Advances in Computational Scattering

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Scattering is the study of the interaction of waves with obstacles. These obstacles could be anything from gratings, to tumours, to ships; the waves could be electromagnetic, elastic, or acoustic. This is a very well-established field of study, mathematically, but only a limited number of exterior scattering problems can be solved analytically.

In recent years, many engineers, computational scientists and numerical analysts have investigated numerical algorithms to simulate scattering, including (but not limited to) the use of integral equations, finite element methods, series methods, geometrical optics, absorbing layers and spectral methods. These developments have helped to make computational scattering algorithms indispensible in several industries for design purposes. Many deep mathematical questions have also been raised as a consequence of this development. The overarching principle and the central challenge in computational scattering is to approximate the scattered wave as accurately and efficiently as possible. Indeed, one may identify the major open problems in the field as the development of high-frequency, high-accuracy algorithms; efficient and accurate absorbing boundary conditions; and preconditioners for discretizations of exterior scattering problems. Regardless of the specific algorithms one may use to study scattering, these issues must be confronted head-on.

This workshop aimed to bring together experts in computational scattering with a view to cross-fertilization and communication. The format included a few overview-style talks each day, followed by informal discussion periods. These discussions were particularly important since the academics working in computational scattering appear to be evolving a subject in seemingly parallel directions, without much interaction. The hope was that participants would learn about other techniques being used to study exterior scattering, discuss common issues and open problems, and hopefully form cross-discipline collaborations.

The workshop was successful in achieving many of its goals. The talks provided an exciting snapshot of the current state-of-the-art in computational scattering. This forum provided a particularly suitable place for students entering the field to gain an overview of the subject area; one of the workshop highlights was the number of informal introductory lectures given by eminent mathematicians to the graduate students.

1 Computational scattering: basic ideas and workshop themes

Computational scattering theory is the study of algorithms to approximate wave-obstacle interactions. The governing equations might be the scalar wave equation (acoustic scattering), Maxwell's equations (electromagnetic scattering) or nonlinear PDE such as those arising in gravitational waves; the obstacles under study are either bounded in space, or are akin to diffraction gratings. A typical assumption is that all nonlinearities are compactly supported in space, allowing for simpler physics far from the obstacle. One may be interested in the propagation of the resulting scattered wave in a waveguide or in all of space. The goal is to compute approximations to this scattered wave, given information about the incident wave, the obstacle, and the medium of propagation. Necessarily, one must also study the mathematical properties of the approximation procedure, which in turn cannot be seperated from the PDE at the continuous level.

Frequently scattering problems are posed in a frequency-domain formulation. Looking for time-harmonic solutions, $F(x,t) = e^{i\omega t} f(x)$, one is led to a time-independant PDE. We illustrate the idea in the context of the frequency-domain formulation of Maxwell's equations. Let Ω be a bounded region in $\mathbb{R}^3$. A perfect conductor occupies the region Ω. By taking the Fourier transform of Maxwell's equations (Ampere's law and Faraday's law) we are lead to the system

$$i\omega\epsilon E(x) + curl\, H(x) - \sigma E = 0, \qquad x \in \mathbb{R}^N \setminus \Omega \tag{1}$$

$$-i\omega\mu H(x) + curl\, E(x) = F, \qquad x \in \mathbb{R}^N \setminus \Omega. \tag{2}$$

Here ϵ and μ are respectively the permittivity and permeability of the medium, which may vary in space. The transform variable is ω, while the (rescaled) fields E and H correspond to the Fourier transforms of the electric and magnetic fields, and F is a source term including information about applied current densities. To close the system, one needs to prescribe boundary conditions on the obstacle Ω, and some conditions at spatial infinity. The latter conditions are referred to as the Silver-Müller conditions. One can eliminate the magnetic field H, and rewrite the system above as a second-order problem. Since we are considering scattering from a perfect obstacle, we can write the Silver-Muller conditions in terms of E^s, the scattered field; the total field $E(x) = E^s(x) + E^i(x)$ for some prescribed incident field E^i. We are finally lead to the following system:

$$\nabla \times (\mu^{-1}\nabla \times E) - k^2\epsilon E = F, \qquad x \in \mathbb{R}^N \setminus \Omega \tag{3}$$

$$E = E^i + E^s, \qquad x \in \mathbb{R}^N \setminus \Omega \tag{4}$$

$$E \times \nu = 0, \qquad x \in \partial\Omega \tag{5}$$

$$\lim_{r\to\infty} r((\nabla \times E^s) \times \hat{r} - i\omega E^s) = 0, \qquad r \to \infty. \tag{6}$$

Even for this simple model, several observations can be made. First, unless Ω is a very simple shape, and the material coefficients are constant, we cannot analytically compute the field $E(x)$, and must resort to numerical simulation. Second, the field $E^s(x)$ occupies an infinite computational region, $\mathbb{R}^3 \setminus \Omega$. This region must be appropriately truncated in order to allow for computations; any truncation strategy must be analyzed for its effect on the accuracy of approximations. While the governing PDE has at most one solution thanks to the Silver-Muller condition, the operator $\nabla \times (\mu^{-1}\nabla \times \cdot) - k^2\epsilon\cdot$ is not coercive; it is well-known that in the interior of cavities, Maxwell's equations permit resonances. Any truncation strategy must take this possibility into account. The choice of boundary condition one prescribes to truncate the region thus plays an important role in the success of the numerical method. Depending on the nature of the boundary condition employed, we refer to them as non-reflecting, absorbing, perfectly matched layers, etc. For the purpose of this meeting we referred to such conditions collectively as **artificial boundary conditions**. **Xavier Antoine, Thomas Hagstrom, Eric Luneville, David Nicholls, Nilima Nigam and Sergey Sadov** spoke on this topic.

Third, the wave number k sets a length-scale called the *wavelength* $\lambda \equiv \frac{1}{k}$. As the wave number k increases, this characteristic scale, becomes smaller. For instance, to accurately resolve a periodic function in $1-D$, anywhere between 3-10 mesh points per wavelength are required. Now consider the scattering of a 30 Gigahertz incident wave, such as those used in high-speed microwave radio relays. This sets a length scale at the order of millimeters. If the scattering obstacle has a radius 10 meters, with complicated geometrical features or electromagnetic properties, one requires billions of mesh points even just to resolve the scattered wave in a thin layer around the obstacle. A major goal is to avoid resolving such small scales while performing computations involving large, complex obstacles; this is an *extremely* challenging task. Indeed, off-the-shelf packages do not suffice in most such situations, and much work is being done in developing novel discretization methods suited for scattering problems. **Jean-Davide Benamou, Anne-Sophie Bonnet-Ben Dhia, Oscar Bruno, Simon Chandler-Wilde, Joseph Coyle, Leszek Demkowicz, Paul Martin, Peter Monk, Jie Shen, Symon Tsynkov and Tim Warburton** spoke on the topic of **accurate discretizations and high-frequency calculations**.

Next, since the governing PDE is not positive-definite, one should not expect any linear system arising from a discretization process to be positive-definite. In practice one can imagine very large linear systems which need to be solved iteratively; the development of **preconditioning strategies** would significantly impact the size of problems one can attack. **Robert Beauwens, Annalisa Buffa, Matthias Maiscak, and Jean-Claude Nedelec** described recent work in the area.

Finally, the inverse problem related to this model- determining the location of the obstacle, and/or the permittivity and permeability of the medium near the obstacle based on the observed scattered wave - is an ill-posed problem. Since the invention of radar, scientists and engineers have striven not only to detect but also to identify unknown objects through the use of electromagnetic waves. Any success in this direction has potentially huge impact in application areas from medical imaging to seismic exploration. Current progress was reported by **David Colton, Fioralba Cakoni and George Hsiao**

2 Workshop Themes, recent work and open problems

The workshop was intended to review the current state-of-the-art in computational scattering, and also to discuss future directions for the community to investigate. To focus the discussion, the workshop was organized around three major themes: artificial boundary conditions, high-frequency computations, and preconditioning. Some recent work on inverse scattering was also discussed.

2.1 Absorbing and artificial boundary conditions

When finite difference, finite element or spectral methods are used to resolve the scattered wave near the obstacle, the computational region must be restricted to be finite. This truncation is achieved by means of absorbing or exact boundary conditions. These conditions can be implemented in various ways, e.g. by using boundary integral equations, series implementations, or the perfectly matched layer of Berenger. No matter which techniques are used, the goal is to obtain as accurate an approximation to solutions of the original scattering problem, as efficiently as possible. Unfortunately, these are competing requirements. There are significant implementation and/or accuracy issues which remain open problems. The construction of high-accuracy artificial boundary conditions in the time-domain is particularly important for applications. It is, however, a complex endeavour to balance the needs of accuracy in space and time with the requirements of efficiency (memory and computation).

Xavier Antoine reviewed recent developments in the technique of *on-surface radiation conditions* with regards to the challenging problem of simulating high-frequency acoustic and electromagnetic scattering problems. He also discussed the development of accurate and local artificial boundary conditions for smooth geometries and the construction of well-posed and well-conditioned integral equations for the iterative solution of high-frequency scattering problems.

Thomas Hagstrom reviewed the state-of-the-art in the construction, analysis, and application of arbitrarily-accurate radiation boundary conditions for time-domain simulations. Specific topics included: (i.) Experiments with nonlocal boundary conditions employing efficient compressions of the time-domain kernels; (ii.) Reformulated local boundary condition sequences and their use in polygonal domains and stratified and anisotropic media; (iii.) Speculations on potential improvements of the local boundary condition sequences and extensions to inhomogeneous media and nonlinear problems.

In an acoustic waveguide, assumed to be semi-infinite along one propagation axis, one can easily construct from the spectral theory of a simple transverse operator an “exact” transparent condition. More precisely, such a condition is based on an explicit diagonalisation of the Dirichlet to Neuman operator. The situation for Maxwell’s equations is more intricate. Indeed, the operator which associates the electrical field to its derivative (equivalent to a Dirichlet to Neuman operator) is not implemented because the transverse and longitudinal Maxwell operators remains coupled and no explicit diagonalisation may be performed. In a talk by **Eric Luneville**, a new transparent condition in a two dimensional case for the regularized Maxwell equations was proposed. The BC was based on the diagonalization of an operator which involves mixed unknowns, e.g. the coupling of the electric tangential component and the divergence of the electric field, or the coupling of electric normal component and the rotational of the electric field. Unfortunately, this transparent condition requires one to deal with a mixed variational formulation where, for example, the divergence on the transparent boundary appears as a new unknown of the problem. However, this formulation is well-posed and its approximation by Lagrange finite elements is convergent. This approach is an alternative way to other methods such that integral equation or Perfectly Matched Layer techniques. It is of interest to point out that it appears as a theoretical tool in the proof of convergence of PML techniques too. Such transverse decompositions are also related to modal approximation. This approach may also be used for elastodynamic problems. In that case, the spectral theory of the transverse operator is not obvious.

Boundary perturbation methods are among the most classical techniques for approximating scattering returns from irregular obstacles. Despite a history which dates to Rayleigh's calculations in the nineteenth century, their convergence, stability, and capabilities were, for almost a century, misunderstood. The work of Bruno & Reitich not only placed these methods on a secure theoretical foundation, but also provided fast, high-order computational strategies. Subsequent work by **David Nicholls** has further clarified the properties and limitations of these methods, and suggested new algorithms to achieve high-order approximations in a rapid and numerically stable manner. Nicholls gave an overview of these boundary perturbation methods and discussed recent enhancements.

Nilima Nigam presented some recent work on artificial boundary conditions for the scattering of elastic waves from bounded obstacles, including extensions of the boundary perturbation approach of Bruno and Reitich, as well as investigations into an overlapping Schwarz domain decomposition method.

The unique solvability of an exterior Dirichlet problem implies the existence of an operator that maps the Dirichlet data (function on the obstacle boundary) to the normal derivative of the solution (another function on the boundary). The Dirichlet-to-Neumann map thus defined is a boundary pseudodifferential operator of order 1. In 2D problems, the boundary is one-dimensional, usually diffeomorphic to a circle, and the DtN can be exactly (without truncation by order) described by a discrete symbol, which is a function of three parameters: boundary parameter s, Fourier series index (discrete momentum) n, and the wavenumber k. As k goes to infinity, the symbol has a nice asymptotic behaviour uniformly in s and n. This idea was discussed by **Sergey Sadov**, who described a reformulation of this asymptotic property as a microlocal refinement of the Kirchhoff approximation.

2.2 High frequency methods and novel discretization techniques

The conditioning and accuracy of most discretization techniques for scattering problems depend crucially on the wave number of the incident wave. In addition, there are algorithms suitable for moderate frequency scattering, and others appropriate for geometrical optics. A key challenge in this field remains the development and analysis of an algorithm which works over a large range of frequencies, and whose performance can be controlled independant of the frequency. In this workshop developments of new high-accuracy methods suitable for a large range of wavenumbers were discussed.

The high frequency asymptotic representation of wavefields (Geometrical Optics in its simple form) is a computationally attractive approach because the discretization is, to a large extent, independent of the frequency. Unfortunately this technique has both theoretical and practical limitations. There has been much work in combining or coupling the usual "frequency aware" (or "full") wavefield and "asymptotic techniques". **Jean-David Benamou** spoke on numerical microlocal analysis, applied to scattering problems. While it is easy to compute a full wavefield representation from its (constructive) asymptotic representation, the opposite extraction (or "analysis") from a given wavefield of its frequency-independent asymptotic representation is far from obvious. He presented a numerical method which, given an analytical or numerical solution of the Helmholtz equation in a neighborhood of a fixed observation point, and assuming that the geometrical optics approximation is relevant, determines at this point the number crossing rays and computes their directions and associated complex amplitudes.

There has been another large body of work on high-frequency methods, which are based on integral equations, high-order integration, fast Fourier transforms and highly accurate high-frequency methods. These can be used in the solution of problems of electromagnetic and acoustic scattering by surfaces and penetrable scatterers — even in cases in which the scatterers contain geometric singularities such as corners and edges. The solvers exhibit high-order convergence, they run on low memories and reduced operation counts, and they result in solutions with a high degree of accuracy. They require, among other tools, accurate representations of obstacle surfaces. A new class of high-order surface representation methods was discussed by **Oscar Bruno**, which allows for accurate high-order description of surfaces from a given CAD representation. These methods are employed in conjunction with a class of high-order, high-frequency methods using integral equations which was developed recently. The talk ended with a description of a general and accurate computational methodology which is applicable and accurate for the whole range of frequencies in the electromagnetic spectrum.

An important aspect of the numerical analysis of scattering algorithms is the precise dependence of their accuracy and conditioning on the frequency. There are many open questions in this direction, some of which have motivated the design of new algorithms. **Simon Chandler-Wilde** gave an overview of recent work on boundary element methods for high frequency scattering problems. He first described what was known about the dependence of the conditioning of boundary integral equations on frequency and on the choice of coupling parameters in combined layer-potential formulations. He next discussed attempts to reduce the number of degrees of freedom by incorporating some of the oscillatory behaviour of the solution in the basis functions used in the boundary element method. His talk contained several open problems.

Often the modeling of the complex physics involved in a scattering problem leads to mathematical challenges. **Anne-Sophie Bonnet-Ben Dhia** described work on acoustic scattering in the presence of a mean flow. This was work motivated by the need to develop noise-reducing technologies for planes, particularly in the neighborhood of the airports. Unfortunately, there exists no satisfactory way to solve the Linearized Euler Equations in the harmonic regime and in unbounded domains; a major effort in this current work involves developing a well-posed model. Bonnet-Ben Dhia's work consists in solving a linearized equation, set on the perturbation of displacement, the so-called Galbrun's equation. An augmented formulation of this process was proposed, which includes a non-local (in space) term, linked to the convection of vortices along the stream lines. This is then combined with a perfectly matched layer to truncate the region.

2.3 Finite and spectral elements

The workshop also brought together researchers who used finite element or spectral element techniques in the study of wave propagation. Since the solutions are quite oscillatory, the "standard" strategies are severely limited in terms of efficiency; speakers presented novel discretization techniques which took into account the particular behaviour of scattered waves and which ameliorated some of the difficulties which plague existing techniques.

For scattering by complicated obstacles or in the presence of inhomogenous media, the use of nonuniform meshes can confer many advantages. However, the construction and implementation of hierarchic finite element bases on unstructured tetrahedral meshes poses challenges at the computational and analytical level, especially where a non-uniform order of approximation may be utilized. Enforcing the appropriate conformity properties of the approximation across element interfaces is typically a difficult task in this case, and recent work on this problem was presented by **Joseph Coyle**. He first related the problem to the intrinsic orientation of the edges and faces as well as the global numbering of the basis functions. Observing that an appropriate reordering of the local numbering of the vertices allows any global tetrahedron to be reduced to one of two possible reference tetrahedra that leads the way for the construction of the hierarchic bases where ease of implementation is not sacrificed.

The theory of hp-discretizations for Maxwell problems was reviewed by **Leszek Demkowicz**, who summarized the main points of the projection-based interpolation theory, convergence results for Maxwell eigenvalues and recent results on the existence of polynomial preserving extension operators in H(curl) and H(div) spaces. He then spoke on the subject of goal-oriented hp-adaptivity, presenting an extension of the original, energy-based hp-algorithm and its applications to borehole logging EM simulations. Finally, he discussed the impact of automatic hp-adaptivity in simulations involving the use of PML. The automatic reproduction of "boundary layers" by the hp-adaptivity significantly reduces the tedious design and tuning of PML's.

Although direct scattering problems in cavities and waveguides are typically linear and well-posed, they are difficult to solve numerically because the oscillatory nature of the solution forces the use of large numbers of degrees of freedom in the numerical method, and the resulting linear system defies standard approaches such as multigrid. This is a particular problem at high frequencies when the scatterer spans many wavelengths. In an effort to improve the efficiency of a volume based approach as the frequency increases and to allow the solution of problems at widely different frequencies on a single grid, **Peter Monk** described his recent work in the use of plane waves as a basis for approximating the scattered field. These are used in a discontinuous Galerkin scheme based on a tetrahedral finite element mesh. This method is termed the Ultra Weak Variational Formulation (UWVF) by its originators O. Cessenat and B. Despres. The use of the Perfectly Matched Layer or Fast Multipole Method to improve the artificial boundary condition needed by the method was also discussed. Interestingly the linear system from the UWVF is easier to solve than the one arising from the finite element method, and this allows a simple parallel implementation of the method. The method has been validated on a variety of problems, and extended to the acoustic-elastic fluid-structures problem.

The use of spectral methods in wave scattering is a very active field of research. **Jie Shen** present an efficient and stable spectral algorithm and their numerical analysis for the Helmholtz equation in exterior domains. The algorithm couples a boundary perturbation technique with a well-conditioned spectral-Galerkin solver based on an essentially exact Dirichlet-to-Neumann operator. Error analysis as well as numerical results were presented to show the accuracy, stability, and versatility of this algorithm.

Recent investigations of the spectral properties of the discrete Discontinuous Galerkin (DG) operators have revealed important connections with their continuous Galerkin analogs. Theoretical and numerical results, which demonstrate the correct asymptotic behavior of these methods and precludes spurious solutions under mild assumptions, were presented by **Tim Warburton**. Given the suitability of DG for solving Maxwell's equations and their ability to propagate waves over long distance, it is natural to seek effective boundary treatments for artificial radiation boundary conditions. A new family of far field boundary conditions were introduced which gracefully transmit propagating and evanescent components out of the domain. These conditions are specifically formulated with DG discretizations in mind, however they are also relevant for a range of numerical methods.

2.4 Special techniques

As mentioned earlier, there has been much work recently in the development of specifically tailored techniques for wave scattering problems. Examples of such work include the use of asymptotic formulae derived using classical techniques, and Huygen's principle.

Paul A. Martin provided the first classical derivation of the Lloyd-Berry formula (published in 1967) for the effective wavenumber of an acoustic medium filled with a sparse random array of identical small scatterers. The approach clarifies the assumptions under which the Lloyd-Berry formula is valid. More precisely, an expression for the effective wavenumber was derived, assuming the validity of Lax's quasicrystalline approximation but making no further assumptions about scatterer size. In the limit of vanishing scatterer size it was shown that the Lloyd-Berry formula is recovered. We have also obtained a similar formula in two dimensions. The methods employed should extend to analogous electromagnetic and elastodynamic problems.

Among the well-known challenges that arise when computing the unsteady wave fields is the deterioration of numerical schemes over long time intervals (error buildup) and the unboundedness of the domain of definition. The latter is typical for many applications, e.g., for the scattering problems, when the waves are radiated toward infinity. In the literature, a standard way to deal with the first issue is to increase the order of accuracy (quite independently, paraxial approximations can be employed), whereas the second issue requires truncation of the domain and setting of artificial boundary conditions (ABCs). According to conventional wisdom, exact ABCs for multidimensional unsteady problems are nonlocal not only in space but also in time, and the extent of temporal nonlocality continually increases as time elapses. It turns out, however, that in many cases both types of difficulties can be addressed using a unified approach based on exploiting the Huygens's principle. The propagation of waves is said to be diffusionless, and the corresponding governing PDE (or system) is said to satisfy the Huygens principle, if the waves due to compactly supported sources have sharp aft fronts. The areas of no disturbance behind the aft fronts are called lacunae. Diffusionless propagation of waves is rare, whereas its opposite - diffusive propagation with after-effects is common. Nonetheless, lacunae can still be observed in a number of important applications, including acoustics and electromagnetism. The key idea of using lacunae for computations is that any finite size region falls behind the propagating aft front, i.e., right into the lacuna, after a finite interval of time. In other words, any given feature of the solution will only have a finite predetermined lifespan on any fixed domain of interest. By incorporating these considerations into a numerical scheme, one can make its grid convergence uniform in time. The same considerations facilitate design of exact unsteady ABCs with only fixed and limited (non-increasing) extent of temporal nonlocality. At the workshop, **Symon Tsynkov** described recent progress made in constructing the lacunae-based numerical schemes for the d'Alembert equation, as well as for the linearized Euler equations and the Maxwell equations. He also discussed different physical models from the standpoint of existence of the lacunae and showed in some interesting cases that are technically speaking diffusive, e.g., the propagation of electromagnetic waves in dilute plasma, lacunae can still be identified in the solutions in some approximate sense.

2.5 Preconditioning strategies

The efficient solution of the linear systems obtained as a consequence of the discretization of exterior scattering problems is an open problem, since these systems are typically dense. Canned preconditioning techniques have been rather unsuccessful. Part of the difficulty in the preconditioning of frequency-domain problems lies in the indefinite natue of the associated linear systems. **Robert Beuwens** gave an overview of the principles behind complex iterative schemes, used to solve large sparse linear systems of equations. He discussed two kinds of methods, which are often used in combination: preconditioning methods and convergence acceleration methods. Preconditioning methods aim at building an approximate system close to the one to be solved but which is inexpensive to solve both in terms of computing time and memory requirements. Convergence acceleration methods are used to transform slowly converging sequences or even diverging sequences into rapidly converging sequences. Acceleration techniques popular today include the polynomial acceleration or Krylov subspace methods as basic blocks in the building of elaborate preconditioners. The talk concluded with recent developments concerning multi- level and recursive ordering methods on the one hand and the parallelization of preconditioned Krylov subspace methods on the other hand.

Preconditioning techniques have recently been developed for boundary integral equations used in this context; there is a pressing need for a systematic preconditioning strategy for other algorithms as well. The use of Calderon projections in the study of integral equations suggests the use of operator-level preconditioners, where the continuous problem is preconditioned by application of suitable pseudo-differential operators. Discretization is performed only after this preconditioning. The electric field integral equation (EFIE) arises in the scattering theory for harmonic electromagnetic waves. **Annalisa Buffa** described an optimal preconditioning technique for the conforming Galerkin approximation of the EFIE via Raviart-Thomas finite elements. At the continuous level, Calderon formulas provide an explicit representation of the inverse operator of the electric field integral operator up to compact pertubations. A stable discretization of the Calderon formula was presented, and then an optimal preconditioner for the linear system which arises from the Galerkin discretization of the EFIE was shown.

Jean-Claude Nedelec also spoke on preconditioning the Maxwell integral equations using Calderon identities

Starting from the well known combined boundary integral formulations due to Brakhage/Werner and Burton/Miller **Olaf Steinbach** reviewed existing modifications which are needed for the numerical analysis in the correct function spaces. While most of the proposed modifications rely on a compactness argument, the current work involved an alternative approach, which leads to a stable approximation scheme.

The symmetric coupling of finite elements and boundary elements for electromagnetic problems results in highly ill-conditioned linear systems of equations. **Matthias Maischak** presented a block-preconditioner for the GMRES method which is based on domain decomposition methods applied to the “FEM-part” and the “BEM-part” separately and analysed the eigenvalue distribution of the preconditioned system. It was shown that the efficiency of this method only depends on the ratio of coarse grid mesh size and the overlap. Numerical examples for the eddy-current problem underline the efficiency of this method.

2.6 Inverse problems

While describing important applications of scattering theory, one is naturally lead to consider inverse problems. Important inverse problems include the reconstruction of biologically relevant information from medical tomography data, the location of hydrocarbons based on seismic imaging information, and the detection of mines. Mathematically, inverse problems in scattering pose severe challenges due to their ill-posed nature.

Fioralba Cakoni spoke on mathematical and computational aspects of inverse Electromagnetic Scattering Problems, specifically as it pertains to synthetic aperture radar (SAR). SAR suffers from limitations arising from the incorrect model assumptions which ignore both multiple scattering and polarization effects. The main theme of this talk was the use of a qualitative method, the linear sampling method, to solve inverse electromagnetic scattering problems. Cakoni first introduced the main mathematical ideas of the linear sampling method for the simple case of electromagnetic scattering by a perfect conductor. She next showed how to use the technique to find both the shape and the surface impedance of a partially coated perfect conductor without knowing a priori whether the obstacle is coated. In the case of an inhomogeneous background, she presented a new method which avoids the need to compute the Green’s function of the background media.

Numerical examples showed the validity of this approach.

Some recent developments in inverse scattering were described by **David Colton**, who also discussed a major open problem in the field.

Scattering theory in periodic structures has many applications in micro-optics. The treatment of the inverse problem, recovering the periodic structure or the shape of the grating profile from the scattered field, is useful in quality control and design of diffractive elements with prescribed far field patterns. **George Hsiao** discussed an inverse diffraction grating problem to recover a two-dimensional periodic structure from scattered waves measured from above and below the structure. The problem was reformulated as an optimization problem including regularization terms. The solution is obtained as the minimizer of the optimization problem, where the objective function consists of three terms: the residual of the Helmholtz equation, the deviation of the computed Rayleigh coefficients from the measured data, and the regularization term to cope with the ill-posedness of the inverse problem. He then described solvability and parameter sensitivity of the algorithm, and showed some numerical experiments validating the approach.

3 Presentation Highlights

The workshop brought together experts in a variety of computational techniques, with a focus on exterior scattering problems. In addition, graduate students and postdoctoral fellows were invited, to establish connections with established mathematicians. To optimize research interaction, several different activities were planned:

- 30 minute lectures by experts
- Poster presentations by graduate students and postdocs: the posters were on display for the duration of the workshop in the coffee room area. Since this area was heavily utilized during breaks, the students and postdocs got several opportunities to discuss their work with other mathematicians. We actually recommend this format for poster sessions for future workshops; the younger mathematicians were very appreciative of the extended opportunity to showcase their research.
- Two panel discussions: At the end of Day 2 and Day 4 of the workshop, panel discussions were held on integral equation methods and finite element methods respectively. These lively discussions included presentations of open problems, discussions of key challenges and suggestions for future research.
- Informal lectures: several expert mathematicians volunteered to give informal lectures to the graduate students. Particularly given the range of mathematical expertise at the workshop, this was a very valuable opportunity for the students.

3.1 Poster presentations

- **Binford, Tommy** (Rice University)
  Title: *Experiments with a Dirichlet to Neumann Map for High Order Finite Elements*
  For electromagnetic scattering problems, the number of degrees of freedom to acheive a desired accuracy can be prohibitively large depending on the domain. Artificial boundary methods are a powerful tool for treating radiation conditions while preserving the physical behavior with fewer degrees of freedom. Work by Nicholls & Nigam on Dirichlet to Neumann maps has provided a method of handling the radiation condition for perturbed simple geometries such as a circular boundary. In this poster, Binford showed experiments where one applies a high order finite element method in conjunction with a Dirichlet to Neuman map to solve Helmholtz' equation for a right circular cylindrical scatterer with different perturbations of a circular artificial boundary away from the scattering object.
- **Ecevit, Fatih** (Max Planck Institute)
  Title: *High-frequency asymptotics and convergence of multiple-scattering iterations in two-dimensional scattering problems*
  One of the main difficulties in high-frequency electromagnetic and acoustic scattering simulations is

that any numerical scheme based on the full-wave model entails the resolution of the smallest wavelength. It is due to this challange that simulations involving even very simple geometries are beyond the reach of classical numerical schemes. Ecevit presented an analysis of a recently proposed integral equation method for the solution of high-frequency electromagnetic and acoustic scattering problems that delivers *error-controllable solutions in frequency-independent computational times*. Within single scattering configurations the method is based on the use of an appropriate ansatz for the unknown surface densities and on suitable extensions of the method of stationary phase. The extension to multiple-scattering configurations, in turn, is attained through consideration of an iterative (Neumann) series that successively accounts for multiple reflections. Here we derive a high-frequency asymptotic expansion of the successively induced currents in this latter procedure and, within this context, we derive an estimate for its convergence rate. As we show, this rate is explicitly computable and it depends solely on geometrical characteristics; in particular, it is independent of the specific incidence of radiation. Numerical results confirm the accuracy of this high-frequency estimate for the case of several interacting structures.

- **Han, Young-Ae** (Caltech)
  Title: *A Continuation Method for high-order parametrization of arbitrary surfaces*
  In this poster, a super-algebraically convergent technique to approximate complicated surfaces in 3-D using locally smooth functions was presented. The method accurately renders geometric singularities such as edges and corners. The approach was based on continuing each smooth branch of a piecewise-smooth function into a new function which, defined on a larger domain, is both smooth and periodic. These "continuation functions" have Fourier coefficients that decay super-algebraically, and thus result in high-order approximations of the given function throughout its domain of definition. Among other benefits, this approach resolves the Gibbs phenomenon. Examples showing the success of this strategy were also shown.

- **Kurtz, Jason** (U. Texas at Austin)
  Title: *Fully-Automatic hp-Adaptivity for Acoustic and Electromagnetic Scattering in 3D*
  Two popular strategies for studying exterior scattering problems are coupled FEM-PML or FEM-Infinite element methods. This work describes an adaptive hp refinement algorithm for both strategies which yields exponential convergence in the energy norm. The hp-adaptive method is ideally suited for scatterers with geometric singularities and/or for discretizations truncated by a perfectly matched layer. Three crucial implementation issues were addressed in the poster: namely, fast integration of element stiffness matrices, a domain-decomposition multi-frontal solver, and a "telescoping" solver for a sequence of locally nested meshes. Computational results were presented for both PML and infinite element truncations.

- **Sifuentes, Josef** (Rice University)
  Title: *GMRES performance in integral equation methods for scattering by inhomogeneous media* Discretizations of integral equation techniques lead to linear systems which are solved iteratively (typically using GMRES). The number of iterations increases considerably with wave number.The poster described recent investigations into the wave-number dependence of the spectrum of the discretized integral operator. This line of research will eventually lead to better preconditioning strategies.

4 Open problems and future directions

One of the big successes of this workshop was due to the scientific generosity of the participants, who not only provided clear expositions on their work, but also detailed open problems and future directions they believed to be of significance. Some of these were reiterated during the two panel discussions (summarized below) and informal talks.

Over the course of the workshop, the participants identified some major directions for future research. Problems which need theoretical and analytical work include careful investigations into wave-number dependent error analysis of existing algorithms, and preconditioning strategies. At the computational level, the community felt the need to develop benchmark problems to test algorithms, and demonstrate the effectiveness of computational strategies on scattering from complex structures and physics.

Another concern which was shared was the overwhelming effort required in meshing complex geometries. It is estimated that of the total time spent on studying scattering problems in an engineering context, developers spend around 80% of their time on describing the geometry and implementing meshes, and only 20% on the actual simulation. While no consensus emerged on how best to deal with this problem, it became clear that for newer algorithms to become widely applicable, they had to account for this bottleneck.

To get a full flavour of the range of open problems suggested, we encourage the interested reader to look at the website:

`http://www.math.mcgill.ca/nigam/BANFF/front.php`

This website contains many of the talks, and links to participant websites and papers.

4.1 Integral equation techniques

- It is well-known that most numerical methods for scattering problems require a mesh which can resolve the incident wave. This means, in particular, that the size of the mesh grows with the wave number k. However, in some situations this may not be necessary. For example, the scattering of a high frequency wave off a convex smooth obstacle should not require such high numerical resolution. An open problem is to characterise the scattering problems for which O(1) discretizations are possible as $k \to \infty$. Does the convexity of the scattering object play an important role, is smoothness of material properties crucial?

- Integral equation techniques rely on the fast and accurate quadrature of oscillatory kernels. This poses interesting problems in the theory of quadrature, not just restricted to scattering. For example, how should one deal with oscillatory integrals, particularly in complex 3-D geometries, in O(1) computational time, without sacrificing accuracy?

- A major open area of investigation remains the hunt for good preconditioners in the twin limit as mesh size $h \to 0$ and wave number $k \to \infty$.

- Geometrical optics is a powerful tool for studying very high frequency scattering. While developing numerical algorithms suitable for a range of frequencies, it would be desirable to incorporate ideas from geometrical optics to deal with the high frequency range. An application would be, for example, acoustic muffling problems, where an integral equation solver may be appropriate for the object, and geometrical optics suffices to capture the large-scale and atmospheric effects.

- An important open area in the numerical analysis of scattering algorithms concerns estimates (above and below) of condition numbers for integral equations for general objects. Some results are known on simple geometries, but these need to be extended.

- A specific question in the numerical analysis of integral equation techniques is whether the Galerkin method is stable for classical Brakhage-Werner integral equations on Lipschitz domains.

- The error analysis of the classical Brakhage-Werner integral predicts a condition number which grows as $O(k^{1/3})$ as $k \to \infty$. This is not reflected in actual computations for a large class of scatterers. Why?

- There exist a profusion of algorithms for scattering, suitable in certain specific frequency regimes. The workshop participants agreed that a key goal is to establish stability for any numerical method uniformly in wave number k.

- Much is known about the physics of wave propagation and interaction in anisotropic and inhomogenous materials. Rather than look for a preconditioner *ab initio*, a fruitful direction of research would involve using knowledge of the physics to design optimal preconditioners.

- While describing a scattering problem in terms of integral equations, one has several choices. Some integral equation formulations are more suitable for computation than others; exploiting this requires a detailed understanding of the spectral properties of various integral equations.

- A valuable contribution from the community would be a set of non-trivial computational examples, showing the efficacy of integral equation based methods. At present, open-source software for boundary integral equations is not as well-developed as it's finite element analog.

- There are some situations where integral equation methods are both natural and more efficient than volumetric discretizations. An important project would be to classify the problems on which one should use integral equation methods.

- Domain decomposition methods are powerful tools which enable parallelization of computation, particularly for large obstacles. Communication between domains occurs via Stekhlov-Poincaré maps, which are accurately described in terms of integral operators. More investigation is needed into optimal combinations of integral equation methods and domain decomposition techniques.

- The use of integral equations of the second kind to solve exterior scattering problems is popular, in particular since the integral operators involved are not singular. Standard boundary element techniques do not always seek approximations in the correct Sobolev spaces. Indeed, integral equation techniques are quite versatile, and performing discretizations appropriately will allow for a wider range of problems to be solved.

- Integral equation methods lead to dense matrices; a lot of attention has been paid recently to operator-level preconditioning to improve the computational efficiency of these methods. Calderon projections offer many possibilities in terms of reformulations of integral equations; these need to be further examined for their computational suitability. Upon preconditioning with these projections, an integral equation of form $Bx = F$ can be transformed to one of type

  $$ABx = (I - K)x = AF.$$

  A closer theoretical investigation of the compact operator K is required for various projection methods. In particular, what is the behaviour of these projections at the discrete level, in the presence of meshes with high aspect ratios?

- At the discrete level, both storage and efficient computation of the linear systems arising from integral equation methods poses challenges. One fruitful direction of work which needs more development is the use of algebraic approximation methods and hierarchical matrices in this context. It is, for example, not obvious how one should precondition a system arising from the use of an adaptive mesh.

4.2 Volumetric discretization techniques and artificial boundary conditions

- Multigrid techniques for scattering require that the coarsest grid resolve the wavelength of the incident wave. This is too severe a restriction for this method to be practical at high frequencies; a variant of a multilevel technique which is genuinely independent of frequency is required. Similarly, while domain decomposition techniques are gaining popularity, the dependence of their performance on wavenumber is not clearly described.

- Scattering problems which involve wires or thin structures are notoriously difficult to solve, but applications involving wires and antennae are very important. For example, one may wish to study the electromagnetic fields inside the fuselage and body of an airplane, with the goal of reducing it's signature. In such applications, actually meshing to the level of the wire, while simultaneously capturing the large-scale object, will require either an extremely large mesh or a highly graded one. Existing algorithms need to be tested against benchmark problems involving wires, and we need to develop other algorithms if required.

- Plane-wave time-domain discretization techniques are gaining popularity. Here, one approximates the scattered field using plane wave basis functions. These algorithms need to be rigorously analysed for their convergence and stability properties. It has already been noticed that plane-wave techniques can be cheaper and more accurate than methods reliant on trigonometric or polynomial basis functions, provided one has some a priori knowledge of the direction of the wave to be approximated. The use of other special basis functions, to enable high-order calculations in an inexpensive fashion, also needs to be further investigated.

- In practice, the description of obstacle shapes or the incident wave requires the use of stochastic parameters and shapes. Few high-order methods currently exist for studying stochastic scattering problems; this field provides a wealth of open problems.
- As for the study of Integral Equation based methods, the error analysis of volumetric algorithms rarely includes explicit dependence on the frequency for quantities of interest. A major theoretical undertaking would be to develop tools to evaluate the dependence upon the frequency.
- Volumetric solvers, when coupled with appropriate boundary conditions, can lead to essentially sparse systems, which unfortunately are not positive-definite. A major open problem remains the construction of efficient solution techniques at the discrete level, perhaps using low-frequency or elliptic problems as preconditioners.
- Current convergence and stability results on vector-type finite element techniques for scattering do not extend to highly anisotropic meshes or materials. Since high-contrast and strongly anisotropic materials occur in practice, a careful study of numerical methods in this context is required. Indeed, effective *a posteriori* error estimates are not available, making adaptive meshes difficult to implement.
- An interesting question arises in the study of electromagnetic scattering: since the solutions of Maxwell's equation obey the Gauss, Ampere and Faraday laws. Should finite element approximations obey these at the element level? Is there any room for "fully compatible discretization" of electromagnetic waves?
- hp-adaptive finite element techniques can be very efficient, particularly when the scatterer or the medium has several scales, near-singular geometric features, or strong anisotropies. A rigorous error analysis of such methods for a variety of scattering problems remains an open challenge.
- The perfectly matched layer of Berenger has been very successful in certain contexts. Is there a stable PML for all symmetric hyperbolic systems? What about the PML for anisotropic elastic scattering: Is it stable?
- Exact boundary conditions are exact implementations of the Stekhlov-Poincaré maps on a truncating boundary. Is there a purely local (in space and time) exact boundary condition for the wave equation in the time domain?

This list of open problems by no means exhausts the issues brought up during the workshop; several more technical questions were presented in the actual talks and posters, for which we refer the reader to the associated website.

5 Participants

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