

# Integral Equations Methods: Fast Algorithms and Applications

Dec. 8 – 13, 2013

## MEALS

\*Breakfast (Buffet): 7:00–9:30 am, Sally Borden Building, Monday–Friday

\*Lunch (Buffet): 11:30 am–1:30 pm, Sally Borden Building, Monday–Friday

\*Dinner (Buffet): 5:30–7:30 pm, Sally Borden Building, Sunday–Thursday

Coffee Breaks: As per daily schedule, in the foyer of the TransCanada Pipeline Pavilion (TCPL)

**\*Please remember to scan your meal card at the host/hostess station in the dining room for each meal.**

## MEETING ROOMS

All lectures will be held in the lecture theater in the TransCanada Pipelines Pavilion (TCPL). An LCD projector, a laptop, a document camera, and blackboards are available for presentations.

## SCHEDULE

You are welcome to schedule lectures as you see fit, as long as you adhere to the meal times (noted above), coffee break start and end times (noted below) and take into account the "welcome" on Monday morning, the Banff Centre tour at 1:00 pm, and the group photo at 2:00 pm every Monday afternoon.

Please email your finalized schedule and abstracts to BIRS Station Manager [birmsmgr@birs.ca](mailto:birmsmgr@birs.ca) by Thursday morning before your arrival (at the latest) in order to allow for printing and posting to the website.

You are also encouraged to e-mail the schedule to your participants. BIRS provides the option of an electronic mail list in order to facilitate communications with your participants. When you login to the Organizer Interface at <https://www.birs.ca/orgs>, you will be prompted to create an electronic mail list for your workshop. Click "Yes" to create one and receive instructions, or "No" to decline. If you would like more information about our electronic mail lists, please e-mail [help@birs.ca](mailto:help@birs.ca).

### Sunday

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<b>16:00</b>	Check-in begins (Front Desk - Professional Development Centre - open 24 hours)
<b>17:30–19:30</b>	Buffet Dinner, Sally Borden Building
<b>20:00</b>	Informal gathering in 2nd floor lounge, Corbett Hall Beverages and a small assortment of snacks are available on a cash honour system.

## Monday

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<b>7:00–8:45</b>	Breakfast
<b>8:45–9:00</b>	Introduction and Welcome by BIRS Station Manager, TCPL
<b>9:00–12:00</b>	<b>Session: Quadrature</b>
9:00–9:30	Bradley Alpert Efficiency-Enhanced Hybrid Gauss-Trapezoidal Quadrature Rules
9:30–10:00	Johan Helsing A high-order panel-based explicit-split Nystrom scheme for the discretization of singular integral equations and for near field evaluation
10:00–10:30	Coffee Break, TCPL
10:30–11:00	Andreas Kloeckner Fast Algorithms for the Evaluation of Layer Potentials using “Quadrature by Expansion”
11:00–11:30	Zydrunas Gimbutas Interpolation and integration in spaces of singular functions
<b>11:30–13:00</b>	Lunch
<b>13:00–14:00</b>	Guided Tour of The Banff Centre; meet in the 2nd floor lounge, Corbett Hall
<b>14:00</b>	Group Photo; meet in foyer of TCPL (photograph will be taken outdoors so a jacket might be required).
<b>14:30–15:30</b>	Coffee Break, TCPL
<b>15:30–17:00</b>	<b>Session: Fast Algorithms</b>
15:30–16:00	Gregory Beylkin Solving equations using nonlinear approximations
16:00–16:30	Anna-Karin Tornberg The Spectral Ewald method
16:30–17:00	Break
17:00–17:30	Bryan Quaife FMM-based Preconditioners for Second Kind Integral Equations
17:30–18:00	Adrianna Gillman A high-order accurate direct solution technique for acoustic scattering problems in 3D
<b>18:00–19:30</b>	Dinner

## Tuesday

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<b>7:00–9:00</b>	Breakfast
<b>9:00–12:00</b>	<b>Session: Fast Direct Solvers</b>
9:00–9:30	Denis Zorin An $O(N)$ Direct Solver for Integral Equations
9:30–10:00	Eric Michielssen Butterfly/MLMDA-based Direct Solvers
10:00–10:30	Coffee Break, TCPL
10:30–11:00	Eric Darve Fast algorithms for dense linear algebra
11:00–11:30	Kenneth Ho Hierarchical interpolative factorization for integral operators
<b>11:30–13:30</b>	Lunch
<b>14:30–15:30</b>	Coffee Break/Posters, TCPL
<b>15:30–18:00</b>	<b>Session: Wave Applications</b>
15:30–16:00	Alexander Barnett Spectrally accurate direct solution of variable-media scattering problems via impedance maps
16:00–16:30	Naoshi Nishimura Solution of scattering problems for Helmholtz' equation in domains with disturbed periodicity
16:30–17:00	break
17:00–17:30	Timo Betcke The BEM++ boundary element library: Design and applications
17:30–18:00	Zhen Peng Integral Equation Domain Decomposition with Discontinuous Galerkin Discretization for Time-Harmonic Maxwell Equations
<b>18:00–19:30</b>	Dinner

## Wednesday

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<b>7:00–9:00</b>	Breakfast
<b>9:00–12:00</b>	<b>Session: Wave Applications, Continued</b>
9:00–9:30	Charles Epstein The Debye Source Representation for the Beltrami Equation
9:30–10:00	Mike O'Neil An integral equation approach for the numerical calculation of Beltrami (force-free) fields
10:00–10:30	Andrew Christlieb
10:30–14:30	Informal Discussion A High Order A-Stable Wave Propagation Method
<b>11:30–13:30</b>	Lunch
<b>14:30–15:30</b>	Coffee Break, TCPL
<b>15:30–17:00</b>	<b>Session: Fluid Applications</b>
15:30–16:00	George Biros Fast integral equation algorithms for particulate flows
16:00–16:30	Rikard Ojala Accurate bubble and drop simulations in 2D Stokes flow
16:30–17:00	Manas Rachh New integral equation methods for mobility and capacitance problems in elasto- and electrostatics
<b>17:30–19:30</b>	Dinner

## Thursday

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<b>7:00–9:00</b>	Breakfast
<b>9:00 - 16:00</b>	Informal discussion, possibly skiing or exploring Banff Lectures
<b>11:30–13:30</b>	Lunch
<b>14:30–15:30</b>	Coffee Break, TCPL
<b>16:00–17:30</b>	<b>Session: Other Applications</b>
16:00–16:30	Ming Gu Subspace Iteration Randomization and Singular Value Problems
16:30–17:00	Robert Krasny A Treecode-Accelerated Boundary Integral Poisson-Boltzmann Solver for Solvated Proteins
17:00–17:30	Jingfang Huang Mathematical and Numerical Aspects of the Adaptive Fast Multipole Poisson-Boltzmann Solver
<b>18:00–19:30</b>	Dinner

## Friday

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<b>7:00–9:00</b>	Breakfast
<b>9:00</b>	Informal Discussions
10:00–11:00	Coffee Break, TCPL
<b>11:30–13:30</b>	Lunch
<b>Checkout by 12 noon.</b>	

\*\* 5-day workshop participants are welcome to use BIRS facilities (BIRS Coffee Lounge, TCPL and Reading Room) until 3 pm on Friday, although participants are still required to checkout of the guest rooms by 12 noon. \*\*

# Integral Equations Methods: Fast Algorithms and Applications

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## ABSTRACTS

Speaker: **Bradley Alpert**

Title: *Efficiency-Enhanced Hybrid Gauss-Trapezoidal Quadrature Rules*

Abstract: Several years ago quadrature rules for smooth functions and functions with algebraic or logarithmic singularities were introduced and have since been employed successfully by several groups in the solution of integral equations on closed curves. These rules, like essentially all methods designed for high order convergence, deliver accuracy that depends strongly on the effective bandlimit of the integrand.

Here we introduce new quadrature rules, targeting the same function classes, but tailored for uniformly high accuracy from low frequency up through a bandlimit proportional to the number of quadrature nodes. The effect is significantly enhanced efficiency, so that fewer points to approximate an integral, and fewer unknowns to solve an integral equation, are generally needed to achieve a prescribed accuracy. We present the formulation, implementation, and performance of these rules.

Speaker: **Alexander Barnett**

Title: *Spectrally accurate direct solution of variable-media scattering problems via impedance maps.*

Abstract: Time-harmonic scattering from a bounded 2D region in which the wave speed varies smoothly in space has applications including ultrasound imaging, underwater acoustics, and quantum mechanics. We present an algorithm which constructs the interior Dirichlet-to-Neumann (DtN) map for the region by bottom-up recursive merges of impedance-to-impedance (ItI) maps on a quadtree of boxes. These ItI maps are approximated on the smallest (leaf) boxes via spectral collocation. Since the ItI map is unitary the method is robust (immune to interior resonances). We couple the DtN and the radiation condition on the boundary of the region to get a 2nd kind integral equation. Thus problems 100 wavelengths in size can be solved to 9 digit accuracy in a few minutes on a workstation; each new incident wave requires a fraction of second per solve. Joint work with Adrianna Gillman and Gunnar Martinsson.

Speaker: **Timo Betcke**

Title: *The BEM++ boundary element library: Design and applications*

Abstract: BEM++ ([www.bempp.org](http://www.bempp.org)) is an ongoing project to develop an open-source, versatile Galerkin boundary element library for a range of applications in electrostatics, acoustics, and computational electromagnetics. The core of the library is developed in C++, with almost all functions accessible from a simple to use Python interface. The library makes use of H-Matrix acceleration and preconditioners. FMM support is in development. Systems of boundary integral equations are naturally supported, and C++ and Python interfaces to Trilinos provide a range of iterative solver options. In this talk we will give an overview of the library by demonstrating the solution of several relevant and interesting application problems, covering acoustics, electromagnetics, diffuse optics, and time-domain problems.

Speaker: **Gregory Beylkin**

Title: *Solving equations using nonlinear approximations*

Abstract: A typical approach to solving partial differential or integral equations is to approximate their solution via a fixed (perhaps, an adaptive) basis and then find the coefficients of the representation. Nonlinear approximations assume that the solution can be efficiently expressed via a linear combination of functions chosen from a set much larger than a basis. We then seek an optimal (or near optimal) representation of the solution in this form satisfying the underlying equations. While there are some advantages in using nonlinear approximations in low dimensions, the need to switch away from the usual representations via bases (or via sampling) becomes clear when considering equations in high dimensions. A fixed basis

approach leads to an exponential growth of computational complexity with the increase of dimensionality whereas nonlinear approximations offer a path to avoid the so-called "curse of dimensionality". The difficulty now shifts to constructing stable numerical algorithms for optimizing representations of solutions in the process of solving the underlying equations. Perhaps the first attempt to use nonlinear approximations was in quantum chemistry and originates in the seminal papers of Boys, Longstaff and Singer (1960). The authors used linear combinations of Gaussians whose exponents and coefficients were optimized (in the process of constructing solutions) via Newton's method. Unfortunately, such approach turned out to be practical only for very small molecules. Consequently, construction of spatial orbitals has been traditionally performed off-line and the resulting sets of functions used as a fixed basis. More recent multiresolution approaches (e.g., via multiwavelets), use a dynamically refined selection of basis functions to represent spatial orbitals. However, since the basis functions do not resemble the spatial orbitals, multiresolution methods require a relatively large number of parameters in the resulting representations. We have developed an approach similar (in spirit) to the original papers (already mentioned) but using a completely different type of algorithms. These algorithms are designed specifically to optimize representations via exponentials or Gaussians, the basic components in the construction. The talk will describe relevant algorithms for optimization and the progress in solving equations of quantum chemistry via the new approach.

Speaker: **George Biros**

Title: *Fast integral equation algorithms for particulate flows*

Abstract: In this talk I will present recent work on algorithms for simulation of particulate flows: (1) implicit solvers and adaptive time stepping for accurate simulations, (2) preconditioners for the related integral equations, (3) spatial adaptivity, and (4) coarse scaling. This is joint work with Bryan Quaife and Dhairya Malhotra.

Speaker: **Andrew Christlieb**

Title: *A High Order A-Stable Wave Propagation Method*

Abstract: The goal of this work is the development of a low storage implicit Maxwell solver for application to problems in plasma physics. The key issue motivating this work is the vast scale separation in temporal scales in these problems. The two common approaches are sub-cycling and the introduction of implicit methods. The problem with sub-cycling is the time and loss of accuracy do to hundreds of EM solves per single time step of the plasma species whereas the issue with implicit solvers is the time associated with inversion of the matrix.

In recent work, we developed a new A-stable approach to wave propagation problems based on the Method of Lines Transpose (MOL<sup>T</sup>) formulation combined with alternating direction implicit (ADI) schemes. Because our method is based on an integral solution of the ADI splitting of the MOL<sup>T</sup> formulation, we are able to easily embed non-Cartesian boundaries and include point sources with high accuracy. Further, we developed an efficient  $O(N)$  convolution algorithm for rapid evaluation of the kernels. We have demonstrated the utility of this method by applying it to a range of problems with complex geometry, including cavities with cusps.

However, one of the well-known drawbacks of ADI methods is the high degree of dispersion that they introduce. Furthermore, the Dahlquist barrier is a well-known theorem which prevents the construction of a scheme of order higher than 2, which remains unconditionally stable. We note that this barrier can be removed if the scheme is not a linear multistep scheme.

In this work, we present several important modifications to our recently developed wave solver. We obtain a family of wave solvers which are unconditionally stable, accurate of order  $2P$ , and require  $O(NP)$  operations per time step, where  $N$  is the number of spatial points. We obtain these schemes by including higher derivatives of the solution, rather than increasing the number of time levels, thus removing the Dahlquist barrier. The novel aspect of our approach is that the higher derivatives are constructed using successive applications of the convolution operator, which does not formally change the size of the stencil. One way to view this method is to consider it through the lens of defect correction, as with each application of the convolution kernel, we are eliminating the next highest error term.

We develop these schemes in one spatial dimension, and then extend the results to higher dimensions, by reformulating the ADI scheme to include recursive convolution. Thus, we retain a fast, unconditionally stable scheme, which does not suffer from the large dispersion errors characteristic to the ADI method. We demonstrate the utility of the method by applying it to a host of wave propagation problems. In our future work we plan to combine these methods with mesh based and particle based Vlasov solvers. Co-Authers: Matt Causley, Yaman Guclu, Eric Wolf

Speaker: **Eric Darve**

Title: *Fast algorithms for dense linear algebra*

Abstract: We will be presenting novel algorithms to solve dense linear systems  $Ax = b$  in  $O(N)$  floating point operations for matrices  $A$  of size  $N \times N$ . Such matrices arise in the context of integral equation methods. The new algorithms have the potential to replace classical iterative solvers, such as GMRES and Conjugate Gradient methods. Their computational cost is competitive and scales linearly with the problem size. In addition, being based on direct LU factorization, they do not require preconditioners, which are hard to derive in some cases. This work is based on hierarchical matrices ( $H$  and  $H^2$ ) and relies on the low-rank structure of various sub-blocks in the matrix, for its acceleration.

Speaker: **Charles Epstein**

Title: *The Debye Source Representation for the Beltrami Equation*

Abstract: Epstein and Greengard recently introduced a new representation, called the Debye Source Representation, for solutions of the time harmonic Maxwell Equations (THME[k]) with very good analytic and numerical attributes. We show that the space of solutions to the THME[k] has a natural complex structure. The eigenspaces are solutions to the Beltrami equations:  $\text{curl } E = \pm kE$ . The Debye representation uniformizes this complex, which leads to an effective numerical method for solving the Beltrami equation. This work is joint with Leslie Greengard and Michael O'Neil.

Speaker: **Adrianna Gillman**

Title: *A high-order accurate direct solution technique for acoustic scattering problems in 3D*

Abstract: This talk will describe an accelerated direct solver for the integral equations that model acoustic scattering in 3D. For many problems of interest, iterative methods require thousands of iterations to converge. As an alternative, we couple a high-order Nystrom discretization with a robust direct solver which is resistant to the issues that plague iterative schemes. The result is a hierarchically constructed scattering matrix that is (frequently) much smaller than the original system and achieves high accuracy. Often the method attains  $O(N^{1.5})$  complexity where  $N$  is the number of discretization points. Numerical results will illustrate the performance of the method. This is a joint work with James Bremer and Per-Gunnar Martinsson.

Speaker: **Zydrunas Gimbutas**

Title: *Interpolation and integration in spaces of singular functions*

Abstract: In this talk, we present a simple scheme for the stable interpolation and integration in spaces of singular functions in one and higher dimensions. 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 obtained interpolation nodes can be further post-processed to yield Gaussian-like quadrature rules. The scheme can be viewed as a generalization of the Lagrange interpolation formula for singular functions in one and higher dimensions. We illustrate the performance of the approach with several numerical examples. This is joint work with Vladimir Rokhlin.

Speaker: **Johan Helsing**

Title: *A high-order panel-based explicit-split Nystrom scheme for the discretization of singular integral equations and for near field evaluation.*

Abstract: I discuss how to implement a high-order accurate panel-based partially explicit-split Nystrom

quadrature scheme for the discretization of singular integral equations on curves in the plane. Accurate evaluation of potential fields close to the boundaries where their sources are situated is also discussed. I show examples for integral equations associated with axisymmetric interior Helmholtz problems. This involves integral operators with both logarithmically-singular and Cauchy-singular parts. The relative accuracy in plots of resonant fields is, typically, 14-15 digits everywhere in the computational domain.

Speaker: **Kenneth Ho**

Title: *Hierarchical interpolative factorization for integral operators*

Abstract: We present some recent results on the efficient factorization of matrices associated with non-oscillatory integral operators in 2D and 3D. In contrast to the 1D case, such matrices exhibit considerable rank growth in their off-diagonal blocks when compressed using standard hierarchical schemes. We combat this with explicit dimensional reductions via geometric reclustering and additional compression. The resulting ranks are much better behaved, yielding essentially linear costs to construct, apply, and invert the factorization. Our method is fully adaptive and can handle both boundary and volume problems. This is joint work with Lexing Ying.

Speaker: **Jingfang Huang**

Title: *Mathematical and Numerical Aspects of the Adaptive Fast Multipole Poisson-Boltzmann Solver*

Abstract: This talk summarizes 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. Possible strategies to further improve the efficiency, accuracy and applicability of the AFMPB solver to large-scale long-time molecular dynamics simulations are discussed, and numerical results are presented to demonstrate the potential of the solver.

Speaker: **Andreas Kloeckner**

Title: *Fast Algorithms for the Evaluation of Layer Potentials using ‘Quadrature by Expansion’*

Abstract: Quadrature by Expansion, or ‘QBX’, is a systematic, high-order approach to singular quadrature that applies to layer potential integrals with general kernels on curves and surfaces. Being based on a scheme for close evaluation due to Barnett, the scheme provides a unified evaluation capability for layer potentials. This talk discusses algorithmic options for using QBX within a variant of the Fast Multipole Method. A method is presented that preserves accuracy, generality and close evaluation capability while only requiring a relatively modest increase in computational cost in comparison to a point-to-point FMM. In addition, an optionally GPU-accelerated set of open-source software libraries is discussed that implements the proposed method.

Speaker: **Robert Krasny**

Title: *A Treecode-Accelerated Boundary Integral Poisson-Boltzmann Solver for Solvated Proteins*

Abstract: We present a treecode-accelerated boundary integral (TABI) solver for electrostatics of solvated proteins described by the linear Poisson-Boltzmann equation. The method uses a well-conditioned boundary integral formulation for the electrostatic potential and its normal derivative on the molecular surface. The surface is triangulated by MSMS and the integral equations are discretized by centroid collocation. The linear system is solved by GMRES and the matrix-vector product is carried out by a Cartesian treecode which reduces the cost from  $O(N^2)$  to  $O(N \log N)$ , where  $N$  is the number of faces in the triangulation. The code is applied to two test cases, the Kirkwood sphere and a medium sized protein. We compare TABI results with those obtained using the grid-based APBS code, in terms of error, CPU run time, and memory usage, and we also present parallel TABI simulations. The TABI solver exhibits good serial and parallel performance combined with relatively simple implementation, efficient memory usage, and geometric adaptability. This is joint work with Weihua Geng (Southern Methodist University).

Speaker: **Eric Michielssen**

Title: *Butterfly/MLMDA-based Direct Solvers*

Abstract: We have demonstrated a new direct integral equation solver for high-frequency electromagnetic analysis that derives from butterfly/multilevel matrix decomposition algorithm (MLMDA) compression schemes. Current direct solvers all leverage H-matrix techniques, that is, they exploit the low-rank nature of blocks of inverse matrices discretizing integral operators. Unfortunately, this low-rank property only manifests for (i) electrically small, (ii) volumetric, (iii) and elongated/quasi-planar scatterers. That is, direct solvers that leverage low-rank notions fail when applied to high-frequency analysis of electromagnetic scattering from arbitrarily shaped surfaces. The new butterfly/MLMDA solver remedies this situation.

The new direct integral equation solver utilizes MLMDA/butterfly schemes for compressing the LU factors of MoM matrices. The solver has three important features of note. (i) The solver bypasses all low rank compression steps of its predecessor (G. Han, H. Jun, and E. Michielssen, "On MLMDA/Butterfly compressibility of inverse integral operators," IEEE Antennas and Wireless Propagation Letters, vol. 12, pp. 31-34., 2013) and operates directly on butterfly-compressed blocks. The latter is achieved using new randomized schemes for rapidly adding and multiplying butterfly-compressed operators. (ii) The solver executes in parallel, using a hybrid OpenMP-MPI strategy to accelerate the hierarchical inverse/decomposition of the MoM matrix. Despite the inherently sequential nature of this operation, the solver exhibits excellent scaling properties up to several hundred processors. (iii) The solver applies to large-scale 3D analysis and was implemented to invert a combined field (as opposed to a simple electric field) integral operator.

The solver has been shown capable of inverting integral equation matrices that discretize combined field integral equations modeling scattering from electrically large structures involving 15 million unknown on a small cluster using just a few hours of CPU time. For problems of this size, the back substitution time, i.e. the solve time per right hand side following the LU decomposition is roughly 30 seconds, far smaller than the time required by iterative fast multipole solvers.

We note that while proven very effective, the compressibility of blocks of LU factors of matrices discretizing high-frequency integral operators via Butterfly/MLMDA schemes remains an experimental observation. Current research is aimed at developing a theoretical framework that fully justifies the use of this approach.

Speaker: **Naoshi Nishimura**

Title: *Solution of scattering problems for Helmholtz' equation in domains with disturbed periodicity*

Abstract: In engineering one sometimes has to deal with objects in which some components are missing in otherwise completely periodic structures. We are interested in the wave scattering by this type of structures having disturbed periodicity. This talk presents a fast method of solution for scattering problems associated with such structures for Helmholtz' equation in 2D. The solution process of this problem using the Floquet transform requires the evaluation of an integral whose integrand depends on solutions of certain periodic boundary value problems. We apply a periodic version of fast multipole method to compute this integrand which, however, may vary very quickly or may have singularities due to the presence of the resonance anomalies. We propose to use Sakurai-Sugiura projection method, which is one of solvers for nonlinear eigenvalue problems, to locate these anomalies. We also propose effective ways to accelerate the convergence of certain equations to be solved on the boundaries of missing scatterers. With J. Morita, Graduate School of Informatics, Kyoto University, Japan

Speaker: **Rikard Ojala**

Title: *Accurate bubble and drop simulations in 2D Stokes flow*

Abstract: This talk will be on moving interfaces and free boundaries in two dimensional Stokes flow, where the flow is due to surface tension. For such flows in the Stokesian regime, with small Reynolds numbers, the resulting linear governing equations can be recast as an integral equation. This is a well-known and widely used fact. What is frequently overlooked, however, 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. We will discuss how to apply a general special quadrature approach to resolve this problem. The result is a robust and

accurate solver capable of handling a wide range of bubble and drop configurations. An example of a fairly complex drop setup that can be treated is displayed below.

Speaker: **Mike O’Neil**

Title: *An integral equation approach for the numerical calculation of Beltrami (force-free) fields*

Abstract: Beltrami (force-free) fields are those vector fields which are proportional to their own curl:  $\text{curl}(\mathbf{B}) = k\mathbf{B}$ , with "k" a scalar. Beltrami fields arise in several different areas of applied mathematics and physics. For example, in fluid dynamics, Beltrami flows are those flows whose velocity and vorticity are parallel. In plasma physics, magnetic Beltrami fields inside a confinement device at equilibrium arise via Lorentz force balancing. In this talk, I will describe recently developed integral equation methods for calculating Beltrami fields, paying special attention to axially-symmetric geometries (with problems in plasma physics in mind). By viewing Beltrami fields as special-case time-harmonic Maxwell fields (with wavenumber "k"), their calculation can be reduced to a boundary integral equation similar to those found in electromagnetics. Using the previously introduced generalized Debye source formulation of electromagnetic fields, robust representations of Beltrami fields and well-conditioned integral equations are immediate consequences.

Speaker: **Zhen Peng**

Title: *Integral Equation Domain Decomposition with Discontinuous Galerkin Discretization for Time-Harmonic Maxwell Equations*

Abstract: Surface integral equation (SIE) methods have shown to be effective in solving electromagnetic wave scattering and radiation problems. It is mainly due to the fact both the analysis and unknowns reside only on the boundary surfaces of the targets. However, applications of the SIE methods often lead to dense and ill-conditioned matrix equations. The efficient and robust solution of the SIE matrix equation poses an immense challenge. This talk will discuss some recent progress in SIE methods for solving time-harmonic Maxwell equations. The first topic is domain decomposition for surface integral equations via multi-trace formulation. The entire computational domain is decomposed into a number of non-overlapping sub-regions. Each local sub-region is homogeneous with constant material properties and described by a closed surface. Through this decomposition, we have introduced at least two pairs of trace data as unknowns on interfaces between sub-regions (multi-trace formulation). This multi-trace feature admits two major benefits: the localized surface integral equation for the homogeneous sub-region problem is amenable to operator preconditioning; the resulting linear systems of equations readily lend themselves to optimized Schwarz methods. A discontinuous Galerkin surface integral equation method is proposed for the numerical solution of sub-regions. The main objective of this work is to allow the implementation of the combined field integral equation (CFIE) using square-integrable,  $\mathbf{L}^2$ , trial and test functions without any considerations of continuity requirements across element boundaries. Due to the local characteristics of  $\mathbf{L}^2$  vector functions, it is possible to employ non-conformal surface discretizations of the targets. Furthermore, it enables the possibility to mix different types of elements and employ different order of basis functions within the same discretization. Therefore, the proposed method is highly flexible to apply adaptation techniques. The capability of these methods is illustrated through several real-world applications, including EMI/EMC analysis of multiple antennas installed on a high-definition mock-up aircraft, and electromagnetic scattering from a complex composite unmanned aerial vehicle.

Speaker: **Bryan Quaife**

Title: *FMM-based Preconditioners for Second Kind Integral Equations*

Abstract: The discretization of a second kind integral equation with a smooth boundary results in a linear system that can be solved with a mesh-independent number of GMRES iterations. However, when the geometry has regions of high curvature or other complications, the number of GMRES iterations does depend on the number of discretization points, N, until N is quite large. In many applications, such a cost is prohibitively expensive.

I will summarize different preconditioners (single-grid, multigrid, approximate sparse inverses) that have appeared in the literature. Then, I will propose a new class of preconditioners based on an FMM-

based spatial decomposition of the double-layer potential. I will demonstrate mesh-independence for two-dimensional geometries whose curvature ranges over several orders of magnitude. Possible extensions of this work include three dimensions and first-kind integral equations.

Speaker: **Manas Rachh**

Title: *New integral equation methods for mobility and capacitance problems in elasto- and electrostatics*

Abstract: The capacitance matrix in electrostatics relates the potentials of a given configuration of perfect conductors to the charges induced on them. The inverse of this matrix is called the elastance matrix. Existing integral equation formulations for the elastance problem involve solving a modified Dirichlet problem. This results in solving a bordered linear system with  $N + M$  unknowns where  $N$  is the number of discretization points and  $M$  is the number of boundary components (which can be ill-conditioned for large  $M$ ). Integral equation methods for computing grand mobility tensors for rigid bodies in a Stokesian fluid encounter similar issues. In this talk, we will describe a second kind integral formulation for applying the elastance matrix which involves a Neumann problem, eliminating the requirement for auxiliary unknowns. We extend this idea to the computation of the grand mobility tensor.

Speaker: **Anna-Karin Tornberg**

Title: *The Spectral Ewald method*

Abstract: The Spectral Ewald (SE) method is a spectrally accurate fast FFT based summation method that has been developed for electrostatics and Stokes flow. For electrostatics, we have implemented the SE method within GROMACS, a widely used molecular dynamics simulation tool, and we present comparisons to the state-of-the-art electrostatic methods SPME and P3M that are available within GROMACS. We also discuss the framework for deriving so called Ewald summation formulas and the design of the SE method for different kernels and different assumptions on periodicity.

Speaker: **Denis Zorin**

Title: *An  $O(N)$  Direct Solver for Integral Equations*

Abstract: An efficient direct solver for volume integral equations with  $O(N)$  complexity for a broad range of problems is presented. The solver relies on hierarchical compression of the discretized integral operator, and exploits that off-diagonal blocks of certain dense matrices have numerically low rank. Technically, the solver is inspired by previously developed direct solvers for integral equations based on "recursive skeletonization" and "Hierarchically Semi-Separable" (HSS) matrices, but it improves on the asymptotic complexity of existing solvers by incorporating an additional level of compression. The resulting solver has optimal  $O(N)$  complexity for all stages of the computation, as demonstrated by both theoretical analysis and numerical examples. The computational examples further display good practical performance in terms of both speed and memory usage. In particular, it is demonstrated that even problems involving  $10^7$  unknowns can be solved to precision  $10^{-10}$  using a simple Matlab implementation of the algorithm executed on a single core.

## POSTER ABSTRACTS

Speaker: **Amirhossein Aminfar**

Title: *A Fast Multifrontal Method for Finite Element*

Abstract: In this poster we first introduce the multifrontal method as the state of the art algorithm for solving sparse finite element matrices. Next, we give a brief overview of the two different approaches we took to arrive at fast block low-rank dense solvers, namely, fast dense solvers by factorization and fast dense solver by extended sparsification. Finally, we demonstrate how fast block-low-rank dense solvers can be used to accelerate the multifrontal solve process by considering the stiffness matrix for the heat equation in a turbine blade geometry. Joint with Eric Darve.

Speaker: **Travis Askham**

Title: *On the discretization of integral equations for divergence-form PDEs with internal layers*

Abstract: We investigate the behavior of integral formulations of variable coefficient elliptic partial differential equations (PDEs) in the presence of steep internal layers. In one dimension, the equations that arise can be solved analytically and the condition numbers estimated in various  $L_p$  norms. We show that high-order accurate Nyström discretization leads to well-conditioned finite dimensional linear systems if and only if the discretization is both norm-preserving in a correctly chosen  $L_p$  space and adaptively refined in the internal layer. Joint with Leslie Greengard.

Speaker: **Aditi Ghosh**

Title: *Fast Iterative Methods for The Variable Diffusion Coefficient Equation in a Unit Disk*

Abstract: Variable coefficient diffusion equation has widespread applications in many areas of Engineering and Industrial research like the flow in porous media and Tomography. We present here fast, iterative methods to solve this equation with applications to the Ginzburg Landau equation. Our technique is based on solution of Poisson and Helmholtz equation in a unit disc using fast FFT and recursive relations. The performance of this fast method is illustrated with some numerical examples. Joint with Prabir Daripa.