of the wavefront outside the sphere, the computation can be greatly improved.

Up to now, convolution quadrature based discretization of time domain integral equations has only been considered for linear problems. However **Lehel Banjai** in his talk on *Time-domain boundary integral treatment of the wave equation with a non-linear impedance boundary condition* showed how to formulate and analyze a fully discrete approximation to a non linear problem in which the non-linearity appears in the boundary condition. This opens a new class of problems to analysis and computation.

3.2 Volume Solvers

One of the most demanding applications of time domain methods is seismic wave propagation which involves solving the elastic or acoustic wave equation in large volumes with highly variable coefficients. In her presentation *High-order numerical schemes for imaging the subsurface*, **Helene Barucq** showed how a combination of high order Symmetric Interior Penalty Discontinuous Galerkin (SIPG) finite element methods with a careful choice of fluxes and explicit time stepping leads to an efficient solver for elastic and acoustic wave equations.

Other time-stepping methods could also have attractive properties. **Martin Gander**, in a talk entitled *Space-Time Decomposition Methods* discussed how to parallelize in time. Usually the solution of the wave equation is thought of as a serial algorithm stepping from one time step to the next, but a truly parallel approach could greatly speed up calculations.

Continuing in the theme of improved time-stepping, **Andrea Moiola** described a novel approach that use exact solutions of the wave equation to construct a Trefftz space-time discontinuous Galerkin method. A more classical approach to developing high order (8th to 10th order!) integrators was taken by **Maria Moreta** in her talk on *Multistep cosine methods: numerical resolution of second order in time equations*.

Often when simulating wave interactions with complex geometric structures the ratio of diameter of the smallest element in the mesh to the largest can be very large. Since explicit time integrators are fast but the time step is constrained by the minimum space-step size, it is interesting to develop methods that can handle small elements without a crushing decrease in the global timestep size. In her talk on *Locally implicit time integration for linear Maxwell's equations*, **Marlis Hockbruch** showed a new method that switches between using an explicit solver on large elements and an implicit solver on smaller elements. She proved that such methods are stable and convergent.

Discontinuous Galerkin methods for discretizing in space can also benefit from further development according to **Tom Hagstrom** in his talk on *Some New Formulations of DG Methods for Wave Equations*. It is well-known that high order SIPG methods with standard leapfrog timestepping have a very stringent constraint on the time step size compared to the minimum space step. Understanding the source of this constraint can produce new discretizations that have better time stepping properties.

The need for high order discretizations in space to solve time harmonic problems was underlined by **Stefan Sauter** who spoke on *Stability and Convergence Analysis for Galerkin-type discretizations of the Helmholtz equation for constant and variable wave speed*. It is now possible to analyze time harmonic problems with variable wave speeds and show how increasing polynomial degree can counter the pollution effect of dispersion as the frequency of the wave increases.

3.3 Mesh Truncation and Absorbing Boundary Conditions

The problem of providing a transparent or absorbing boundary condition on the boundary of the finite computational domain used by finite element or finite difference methods can be solved by using a matched FEM-BIE formulation as mentioned earlier, but a far more common approach is to modify the equation in a layer around the computational domain and use a perfectly matched layer or PML. However the PML equations defy easy analysis. During her talk *Matched layers and Transmission problems*, **Laurence Halpern** discussed well-posedness of the PML boundary value problem in practical cases when the coefficients in the PML are discontinuous. A complete proof of convergence of the fully discrete PML problem remains an open problem.

In more complex media, such as certain time domain elasticity problems involving anisotropic media, the standard PML becomes unstable. This is also true for negative index metamaterials, an important class of dispersive media (in which the coefficients in the wave equation are frequency dependent). **Patrick Joly** discussed *Time Domain Perfectly Matched Layers for electromagnetic wave propagation in negative index materials* and proved that the classical PML is unstable and then proposed a new PML suitable for such materials. Numerical experiments using the standard Drude model demonstrated the method. This is important, for example, for modeling metals at optical frequencies.

The coupling of FEM and TDBIE was considered by **Giovanni Monegato** in *Some recent developments on the applications of space-time boundary integral equations and convolution quadratures*. He advocated the use of TDBIE as transparent boundary conditions on the artificial boundary arising in the finite element method. Examples included multiple scattering/multiple sources and rotating domains.

3.4 Advanced Methods and Applications

Several speakers touched on more exotic problems or algorithms. In his talk on *Multiscale method for the wave equation in heterogenous media*, **Assyr Abdulle** discussed a local orthogonal decomposition method for approximating the wave equation in highly heterogeneous media. This multiscale method is intended to account for sub-wavelength inhomogeneity in a medium (for example oscillations in ϵ_r) by using a localized fine mesh solution to correct a coarser scale global solver. Such methods have important applications in photonics.

Continuing the theme of solving wave propagation problems in complex media, **Jichun Li** talked on the *Mathematical analysis and time-domain finite element modeling of invisibility cloaks with metamaterials*. Using exotic choices of ϵ_r (and a variable permeability μ_r) it is possible to construct a medium which shields its interior from probing external waves (an invisibility cloak). Numerical simulations require the use of frequency dependent coefficients in the wave equation which substantially complicates the numerical analysis.

Two further talks illustrate the breadth of applications in this area. Presenting on *Convolution quadrature for the linear Schrodinger equation*, **Jens Markus Melenk** showed how convolution quadrature techniques could be used to analyze a numerical approximation to the Schroedinger equation. In particular he showed that it is possible to construct transparent or absorbing boundary conditions via BEM-FEM coupling based on the use of implicit Runge-Kutta methods to discretize in time.

In a different direction **Ralf Hiptmair** spoke on *Discretizing the Advection of Differential Forms* where the basic model problem involves simulating slowly varying electromagnetic fields in the presence of a conducting moving fluid. By using exterior calculus this problem and other problems involving medium can be put in a common framework and discretize via a semi-Lagrangian approach and a stabilized Galerkin approach.

3.5 Inverse Problems

A major application area for computational methods in wave propagation is inverse problems. Typically the goal of inverse problems is to use remote measurements of the scattered wave to determine features such as the shape and composition of unknown scattering objects. A major example we have already mentioned is seismic inverse problem in which it is desired to image the subsurface topography of the earth using reflected elastic waves initiated on the surface.

Three talks in the conference focused on inverse problems. During her talk on *Time-dependent wave splitting and source separation*, **Marie Kray** presented a new algorithm for the classical inverse problem of source separation.

Also in the time domain, during his talk *Acoustic localisation of coronary artery disease*, **Simon Shaw** presented an ambitious project to detect atherosclerosis in coronary arteries. The intent is to detect and localize atherosclerosis from weak acoustic signals measured on the chest. A key part of this work is a fast solver for the elastic wave equation.

In a different direction **Chrysoula Tsogka** discussed a problem of detecting objects in an acoustic waveguide. In her talk entitled *Partial array imaging in acoustic waveguides* she developed a model test problem for detecting an array of point reflectors, and used this model problem to understand an imaging algorithm based on back propagation.

4 Scientific Progress Made

The scientific progress made at such a workshop cannot be assessed immediately after the workshop, but will become visible in the next years by the publications that originated from it, and possibly in the next decades by the enduring positive effects it may have had on the research direction and careers of younger participants. Senior participants confirm that workshops of precisely this type — bringing together a group of at most 50 dedicated researchers from different research directions centering on a common topic in an inspring atmosphere — have the greatest potential of such long-lasting effects on scientific progress in a field.

As one participant put it concisely in her comment on the BIRS questionnaire: "The workshop was excellent and very useful to activate contacts and collaborations I wouldn't have had otherwise. I had the opportunity to discuss with different researchers working in my area of expertise and came back home with several new ideas and prospectives for future research. I also got important feedback on my most recent research and the environment and infrastructure were optimal." It can be safely assumed that this experience is shared by most of the participants of this workshop.

5 Outcome of the Meeting

The workshop succeeded in its primary goal to bring together experts in time domain integral equations, time domain volume techniques, linear system solvers and absorbing boundary conditions in order to explore the strengths and weakness of the various approaches in a collaborative environment. Researchers from these groups are very rarely together in one venue.

There has been much exciting progress recently in each of the different areas of wave propagation covered by this workshop. This raises fundamentally important questions about the "best" strategy for solving different types of problems; in particular, about the relative merits of the BIE and PDE approaches for time domain problems. The workshop provided new insight on these questions and created new collaborations and contacts between reserachers approaching the subject from different directions.

The list of participants included eleven females and ten younger researchers. We were committed to training younger talent and achieving appropriate representation of women. The final participant list included several post-docs and even advanced graduate students appropriately chosen later in the process. One of the participants noted in an e-mail "Thank you very much for the invitation to the excellent workshop last week. I learned a lot from it, found it very valuable and enjoyed the whole event. I also appreciated that the gender balance was very good - that is not so easy to achieve.".

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