Midwest Numerical Analysis Day

University of Michigan, Ann Arbor

May 20-21, 2022

Contents

Invited Speakers

Daniela Calvetti (Case Western Reserve University)
Yingda Cheng (Michigan State University)
Peijun Li (Purdue University)
Lothar Reichel (Kent State University)
Li Wang (University of Minnesota)
Zhimin Zhang (Wayne State University)

Organizing Committee

Mariana Carrasco-Teja
Krishna Garikipati
Robert Krasny
Christina Ruhfel
Divakar Viswanath

Sponsors

Department of Mathematics
Michigan Center for Applied and Interdisciplinary Mathematics (MCAIM)
Michigan Institute for Computational Discovery and Engineering (MICDE)

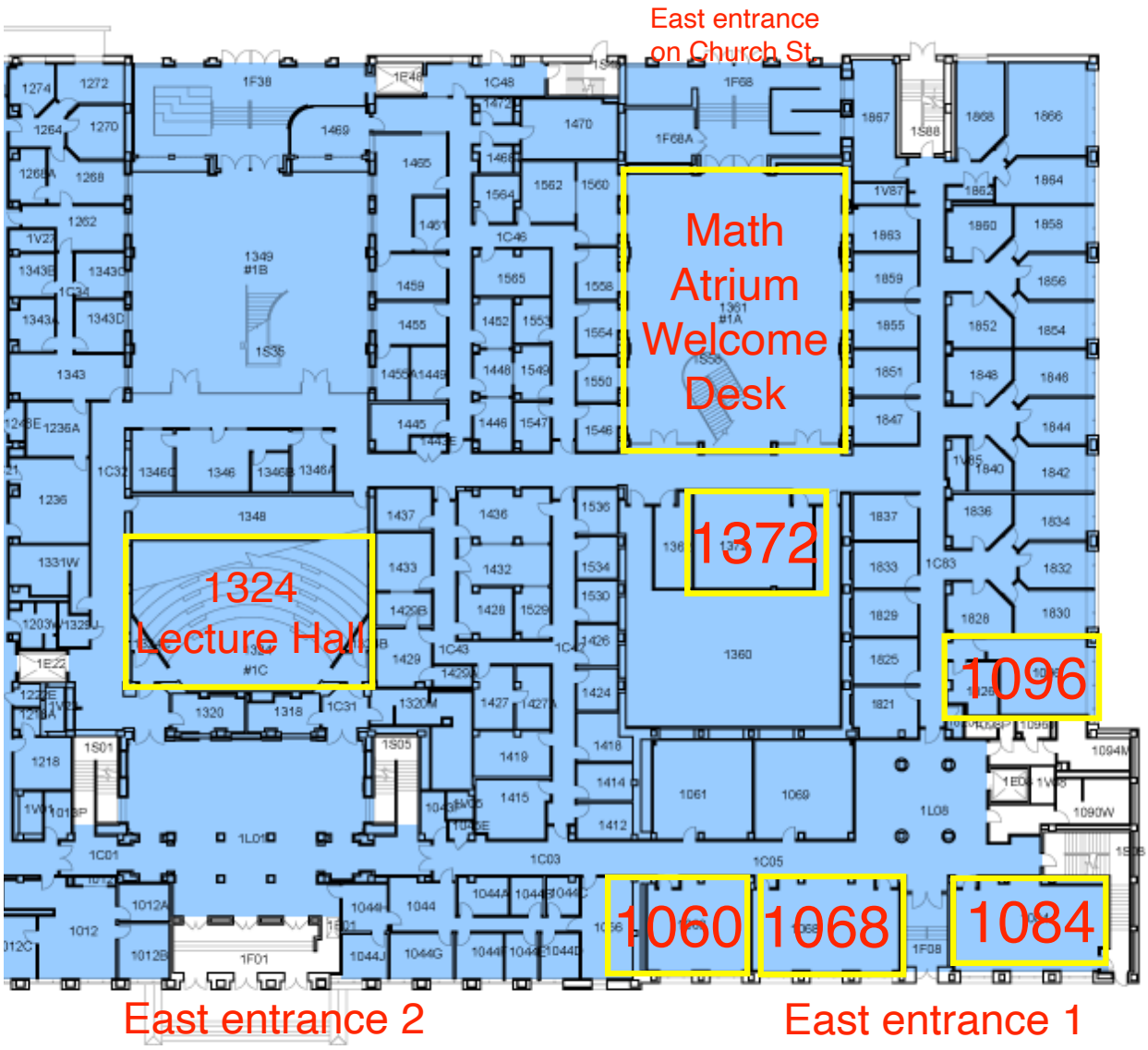
Future MWNADs

2023, Iowa State University, Jue Yan
2024, University of Iowa, Weimin Han
2025, University of Nebraska-Lincoln, Huijing Du

1 Program

Friday		
1:00pm	Check In	Math Atrium
1:50pm	Welcome	1324 EH
	Lydia Bieri, Director, MCAIM	
	Krishna Garikipati, Director, MICDE	
2:00pm	Invited Talk: Daniela Calvetti	1324 EH
3:00pm	Invited Talk: Yingda Cheng	1324 EH
4:00pm	Coffee Break, Poster Session	Math Atrium
4:30pm	Contributed Talk Session F1	1060 EH
	Contributed Talk Session F2	1068 EH
	Contributed Talk Session F3	1084 EH
	Contributed Talk Session F4	1096 EH
Saturday		
8:00am	Breakfast	Math Atrium
9:00am	Invited Talk: Li Wang	1324 EH
10:00am	Invited Talk: Lothar Reichel	1324 EH
11:00am	Coffee Break	Math Atrium
11:30am	Contributed Talk Session S1	1060 EH
	Contributed Talk Session S2	1068 EH
	Contributed Talk Session S3	1084 EH
	Contributed Talk Session S4	1096 EH
	Contributed Talk Session S5	remote (1372 EH)
12:30pm	Lunch	Math Atrium
2:00pm	Invited Talk: Zhimin Zhang	1324 EH
3:00pm	Invited Talk: Peijun Li	1324 EH
4:00pm	Coffee Break	Math Atrium
4:30pm	Contributed Talk Session S6	1060 EH
	Contributed Talk Session S7	1068 EH
	Contributed Talk Session S8	1084 EH
	Contributed Talk Session S9	remote (1372 EH)

2 East Hall Map



3 Schedule of Talks

3.1 Invited talks (1324 EH)

Friday 2pm, **Daniela Calvetti**, Case Western Reserve University
Better Together: The Partnership of Bayesian Inference and Numerical Analysis in the Solution of Inverse Problems

Friday 3pm, **Yingda Cheng**, Michigan State University
Sparse Grid Discontinuous Galerkin (DG) Methods for High Dimensional PDEs

Saturday 9am, **Li Wang**, University of Minnesota
Variational Computational Methods for Gradient Flow

Saturday 10am, **Lothar Reichel**, Kent State University
Error Estimates for Golub-Kahan Bidiagonalization with Tikhonov Regularization for Ill-posed Operator Equations

Saturday 2pm, **Zhimin Zhang**, Wayne State University
Efficient Spectral Methods and Error Analysis for Nonlinear Hamiltonian Systems

Saturday 3pm, **Peijun Li**, Purdue University
Inverse Random Source Problems for Wave Equations

3.2 Friday contributed talks

Session F1, DG methods, 1060 EH

Yue Kang, Michigan Technological University
Bound-preserving discontinuous Galerkin methods with second-order implicit pressure explicit concentration time marching for compressible miscible displacements in porous media

Fangyao Zhu, Michigan Technological University
Discontinuous Galerkin methods with Patankar time discretization for chemical reacting flow

Tamas Horvath, Oakland University
Sliding grid techniques for Space-Time Hybridizable Discontinuous Galerkin methods

Session F2, Integral equations, 1068 EH

Yue Cao, Illinois Institute of Technology
Kernel free boundary integral method and its application

Somveer Singh, Indian Institute of Technology BHU Varanasi, India
Numerical analysis of nonlinear weakly singular integro-partial differential equations arising from viscoelasticity

Lei Wang, University of Wisconsin, Milwaukee
Application of the Barycentric Lagrange Treecode for Computing Correlated Random Displacements Using the Spectral Lanczos Decomposition Method

Session F3, Wave propagation, 1084 EH

Zhichao Peng, Michigan State University
EM-WaveHoltz: a flexible frequency-domain Maxwell solver built from time-domain solvers

Yann-Meing Law, Michigan State University
The Hermite-Taylor Correction Function Method for Maxwell's Equations

Yang Yang, Michigan Technological University
Stability analysis of the Eulerian-Lagrangian finite volume methods for nonlinear hyperbolic equations in one space dimension

Session F4, Multiscale, geometric, and exponential methods, 1096 EH

Siu Wun Cheung, Lawrence Livermore National Laboratory
Multiscale and numerical upscaling methods for physical processes in high contrast heterogeneous porous media

Jiahui Chen, Michigan State University
Evolutionary de Rham-Hodge method

Van Hoang Nguyen, Mississippi State University
Efficient exponential methods for genetic regulatory systems

3.3 Saturday morning contributed talks

Session S1, DG methods, 1060 EH

Mahboub Baccouch, University of Nebraska at Omaha
A local discontinuous Galerkin method for elliptic problems on Cartesian grids: Superconvergence, a posteriori error estimation, and adaptivity

Andrés Galindo Olarte, Michigan State University
Accuracy enhancement of discontinous Galerkin solutions for Vlasov-Maxwell equations

Devina Sanjaya, University of Tennessee, Knoxville
Global mesh optimization: Is it worth the cost?

Session S2, Biological modeling, 1068 EH

Dexuan Xie, University of Wisconsin-Milwaukee
A new nonlinear iterative scheme for solving a nonuniform size modified Poisson-Boltzmann ion channel model

Zhen Chao, University of Michigan
Integral method for solving one-dimensional Poisson-Nernst-Planck ion channel model

Will Zhang, University of Michigan
Fractional Viscoelastic Modeling of Cardiovascular Soft Tissues

Session S3, High-order methods, 1084 EH

Luan Vu Thai, Mississippi State University
High-order efficient multirate infinitesimal step-type methods

Trky Alhsmy, Mississippi State University
High-order adaptive exponential Runge-Kutta methods

Qicang Shen, University of Michigan
High-order accurate solution of the spatial kinetics problem for nuclear reactor simulation using the spectral deferred correction method

Session S4, Inverse problems, statistical methods, 1096 EH

Ying Liang, Purdue University
Least-squares method for recovering multiple medium parameters

Neophytos Charalambides, University of Michigan
Orthonormal Sketches for Secure Coded Regression

Session S5, Saturday morning, remote from 1372 EH

Songting Luo, Iowa State University
A Fixed-point Iteration Method for High Frequency Helmholtz Equations

Xiaoming He, Missouri University of Science and Technology
PIFE-PIC: Parallel Immersed-Finite-Element Particle-in-Cell for 3-D kinetic simulations of plasma-material interactions

Ahmed Al-Taweel, University of Arkansas at Little Rock
A stabilizer free weak Galerkin finite element method with supercloseness of order two

3.4 Saturday afternoon contributed talks

Session S6, Reduced order modeling, 1060 EH

Jörn Zimmerling, University of Michigan
Reduced order model approach to inverse scattering

Siddhartha Srivastava, University of Michigan
Non-local calculus on graphs with application to reduced order modeling

Jovan Zigic, Virginia Polytechnic Institute and State University
A Splitting Approach to Dynamic Mode Decomposition of Nonlinear Systems

Session S7, Phase-field modeling, 1068 EH

Zachary Candelaria, Virginia Polytechnic Institute and State University
Phase-Field Modeling of Oscillatory Wetting Phenomena with Contact Angle Hysteresis

Min-Jhe Lu, Illinois Institute of Technology
Mechano-chemical Tumor Models: An Energetic Variational Approach

Ziyang Huang, University of Michigan
Modeling multiphase problems with the consistent and conservative Phase-Field method

Session S8, Parallel computing, Newton's method, 1084 EH

Zachary Miksis, University of Notre Dame
Parallel implementation of a sparse grid fast sweeping WENO method for Eikonal equations

Zhonggang Zeng, Northeastern Illinois University
Newton's iteration at nonisolated solutions

Emmanuel Djegou, Missouri University of Science and Technology
To be determined.

Session S9, Saturday afternoon, remote from 1372 EH

Chunmei Wang, University of Florida
A New Numerical Method for Div-Curl Systems with Low Regularity Assumptions

Chenyang Cao, Purdue University
A fast stable matrix form to some transforms

Jiguang Sun, Michigan Technological University
Local estimators and Bayesian inverse problems with non-unique solutions

4 Abstracts of Invited Talks

Daniela Calvetti
Case Western Reserve University

Better Together: The Partnership of Bayesian Inference and Numerical Analysis in the Solution of Inverse Problems

The numerical solution of inverse problems where the number of unknowns exceeds the available data is a notoriously difficult problem. Regularization methods designed to overcome the paucity of data penalize candidate solutions for unlikely or undesirable features. Discretization level of the underlying continuous problem can also be used to improve the accuracy of the computed solution. In this talk we show how recasting the inverse problems within the Bayesian framework makes it possible to express via a probability density function features believed to characterize the solution in a way that interfaces naturally with state of the art computational schemes. In that context, we will present an efficient computational scheme for the recovery of sparse solutions, where the sparsity is encoded in terms of hierarchical models whose parameters can be set to account for the sensitivity of the data to the solution. The computations can be organized as an inner-outer iteration scheme, where a weighted linear least squares problem is solved in the inner iteration and the outer iteration updates the scaling weights. When the least squares problems are solved approximately by the Conjugate Gradient method for least squares (CGLS) equipped with a suitable stopping rule, typically the number of CGLS iterations quickly converges to the cardinality of the support, thus providing an automatic model reduction. Computed examples will illustrate the performance of the approach in a number of applications.

Yingda Cheng
Michigan State University

Sparse Grid Discontinuous Galerkin (DG) Methods for High Dimensional PDEs

In this talk, I will introduce adaptive sparse grid DG methods, and discuss their applications in solving high dimensional PDEs, including kinetic equations, Hamilton-Jacobi equations, etc. The methods, which combine the advantages of sparse grid and DG approach, are shown to be particularly effective for high dimensional transport equations.The methods are constructed using multiwavelets of various kinds. We prove stability and accuracy for model equations. Adaptivity is incorporated for time evolution problems. Benchmark test results are shown.

Peijun Li
Purdue University

Inverse Random Source Problems for Wave Equations

Motivated by significant applications, the inverse source problem remains an important and active research subject in inverse scattering theory. The inverse random source problem refers to the inverse source problem that involves uncertainties, and is substantially more challenging than its deterministic counterpart.

In this talk, our recent progress will be discussed on inverse source problems for the stochastic wave equations. I will present a new model for the random source, which is assumed to be a microlocally isotropic Gaussian random field such that its covariance operator is a classical pseudo-differential operator. The well-posedness and regularity of the solution will be addressed for the direct problem. For the inverse problem, it is shown that the principal symbol of the covariance operator can be uniquely determined by the high frequency limit of the wave field at a single realization. I will also highlight some ongoing and future projects in the inverse random potential and medium problems.

Lothar Reichel
Kent State University

Error Estimates for Golub-Kahan Bidiagonalization with Tikhonov Regularization for Ill-posed Operator Equations

Linear ill-posed operator equations arise in various areas of science and engineering. The presence of errors in the operator and the data often makes the computation of an accurate approximate solution difficult. We compute an approximate solution of an ill-posed operator equation by first determining an approximation of the operators of generally fairly small dimension by carrying out a few steps of a continuous version of the Golub-Kahan bidiagonalization (GKB) process to the noisy operator. Then Tikhonov regularization is applied to the low-dimensional problem so obtained and the regularization parameter is determined by solving a low-dimensional nonlinear equation. The effect of replacing the original operator by the low-dimensional operator obtained by the GKB process on the accuracy of the solution is analyzed, as is the effect of errors in the operator and data. Computed examples that illustrate the theory are presented. This talk presents joint work with A. Alqahtani, T. Mach, and R. Ramlau.

Li Wang
University of Minnesota

Variational Computational Methods for Gradient Flow

In this talk, I will introduce a general variational framework for nonlinear evolution equations with a gradient flow structure, which arise in material science, animal swarms, chemotaxis, and deep learning, among many others. Building upon this framework, we develop numerical methods that have built-in properties such as positivity preserving and entropy decreasing, and resolve stability issues due to the strong nonlinearity. Two specific applications will be discussed. One is the Wasserstein gradient flow, where the major challenge is to compute the Wasserstein distance and resulting optimization problem. I will show techniques to overcome these difficulties. The other is to simulate crystal surface evolution, which suffers from significant stiffness and therefore prevents simulation with traditional methods on fine spatial grids. On the contrary, our method resolves this issue and is proved to converge at a rate independent of the grid size.

Zhimin Zhang
Wayne State University

Efficient Spectral Methods and Error Analysis for Nonlinear Hamiltonian Systems

We investigate efficient numerical methods for nonlinear Hamiltonian systems. Three polynomial spectral methods (including spectral Galerkin, Petrov-Galerkin, and collocation methods) are presented. Our main results include the energy and symplectic structure preserving properties and error estimates. We prove that the spectral Petrov-Galerkin method preserves the energy exactly and both the spectral Gauss collocation and spectral Galerkin methods are energy conserving up to spectral accuracy. While it is well known that collocation at Gauss points preserves symplectic structure, we prove that the Petrov-Galerkin method preserves the symplectic structure up to a Gauss quadrature error and the spectral Galerkin method preserves the symplectic structure to spectral accuracy. Furthermore, we prove that all three methods converge exponentially (with respect to the polynomial degree) under sufficient regularity assumption. All these aforementioned properties make our methods possible to simulate the long time behavior of the Hamiltonian system. Numerical experiments indicate that our algorithms are efficient.

5 Abstracts of Contributed Talks

Trky Alhsmy
Mississippi State University

High-order adaptive exponential Runge-Kutta methods

Exponential Runge-Kutta (ExpRK) methods have shown to be well-suited for the time discretization of stiff semilinear parabolic PDEs. The construction of stiffly-accurate ExpRK schemes requires solving a system of stiff order conditions which involve matrix functions. So far, methods up to order 5 have been derived by relaxing one or more order conditions (depending on a given order of accuracy). These schemes, however, allow using with constant step sizes only. In this talk, we will derive new and efficient ExpRK schemes of high orders which not only fulfill the stiff order conditions in the strong sense and but also support variable step sizes implementation. Numerical examples are given to verify the accuracy and to illustrate the efficiency of the newly constructed ExpRK schemes.

Ahmed Al-Taweel
University of Arkansas at Little Rock

A stabilizer free weak Galerkin finite element method with supercloseness of order two

The weak Galerkin (WG) finite element method is an effective and flexible general numerical technique for solving partial differential equations. A simple WG finite element method is introduced for second-order elliptic problems. First we have proved that stabilizers are no longer needed for this WG element. Then we have proved the supercloseness of order two for the WG finite element solution. The numerical results confirm the theory.

Mahboub Baccouch
University of Nebraska at Omaha

A local discontinuous Galerkin method for elliptic problems on Cartesian grids: Superconvergence, a posteriori error estimation, and adaptivity

In this talk, we present a local discontinuous Galerkin (LDG) methods for two-dimensional second-order elliptic problems. Convergence properties for the solution and for the auxiliary variable that approximates its gradient are established. We prove that the LDG solution is superconvergent towards a particular projection of the exact solution. The order of convergence is proved to be p +2, when tensor product polynomials of degree at most pare used. Then, we show that the actual error can be split into two parts. The components of the significant part can be given in terms of (p +1)-degree Radau polynomials. We use these results to construct a reliable and efficient residual-type a posteriori error estimates. We prove that the proposed residual-type a posteriori error estimates converge to the true errors in the L2-norm under mesh refinement. The order of convergence is proved to be p+2. Finally, we present a local AMR procedure that makes use of our local and global a posteriori error estimates. We provide several numerical examples illustrating the effectiveness of our procedures.

Zachary Candelaria
Virginia Polytechnic Institute and State University

Phase-Field Modeling of Oscillatory Wetting Phenomena with Contact Angle Hysteresis

A recently published experimental study by Xia and Steen examines the connection between the contact line velocity and contact angle of liquid drops on an oscillating substrate that display contact angle hysteresis. Of particular interest in this experimental study is the analysis of the dependence of contact angle deviation on contact line velocity. Indeed it is found that for small angular displacements, there is a linear relationship between the two. Moreover, the oscillating drop exhibits contact angle hysteresis that is much greater than that measured from quasi-static experiments. Here we use a phase-field model of dynamic wetting which directly includes the contact angle hysteresis to simulate the results of the aforementioned authors. A thorough derivation of the governing equations is presented, starting from the pioneering work of Cahn and Hilliard. Our model is unique due to the explicit inclusion of contact angle hysteresis, a notoriously difficult physical phenomenon to model mathematically. By choosing appropriate parameters, our model can achieve very good agreement with experimental data. Further, we investigate the effects of contact line friction and the hysteresis window, which are otherwise very difficult to explore experimentally.

Chenyang Cao
Purdue University

A fast stable matrix form to some transforms

In this talk, we present a fast stable matrix-version method for evaluating the discretized transforms in one dimension, such as Gaussian transform, Hilbert transform. With the help of exponential expansions and diagonal form of translation, the kernel matrices from these transforms can be quickly approximated into structured matrices called sequentially semiseparable (SSS) matrices. Further, we can transfer SSS matrix representation to hierarchical semiseparable (HSS) matrix representation, which would be a more stable form for evaluating. Numerical experiments will be demonstrated on the performance and accuracy of evaluations.

Yue Cao
Illinois Institute of Technology

Kernel free boundary integral method and its application

We developed a kernel-free boundary integral method (KFBIM) for solving variable coefficients partial differential equations (PDEs) in a doubly-connected domain. We focus our study on boundary value problems (BVP) and interface problems. A unique feature of the KFBIM is that the method does not require an analytical form of the Green's function for designing quadratures, but rather computes boundary or volume integrals by solving an equivalent interface problem on Cartesian mesh. The method has second-order accuracy in space, and its complexity is linearly proportional to the number of mesh points. Numerical examples demonstrate that the method is robust for variable coefficients PDEs, even for cases when diffusion coefficients ratio is large and when two interfaces are close. We also develop two methods to compute moving interface problems whose coefficients in governing

equations are spatial functions. Variable coefficients could be a non-homogeneous viscosity in Hele-Shaw problem or an uptake rate in tumor growth problems. The methods have second-order accuracy in both space and time. Machine learning techniques have achieved magnificent success in the past decade. We couple the KFBIM with supervised learning algorithms to improve efficiency. In the KFBIM, we apply a finite difference scheme to find dipole density of the boundary integral iteratively, which is quite costly. We train a linear model to replace the finite difference solver in GMRES iterations. The cost, measured in CPU time, is significantly reduced. We also developed an efficient data generator for training and derived an empirical rule for data set size.

Zhen Chao
University of Michigan

Integral method for solving one-dimensional Poisson-Nernst-Planck ion channel model

A system of Poisson-Nernst-Planck (PNP) dielectric continuum model has been used to describe the dynamics of ion transport through biological ion channels besides being widely employed in semiconductor industry. Most of the existing literature focus on the finite difference method and finite element method for solving PNP system. In this talk, we employ the integral method with the Gummel iteration method to solve the one-dimensional (1D) steady state PNP system. We describe the 1D steady state PNP model and the implementation of our numerical method. Several numerical examples are presented to show the stability and usefulness of the numerical method, we notice that the integral method with Gummel iteration still works for high electrostatic potential and nonelectroneutral cases without using Slotboom transformation.

Neophytos Charalambides
University of Michigan

Orthonormal Sketches for Secure Coded Regression

We propose a method for speeding up linear regression distributively, while ensuring security. We leverage randomized sketching techniques, and improve straggler resilience in asynchronous systems. Specifically, we apply a random orthonormal matrix and then subsample in blocks, to simultaneously secure the information and reduce the dimension of the regression problem. In our setup, the transformation corresponds to an encoded encryption in an approximate gradient coding scheme, and the subsampling corresponds to the responses of the non-straggling workers; in a centralized coded computing network. We focus on the special case of the Subsampled Randomized Hadamard Transform, which we generalize to block sampling; and discuss how it can be used to secure the data. We illustrate the performance through numerical experiments.

Jiahui Chen
Michigan State University

Evolutionary de Rham-Hodge method

The de Rham-Hodge theory is a landmark of the 20th Century's mathematics and has had a great impact on mathematics, physics, computer science, and engineering. This work introduces an evolutionary de Rham-Hodge method to provide a unified paradigm for the multiscale geometric and topological analysis of evolving manifolds constructed from a filtration, which induces a family of evolutionary de Rham complexes. While the present method can be easily applied to close manifolds, the emphasis is given to more challenging compact manifolds with 2-manifold boundaries, which require appropriate analysis and treatment of boundary conditions on differential forms to maintain proper topological properties. Three sets of unique evolutionary Hodge Laplacians are proposed to generate three sets of topology-preserving singular spectra, for which the multiplicities of zero eigenvalues correspond to exactly the persistent Betti numbers of dimensions 0, 1, and 2. Additionally, three sets of non-zero eigenvalues further reveal both topological persistence and geometric progression during the manifold evolution. Extensive numerical experiments are carried out via the discrete exterior calculus to demonstrate the potential of the proposed paradigm for data representation and shape analysis. To demonstrate the utility of the proposed method, application is considered to the protein B-factor predictions of a few challenging cases for which other existing models do not work well.

Siu Wun Cheung
Lawrence Livermore National Laboratory

Multiscale and numerical upscaling methods for physical processes in high contrast heterogeneous porous media

Many applications related to subsurface formations requires accurate numerical simulations in high contrast heterogeneous porous media, in which the material properties within fractures can have a large difference from the material properties in the background media, which can also contain highly heterogeneous and high contrast regions. These large contrasts in material properties and the complex geometries of the fractures lead to difficulties in traditional numerical simulations due to the fact that solutions contain various scales and resolving these scales requires huge computational costs. In this talk, we will discuss the development of several multiscale and upscaling methods for physical processes in high contrast heterogeneous porous media, which aims at efficiently compute numerical approximations by formulating coarse-scale equations for dominant components of the solution representation. Using the concepts of model order reduction and localized energy minimization, we develop multiscale and numerical upscaling methods which significantly reduces the problem size and exhibits convergence with respect to the coarse mesh size. We will discuss recent developments in multiscale methods, such as online adaptivity and iterative oversampling techniques in basis constructions.

Emmanuel Djegou
Missouri University of Science and Technology

To be determined.

To be determined.

Andrés Galindo Olarte
Michigan State University

Accuracy enhancement of discontinous Galerkin solutions for Vlasov-Maxwell equations

In this talk, we will establish negative-order estimates for the accuracy of discontinuous Galerkin (DG) approximations to smooth solutions for the Vlasov-Maxwell (VM) system of equations. For the approximated solutions, we are able to extract this "hidden accuracy" through the use of a Smooth-Increasing Accuracy-Conserving (SIAC) filter which is a convolution kernel that is composed of a linear combination of B-splines. We provide rigorous error estimates for the DG solutions that show improvement to $(2k + 1/2)$-th order in the negative-order norm.

Xiaoming He
Missouri University of Science and Technology

PIFE-PIC: Parallel Immersed-Finite-Element Particle-in-Cell for 3-D kinetic simulations of plasma-material interactions

In this presentation, we present a recently developed particle simulation too PIFE-PIC, which is a novel three-dimensional (3-D) Parallel Immersed-Finite-Element (IFE) Particle-in-Cell (PIC) simulation model for particle simulations of plasma-material interactions. This framework is based on the recently developed non-homogeneous electrostatic IFE-PIC method, which is designed to handle complex plasma-material interface conditions associated with irregular geometries using a Cartesian-mesh-based PIC. Three-dimensional domain decomposition is utilized for both the electrostatic field solver with IFE and the particle operations in PIC to distribute the computation among multiple processors. A simulation of the orbital-motion-limited (OML) sheath of a dielectric sphere immersed in a stationary plasma is carried out to validate PIFE-PIC and profile the parallel performance of the code package. Parallel efficiency up to approximately 110 superlinear speedup was achieved for strong scaling test. Furthermore, a large-scale simulation of plasma charging at a lunar crater containing 2 million PIC cells (10 million FE/IFE cells) and about 1 billion particles, running for 20,000 PIC steps in about 154 wall-clock hours, is presented to demonstrate the high-performance computing capability of PIFE-PIC.

Tamas Horvath
Oakland University

Sliding grid techniques for Space-Time Hybridizable Discontinuous Galerkin methods

The Space-time Discontinuous Galerkin (ST-DG) method is an excellent method to discretize problems on deforming domains. This method uses DG to discretize both the spatial and temporal directions, allowing for an arbitrarily high order approximation in space and time. We present a higher-order accurate Embedded-Hybridized Discontinuous Galerkin method for fluid-rigid body interactions. We apply a sliding grid technique or rotational movement that can handle arbitrary rotation. The numerical examples will include galloping and fluttering motions.

Ziyang Huang
University of Michigan

Modeling multiphase problems with the consistent and conservative Phase-Field method

In the presentation, I will introduce the consistent and conservative Phase-Field method that addresses issues of coupling the Phase-Field modeling techniques to hydrodynamics, mass or heat transfer, and phase changes. Thanks to the proposed consistency conditions, the method results in multiphase models that enjoy not only the conservation of mass and momentum, but also the kinetic energy conservation and Galilean invariance, independent of the choice of the Phase-Field models to capture the interfaces or of the number and material properties of the phases. As a result, the mechanical and thermal equilibrium is guaranteed for arbitrarily large ratios of density and thermal capability. In the method, a volume distribution algorithm is developed to eliminate the production of fictitious phases, local voids, or overfilling, but simultaneously ensure the conservation and boundedness of the Phase-Field function.

Yue Kang
Michigan Technological University

Bound-preserving discontinuous Galerkin methods with second-order implicit pressure explicit concentration time marching for compressible miscible displacements in porous media

In this talk, I will introduce the bound-preserving interior penalty discontinuous Galerkin (IPDG) methods with a second-order implicit pressure explicit concentration (SIPEC) time marching for the coupled system of two-component compressible miscible displacements. The SIPEC method is based on the traditional second-order strong-stability-preserving Runge-Kutta (SSP-RK2) method. The main idea is to treat the pressure equation implicitly and the concentration equation explicitly. However, this treatment would result in a first-order accurate scheme. Therefore, we propose a correction stage to compensate for the second-order accuracy in each time step. We can deal with the velocity in the diffusion term explicitly to avoid correction of the diffusion term. Also, we need to ensure that the bound-preserving technique for the convection and source terms can be applied when the correction stage has been established. In fact, in the correction stage, the new approximation to the concentration can be chosen as the numerical solution in the previous stage, so the numerical cell averages are positivity-preserving. Numerical experiments will be given to demonstrate that the proposed scheme can reduce the computational cost significantly.

Yann-Meing Law
Michigan State University

The Hermite-Taylor Correction Function Method for Maxwell's Equations

Hermite-Taylor methods are high-order methods for hyperbolic problems that rely on a Hermite interpolation procedure in space and a Taylor method in time. The stability condition

of these methods depends only on the largest wave-speed, independent of the order. However, the treatment of general boundary conditions is still a challenge since these methods require not only to know the electromagnetic fields on the boundary but also their m first derivatives in space to achieve a $(2m+1)$-order method. In this talk, we investigate the Correction Function Method (CFM) to seek all the needed information on the boundary in the Hermite-Taylor setting. The CFM relies on the minimization of a functional based on Maxwell?s equations. This minimization problem has to be solved for only some nodes in the vicinity of the boundary at each time step. Numerical examples in 1-D and 2-D are performed and the expected convergence order is observed for reasonable values of m.

Ying Liang
Purdue University

Least-squares method for recovering multiple medium parameters

We present a two-stage least-squares method for inverse medium problems of reconstructing multiple unknown coefficients simultaneously from noisy data. A direct sampling method is applied to detect the location of the inhomogeneity in the first stage, while a total least-squares method with a mixed regularization is used to recover the medium profile in the second stage. The total least-squares method is designed to minimize the residual of the model equation and the data fitting, along with an appropriate regularization, in an attempt to significantly improve the accuracy of the approximation obtained from the first stage. We shall also present an analysis on the well-posedness and convergence of this algorithm. Numerical experiments are carried out to verify the accuracies and robustness of this novel two-stage least-squares algorithm, with high tolerance of noise in the data.

Min-Jhe Lu
Illinois Institute of Technology

Mechano-chemical Tumor Models: An Energetic Variational Approach

The building of the mechano-chemical tumor models aims to understand how the two key factors of (1) the mechanical interaction between the tumor cells and their surroundings, and (2) the biochemical reactions in the microenvironment of tumor cells can influence the dynamics of tumor growth. The mechanical interaction, realized by pressure or force between cells, is in view of the experimental discovery of microskeletons within cells, which give them mechanical strength. The biochemical reactions are involved with chemical species which either supply tumor with nutrients or change the cell cycle events of a tumor cell population. In this talk I will demonstrate how we apply the Energetic Variational Approach to build such models. The numerical simulation results in both sharp interface and diffuse interface (phase-field) formulation will also be given. This is a joint work with Prof. Chun Liu, Prof. John Lowengrub, Prof. Shuwang Li, Dr. Yiwei Wang and Dr. Huaming Yen.

Songting Luo
Iowa State University

A Fixed-point Iteration Method for High Frequency Helmholtz Equations

In order to obtain globally valid solutions for high frequency Helmholtz equations efficiently without "pollution effect", we will transfer the problem into a fixed-point problem related to an exponential operator, and the associated functional evaluations are achieved by unconditionally stable operator-splitting based pseudospectral schemes such that large step sizes are allowed to reach the approximated fixed point efficiently for prescribed accuracy requirement. Both two-dimensional and three-dimensional numerical experiments are presented to demonstrate the method.

Zachary Miksis
University of Notre Dame

Parallel implementation of a sparse grid fast sweeping WENO method for Eikonal equations

Fixed-point fast sweeping methods are a class of explicit iterative methods developed in the literature to efficiently solve steady state solutions of hyperbolic PDEs. They are explicit and do not involve inverse operation of any nonlinear local system. Hence they are robust and flexible, and have been combined with high order WENO schemes to solve various hyperbolic PDEs in the literature. For multidimensional nonlinear problems, high order fixed-point fast sweeping WENO methods still require quite large amount of computational costs. We apply sparse-grid techniques, a naturally parallelizable and effective approximation tool for multidimensional problems, to reduce the computational costs of fixed-point fast sweeping WENO methods. Here we focus on a robust Runge-Kutta (RK) type fixed-point fast sweeping WENO scheme with third order accuracy for solving Eikonal equations, an important class of static Hamilton-Jacobi (H-J) equations. Numerical experiments on solving multidimensional Eikonal equations in parallel are performed to show that the sparse grid computations of the scheme achieve large savings of CPU times, and at the same time maintain comparable accuracy and resolution with those on corresponding regular single grids. This work is by Zachary Miksis and Yong-Tao Zhang.

Van Hoang Nguyen
Mississippi State University

Efficient exponential methods for genetic regulatory systems

In recent years, gene regulatory networks (GRNs) have attracted a lot of interest as they play a crucial role in modeling the protein regulation processes. Among many numerical schemes which were introduced for simulating these systems, the classical fourth-order Runge-Kutta method (RK4) has been often used. When simulating GRNs, it is difficult to characterize some important properties of the system, such as stability and phase properties. Very recently, splitting methods, exponentially fitted two-derivative Runge-Kutta (EFTDRK) methods and classical exponential Runge-Kutta (ExpRK)-type methods have been also considered. In this work, we propose a class of partitioned ExpRK methods and exponential Rosenbrock methods for the simulation of genetic regulatory systems. Moreover, we also investigate the stability and phase properties of the proposed schemes. Finally, based on a set of benchmark test problems including two- and three-gene systems, we demonstrate the accuracy and efficiency of the newly derived methods in comparison with several popular schemes. This talk is based on a joint work with Vu Thai Luan and Julius Ehigie.

Zhichao Peng
Michigan State University

EM-WaveHoltz: a flexible frequency-domain Maxwell solver built from time-domain solvers

Two main challenges to design efficient iterative solvers for the frequency-domain Maxwell equations are the indefinite nature of the underlying system and the high resolution requirements. Scalable parallel frequency-domain Maxwell solvers are highly desired. This talk will introduce the EM-WaveHoltz method which is an extension of the recently developed Wave-Holtz method for the Helmholtz equation to the time-harmonic Maxwell equations. Three main advantages of the proposed method are as follows. (1) It always results in a positive definite linear system. (2) Based on the framework of EM-WaveHoltz, it is flexible and simple to build efficient frequency-domain solvers from current scalable time-domain solvers. (3) It is possible to obtain solutions for multiple frequencies in one solve. The formulation of the EM-WaveHoltz and analysis in the continuous setting for the energy conserving case will be discussed. The performance of the proposed method will be demonstrated through numerical experiments.

Devina Sanjaya
University of Tennessee, Knoxville

Global mesh optimization: Is it worth the cost?

Global mesh optimization is a natural approach when we view meshing as a method to connect geometry nodes, construct valid mesh elements of certain types, and arrange these elements to cover the entire computational domain. From this viewpoint, we can easily see that the effect of one node movement will propagate not only to all of the neighboring elements, but also to the entire domain. Hence, one may argue that global mesh optimization is simply too expensive and impractical. However, if we were to overcome the cost barrier, global mesh optimization could significantly improve the accuracy and robustness of computational simulations, closely couple multiple mesh adaptation techniques, eliminate heuristics in meshing, and fully automate meshing procedures. In this talk, I will describe several ongoing efforts in developing effective optimization problem formulations and architectures as well as identify the main challenges. The talk will be presented in the context of high-order, finite-element meshes, and in this context, one may view global mesh optimization as a way to capture the global coupling between the optimal placement of element?s vertices and high-order geometry nodes within the computational domain. The ultimate goal is to build an automated, high-order meshing suite for maximizing the accuracy and robustness of computational fluid dynamics (CFD) simulations while efficiently using the high-performance computing (HPC) systems to reduce human workload.

Qicang Shen
University of Michigan

High-order accurate solution of the spatial kinetics problem for nuclear reactor simulation using the spectral deferred correction method

Solving initial value problems with high-order methods receives considerable attention in many fields because these methods can potentially improve the accuracy of the simulation results with lower computational cost than low-order methods. Most methods, however, are either complicated to implement or unstable when the order of accuracy is high. The Spectral Deferred Correction (SDC) method is a stable, robust, and efficient high-order time-integration scheme capable of an arbitrary order of accuracy. We apply the SDC method to solve the time-dependent diffusion equation of the spatial kinetics problem of the nuclear reactor. We will present how we combine the SDC with the common-used low-order methods for modeling the spatial kinetics models. Numerical results will be presented. The investigations made here can provide the foundation for future investigations on simulating the neutron transport problem using the high-order methods both for the spatial discretization and time integration.

Somveer Singh
Indian Institute of Technology BHU Varanasi, India

Numerical analysis of nonlinear weakly singular integro-partial differential equations arising from viscoelasticity

An efficient matrix method is presented for the solution of non-linear weakly singular partial integro-differential equation (SPIDE) arising from viscoelasticity subject to the given initial and boundary conditions. The method is based on the operational matrices of Legendre wavelets. By implementing the operational matrices of Legendre wavelets, the given intero-PDE is reduces to the system of nonlinear equations. Some useful results concerning the convergence and error estimates associated to the suggested scheme are presented. Illustrative examples are provided to show the effectiveness and accuracy of proposed numerical method.

Siddhartha Srivastava
University of Michigan

Non-local calculus on graphs with application to reduced order modeling

Due to the expense and complexity of numerically solving Partial Differential Equations (PDE), high fidelity simulations do not lend themselves to typical engineering design and decision-making, which must instead rely on reduced-order models. We present an approach to reduced-order modeling that builds off recent graph-theoretic work for representation, exploration, and analysis on computed states of physical systems [1]. This graph-theoretic framework consists of representing a physical system with a discrete manifold, where high fidelity and high dimensional states are mapped to vertices on a graph, with a lower-dimensional state vector associated with each vertex. Weighted edges between vertices can then be assigned, or found through graph-theoretic principles, indicating relationships or transitions between states and the magnitude of such correlations. We extend a non-local calculus on finite weighted graphs [2] to build models by exploiting polynomial expansions and the Taylor series, making graph-based representation amenable to modeling the PDE system. We analyze the consistency of the non-local derivatives in this setting, a crucial requirement for numerical applications. We show that the weight of the graph can be fine-tuned to achieve arbitrary order of accuracy in any number of dimensions without any assumptions

of symmetry in the underlying data. Finally, applications of the method are demonstrated by extracting reduced-order models in the form of ordinary differential equations from parabolic partial differential equations of progressive complexity.

[1] Banerjee, R., et al. "A graph theoretic framework for representation, exploration and analysis on computed states of physical systems." Computer Methods in Applied Mechanics and Engineering 351 (2019): 501-530.

[2] Gilboa, Guy, and Stanley Osher. "Nonlocal operators with applications to image processing." Multiscale Modeling & Simulation 7.3 (2009): 1005-1028.

Jiguang Sun

Michigan Technological University

Local estimators and Bayesian inverse problems with non-unique solutions

The Bayesian approach is effective for inverse problems. The posterior density distribution provides useful information of the unknowns. However, for problems with non-unique solutions, the classical estimators such as the maximum a posterior (MAP) and conditional mean (CM) are not suitable. We introduce two new estimators, the local maximum a posterior (LMAP) and local conditional mean (LCM). A simple algorithms based on clustering to compute LMAP and LCM is proposed. Their applications are demonstrated by three inverse problems: an inverse spectral problem, an inverse source problem, and an inverse medium problem.

Luan Vu Thai

Mississippi State University

High-order efficient multirate infinitesimal step-type methods

Multirate time integrators use different time steps for integrating different components of multiphysics systems, thereby increasing computational efficiency over classical time integration methods. So far, multirate schemes of orders up to four have been proposed in the literature such as MIS or MRI-GARK methods. Their derivations, however, require solving a complicated set of coupling and decoupling order conditions, which pose difficulties to construct higher orders. In this talk, we propose a new family of high-order multirate time integrators based on recent developed exponential Runge-Kutta/Rosenbrock methods, thereby named MERK/MERB methods. They can be classified as MIS-type methods. Their rigorous convergence analysis was carried out. Schemes up to order 6 have been constructed in an elegant way. Moreover, these new schemes allow to use a smaller number of modified differential equations in each step when compared to existing MIS or MRI-GARK of the same orders. Numerical experiments are given to demonstrate the accuracy and efficiency of the newly derived MERB schemes.

Chunmei Wang

University of Florida

A New Numerical Method for Div-Curl Systems with Low Regularity Assumptions

The speaker will present a numerical method for div-curl systems with normal boundary conditions by using a finite element technique known as primal-dual weak Galerkin (PDWG). The PDWG finite element scheme for the div-curl system has two prominent features in that it offers not only an accurate and reliable numerical solution to the div-curl system under the low Hα-regularity ($\alpha > 0$) assumption for the true solution, but also an effective approximation of normal harmonic vector fields regardless the topology of the domain.

Lei Wang
University of Wisconsin, Milwaukee

Application of the Barycentric Lagrange Treecode for Computing Correlated Random Displacements Using the Spectral Lanczos Decomposition Method

In Brownian Dynamics simulations, correlated random displacements $\mathbf{g} = \sqrt{D}\mathbf{z}$ can be computed using the Spectral Lanczos Decomposition Method (SLDM), where D is the diffusion matrix based on the Rotne-Prager-Yamakawa tensor and $\mathbf{z}$ is a normal random vector. Each step of the SLDM requires computing a matrix-vector product $D\mathbf{q}_k$, where $\mathbf{q}_k$ is the kth Lanczos vector. The present work applies the barycentric Lagrange treecode (BLTC) to accelerate the matrix-vector product in the SLDM. Numerical results show the performance of the SLDM-BLTC in serial and parallel simulations.

Dexuan Xie
University of Wisconsin-Milwaukee

A new nonlinear iterative scheme for solving a nonuniform size modified Poisson-Boltzmann ion channel model

The nonuniform size modified Poisson-Boltzmann ion channel (nuSMPBIC) model is difficult to solve numerically due to that it is not only an exponentially nonlinear system with strong solution singularity but also involves an interface boundary value problem defined in a box domain with three complex regions (an ion channel protein region, a solvent region, and a membrane region) and multiple nonlinear algebraic equations defined on the solvent region only. To overcome these numerical difficulties, we recently developed novel iterative technique and an effective nonlinear iterative scheme for solving the nuSMPBIC model. Moreover, this new scheme has been implemented as a finite element program package, which works for an ion channel protein with a three-dimensional molecular structure and a mixture solution of multiple ionic species with distinct ion sizes. In this talk, I will describe the construction of this new scheme. I then will report numerical results to demonstrate the fast convergence of the new nonlinear iterative scheme and the high performance of the nuSMPBIC finite element software. This work is partially supported by the Simons Foundation, USA, through research award 711776.

Yang Yang
Michigan Technological University

Stability analysis of the Eulerian-Lagrangian finite volume methods for nonlinear hyperbolic equations in one space dimension

In this talk, we construct a novel Eulerian-Lagrangian finite volume (ELFV) methods for nonlinear scalar hyperbolic equations in one space dimension. It is well known that the exact solutions to such problems may contain shocks though the initial conditions are smooth, and direct numerical methods may suffer from restricted time step sizes. To relieve the restriction, we propose the ELFV method, where the space-time domain was partitioned based on the characteristics that originated from the cell interfaces in the spatial domain. Unfortunately, to avoid the intersection of the characteristics, the time step sizes are still limited. To fix this gap, we detect ETCs and carefully design the influence region of each ETC within which the cells are merged together to form a new one. Then with the new partition of the space-time domain, it is possible to gain larger time step sizes. Moreover, we theoretically prove that the proposed first-order scheme with Euler forward time discretization is total-variation-diminishing and maximum-principle-preserving. Numerical experiments verify the optimality of the designed time step sizes.

Zhonggang Zeng
Northeastern Illinois University

Newton's iteration at nonisolated solutions

The textbook Newton's iteration has been unnecessarily restricted to isolated solutions of square systems with nonsingular Jacobian. As a recent discovery, Newton's iteration can easily be applied to nonsquare systems with nonisolated solutions and rank-deficient Jacobians while maintaining quadratic convergence. This talk will elaborate on the extension of Newton's iteration, its quadratic convergence on nonisolated solutions, and a wide range of applications in solving of nonlinear systems of equations.

Will Zhang
University of Michigan

Fractional Viscoelastic Modeling of Cardiovascular Soft Tissues

While experimental evidence shows that the mechanical response of most tissues is viscoelasticity, current biomechanical models used in computational studies often assume only hyperelasticity. Fractional viscoelastic constitutive models have been successfully used in literature to capture the material response. However, the translation of these models into computational platforms remains limited due to a computational cost that is $O(N_T^2)$ and a storage cost that is $O(N_T)$ in order to store and integrate historical data. We developed a novel numerical approximation to the Caputo derivative which exploits a recurrence relation to give a computational cost that is $O(N)$ and a storage cost that is fixed over time. We used this approach to extend the conventional analysis of residual stress in aortic soft tissues by considering the effects of viscoelasticity. A substantial portion viscoelastic tissue is necessary to capture the long-term dynamics of the residual stress experiment. In addition, the results show that conventional estimates of residual stress are over-estimated a factor of 2 and that viscoelasticity is necessary to accurately estimate residual strain. Using this approach, we developed a fractional viscoelastic model for myocardium that improves the quality of fit compared to current models in the literature. We analyzed the numerical properties of this approach using simplified examples and application in simulations of the right ventricle. These results demonstrates that fractional viscoelasticity has enormous potential for facilitating the analysis of viscoelastic properties of soft biological tissues in computational problems.

Fangyao Zhu
Michigan Technological University

Discontinuous Galerkin methods with Patankar time discretization for chemical reacting flow

I will talk about bound-preserving modified Patankar scheme with discontinuous Galerkin (DG) methods for chemical reactive flows. For this problem, the physical density and pressure must be kept positive. We start from production-destruction equations. Using the idea of the high order modified Patankar Runge-Kutta, we adapt it to multi-step method. Coupled with this time integration method, we use bound-preserving discontinuous Galerkin method in space to preserve those physical properties. Numerical examples will be shown.

Jovan Zigic
Virginia Polytechnic Institute and State University

A Splitting Approach to Dynamic Mode Decomposition of Nonlinear Systems

Reduced-order models have long been used to understand the behavior of nonlinear partial differential equations. Naturally, reduced-order modeling techniques come at the price of computational accuracy for a decrease in computation time. Optimization techniques are studied to improve either or both of these objectives and decrease the total computational cost of the problem. This talk focuses on the dynamic mode decomposition (DMD) applied to nonlinear PDEs with periodic boundary conditions. It provides a study of a newly proposed optimization framework for the DMD method called the Split DMD.

Jörn Zimmerling
University of Michigan

Reduced order model approach to inverse scattering

In this talk, we approach imaging problems from the angle of reduced order modeling. We consider an inverse scattering problem, where data are gathered by arrays of sensors that probe an unknown heterogeneous medium with waves and measure the scattered returns. Rather than asking the question "which scattering medium could have caused the measured wave returns" directly, we first construct a reduced-order model from the measured data. Using this reduced order model, we can approximate the field inside the unknown medium. Using these internal waves, we propose novel qualitative and quantitative approaches to solve inverse scattering problems and locate scatters.

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6 Posters

Ali Akhtari
University of Michigan - Dearborn

Magnetoconvection in a long vertical enclosure with walls with finite electrical conductivity

First results of implementation of a new solver for magnetohydrodynamic flows of liquid metals with natural convection are presented. A nearly fully conservative finite-difference scheme, which is known to improve accuracy and efficiency of simulations in the case of strong magnetic field effects, is combined with a tensor-product-Thomas solution of elliptic problems. The method is adapted to flows in domains with thin walls of finite electric conductivity and validated for a magnetoconvection flow in a long vertical box. The effects of wall electrical conductivity and the strength of the magnetic field are explored.

Vishwas Goel
University of Michigan

Simulation-based Optimization of the HOLE Architecture to Enable Fast Charging in Energy-Dense Li-ion Batteries

Li-ion batteries that are used in electric vehicles (EVs) primarily suffer from three main issues - limited capacity, slow charging, and fire outbreaks. The issue of limited capacity can be solved by designing energy-dense batteries, which entails the use of thick electrodes with low porosity. However, such an electrode design proves to be too tortuous for the transport of Li-ions with the electrode, which limits the charging rate. Furthermore, a graphite anode (most common anode material) based on this design is highly susceptible to Li-plating under fast charging conditions. Thus, it can be said that all three issues cannot be overcome by employing the conventional electrode design. To overcome these challenges, we have developed the Highly Ordered Laser-patterned Electrode (HOLE) architecture, which enables fast charging (6C) in energy dense electrodes ($\sim$ 3 mAh/cm2) while eliminating the Li plating susceptibility, and thereby, solving the Li-plating caused fire outbreak issues in conventional Li-ion batteries.

Spencer Lee
Michigan State University

Numerical Methods for Highly Oscillatory Problems in Quantum Computing

We present a numerical methods tailored for Schrödinger equations with time dependent Hamiltonians and rapidly oscillating solutions, such as those arising in the modeling of controlled qudits. Our method discretizes the Picard form of the ordinary differential equation (ODE) by Filon quadrature. The method is implicit but the size of the linear system is always the dimension of the ODE independent of order. We illustrate that the new method is superior to the classic RK4 method.

Robert Malinas
University of Michigan

Change Detection for High-Dimensional Covariance Using Random Matrix Theory

Time series data often violates stationarity assumptions that are crucial to the success of most analysis methods. We introduce a novel test of stationarity based on random matrix theory. The test uses the spectral distribution of the sample covariance to detect deviations from second-order stationarity under the single change point model: the covariance matrix changes once over the observation interval. Using random matrix theory and free probability, we develop a statistic that is asymptotically zero for all indices under the null hypothesis under which no change is present. Furthermore, we show that the statistic is asymptotically maximized at the true change point with high probability under the alternative hypothesis. This yields a procedure by which we can detect a change in covariance by thresholding and subsequently estimate the change point by maximizing the statistic over the observed indices.

Som Phene
University of Michigan Ann Arbor

Perturbed Steklov Eigenvalues via Asymptotic Analysis

We detect presence of impurities in a material by calculating Asymptotic series for Steklov Eigenvalue expansion.

Amit Rotem
Michigan State University

The WaveHoltz Heterogeneous Multiscale Method

We present the WaveHoltz Heterogeneous Multiscale Method (HMM), an iterative method for efficiently computing the homogenized solution to the Helmholtz equation with highly oscillatory variable coefficients that would make a direct numerical simulation prohibitively expensive. Unlike other numerical methods for the Helmholtz equation which directly discretize in the frequency domain, the WaveHoltz method discretizes in the time domain and iterates on the wave-equation. The WaveHoltz operator has many benefits: it is positive definite, has a bounded condition number, and is highly parallelizable. We solve the wave-equation within the WaveHoltz iteration via the HMM which finds the homogenized solution to the wave-equation with highly oscillatory coefficients without having to resolve the high-frequency information on the entire domain. When combined the WaveHoltz HMM is a highly efficient iterative method for computing the homogenized solution to the Helmholtz equation and has the additional benefit that, when compared to other multiscale methods which directly solve the elliptic problem, WaveHoltz HMM does not introduce additional error from artificial numerical boundary conditions.

Marc Tunnell
Grand Valley State University

bf Fast Gaussian Process Emulation of Mars Global Climate Model

The NASA Ames Mars Global Climate Model (MGCM) software has been in steady use at NASA for decades and was recently released to the public. This model simulates the complex interactions of various weather cycles that exist on Mars, namely the Dust Cycle, the CO2 Cycle, and the Water cycle. Utilized by NASA, the MGCM is used to help understand their empirically observed data through the use of sensitivity studies. However, these sensitivity studies are computationally taxing, requiring weeks to run. To address this issue, we have developed a surrogate model using Gaussian processes (GP) that can emulate the output of this model with relatively small amounts of data in a reduced amount of time (on the order of minutes). We demonstrate the effectiveness of our emulator using backward error analysis.