Modern Advances in Computational and Applied Mathematics: A workshop in honor of the birthdays of Charles L. Epstein and Leslie Greengard

POSTER SESSIONS

Note: In order to promote early dissemination and discussion of their research, we have deliberately placed most junior poster presenters on Friday, and more senior on Saturday. (However, which day you are on should in no way be taken as a comment on research quality, or for that matter, your age!) Within each day, ordering is alphabetical. Poster spots are first come, first serve, and poster presenters are responsible for setting up and/or taking down their posters in time for the next day.

Friday June 9: 3:15-4:45pm, Henry R. Luce Hall Room 202

1. **Ludvig Af Klinteberg** (KTH, Stockholm, Sweden).

   Automatic parameter selection in QBX

   Quadrature by expansion (QBX) is a promising method for the evaluation of singular and nearly singular layer potentials. The method does however introduce two new errors, which in turn depend on several new parameters. These must be correctly chosen for the computations to be efficient. We have developed a scheme that simplifies the parameter selection problem, by setting parameters on the fly while trying to maintain the errors below a target tolerance. This is based on a method for accurately estimating quadrature errors, which allows us to monitor the error in the coefficients of the local expansion used by QBX.

2. **Jordan Angel** (Rensselaer Polytechnic Institute).

   High-order upwind scheme for second-order Maxwell's Equations

   We present a high-order upwind scheme for the 2D and 3D time-domain Maxwell's equations in second-order form on curvilinear and overlapping grids. The scheme is demonstrated to be stable without the need of additional artificial dissipation usually required by centered finite difference schemes. Stability on overlapping grids is demonstrated by conducting a careful parameter space search to look for unstable solutions. Numerical results confirm the high order of convergence and stability without artificial dissipation.

3. **Huthaifa Ashqar** (Virginia Tech).

   Smartphone Transportation Mode Recognition Using a Hierarchical Machine Learning Classifier and Pooled Features from Time and Frequency Domains

This study proposes a new hierarchical framework classifier that increases the overall accuracy of classifying transportation modes. The study also investigates the possibility of improving classification accuracy by extracting new frequency domain features. The proposed framework has two layers. The first layer contains a multiclass classifier that discriminates between five transportation modes. The second layer consists of binary classifiers that differentiate between two chosen modes from the first layer. In addition, the proposed framework combined the new extracted features with traditionally used time domain features in a big pool. Results show that the classification accuracy of the proposed framework outperforms traditional classification approaches. Using this approach, classification accuracy for the same data set increased from 95.10% to 97.02%.

4. **Lukas Bystricky** (Florida State University).

   Modeling 2D Rigid Body Motion Using Boundary Integral Equations

   Understanding macroscopic properties of suspensions can be aided by a detailed understanding of the motion of the suspended particles. This poster will investigate modeling the motion of suspended rigid particles in confined and unconfined domains. We will use the results to make predictions of certain macroscopic properties of the bulk fluid, for example the viscosity.

5. **Anil Damle** (University of California, Berkeley).

   Robust and efficient multi-way spectral clustering

   A common question arising in the study of graphs is how to partition nodes into well-connected clusters. One standard methodology is known as spectral clustering and utilizes an eigenvector embedding as a staring point for clustering the nodes. Given that embedding, we present a new algorithm for spectral clustering based on a column-pivoted QR factorization. Our method is simple to implement, direct, scalable, and requires no initial guess. We also provide theoretical justification for our algorithm and experimentally demonstrate that its performance tracks recent information theoretic bounds for exact recovery in the stochastic block model.

6. **Fuhui Fang** (UNC Chapel Hill).

   Hierarchical Orthogonal Matrix Generation and Matrix-Vector Multiplications in Rigid Body Simulations

   We apply the hierarchical modeling technique and study some numerical linear algebra problems arising from the Brownian dynamics simulations of biomolecular systems where molecules are modeled as ensembles of rigid bodies. Given a rigid body p consisting of n beads, the $6 \times 3n$ transformation matrix Z that maps the force on each bead to p translational and rotational forces (a 6×1 vector), and V the row space of Z, we show how to explicitly construct the $(3n-6) \times 3n$ matrix $\tilde{Q}$ consisting of $(3n-6)$ orthonormal basis vectors of $V^{\perp}$ (orthogonal complement of V) using only $O(n \log n)$ operations and storage. For applications where only the matrix-vector multiplications $\tilde{Q}\vec{v}$ and $\tilde{Q}^T\vec{v}$ are needed, we introduce asymptotically optimal $O(n)$ hierarchical algorithms without explicitly forming $\tilde{Q}$. Preliminary numerical results are presented to demonstrate the performance and accuracy of the numerical algorithms.

7. **Md. Kamrul Hasan** (Marquette University).

   Color space analysis of image for best prediction using machine learning algorithm

In image analysis, researchers use different color spaces like red, green, blue (RGB), hue, saturation, and blue (HSV), etc. For better prediction, we use red color or green color intensity values of the image using machine learning algorithm. But, we know that we many other color space which are also necessary for image analysis. So, the research question is which color space or mixed of color space is very much essential for any particular image processing system. In this poster, we will show some preliminary result where different color space is giving various results.

8. **Aarti Jajoo** (Baylor College of Medicine).

   Patterns of Correlated DNA Methylation in Severe Malnutrition

   Severe Childhood Malnutrition (SCM) occurs in two distinct forms: Edematous SCM (ESCM) with higher mortality and Non-edematous SCM (NESCM) with less mortality. Phenotypic differences between the 2 forms are very apparent but the pathogenic factors causing these disparities are still unknown. Differences in the genome-wide DNA methylation levels between the two forms has been observed. We have also identified variation in correlation of methylation level in nearby sites within individuals across the two forms. These inter-relational methylation structures are described in the literature, but their consistency across individuals, their underlying meaning, and potential phenotypic consequences have still remained unexplored. We will discuss the mathematical and statistical aspects of capturing and characterizing these variations and the challenges faced in the process. We will present results for acute and recovered individuals using our algorithm on 450k (sites) methylation chip data.

9. **Jiahua Jiang** (University of Massachusetts Dartmouth).

   Offline-Enhanced Reduced Basis Method through adaptive construction of the Surrogate Parameter Domain

   Classical Reduced Basis Method (RBM) is a popular certified model reduction approach for solving parametrized partial differential equations. However, the large size or high dimension of the parameter domain leads to prohibitively high computational costs in the offline stage. In this work we propose and test effective strategies to mitigate this difficulty by performing greedy algorithms on surrogate parameter domains that are adaptively constructed. These domains are much smaller in size yet accurate enough to induce the solution manifold of interest at the current step. In fact, we propose two ways to construct the surrogate parameter domain: Successive Maximization Method and Cholesky Decomposition Method. The algorithm is capable of speeding up RBM by effectively alleviating the computational burden in offline stage without degrading accuracy, assuming that the solution manifold has low Kolmogorov width. We demonstrate the algorithm's effectiveness through numerical experiments.

10. **Jason Kaye** (Courant Institute, NYU).

    Integral Equation Method for the First Passage Problem on the Sphere

    The first passage time (FPT) problem, which arises in models of various stochastic processes in cell biology, asks the expected time which a particle diffusing in a domain takes to leave through a set of patches on the boundary. The passage time may be computed as the solution to a Poisson problem of mixed Dirichlet–Neumann type, the singular nature of which leads to challenges as the number of patches grows and their size shrinks. We introduce a method which solves the FPT problem in the interior and exterior of a sphere with many small patches on its surface. The method uses the Neumann Green's function for the sphere to reduce the problem to an integral equation on the patches. The singular nature of the solution is captured by solving the single-patch problem. The many-patch problem is then solved by multiple scattering methods, and the resulting iteration is accelerated by an FMM. We use the method to study the FPT as the number, size, and arrangement of the patches is varied.

11. **Nicholas Knight** (Courant Institute, NYU).

    Butterflies in Layered Media

    We present an algorithm for electromagnetic scattering calculations in layered media by use of butterfly-accelerated Sommerfeld integrals. In the time-harmonic setting, representing electromagnetic fields by generalized Debye sources (and their Fourier transforms) along media interfaces efficiently decouples several unknowns, and leads to a representation whose evaluation is amenable to acceleration via a butterfly algorithm. When coupled with an iterative solver, the corresponding integral equation formulation can be efficiently solved.

12. **Roy Lederman** (Princeton University).

    A Representation Theory Perspective on Simultaneous Alignment and Classification

    One of the difficulties in 3D reconstruction of molecules from images in single particle Cryo-Electron Microscopy (Cryo-EM) is heterogeneity in samples: in many cases, the samples contain a mixture of molecules or conformation. Many existing algorithms are based on iterative approximations of the molecules in a non-convex optimization that is prone to reaching suboptimal local minima, others require an alignment in order to perform classification, or vice versa. The recently introduced Non-Unique Games framework provides a representation theoretic approach to studying problems of alignment over compact groups, and offers convex relaxations for alignment problems which are formulated as semidefinite programs with certificates of global optimality under certain circumstances. We propose to extend Non-Unique Games to the problem of simultaneous alignment and classification with the goal of simultaneously classifying Cryo-EM images and aligning them within their respective classes.

13. **William Leeb** (Princeton University).

    PCA from noisy, high-dimensional, corrupted observations

    We study the spiked covariance model when the measurements have undergone a "diagonal modulation". This includes data with missing entries and blurred images. We derive the asymptotic limits of the eigenvalues and principal components for this data. We apply these new results to several statistical problems, including singular value shrinkage and Wiener filtering. This is joint work with Edgar Dobriban and Amit Singer.

14. **Yingzhou Li** (Stanford University).

    Distributed-memory hierarchical interpolative factorization

    The hierarchical interpolative factorization (HIF) offers an efficient way for solving or preconditioning elliptic partial differential equations. By exploiting locality and low-rank properties of the operators, the HIF achieves quasi-linear complexity for factorizing the discrete positive definite elliptic operator and linear complexity for solving the associated linear system. In this poster, the distributed-memory HIF (DHIF) is introduced as a parallel and distributed-memory implementation of the HIF. The DHIF organizes the processes in a hierarchical structure and keep the communication as local as possible. Extensive numerical examples are performed on the NERSC Edison system with up to 8192 processes. The numerical results agree with the complexity analysis and demonstrate the efficiency and scalability of the DHIF.

15. **F. Patricia Medina** (Worcester Polytechnic Institute).

    Mathematical treatment and simulation for a methane hydrate model

    The computational simulation of Methane Hydrates (MH), an ice-like substance abundant in permafrost regions and in subsea sediments, is useful for the understanding of their impact on climate change as well as a possible energy source. We consider a simplified model of MH evolution which is a scalar nonlinear parabolic PDE with two unknowns, solubility, and saturation, bound by an inequality constraint. We extend the theory of monotone operators to the present case of a spatially variable constraint. Part of our posterior work extended the computational model and analysis to include more variables such as salinity, pressure, temperature, and gas phase saturation, as well as in considering realistic scenarios such as those that may occur in ocean observatories along Hydrate Ridge and Cascadia Margin.

16. **Oleksandr Misiats** (Courant Institute, NYU).

    Convex Duality in Nonconvex Variational Problems

    We consider the minimization problem which models martensitic (diffusionless) phase transitions in rectangular domains. Physical experiments suggest that if opposite phases are present at opposite sides, the transition has a form of a zig-zag wall. My poster addresses the mathematical model of this phenomenon, which involves the minimization of singularly perturbed 2D and 3D elastic energies with phase constraints. By means of sharp upper and lower bounds, we show that the experimentally observed zig-zag structure provides optimal energy scaling law. Despite the fact that the problem is highly nonconvex due to the presence of nonconvex phase constraints and the singular perturbation, I will describe a relaxation method which allows to use the convex duality technique for the purpose of obtaining a sharp lower bound.

17. **Qi Tang** (Rensselaer Polytechnic Institute).

    A Stable FSI Algorithm for Rigid Bodies and Incompressible Flows

    A stable added-mass/added-damping partitioned algorithm is developed for fluid-structure interaction (FSI) problems involving viscous incompressible flow and rigid bodies. The algorithm remains stable, without sub-iterations, even for light rigid-bodies when added-mass and viscous added-damping effects are large. A fully second-order accurate implementation of the scheme is developed based on a fractional-step method for the incompressible Navier-Stokes equations and overlapping grids to handle the moving geometry. A number of difficult benchmark problems in 2D and 3D will be presented to verify the proposed algorithm.

18. **James Vogel** (Purdue University).

    Applications of Superfast Divide-and-Conquer Eigensolvers

    The superfast divide-and-conquer eigenvalue algorithm (V, Xia, Cauley, Balakrishnan, SISC 2016) utilizes the eigenvector structure of symmetric hierarchical semiseparable (HSS) matrices and acceleration via the fast multipole method (FMM) to accurately compute the eigendecomposition for a large class of matrices in near-linear time and storage complexity.

We show how this algorithm can be leveraged as a subroutine to greatly accelerate many important algorithms in science and engineering. Some of these applications include electronic structure calculation, medical imaging, optimal control, structural dynamics, and fast PDE solvers. We also show some recent selected improvements to algorithm generalization, analysis, and high-performance implementation.

19. **Yabin Zhang** (Rice University).

    A fast direct solver for boundary value problems with locally-perturbed geometries

    Many problems in science and engineering can be formulated as integral equations with elliptic kernels. In particular, in optimal control and design problems, the domain geometry evolves and results in a sequence of discretized linear systems to be constructed and inverted. While the systems can be constructed and inverted independently, the computational cost is relatively high. In the case where the change in the domain geometry for each new problem is only local, i.e. the geometry remains the same except within a small subdomain, we are able to reduce the cost of inverting the new system by reusing the pre-computed fast direct solvers of the original system. The resulting solver only requires inexpensive matrix-vector multiplications, thus dramatically reducing the cost of inverting the new linear system. Numerical results demonstrate the performance of the solver.

Saturday June 10: 3:15-4:15pm, Henry R. Luce Hall Room 202

20. **Bedros Afeyan** (Polymath Research Inc).

    Multiscale Adaptive Methods for Modeling Vlasov Plasmas

    We describe a number of strategies for solving the Vlasov–Poisson system of equations using both particle and continuum models. In fact, we merge the distinction between the two by resorting to adaptive, multi-scale methods which use elements of both. We demonstrate the utility of these approaches by comparing them to both traditional particle methods and to traditional fixed-grid methods. Self-organization of high energy density plasmas far from equilibrium when injected with coherent radiation is what we seek. These methods organically give rise to reduced descriptions and model selection, wherever possible.

21. **Tamir Bendory** (Princeton University).

    (may be moved to Friday)

    Bispectrum Inversion with Application to Multireference Alignment

    We consider the problem of estimating a signal from multiple noisy translated versions of itself, called multireference alignment. Existing methods rely on estimating the relative translations, which is impossible in a low signal-to-noise ratio regime. To overcome this fundamental barrier, we suggest estimating the signal directly using features that are invariant to translations. Specifically, we estimate the signals Fourier magnitudes and phases from the mean power spectrum and bispectrum of the observations, respectively. We then propose a variety of algorithms to estimate the Fourier phases from the bispectrum. Our main method consists of a non-convex local optimization algorithm over the smooth manifold of phases. Empirically, in the absence of noise, the non-convex algorithm appears to converge to the target signal regardless of initialization. Numerical experiments demonstrate that the invariant feature approach is superior over alignment-based methods in high noise regimes.

22. **Yanlai Chen** (University of Massachusetts Dartmouth).

    Ultra-efficient Reduced Basis Method and Its Integration with Uncertainty Quantification.

    Models of reduced computational complexity is indispensable in scenarios where a large number of numerical solutions to a parametrized problem are desired in a fast/real-time fashion. Thanks to an offline-online procedure and the recognition that the parameter-induced solution manifolds can be well approximated by finite-dimensional spaces, reduced basis method (RBM) and reduced collocation method (RCM) can improve efficiency by several orders of magnitudes. The accuracy of the RBM solution is maintained through a rigorous a posteriori error estimator whose efficient development is critical and involves fast eigensolves.

    After giving a brief introduction of the RBM/RCM, this poster will show our recent work on significantly delaying the curse of dimensionality for uncertainty quantification, and new fast algorithms for speeding up the offline portion of the RBM/RCM by around 6-fold.

23. **Johan Helsing** (Lund University, Sweden).

    High-order convergent and accurate electromagnetic solvers for Lipschitz domains

    We present an integral equation based numerical solver for electromagnetic problems in domains with corners, sharp edges, and conical tips. The solver is free from tailor-made special basis functions and precomputed quadratures. Rather, it relies on standard Nyström discretization with underlying adaptive panel-based Gauss–Legendre quadrature. In tandem with that, recursively compressed inverse preconditioning (RCIP) acts as a fast direct solver in regions with troublesome geometry. Thanks to this acceleration, problems in Lipschitz domains can be solved essentially with the same speed and accuracy as problems in smooth domains. Examples include high-wavenumber eigenproblems for axially symmetric microwave cavities with piecewise smooth and perfectly conducting surfaces; whispering gallery modes and general resonances of dielectric objects in vacuum; and the spectral measure of the polarizability tensor of rectangles, rectangular cuboids, and snow-cone shaped inclusions.

24. **Shidong Jiang** (New Jersey Institute of Technology).

    Accurate evaluation of unsteady Stokes layer potentials in complex moving geometries

    We present a new scheme for the accurate evaluation of unsteady Stokes layer potentials in complex moving geometries. The scheme splits the layer potentials into two parts — a singular local part that contains the temporal integration from $t - dt$ to t and a smooth history part that contains the temporal integration for 0 to $t - dt$. The leading asymptotic term of the local part is analysed in detail and the remaining part is discretized via a global quadrature after a change of variable. The performance of the scheme is demonstrated via several numerical examples.

25. **Shilpa Khatri** (University of California, Merced).

    Local analysis for close evaluation of layer potentials

    Accurate evaluation of layer potentials near boundaries and interfaces are needed in many applications, including fluid-structure interaction problems and near-field scattering problems. A classical method to approximate the solution everywhere in the domain consists of using the same quadrature rule (Nyström method) used to solve the underlying boundary integral equation. This method is problematic for evaluations close to boundaries and interfaces. For a fixed number, N, of quadrature points, this method incurs a non-uniform error with $O(1)$

errors in a boundary layer of thickness $O(1/N)$. Using an asymptotic expansion of the associated kernel, we remove this $O(1)$ error without having to use high-order Nyström methods. To demonstrate this method, we consider the interior and exterior Laplace problems.

26. **Andreas Kloeckner** (University of Illinois at Urbana-Champaign).

    Accuracy and Applicability of Quadrature by Expansion

    The rapid evaluation of layer and volume potentials forms the cornerstone of the numerical solution of PDEs with the help of integral equation methods. Quadrature by Expansion is an effective method for evaluating these potentials with high order accuracy up to controlled precision. To do so, the method relies on series expansions of the potential. I show recent results from the study of the approximation properties of the method as well as its potential for practicality in large-scale calculations.

27. **Christian Müller** (Flatiron Institute).

    Proximal algorithms for high-dimensional penalized statistical estimation

    In statistics, the task of simultaneously estimating a regression vector and an additional model parameter is often referred to as concomitant estimation. Huber introduced a generic method for formulating "maximum likelihood-type" estimators (or M-estimators) with a concomitant parameter from a convex criterion. In this contribution, we provide a generic proximal algorithmic approach for solving convex optimization problems associated with the class of penalized concomitant M-estimators. This class of estimators includes the scaled Lasso and the TREX as special cases. We present novel proximity operators arising from different concomitant estimators and show their applicability in standard proximal algorithm schemes. We illustrate both the algorithmic performance of the optimization routines and the statistical performance of the different estimators on selected synthetic and real-world examples.

28. **Kostas Mylonakis** (Aristotle University of Thessaloniki), **Nikos Pitsianis** and **Xiaobai Sun** (Duke).

    The Fast Multipole Method in Three Decades

    In three decades, the Fast Multipole Method (FMM) by Vladimir Rokhlin and Leslie Greengard has made a profound influence in applied mathematics and extensive impact on scientific inquiries by and large. To applied mathematics, the FMM carries the analysis-based principles and instructions used to design, develop and analyze fast, accurate and robust algorithms, with adaptation in the formulation and computation to domain-specific models and data. To scientific studies, the FMM has enabled and advanced numerous inquiries that were previously intractable in computation. Moreover, the FMM fosters a new generation of multi-disciplined researchers and forges closer connections among mathematical and scientific studies as well as communities. This poster is a glimpse of the immeasurable influence and impact of the FMM, in terms of citation and collaboration, over near and far geodesic distance and over time, using limited information and processing resources.

29. **Santosh Kumar Nanda** (Thapar University, Patiala, India).

    High-order numerical approximation of population age density model

    The main objective of this work is to design a higher order IMEX-WENO (implicit-explicit weighted non-oscillatory) scheme for solving a population age density model with nonlinear growth, mortality rates, reproduction rate. The main complication in this model is the presence of global terms in the coefficients and boundary condition. We carefully design numerical approximation to these global and boundary conditions to ensure high order accuracy. We presented numerical examples to show the performance of design scheme and compare it with lower order scheme.

30. **Zhen Peng** (University of New Mexico).

    Stochastic Integral Equation Methods for Wave Chaotic Analysis

    This work concerns a quantitative statistical analysis accounting for the uncertainty in complex wave-chaotic systems. The primary contributions are twofold: (i) a novel stochastic Greens function method for wave interaction with wave-chaotic media, which quantitatively describes the universal statistical property of chaotic systems through random matrix theory (RMT); (ii) a hybrid deterministic and stochastic formulation, in which small components (electronics, antennas, etc.) in the computational domain are modeled using first-principles and large portions (cavity enclosures, scattering environments, etc.) are modeled statistically.

31. **Jun Wang** (Courant Institute, NYU).

    Fast Methods for the Evaluation of Heat Potentials in Moving Geometry

    We present a hybrid asymptotic numerical method for the accurate evaluation of single and double layer heat potentials in two dimensions. These are non-local integral operators in space-time and require fast algorithms to handle the history part efficiently. In order to design high order accurate rules, however, it is the local-in-time component of the heat potential that gives rise to numerical difficulties. Our scheme requires only a local asymptotic calculation plus several boundary integrals with a Gaussian kernel, which can be accelerated by a new version of the fast Gauss transform.