MID-ATLANTIC NUMERICAL ANALYSIS DAY

A one-day conference on Numerical Analysis and Scientific Computing for graduate students and post-doctorates from the Mid-Atlantic region

Department of Mathematics

Friday, November 10, 2023 | Philadelphia, PA

Organizers: Benjamin Seibold and Daniel B. Szyld

Temple University

Schedule (Friday, November 10, 2023)

9:15am–9:50am	Registration and Breakfast (provided)
9:50am–10:00am	Opening Remarks
10:00am–11:00am	**Presentations** (Discretization, Interpolation, Sampling)
11:00am–11:20am	*Coffee Break*
11:20am–12:00pm	**Presentations** (Numerical Linear Algebra)
12:00pm–1:30pm	Posters and Lunch (provided)
1:30pm–2:30pm	**Keynote Lecture** (Lois Curfman McInnes)
2:30pm–2:45pm	*Coffee Break*
2:45pm–3:25pm	**Presentations** (Model Reduction)
3:25pm–3:45pm	*Coffee Break*
3:45pm–4:45pm	**Presentations** (Applications)
4:45pm–5:55pm	Closing Remarks
5:30pm–7:30pm	Group Dinner (attendance optional)

Speakers

Discretization, Interpolation, Sampling (10:00am~11:00am)

GUILLAUME BONNET, UNIV. OF MARYLAND, COLLEGE PARK
   Monotone discretization of degenerate elliptic equations using Voronoi's first reduction of quadratic forms

RICHARD CONNOR GREENE, NJIT
   Efficient polynomial interpolation on the square and cube

SHANYIN TONG, COLUMBIA UNIVERSITY
   Large deviation theory-based adaptive importance sampling for rare events in high dimensions

Numerical Linear Algebra (11:20am~12:00pm)

SARAH GIFT, DREXEL UNIVERSITY
   Real factorization of PSD matrix polynomials

ANDREW HIGGINS, TEMPLE UNIVERSITY
   Analysis of randomized Householder-Cholesky QR

Posters and Demos (12:00pm~1:30pm)

AHMET KAAN AYDIN, UNIVERSITY OF MARYLAND, BALTIMORE COUNTY
   Several robust model reductions for the boundary feedback stabilization of fully magnetic piezoelectric smart beams

LUKE EVANS, FLATIRON INSTITUTE
   Target measure diffusion maps: Sharp error analysis and spatial subsampling

GABRIEL PROVENCHER LANGLOIS, NEW YORK UNIVERSITY
   Robust sparse regression using Hamilton-Jacobi equations, gradient inclusions and screening rules

RISHAD ISLAM SHANTHO, LEHIGH UNIVERSITY
   Analysis of exact and approximate map for linear systems arising in discretized PDEs

JACOB WOODS, NOUR KHOUDARI, MENGSHA YAO, and NICOLE ZALEWSKI, TEMPLE UNIVERSITY
   Swarming and instabilities in multi-agent systems

JIAXING LIANG, UNIVERSITY OF MARYLAND
   Efficient Computational Algorithms for Magnetic Equilibrium in a Fusion Reactor

Keynote Lecture (1:30pm~2:30pm)

LOIS CURFMAN MCINNES, ARGONNE NATIONAL LIBRARY

Lear Scientific software ecosystems and communities: Why we need them and how each of us can help thrive

Model Reduction (2:45pm~3:25pm)

SEAN JOSEPH REITER, VIRGINIA TECH

Generalizations of data-driven balancing: What do you need to sample for different balancing-based reduced models?

MICHAEL S. ACKERMANN, VIRGINIA TECH

Frequency-based reduced order models from purely time-domain data

Applications (3:45pm~4:45pm)

QINYING CHEN, UNIVERSITY OF DELAWARE

2D fluid model and simulations for evaporation-driven tear film thinning

KIERA ELOISE KEAN, TEMPLE UNIVERSITY

Moment methods for advection on networks and applications in life cycle models

RUJEKO CHINOMONA, TEMPLE UNIVERSITY

StaRMAP: Simple, efficient, and flexible simulation software for radiation transport

Abstracts of Talks

Discretization, Interpolation, Sampling (10:00am–11:00am)

GUILLAUME BONNET, UNIV. OF MARYLAND, COLLEGE PARK

Monotone discretization of degenerate elliptic equations using Voronoi's first reduction of quadratic forms

Degenerate elliptic equations are a class of second-order equations whose analysis relies on the maximum principle. A natural requirement for discretizations of such equations is to satisfy a property of monotonicity. This property can be seen as a nonlinear generalization of the Z-matrix property in linear algebra, and leads to a discrete maximum principle. I will show how a matrix decomposition based on Voronoi's first reduction, a tool originating from the theory of low-dimensional lattice geometry, can be used to build efficient monotone discretizations of anisotropic or nonlinear second-order operators. I will then present an application to the Monge-Ampère equation arising in fields such as optimal transport and nonimaging optics. In this setting, some obstructions prevent the direct application of the standard theory of monotonicity. I will explain how they can be overcome, and show some numerical results in the context of far-field refractor design.

RICHARD CONNOR GREENE, NJIT

Efficient polynomial interpolation on the square and cube

Polynomial interpolation is a ubiquitous tool in numerical analysis. We present a method for deriving collocation points that attain faster convergence in integration and interpolation errors than standard tensor-product Chebyshev points in 2 and 3 dimensions, with ready generalization to higher dimensions. The natural polynomial basis associated to the points is efficient in "Euclidean" degree, which is the relevant measure for interpolating or integrating a generic analytic function. In addition to this efficiency advantage, there are natural algorithms based on the fast Fourier transform for working with the points; the conversion of point values to polynomial basis coefficients (and vice versa) can be performed in $O(n \log n)$ time. We compare the results of interpolating and integrating with these points to other "reduced" sets of points, including the "Padua" points and sparsified tensor-product points.

SHANYIN TONG, COLUMBIA UNIVERSITY

Large deviation theory-based adaptive importance sampling for rare events in high dimensions

Rare and extreme events are infrequent but have severe consequences. Estimating the probability of such events can inform strategies that mitigate their effects. However, calculating small probabilities is hard, particularly when involving complex dynamics and high-dimensional random variables. In this talk, I will discuss our proposed method for accurately estimating rare event or failure probabilities for expensive-to-evaluate numerical models in high dimensions. The proposed approach combines ideas from large deviation theory and adaptive importance sampling. The importance sampler uses a cross-entropy method to find an optimal Gaussian biasing distribution, and reuses all samples made throughout the process for both, the target probability estimation and for updating the biasing distributions. Large deviation theory is used to find a good initial biasing distribution through the solution of an optimization problem. Additionally, it is used to identify a low-dimensional subspace that is most informative of the rare event probability. This subspace is used for the cross-entropy method, which is known to lose efficiency in higher dimensions. We compare the method with a state-of-the-art cross-entropy-based importance sampling scheme using three examples: a high-dimensional failure probability estimation benchmark, a problem governed by a diffusion partial differential equation, and a tsunami problem governed by the time-dependent shallow water system in one spatial dimension.

SARAH GIFT, DREXEL UNIVERSITY
Real factorization of PSD matrix polynomials

Suppose $Q(x)$ is a real nxn regular symmetric positive semidefinite matrix polynomial. Then it can be factored as $Q(x) = G(x)^T G(x)$ where $G(x)$ is a real nxn matrix polynomial with degree half that of $Q(x)$ if and only if $\det(Q(x))$ is the square of a nonzero real polynomial. We provide a detailed algorithm for computing the factorization, rooted in finding a skew-symmetric solution to a modified algebraic Riccati equation $XSX - XR + R^T X + P = 0$, where P,R,S are real nxn matrices with P and S real symmetric.

ANDREW HIGGINS, TEMPLE UNIVERSITY
Analysis of randomized Householder-Cholesky QR

CholeskyQR2 and shifted CholeskyQR3 are two state-of-the-art algorithms for computing tall-and-skinny QR factorizations since they attain high performance on current computer architectures. However, to guarantee stability, for some applications, CholeskyQR2 faces a prohibitive restriction on the condition number of the underlying matrix to factorize. Shifted CholeskyQR3 is stable but has 50% more computational and communication costs than CholeskyQR2. In this paper, a randomized QR algorithm called Randomized Householder-Cholesky (`rand_cholQR`) is proposed and analyzed. Using one or two random sketch matrices, it is proved that with high probability, its orthogonality error is bounded by a constant of the order of unit roundoff for any numerically full-rank matrix, and hence it is as stable as shifted CholeskyQR3. An evaluation of the performance of (`rand_cholQR`) on a NVIDIA A100 GPU demonstrates that for tall-and-skinny matrices, (`rand_cholQR`) with multiple sketch matrices is nearly as fast as, or in some cases faster than, CholeskyQR2. Hence, compared to CholeskyQR2, (`rand_cholQR`) is more stable with almost no extra computational or memory cost, and therefore a superior algorithm both in theory and practice.

AHMET KAAN AYDIN, UNIVERSITY OF MARYLAND, BALTIMORE COUNTY
Several robust model reductions for the boundary feedback stabilization of fully magnetic piezoelectric smart beams

Piezoelectric materials exhibit electric responses to mechanical stress and mechanical responses to electric stress. The electrostatic and magnetizable PDE models, describing the longitudinal oscillations on the beam, with boundary feedback sensors/actuators are known to have exponentially stable solutions. Firstly, a thorough analysis of the maximal decay rate via the optimal choice of feedback sensor amplifiers is discussed. Next, model reductions by standard Finite Differences and Finite Elements are proposed. Indeed, numerical filtering is implemented for each case to eliminate the spurious high-frequency modes. Finally, we propose a recently developed Finite-difference-based model reduction that uniformly retains the exponential decay property of the PDE. This novel model reduction approach is promising for coupled PDE systems of the same sort.

LUKE EVANS, FLATIRON INSTITUTE
Target measure diffusion maps: Sharp error analysis and spatial subsampling

We detail our recent theoretical and numerical developments with the "target measure diffusion maps"(TMDmap) algorithm of Banisch and Trstanova, a modified diffusion map algorithm which reweights to a user-defined "target measure". A key contribution is explicit formulas for the prefactors in the leading order terms of the bias and variance errors for the discrete generator approximated by TMDmap. To our knowledge, this is the first consistency result that enumerates the prefactor from the bias error. We further provide an error analysis of TMDmap applied to the "committor pde", a key boundary value problem in the study of rare events in metastable systems, and theoretically justify why the committor pde is particularly suitable for solving with diffusion maps. We then illustrate these results with a simple post-processing algorithm to obtain quasi-uniform point clouds in moderate dimensions, and an application to molecular dynamics simulations of butane and alanine dipeptide.

GABRIEL PROVENCHER LANGLOIS, NEW YORK UNIVERSITY
Robust sparse regression using Hamilton-Jacobi equations, gradient inclusions and screening rules

Sparse regression models are a cornerstone of statistics and machine learning. In the era of big data, these models depend on robust and efficient optimization algorithms to perform well. State-of-the-art algorithms for many sparse regression models, however, were not traditionally designed to handle big data sets; they often lack scalable parallelism or scale poorly in size, or are prone to produce unreliable numerical results. The lack of scalability makes it challenging to apply variable selection to big data sets, while the lack of robustness may impact both the accuracy and the false discovery rate (FDR) of sparse regression models. These limitations in efficiency and robustness make sparse regression on big data sets essentially impossible without access to adequate and costly computational resources. Without efficient and robust algorithms to minimize monetary and energy costs, these limitations prevent new scientific discoveries.

This project aims to develop new optimization algorithms that overcome the limitations of state-of-the-art algorithms for certain sparse regression models in big data sets. These proposed algorithms rely on developing novel mathematical analyses of sparse regression methods in terms of Hamilton–Jacobi partial differential equations (HJ PDEs), gradient inclusions and exact screening rules for computing sparse regularization paths. These theoretical connections will be leveraged in the following ways:
a) Automatically and numerically perform parameter selection of sparse regression models. b) Control the FDR inherent to sparse regression by combining it with knockoff filters. c) Design efficient implementations for standard CPUs and specialized hardware, e.g., FPGAs, to obtain fast numerical codes.

RISHAD ISLAM SHANTHO, LEHIGH UNIVERSITY
Analysis of exact and approximate map for linear systems arising in discretized PDEs

Generally, discretization of partial differential equations (PDEs) creates a sequence of linear systems $A_k x_k = b_k$, k= 1, 2, ..., N with structured sparsity patterns. When solving these linear systems using iterative solvers, we can use preconditioner updates instead of computing preconditioners for each system from scratch. One such preconditioner update is the Sparse Approximate Map (SAM) (Carr et al., 2021) which is based on sparse approximate inverse and maps one matrix in the sequence to another nearby one for which we have an effective preconditioner. To efficiently compute these preconditioner updates, we seek to compute an optimal sparsity pattern. In this poster, we examine several sparsity patterns for computing the SAM update in an effort to characterize optimal or near-optimal sparsity patterns for linear systems arising from discretized PDEs. These sparsity patterns should allow for enough nonzeros to compute an accurate enough map, without creating too dense of an update that will incur higher costs per iteration of the iterative solver. We focused our attention on level 1 and level 2 neighbors in the graph representation of the matrices A_k based on analysis in (Chow, 2000), as well as an element-wise analysis on the difference matrix between two nearby matrices e.g., $k^{(th)}$ and $(k-1)^{(st)}$ matrix. We extended the existing analysis to show that if our sequence of linear systems satisfies simple subset assumptions, we can characterize properties of the sparsity pattern of the exact map. Additionally, for applications emitting symmetric coefficient matrices, we considered a variation of the sparse approximate map that preserves symmetry.

JACOB WOODS, NOUR KHOUDARI, MENGSHA YAO, and NICOLE ZALEWSKI , TEMPLE UNIVERSITY
Swarming and instabilities in multi-agent systems

Multi-agent systems consist of many interacting natural or artificial entities such as fish schools, birds flocks, robotic swarms, and vehicular traffic flows. Modeling such systems should capture the emergent behaviors and patterns that arise from the local interactions and rules of the agents. An aspect of particular interest is the dynamic instability observed in the swarming behavior of such systems. Traffic waves rising from car-following behavior and birds flocking in defense against predators are examples of such phenomena. In this work, we discuss recent advances in modeling, analysis, and quantification of swarming behavior in 1D and 2D multi-agent systems.

JIAXING LIANG, UNIVERSITY OF MARYLAND
Efficient Computational Algorithms for Magnetic Equilibrium in a Fusion Reactor

My research focuses on equilibrium computations in magnetic confinement fusion devises, specifically in tokomaks, where the plasma's equilibrium configuration depends on the balance between hydrostatic pressure and magnetic forces. This leads to a semi-linear elliptic equation known as the Grad-Shafranov equation. However, the plasma boundary is not known a priori, resulting in a free boundary problem. I am investigating the impact of uncertainties in the current intensities running through the external coils on the plasma confinement. This involves a parameter space with twelve dimensions. Our objective is to approximate the expectation of the plasma field at the equilibrium configuration using the Monte Carlo method. To reduce computational costs of Monte Carlo, we consider a surrogate function constructed with sparse grid stochastic collocation. We assess the accuracy and efficiency of surrogate-based Monte Carlo sampling, demonstrating significant tune reductions ranging from x7 to over x30. Additionally, we explore cost-efficiency through the multilevel Monte Carlo method, focusing on geometry-conforming grids and adaptive grids, obtaining substantial time reductions of up to x200. Lastly, we establish a hybrid approach combining surrogates with multilevel Monte Carlo sampling. leading to remarkable cost reductions by x50 to x300.

Keynote Lecture (1:30pm-2:30pm)

LOIS CURFMAN MCINNES, ARGONNE NATIONAL LIBRARY

Lear Scientific software ecosystems and communities: Why we need them and how each of us can help thrive

Software in high-performance computing (HPC) is a cornerstone of long-term collaboration and scientific progress, but software complexity is increasing due to disruptive changes in computer architectures and the challenges of next-generation science. Thus, the HPC community has the unique opportunity to fundamentally change how scientific software is designed, developed, and sustained—embracing community collaboration toward scientific software ecosystems. This presentation will introduce work in the U.S. Exascale Computing Project, where a varied suite of scientific applications builds on programming models and runtimes, math libraries, data and visualization packages, and development tools that comprise the Extreme-scale Scientific Software Stack (E4S). As an example, we will highlight recent advances in composable solvers in the PETSc library, where innovative algorithms and data structures are helping to achieve scalable performance on extreme-scale architectures. We will also discuss how crosscutting software strategies are increasing developer productivity and software sustainability, thereby mitigating technical risks by building a firmer foundation for reproducible, sustainable science. The presentation will mention complementary community efforts and opportunities for involvement.

SEAN JOSEPH REITER, VIRGINIA TECH

Generalizations of data-driven balancing: What do you need to sample for different balancing-based reduced models?

We present generalizations of the Quadrature-based Balanced Truncation (QuadBT) framework of Gosea, Gugercin, and Beattie to other types of balancing. QuadBT is an entirely `non-intrusive' reformulation of balanced truncation; a classical projection-based model order reduction technique for linear systems. QuadBT is non-intrusive in the sense that it builds approximate balanced reduced-order models entirely from system response data (e.g., transfer function measurements) without the need to reference an explicit state-space realization of the underlying full-order model. We extend this data-driven framework to other types of balancing; namely, balanced stochastic truncation, positive-real balanced truncation, and bounded-real balanced truncation. We show that the data-driven construction of these balanced reduced-order models requires sampling certain spectral factors associated with the system of interest. Several numerical experiments are included to validate our approach.

MICHAEL S. ACKERMANN, VIRGINIA TECH

Frequency-based reduced order models from purely time-domain data

Classically, constructing reduced order models (ROMs) of large scale dynamical systems has required access to internal system matrices. When these quantities are not available, data driven approaches can be used that require access only to input-output data. Frequency-based data-driven methods have been very successful in creating high fidelity ROMs from data, but require access to values (and sometimes derivatives) of the transfer function. These quantities can at times be costly or difficult to obtain, but one may have ample access to time-domain input-output data. In 2020, Burohman et al. introduced a framework to directly calculate transfer function values and derivatives using only time-domain data. We first discuss improvements to this method that allow for a more efficient and robust numerical implementation, which lead to a theoretical result on optimal diagonal scaling of a class of matrices. We then use these improvements to develop an algorithm that extends H2-optimal approximation to purely time-domain data. We also compare the H2-optimal algorithm's performance to other well established frequency based ROM techniques (such as Loewner framework and Vector Fitting) using only time-domain data.

QINYING CHEN, UNIVERSITY OF DELAWARE

2D fluid model and simulations for evaporation-driven tear film thinning

Many parameters affect the dynamics of human tear films, and exact values or ranges for some are not well known. We model tear film dynamics with nonlinear PDEs for the thickness, osmolarity and fluorescein concentration of the tear film. We first explore the tear film thinning and breakup patterns going from spot to streak. We then use proper orthogonal decomposition (POD) technique to find a compact basis for the PDE solution with a circularly symmetric evaporation function. The POD defines compressed dynamics that are used to solve the inverse problem of recovering a more general evaporation function.

KIERA ELOISE KEAN, TEMPLE UNIVERSITY

Moment methods for advection on networks and applications in life cycle models

We discuss low-dimensional moment methods for advective problems on networks of domains. The evolution of a density function is described by a linear advection-diffusion-reaction equation on each domain, combined via advective flux coupling across domains in the network graph, where coefficients vary in time and across domains but they are fixed along each domain. The solution on each domain is frequently close to a Gaussian. We thus study moment methods that track only the three degrees of freedom per domain that define a Gaussian, in contrast to traditional PDE discretization methods that tend to require many more variables per domain.

A simple ODE-based moment method is developed, as well as an asymptotic-preserving scheme. We apply the methodology to an application that models the life cycle of forest pests, calibrated for the spotted lantern fly, an invasive species present in the Eastern USA. We showcase that the moment method, despite its significant low-dimensionality, can successfully reproduce the prediction of the pest's establishment potential, compared to much higher-dimensional computational approaches.

RUJEKO CHINOMONA, TEMPLE UNIVERSITY

StaRMAP: Simple, efficient, and flexible simulation software for radiation transport

The simulation of particle and energy transport through a medium is a fundamental component in various applications, including radiation therapy, plasma physics, nuclear reactors, nuclear medicine, and atmospheric and environmental modeling. However, the inherent complexity of the underlying physics and kinetic equations, coupled with their high-dimensional phase space, presents significant challenges in achieving efficient solutions. The Staggered Grid Radiation Moment Approximation (StaRMAP) computational methodology and open-source software framework addresses some of these challenges. StaRMAP offers a user-friendly approach for solving the radiative transfer equation using moment methods of arbitrary order, while providing a diverse range of moment closures. This flexibility empowers users to tackle intricate problems in a straightforward and adaptable manner. StaRMAP includes multiple benchmark tests, making it a valuable tool for testing, benchmarking, and verification. The software has also gained recognition as a research and educational resource. This presentation highlights the fundamental components of the software, demonstrates its user-friendliness (including the ability to extract key quantities of interest), and showcases ongoing research applications in radiotherapy for cancer treatment. StaRMAP serves as a bridge between complex challenges in radiation transport and practical solutions, making it an indispensable resource for researchers and the wider community.

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