Integral Equations Methods: Fast Algorithms and Applications

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1 Overview of the Field

Integral equations have long been an invaluable tool in the analysis of linear boundary value problems associated with the Laplace and Helmholtz equations, the equations of elasticity, the time-harmonic Maxwell equations, the Stokes equation, and many more. Numerical methods based on integral equations have become increasingly popular, due in large part to the development of associated fast algorithms such as the Fast Multipole Method (FMM) [2]. Many of the core problems arising in electromagnetics, acoustics, solid and fluid mechanics, molecular dynamics, quantum physics and chemistry, and astrophysics can now be solved extremely efficiently using fast integral equation methods (FIEMs). For such problems, this has proven to be game changing: FIEM have enabled the accurate solution of problems far larger than what had previously been imagined possible. Recent hardware developments (GPUs, increased storage capacity, distributed computing, etc) have put us in a position where we could soon see such methods being mainstreamed to the point where it would be possible to perform complex 3D simulations in close to real time on a desktop machine. The impact of such a development would be profound.

2 Recent Developments and Open Problems

In recent years, several advances have raised the possibility that the exceptional performance demonstrated in certain super-computing settings can be made accessible to a much broader audience of researchers relying on scientific computing in their work. Specific advances include:

- Fast operator algebra: The first generation of analysis-based fast algorithms provided tools, such as the FMM, for rapidly applying certain integral operators. These are highly efficient but are limited to a narrow class of operators. In the last ten years, it has been demonstrated that in addition to merely applying an operator rapidly, one can also accelerate the multiplication of operators, inversion of operators, and even computing full or partial spectral decompositions. Thus, it is now possible to handle a much broader class of operators than was previously thought possible.

- Inexpensive storage and multicore processors: Computing architecture is rapidly changing. While it used to be the case that storage and the cost of a single floating-point operation were the principal limiting factors, communication is now emerging as the principal constraint. The reason is the move to parallel and distributed computing, which in turn is driven by the stagnating clock-speed of processors coupled with a shrinking cost per processor. The most extreme manifestation of this shift is perhaps the emergence of components like Graphics Processing Units (GPUs), which contain a very large number of cores each having limited capabilities. The changing computing environment is making many of the currently used numerical algorithms uncompetitive. This creates a demand for new algorithms that are designed from scratch to minimize communication, rather than the number of floating point operations required.

- Randomized algorithms in numerical linear algebra: It has recently been demonstrated that approximate factorizations of matrices of numerically low rank can be constructed very efficiently via certain randomized sampling procedures. This work draws on random matrix theory, functional analysis, and linear algebra, and furnishes computational techniques that are highly efficient, robust, versatile, and of intrinsic mathematical interest. Since many analysis-based fast algorithms rely on the hierarchical splitting of a large matrix into submatrices of numerically low rank, there is an obvious opportunity to incorporate the new randomized sampling algorithms into the fast operator algebra methods to achieve even faster and more versatile algorithms.

- Improved surface representations and discretizations: Real-world applications often involve curves and surfaces with (sometimes thousands of) corners and edges: the interaction of such geometry with the singular kernels of integral operators poses a challenge to accurate solution, particularly in three dimensions. There has been recent progress on high-order surface representations, on the automatic generation of efficient and well-conditioned quadrature schemes for discretizing integral equations, and on evaluation of potential fields close to their sources.

- New and expanding areas of application: Many of the FIEM developed for the classical equations in mathematical physics have increasingly been used as building blocks for solving much more complicated boundary value problems. FIEM have now started to compete with finite element and finite differences in simulating complex systems in science and engineering.

- New mathematical formulations of key boundary value problems: There have been recent breakthroughs in creating a well-conditioned mathematical formulation of the scattering problem for time-harmonic Maxwell equations, in the representation of problems in periodic geometries, and deriving second-kind integral equations for high-order systems of PDEs. Such analytically sound formulations are key to creating software packages that are robust at all user parameters.

3 Presentation Highlights

Presentations where grouped according to five themes:

1. Quadrature methods
2. Fast algorithms
3. Fast direct solvers
4. Wave applications
5. Fluid and other applications

3.1 Quadrature Methods

There were four talks concerning developing efficient high-order discretization schemes for integral equations with singular/hypersingular kernels in complex geometries. The practical application of integral equation methods requires the accurate evaluation of boundary integrals with singular, weakly singular or nearly singular kernels. Historically, these issues have been handled either by low-order product integration rules (computed semi-analytically), by local modifications of a smooth rule, by singularity subtraction/cancellation, by kernel regularization and asymptotic analysis, or by the construction of special purpose "generalized Gaussian" quadrature rules. In the complex analytic case, additional methods have been developed by for off-surface evaluation. It should be noted that in the two-dimensional case, several of these alternatives provide extremely effective schemes, since they all permit local adaptivity and high order accuracy. In this section, we summarize some recent developments on efficient high-order quadrature schemes for discretizing integral equations.

QUADRATURE BY EXPANSION SCHEME: Andreas Klöckner (The University of Illinois at Urbana-Champaign) and his collaborators have developed a new efficient high-order discretization for singular and hypersingular integrals. Quadrature by Expansion (QBX) [8], is a systematic, high-order approach to singular quadrature that applies to layer potential integrals on curves and surfaces whose kernels derive from linear PDE. Being based on a scheme for close evaluation due to Alex Barnett (Dartmouth College), the scheme also provides evaluation of potentials close to the source layer. The scheme is makes use of the assumption that the field induced by the layer potential operator is locally smooth when restricted to either the interior or the exterior. Discontinuities in the field across the boundary are permitted.

QBX is straightforward to implement and applicable to most practically relevant kernels in two and three dimensions. It is compatible with fast hierarchical methods for potential computation, such as the Fast Multipole Method. It provides a simple convergence theory. Open research questions surrounding QBX include adaptivity, a black-box implementation with fast solvers as well as their application for huge problems, the treatment of edges and corners, and a precise quantitative theory of the spectral behavior of layer potential operators discretized by QBX.

PANEL BASED METHODS: Johan Helsing (Lund University, Sweden) and his collaborators have developed a Nyström discretization scheme for boundary integral equations containing singular integral operators [4]. The scheme is panel based and applies to integral equations in the plane. Its advantages compared to competing panel-based schemes include higher-order convergence (16th order), higher achievable accuracy (close to machine precision not just for the integral equation itself but also for fields in the entire computational domain when the underlying mathematical problem is well conditioned), and smaller error constant (the convergence sets in earlier).

SOME OTHER RECENT DEVELOPMENTS: Bradley Alpert (National Institute of Standards and Technology) presented a talk titled "Efficiency-Enhanced Hybrid Gauss-Trapezoidal Quadrature Rules," in which he discussed a new quadrature method that extends his quadrature rules developed several years ago [1] that are in use by several groups. Those quadratures enable accurate integration of singularities present in a variety integral equation problems. The new quadratures, also a form of endpoint-corrected rules, are tailored for uniformly high accuracy.

Zydrunas Gimbutas (National Institute of Standards and Technology) presented a talk titled "Interpolation and Integration in Spaces of Singular Functions". This talk emphasized the need to develop numerical schemes for simultaneous interpolation and integration of singular functions. The interpolative decomposition is used to determine the initial interpolation nodes and the appropriate basis functions are then determined in the least-squares sense. The new scheme is expected to be used in the context of axisymmetric solvers for the Helmholtz equation in three dimensions.

3.2 Fast Algorithms

Three talks were given discussing a broad range of fast algorithms. Gregory Beylkin (The University of Colorado) presented new algorithms for solving equations using nonlinear approximations. These algorithms are designed specifically to optimize representation of solutions via exponentials or Gaussians, the basic components in the construction. His talk described relevant algorithms for optimization and the progress in solving equations of quantum chemistry via this new approach.

Bryan Quaife (The University of Texas at Austin) discussed FMM-based Preconditioners for Second Kind Integral Equations. He proposed a new class of preconditioners using an FMM-based spatial decomposition of the double-layer potential. He demonstrated mesh-independence for two-dimensional geometries whose curvature ranges over several orders of magnitude.

Anna-Karin Tornberg (Royal Institute of Technology, Sweden) presented work on the the Spectral Ewald (SE) method, a spectrally accurate fast FFT-based summation method that has been developed for electrostatics[10] and Stokes flow[9]. For electrostatics, the SE method has been implemented within GROMACS, a widely used molecular dynamics simulation tool. Comparisons to the state-of-the art- electrostatic methods SPME and P3M that are available within GROMACS were presented. The framework for deriving so called Ewald summation formulas and the design of the SE method for different kernels and different assumptions on periodicity was also discussed.

3.3 Fast Direct Solvers

An area of research that is currently seeing very rapid progress concerns the development of ”direct” (as opposed to ”iterative”) solvers for the large systems of linear equations that arise upon the discretization of linear elliptic equations such as, e.g., the Laplace and Helmholtz equations. Over the last several years, a number of researchers have shown that an approximation to the inverse of an $N \times N$ coefficient matrix can often be computed in optimal $O(N)$ time. This is a remarkable development that is likely to have a profound impact on scientific computation. During the workshop, several talks described new and exciting approaches for how such $O(N)$ inversion schemes can be built. Denis Zorin (Courant Institute, New York University) described a technique with strict $O(N)$ complexity designed for integral equations in two and three dimensions; Eric Michielssen (The University of Michigan) described a new scheme that attains $O(N)$ complexity for certain wave problems that had previously been considered outside of reach for direct solvers of this kind; Eric Darve (Stanford University) described an innovative and simplified approach with a broad range of applicability; Kenneth Ho (Stanford University) described an easy-to-implement scheme with applications to both the sparse systems arising upon finite difference discretizations, and to the dense systems associated with integral equations formulations.

3.4 Wave Applications

It became readily apparent during the workshop that fast direct solvers are making exciting advances, especially on the issue of recompression to retain low ranks for 2D surfaces or 3D volume integrals. Several approaches were presented for this. The applications for which they have been implemented are still few, but their potential for problems with multiple right-hand sides is huge, once they become more mature. With three or four groups giving presentations on this, the audience was brought completely up to date (the talks being, as usual, many months more advanced than the preprints).

A wide variety of talks were presented demonstrating that integral equation approaches to wave scattering have continued to make advances, particularly in: quadrature and eigenvalue problems (Johan Helsing), almost-periodic problems (Naoshi Nishimura, Kyoto University), fast-direct solvers (Eric Michielssen, The University of Michigan and Zhen Peng, The University of New Mexico), variable media (Alex Barnett and Adrianna Gillman, Dartmouth College), and software development[11] (Timo Betcke, University College London).

A show-stopper for the week was Eric Michielssen’s new work on using butterfly compression [3] in a fast direct solver for high-frequency electromagnetic scattering, computing 10^4 incident angles from a complex object (an aircraft) around 10^2 wavelengths in size, in around 1 day of CPU time, an unprecedented calculation. Many of the workshop participants became inspired to devote more time to this class of algorithms and to understand why Michielssen’s butterfly fast direct solver works as well as it does. Rigorous analysis for this algorithm remains an open problem.

3.5 Fluids and Other Applications

FIEMs have long provided valuable tools for investigating phenomena which can be modelled by linear equations. These include low-Reynolds-number hydrodynamics, elasto- and electrostatics. There were two talks given on this subject, presenting both state-of-the-art, large-scale calculations and addressing important outstanding technical issues. George Biros (The University of Texas at Austin) presented simulations involving $O(10^7)$ deformable vesicles and discussed recent work on high-order, adaptive, highly stable time-stepping methods as well as near singular integration techniques for dealing with near-collisions [12]. In addition, he discussed a distributed memory fast multipole method for evaluating the volume potentials of the Poisson, low-wave-number Helmholtz and Stokes operators. The performance of these algorithms is truly impressive. They achieve about 530 GFlop/s of double precision performance on a single node on the Stampede platform at the Texas Advanced Computing Center. A problem with 18 *billion* unknowns can be solved in 4.7s on 1024 compute nodes. Dr. Biros also presented a very interesting comparison of parallel versions of the FMM, FFT and high-order multigrid. Using the Poisson problem as a test case, he showed that for non-uniform right hand sides, the FMM is far superior than the other two methods, achieving a factor of 10 speed up over the closest competitor; solutions to problems with a billion unknowns can be computed in a mere second.

Rikard Ojala (Royal Institute of Technology) discussed moving interfaces and free boundaries in two dimensional Stokes flow, where the flow is due to surface tension. A long-standing difficulty in both two and three dimensions is how to deal with interfaces that are close to each other. In this case, the integral kernels are near-singular, and standard quadrature approaches do not give accurate results. Phenomena such as lubrication are then not captured correctly. Dr. Ojala discussed how to apply a general special quadrature approach to resolve this problem.

Manas Rachh (Courant Institute, New York University) discussed a second kind integral formulation for applying the elastance matrix. Existing integral equation formulations for the elastance problem involve solving a modified Dirichlet problem. This results in a system that can be ill-conditioned when the number of boundary components becomes large. This new integral equation formulation involves a Neumann problem, which eliminates this ill-conditioning.

There were two talks discussing Poisson-Boltzmann solvers. Jingfang Huang (The University of North Carolina) summarized the mathematical and numerical theories and implementation details of the Adaptive Fast Multipole Poisson-Boltzmann (AFMPB) solver, including the Poisson-Boltzmann model, boundary integral equation reformulation, surface mesh generation, node-patch discretization, Krylov iterative methods, new version of the fast multipole methods (FMMs), and parallelization on multicore computers. Robert Krasny (The University of Michigan) presented a treecode-accelerated boundary integral (TABI) solver for electrostatics of solvated proteins described by the linear Poisson-Boltzmann equation. The TABI solver exhibits good serial and parallel performance combined with relatively simple implementation, efficient memory usage, and geometric adaptability.

4 Scientific Progress and Outcome of the Meeting

The FIEM research community is a relatively small one, with many of its researchers being geographically isolated. The BIRS workshop was invaluable for keeping this community connected and fostering new collaborations and research directions. This workshop served to foster important cross-pollination (and sometimes heated discussions!) between the US and European groups. These continents have very different styles of algorithm and philosophy, and both learned from the other.

There were many important discussions that occurred during the unstructured sessions of the workshop. These informal discussions were invaluable in identifying important new open problems, generating ideas and fostering interactions between senior and junior researchers. Below is a description of a few of these discussions:

- The importance of having impromptu blackboard discussions/lectures with Vladimir Rokhlin (Yale University) was huge. For all participants, getting Rokhlin's take on ideas, or having him explain a few of his pet projects in person, was felt to be inspirational.

- An important open problem, which was discussed during the workshop, was how to evaluate toroidal harmonics in a fast and reliable way. Toroidal harmonics arise when elliptic PDEs on axisymmetric domains are modeled with integral equations and solved using Fourier-Nyström discretization.

- An ongoing concern in the field of high-order efficient quadratures is the lack of well defined test problems. Bradley Alpert and Johan Helsing discussed establishing a collection of test problems, hosted by NIST. This would facilitate the comparison of new quadrature schemes.

- The quadrature presentations led to numerous follow-up conversations and inquiries. The possibilities for a suite of test problems for integral equation solvers was discussed. Issues include (1) Balance between engaging broadest community of researchers and challenging the most sophisticated algorithms; (2) Balance between simplicity and breadth of coverage of numerical challenges; (3) Include geometric complexities such as sharp corners, near adjacency, and other features? Priorities, key challenges, and likely avenues for progress, for quadrature methods for integral equations on surfaces in three dimensions were also discussed.

The workshop also served to re-energize researchers with new research directions and collaborations. One participant said "I believe everyone at the conference was able to incorporate at least one new method into their current codes". Below are a few concrete examples of how the workshop impacted participants:

- Mike O'Neil learned from interactions with Johan Helsing about partial-explicit kernel-split quadrature rules for axisymmetric Helmholtz problems, and will use them in his research. About this Helsing says, "Mike O'Neil wanted programs that demonstrate how my weight corrections and compensation weights (for logarithmic and Cauchy-type singular kernels) work in practice. I sent him codes just a couple of days ago. This exchange of ideas would probably not have happened without the Banff workshop."
- Helsing has acknowledged BIRS in helping the completion of his recent paper [5]. This was due to questions he got after his talk, and interactions with Barnett.
- Kropinski connected with Helsing and Ojala on their method for solving Laplace's equation with mixed boundary conditions. She has plans on using there methods to study Steklov eigenvalue problems using FIEMs.
- Because of the meeting, Nishimura has started to use fast direct solvers for his problems in almost-periodic media, and to deal with Wood anomalies (after discussion with Barnett).
- Robert Krasny discussed comparing his results with Timo Betcke's BEM++ code
- Jiang, Quaife and Kropinski plan to collaborate with Ho in order to accelerate their integral equation solver for the modified biharmonic equation [7]. This is a critical component to develop FIEM for solving the two dimensional Navier Stokes equations.
- Eric Darve will be writing a book on hierarchical methods and fast algorithms this coming Winter, with Kenneth Ho as a co-author. The workshop was instrumental in recruiting Ho for this work.

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