2014 CBMS-NSF Conference: Fast Direct Solvers for Elliptic PDEs
June 23-29, 2014 at Dartmouth College

Detailed week schedule

Time	**Monday**	**Tuesday**
7:00-9:00	Breakfast (Use meal card at 53 Commons if provided)	
9:00-10:00	Introduction to fast direct solvers for elliptic PDEs The classical Fast Multipole Method (Part I)	The Interpolative Decomposition (ID)
10:00-10:30	Break	
10:30-11:30	The classical Fast Multipole Method (Part II)	Brief introduction to structured matrix algebra. Randomized methods for low-rank approximation
11:30-1:30	Lunch (Use meal card at 53 Commons if provided)	
1:30-4:00	Coding session: Intro to quadrature and BIEs	Outdoor activity
4:00-5:00	Boundary integral equations for boundary value problems and their high-order Nyström quadratures by Alex Barnett	
5:00-6:30	Reception	Dinner (Use meal card at 53 Commons if provided)
6:30-8:00	Dinner (Use meal card at 53 Commons if provided)	

Time	**Wednesday**	**Thursday**
7:00-9:00	Breakfast (Use meal card at 53 Commons if provided)	
9:00-10:00	Fast direct solvers for sparse matrices (Part I)	Boundary Integral Equations - why and how
10:00-10:30	Break	
10:30-11:30	Fast direct solvers for sparse matrices (Part II)	Fast direct solvers for integral equations (Part I)
11:30-1:00	Lunch (Use meal card at 53 Commons if provided)	
1:00-4:00	Coding session.	
4:00-4:30	Tea in Kemeny 300	
4:30-5:30	The Hierarchical Poincare-Steklov scheme by Adrianna Gillman	Inverse Problems in MEG, EEG and Multi-Electrode Recording by Leslie Greengard
5:30-8:00	6:00-10:00 Banquet in DOC pond house	Dinner (Use meal card at 53 Commons if provided)

Time	**Friday**
7:00-9:00	Breakfast (Use meal card at 53 Commons if provided)
9:00-10:00	Fast direct solvers for integral equations (Part II)
10:00-10:30	Break
10:30-11:30	Review and future directions
11:30-1:30	Lunch (Use meal card at 53 Commons if provided)
1:30-2:30	Accelerating Numerical Algorithms of Linear Algebra by Vladimir Rokhlin
2:30-4:00	Lecturers available for questions, etc.

Comments: All lectures and coding sessions will be held in Kemeny 008. Unless otherwise stated please use your meal card (if provided) for dinner. Abstracts for afternoon lectures are provided on page 4.

Detailed weekend schedule

Time	Title	Speaker
Saturday (Kemeny 008)		
7:00-9:00	Breakfast (Use meal card at 53 Commons if provided)	
9:00-9:15	Opening remarks	
9:20-9:50	Recent developments on fast structured linear and eigenvalue solvers	Jianlin Xia *Purdue University*
10:00-10:30	A Black box Inverse Fast Multipole Method	Sivaram Ambikasaran *New York University*
10:30-11:00	Tea in Kemeny 300	
11:00-11:30	A sparse multifrontal solver using hierarchically semi-separable frontal matrices	Pieter Ghysels *Lawrence Berkeley National Lab*
11:40-12:10	Fast Direct Solvers for Integral Equations in 3D: Recent developments and challenges.	Eduardo Corona *New York University*
12:10-2:00	Lunch	
2:00-2:30	A hierarchical multi-Level fast multipole method for multi-scale electromagnetic problems	Zhen Peng *University of New Mexico*
2:40-3:10	A fast direct solver for high frequency scattering from a large cavity in two dimensions	Jun Lai *New York University*
3:10-4:00	Break (Set up posters if participating in poster session)	
4:00-4:40	Q&A with senior people	
5:00-7:00	Poster Session on 3$^{\text{rd}}$ floor of Kemeny Hall	
Sunday (Filene Auditorium)		
7:00-9:00	Breakfast (Use meal card at 53 Commons if provided)	
9:00-9:30	Using a fast solver to accelerate the inverse acoustic scattering problem	Carlos Borges *New York University*
9:40-10:20	The automatic solution of partial differential equations using a global spectral method	Alex Townsend *Oxford University*
10:30-11:00	Preconditioning the 2D Helmholtz equation with polarized traces	Leonardo Zepeda-Núñez *Massachusetts Institute of Technology*
11:00-11:20	Tea outside Filene Auditorium	
11:20-11:50	Communication Complexity of the Fast Multipole Method and its Algebraic Variants	Rio Yokota *King Abdullah University of Science and Technology*
12:00-12:30	On the existence of nonoscillatory phase functions	James Bremer *University of California, Davis*

Comments: Saturday's talks will be Kemeny 008. Sunday's talks will be in Filene Auditorium which is located in the Moore Hall (just north of Kemeny). The poster session will take place on the third floor of Kemeny Hall.
Abstracts for talks are provided on page 5. Abstracts for the poster session are located on page 8.

Abstracts for special lectures

Title: Overview of boundary integral equations for boundary value problems and their high-order Nyström quadratures
Speaker: Alex Barnett
Affiliation: Dartmouth College
Abstract: We review the essentials required to understand and code high-order and spectrally-accurate quadratures for Nyström methods to solve boundary integral equations (BIE). We show how these are used to solve Laplace and Helmholtz BVPs in $\mathbb{R}^2$, and provide pointers to $\mathbb{R}^3$. The lecture is accompanied by a tutorial packet with simple, readable, modular Matlab codes, and theory and coding exercises.

Title: The Hierarchical Poincar-Steklov scheme
Speaker: Adrianna Gillman
Affiliation: Dartmouth College
Abstract: In this talk, we present a high-order accurate discretization technique designed for variable coefficient problems with smooth solutions. The resulting linear system is solved via a fast direct solver with $O(N)$ complexity where N is the number of discretization points. Each additional solve is also $O(N)$ but with a much smaller constant. Unlike fast direct solvers designed for the finite element discretization of PDEs, the constants for the solver do not grow dramatically when the order of the discretization is increased. Numerical results will illustrate the performance of the proposed method. Additionally, we will present a solution technique for free-space scattering problems with locally varying media which utilizes the proposed method.

Title: Inverse Problems in MEG, EEG and Multi-Electrode Recording
Speaker: Leslie Greengard
Affiliation: New York University and The Simons Foundation
Abstract: Electroencephalography (EEG) and magnetoencephalography (MEG) are noninvasive methods for imaging and analyzing electrical activity in the brain. They give rise to ill-posed inverse source localization problems, which we will briefly review. Recent developments in electrode design are making it possible to directly record from a large number of neurons, giving rise to a new class of source localization problems. We will discuss some of the modeling and algorithmic issues which are likely to play a role in this emerging technology for neuroscience. This is joint work with Alex Barnett, Yu Chen, Charlie Epstein and Carlos Borges.

Title: Accelerating Numerical Algorithms of Linear Algebra
Speaker: Vladimir Rokhlin
Affiliation: Yale University
Abstract: I will discuss several new schemes for the solution of large-scale systems of linear algebraic equations, and for related tasks. The schemes are almost (but not quite) iterative, and are meant as a competitor for Conjugate Gradients and related algorithms. The approach will be illustrated with several numerical examples.

Abstracts for weekend workshop

Title: A Black box Inverse Fast Multipole Method
Speaker: Sivaram Ambikasaran
Affiliation: New York University
Abstract: A new fast direct solver for dense linear systems arising out of wide range of applications, integral equations, multivariate statistics, radial basis interpolation, etc., to name a few. *The highlight of this new fast direct solver is that the solver scales linearly in the number of unknowns in all dimensions.* The solver, termed as Black-Box Inverse Fast Multipole Method, works on the same data-structure as the Fast Multipole Method. More generally, the solver can be immediately extended to the class of hierarchical matrices, denoted as $\mathcal{H}^2$ matrices with strong admissibility criteria, i.e., *the interaction between neighboring cluster of particles is full-rank whereas the interaction between particles corresponding to well-separated clusters can be efficiently represented as a low-rank matrix.* The algorithm departs from existing approaches in the fact that throughout the algorithm the interaction corresponding to neighboring clusters are always treated as full- rank interactions. Numerical benchmarks on 1D and 2D manifolds confirm the linear scaling of the algorithm.

Title: Using a fast solver to accelerate the inverse acoustic scattering problems
Speaker: Carlos Borges
Affiliation: New York University
Abstract: We are interested in the reconstruction of the shape of an impenetrable sound-soft obstacle using the far field pattern data produced from the reflection of incident plane waves with different frequencies and incidence directions. This problem is extremely ill-posed and non-linear. To deal with the ill-posedness of the problem, we apply two strategies: on one hand, we introduce a frequency dependent right preconditioner together with an algorithm to produce band limited curves; on the other hand, to further improve the conditioning of the system, we solve the single frequency problem simultaneously using data from plane waves with different directions. The nonlinearity of the problem is dealt with by the use of Newton's method in the single frequency problem. The solution of the inverse scattering problem using the Newton method requires the repeated solution of the direct scattering problem with different source terms. To speed up the computation of the direct scattering problem, we use the fast direct solver HODLR.

Title: On the existence of nonoscillatory phase functions
Speaker: James Bremer
Affiliation: University of California, Davis
Abstract: Many special functions of interest arise as solutions of second ordinary linear differential equations with smoothly varying coefficients. We will explain why solutions of a large class of equations of this type admit approximation via non-oscillatory phase functions, even when the solutions are highly oscillatory. One consequence of this observation is that many highly oscillatory special functions can be evaluated extremely efficiently, and we will present the results of relevant numerical experiments.

Title: Fast Direct Solvers for Integral Equations in 3D: Recent developments and challenges.
Speaker: Eduardo Corona
Affiliation: New York University
Abstract: First, a compressed-block HSS direct solver is presented, highlighting its application to boundary integral equations in 3D. In the light of the recent developments of fast direct solvers in this context, common challenges in performance and storage requirements are discussed. Finally, recent work on an alternative tensor decomposition method is presented.

Title: A sparse multifrontal solver using hierarchically semi-separable frontal matrices
Speaker: Pieter Ghysels
Affiliation: Lawrence Berkeley National Lab
Abstract: We present an implementation of the multifrontal method for the solution of large sparse linear systems, using hierarchically semi-separable (HSS) frontal matrices. These HSS matrices exploit the fact that for many applications arising from partial differential equations, the frontal matrices have off-diagonal blocks of low numerical rank. Low rank compression of those blocks within HSS matrices has the benefit that it limits memory usage due to fill-in and reduces the overall complexity of the solver. The HSS matrices are constructed using an efficient randomized sampling algorithm, in combination with rank-revealing QR decomposition, and partial elimination uses a ULV type decomposition. Depending on the HSS compression tolerance the resulting sparse factorization can be used either as a direct solver or as a preconditioner. We present preliminary results for a parallel implementation; both shared and distributed memory parallelism are considered.

Title: A fast direct solver for high frequency scattering from a large cavity in two dimensions
Speaker: Jun Lai
Affiliation: New York University
Abstract: This talk presents a fast direct solver for an arbitrarily shaped large empty cavity embedded in an infinite perfectly conducting half space. The electromagnetic scattering from the empty large cavity is formulated as a well-conditioned second kind integral equation and the resulting linear system is solved using a fast direct solver. We illustrate the performance of this new scheme with several numerical examples for arbitrarily shaped cavities and for a wide range of frequencies.

Title: A hierarchical multi-level fast multipole method for multi-scale electromagnetic problems
Speaker: Zhen Peng
Affiliation: University of New Mexico
Abstract: A hierarchical multi-level fast multipole method (H-MLFMM) is proposed herein to accelerate the solutions of surface integral equation methods. The proposed algorithm is very suitable for solutions of board-band and multi-scale electromagnetic problems. In the H-MLFMM, two different basis functions are proposed to address two different physics corresponding to the electrical size of the elements. Specifically, for the travelling wave, the plane wave basis functions are considered, inspired by the MLFMM. Whereas in the circuit physics and for the evanescent waves, H-MLFMM employs the so-called skeleton basis functions. Numerical results demonstrate that the H-MLFMM is error controllable and robust for a wide range of applications.

Title: The automatic solution of partial differential equations using a global spectral method
Speaker: Alex Townsend
Affiliation: Oxford University
Abstract: We describe a fast 2D spectral method for the solution of partial differential equations with general boundary conditions defined on rectangular domains, using ideas from low rank approximation of functions and generalized Sylvester matrix equations. Techniques from automatic differentiation and preconditioning are employed to develop an automatic, adaptive, and spectrally accurate PDE solver. The resulting algorithm has been implemented in a new version of the Chebfun2 software system (not yet publicly available), which provides a convenient user interface.

Title: Recent developments on fast structured linear and eigenvalue solvers
Speaker: Jianlin Xia
Affiliation: Purdue University
Abstract: We will discuss a survey of some of our recent developments on new structures, methods, and analysis for structured direct linear and eigenvalue solutions. They include fast direct solution and inversion of 3D discretized elliptic PDEs, matrix-free direct solution and preconditioning, and superfast methods for finding all the eigenvalues of structured matrices. Randomization is extensively used in most of the methods to significantly enhance the flexibility, efficiency, and effectiveness. We will also briefly mention the backward stability and the accuracy control, especially when randomization is involved.

Title: Communication Complexity of the Fast Multipole Method and its Algebraic Variants
Speaker: Rio Yokota
Affiliation: King Abdullah University of Science and Technology
Abstract: Communication becomes the bottleneck for any algorithm as it approaches the limit of its parallel scalability. Therefore, communication complexity is what distinguishes algorithms that scale from ones that do not. It is well known that FMM has O(N) arithmetic complexity, but relatively little attention has been given to its communication complexity. We provide new upper bounds for the communication complexity of FMM, first for the uniform case. We then extend the complexity analysis to the nonuniform case and prove that the same upper bound holds. The complexity analysis is extended even further to the algebraic variants of FMM.

Title: Preconditioning the 2D Helmholtz equation with polarized traces
Presenter: Leonardo Zepeda-Núñez
Affiliation: Massachusetts Institute of Technology
Abstract: We present a domain decomposition solver for the 2D Helmholtz equation, with a special choice of integral transmission condition that involves polarizing the waves into one-way components. This refinement of the transmission condition is the key to combining local direct solves into an efficient iterative scheme, which can then be deployed in a high performance computing environment. The method involves an expensive, but embarrassingly parallel pre-computation of local Green?s functions, and a fast online computation of layer potentials in partitioned low-rank form. The online part has sequential complexity that scales sub-linearly with respect to the number of volume unknowns, even in the high-frequency regime. The favorable complexity scaling continues to hold in the context of low-order finite difference schemes for standard community models such as BP and Marmousi2, where conver- gence occurs in 5 to 10 GMRES iterations.

Abstracts for poster session

Title: Volume Integrals in Complex Geometry
Presenter: Travis Askham
Affiliation: New York University
Abstract: The solution of many problems in scientific computing requires the evaluation of a volume integral over some domain. For free-space problems, the use of an adaptive tree structure with tensor product grids defined on the leaves allows for a simple, lightweight discretization of the integral. When coupled with an FMM, such a discretization can be integrated rapidly. Volume integrals defined on domains with complex geometry cannot be immediately approached in this manner. The main issue is that the boundary of the domain will intersect the interior of many of the boxes in the discretization, much like the cut-cells encountered by finite volume schemes. We discuss function extension as a solution to this problem and present a scheme for computing such an extension.

Title: Hierarchical matrix techniques for the solution of elliptic equations
Presenter: Gustavo Chávez,
Affiliation: King Abdullah University of Science and Technology
Abstract: Hierarchical matrix approximations are a promising tool for approximating low-rank matrices given the compactness of their representation and the economy of the operations between them. Integral and differential operators have been the major applications of this technology, but they can be applied into other areas where low-rank properties exist. Such is the case of the Block Cyclic Reduction algorithm, which is used as a direct solver for the constant coefficients Poisson?s equation. We propose to explore the variable coefficients case, also with Block Cyclic reduction but with the addition of Hierarchical Matrices to represent matrix blocks resulting of the discretization, hence improving the otherwise O(N2) algorithm, into an efficient O(N) algorithm.

Title: GPU Spectral Methods for Elliptic Systems
Presenter: Feng Chen
Affiliation: Brown University
Abstract: We discuss recent efforts to develop GPU-suited spectral methods. First, we review spectral methods and their applications. Then, we introduce a decoupling strategy that maps spectral methods to the Nvidia CUDA programming model. Throughout the presentation we shall describe why we use GPUs and how remarkable speedups can be achieved.

Title: Efficient numerical solution of acoustic and electromagnetic scattering from periodic structures
Presenter: Yuxiang (Larry) Liu
Affiliation: Dartmouth College
Abstract: A lot of modern micro-devices, sensors and solar cells involve the scattering problem from a periodic structure. The scattered wave is governed by Helmholtz equation for acoustic waves or Maxwell equation for electromagnetic waves. The method of fundamental solution (MFS) is an efficient way to solve those kinds of partial differential equations (PDEs). It has exponential convergence when the boundary is smooth. We have developed algorithms to solve the acoustic and electromagnetic scattering problems from various types of objects. For a 3D acoustic wave scattering from a single axisymmetric object with a generic smooth boundary, 13 digits of accuracy can be achieved in around 60 seconds even with high wavenumber $k = 75$ (31 wavelengths in diameter). For a 3D electromagnetic wave scattering from a single axisymmetric object with a generic smooth boundary, we are glad to say that we are able to push the wavenumber as high as $k = 40$ outside and $k = 126$ inside (52 wavelengths in diameter) and still get 8 digits of accuracy. The penalty is that now the program takes around 20 minutes. For a 3D acoustic wave ($k = 10$) scattering from doubly-periodic axisymmetric object with a generic smooth boundary, we are able to get 10 digits in around 8 minutes. Our next goal is to finish the 3D electromagnetic scattering from periodic structures.

Title: Equilibrium Shapes of Planar Bilipid Membranes in Periodic Channels
Presenter: Gary Maple
Affiliation: University of Michigan
Abstract: We derive analytic solutions for the equilibrium shapes of planar bilipid membranes prescribed by the Helfrich energy. We verify them using a boundary integral method that simulates the membrane evolution starting from any arbitrary initial shape. In addition, we analyze the effect of walls in channel flow on the hydrodynamics and the equilibrium shapes using the numerical method.

Title: Vortex roll-up in stratified fluid.
Presenter: Surupa Shaw
Affiliation: University of New Hampshire
Abstract: Recent simulations of a vortex pair in a stratified fluid show that for small Froude number W/Nb ,the vortices disintegrate into internal waves, where W is the vortex strength, b is the vortex spacing, and N is the buoyancy frequency. The kinetic energy loss from the vortex pair in this regime can be remarkably fast, essentially annihilating the coherent vortex pair before any noticeable propagation. If the Froude number is large the vortices remain coherent and propagate as they would in constant density flow. The transition in behavior occurs near a Froude number of unity, but is apparently not a sharp transition, as some wave-making appears to happen for Froude numbers above unity. Here we quantify the wave-making with an integral of the momentum flux around a sequence of circles centered on the vortex pair and moving with it. Numerical solutions are obtained using a spectral method, the flow is treated as Boussinesq and viscous, and the initial conditions are approximately the flow due to a line vortex. The results confirm that the transition is gradual, although the complexity of the wavy flow makes interpretation difficult. These results are related to vortex roll-up in a stratified fluid.

Title: The Effect of Hematocrit on Platelet Adhesion Activity in a Microfluidic Channel
Presenter: Andrew Spann
Affiliation: Stanford University
Abstract: In response to injury, the human body forms a platelet plug along the endothelial layer of blood vessel walls. Although not directly involved in the formation of the platelet plug, the hematocrit (volume fraction) of red blood cells affects the margination of the platelets to the outside of the channel and hence their probability distribution along the channel cross-section. We present boundary integral simulations of red blood cells and platelets in a periodic channel. We compare the performance and parallel scalability of the code with an iterative solver using a particle mesh Ewald sum and a fast direct solver. These simulations show that decreasing the hematocrit of red blood cells leads to a decrease in platelet adhesion activity that corresponds with experimental results of suspensions of red blood cells and platelets in a microfluidic channel.

Title: Reduction of a dense linear system with H2-matrix structure to a linear system with sparse matrix.
Presenter: Daria Sushnikova
Affiliation: Russian Academy of Sciences
Abstract: To construct an H2-representation we use the nested cross approximation that is based on maximum-volume principle for the approximation of low-rank matrices and an iterative scheme for computing a good representor set. Once the H2-matrix is built, we want to solve a linear system with it. We propose a simple approach: we construct an extended sparse matrix from the H2-matrix representation and solve a linear system in such a way that the solution of the original linear system can be recovered. At present we have tested the performance of standard sparse solvers for the extended matrices, but we plan to utilize the specific block structure of it to get better performance.

Title: Isogeometric collocation boundary element methods
Presenter: Matthias Taus
Affiliation: University of Texas at Austin
Abstract: Isogeometric analysis has emerged as a framework for integrating computational geometry and finite element methods. In effect, in isogeometric analysis, interpolation functions widely used in computational geometry are adopted as finite element basis functions. At this stage, there are numerous applications of isogeometric analysis to problems of major practical and scientific significance. The premise of this work is that isogeometric analysis is extremely beneficial for boundary element methods, especially if they are based on collocation discretizations. The main reason is that isogeometric analysis involves smooth basis functions and exact representations of surfaces. In this work we will show that, on smooth surfaces, these properties allow one to represent singular and hyper-singular operators in terms of weakly singular ones, construct high-order approximations without introducing additional degrees of freedom, and formulate integral equations leading to extremely well-conditioned linear algebraic systems. Further, we will show that these results can be extended to non-smooth surfaces using a local refinement strategy. In particular, this approach of local refinement will allow us to develop stable isogeometric collocation boundary element methods on arbitrary surfaces.

Title: Fast and Robust Computation of Laplacian Eigenvalues for Arbitrary Planar Domains
Presenter: Lin Zhao
Affiliation: Dartmouth College
Abstract: The Laplacian spectrum of general multiply-connected planar domains is challenging to obtain with high accuracy. We achieve high accuracy using the determinant of a combined field integral equation discretized with a Nyström scheme, computed by a fast direct solver at a cost of $O(N \log N)$, where N is the number of boundary nodes. We demonstrate our method on a complicated domain. Joint work with Alex Barnett.