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 15, 2019 | Philadelphia, PA

Organizers: Benjamin Seibold and Daniel B. Szyld

Sponsored by the Department of Mathematics, College of Science and Technology, and The Graduate School, Temple University

TEMPLE UNIVERSITY

Schedule

9:15- 9:50	Registration and Breakfast (provided)
9:50-10:00	Opening Remarks
10:00-10:50	Presentations (Numerical Linear Algebra)
10:50-11:10	Coffee Break
11:10-12:00	Presentations (High-Performance Computing)
12:00-1:30	Posters and Lunch (provided)
1:30-2:30	Keynote Lecture (Daniela Calvetti)
2:30-2:45	Coffee Break
2:45-4:00	Presentations (Computational PDE)
4:00-4:15	Coffee Break
4:15-5:05	Presentations (Modelling, Simulation, and Data Science Numerical PDE)
5:05-5:15	Closing Remarks
6:00-8:00	Group Dinner (attendance optional)

Speakers

Numerical Linear Algebra 10:00am-10:50am

ARIELLE CARR, Virginia Tech

An inexact Krylov-Schur algorithm for computing invariant subspaces

VASILEIOS KALANTZIS, IBM Research

Domain decomposition Rayleigh-Ritz approaches for symmetric generalized eigenvalue problems

High-Performance Computing 11:10am-12:00pm

XIAOFENG OU, Purdue University

Stable and efficient matrix version of the fast multipole method

MARCO BERGHOFF, Karlsruhe Institute of Technology, Germany

Design of high-performance computing applications

Posters 12:00pm-1:30pm

ABHIJIT BISWAS, Temple University

Optimal finite volume limiter functions

XIAOFENG CAI, University of Delaware

Eulerian-Lagrangian discontinuous Galerkin method for transport problems and its application to nonlinear Vlasov dynamics

FAYÇAL CHAOUQUI, Temple University

Asynchronous two-level optimized Schwarz method

KAYLA DIANN DAVIE, University of Maryland College Park

Preconditioners for PDE-constrained optimization problems

JOSHUA FINKELSTEIN, Temple University

A new family of exact Langevin integration methods with application toward coarse-grained dynamics

NÉSTOR SÁNCHEZ GOYCOCHEA, Universidad de Concepción, Chile

A priori and a posteriori error analyses of an unfitted HDG method for semi-linear elliptic problems in curved domains

Keynote Speaker: Daniela Calvetti 1:30pm-2:30pm

Daniela Calvetti

Case Western Reserve University

The unreasonable effectiveness of numerical linear algebra in Bayesian inverse problems

Computational PDE 2:45pm-4:00pm

KEVIN ANDREW WILLIAMSON, University of Maryland Baltimore County

Application of adaptive PCM-ANOVA and reduced basis methods to the stochastic Stokes-Brinkman problem

SHANG-HUAN CHIU, New Jersey Institute of Technology

Viscous transport in eroding porous media

SAMUEL FRANCIS POTTER, University of Maryland College Park

Computing the quasipotential for nongradient SDEs in 3D

Modeling, Simulation, and Data Science 4:15pm-5:05pm

RABIE RAMADAN, Temple University

A computational study of the stability of jamitons

MING ZHONG, Johns Hopkins University

Data-driven discovery of emergent behaviors in collective dynamic

Abstracts of Talks

Keynote Speaker

DANIELA CALVETTI, CASE WESTERN RESERVE UNIVERSITY

The unreasonable effectiveness of numerical linear algebra in Bayesian inverse problems

Inverse problems deal with recovering unknown causes from incomplete, noisy indirect observations of their effect. This task may be very difficult even when the observation model is linear, especially if the forward map is very smoothing. In this talk we show how, recently, numerical linear algebra and Bayesian inference have joined forces to provide amazing solutions to a wide range of challenging inverse problems.

Numerical Linear Algebra

ARIELLE CARR, VIRGINIA TECH

An inexact Krylov-Schur algorithm for computing invariant subspaces:

Krylov subspace recycling is a method used to improve convergence of iterative methods applied to sequences of linear systems. In this talk, we incorporate this technique into the Krylov-Schur method in order to determine invariant subspaces of closely related systems. We first show results when using subspace recycling to compute the matrix-vector products within Krylov-Schur. Then, we show how we can recycle previous invariant subspace information, with appropriate updates, for the next, closely related system in order to “warm start” the Arnoldi iteration.

VASILEIOS KALANTZIS, IBM RESEARCH

Domain decomposition Rayleigh-Ritz approaches for symmetric generalized eigenvalue problems:

This talk discusses a parallel domain decomposition Rayleigh-Ritz projection scheme to compute a selected number of eigenvalues (and, optionally, associated eigenvectors) of large and sparse symmetric pencils. The projection subspace associated with interface variables is built by computing a few of the eigenvectors and associated leading derivatives of a zeroth-order approximation of the non-linear matrix-valued interface operator. On the other hand, the projection subspace associated with interior variables is built independently in each subdomain by exploiting local eigenmodes and matrix resolvent approximations. The sought eigenpairs are then approximated by a Rayleigh-Ritz projection onto the subspace formed by the union of these two subspaces. Several theoretical and practical details are discussed, and upper bounds of the approximation errors are provided. Our numerical experiments demonstrate the efficiency of the proposed technique on sequential/distributed memory architectures as well as its competitiveness against schemes such as shift-and-invert Lanczos, and Automated MultiLevel Substructuring combined with p-way vertex-based partitionings.

High-Performance Computing

Xiaofeng Ou, Purdue University

Stable and efficient matrix version of the fast multipole method:

We present the fast multipole method (FMM) in pure matrix language, which is much easier for non-physics background people to understand. As we shall see, multipole/local expansions in FMM are essentially (separable and analytic) low-rank approximation. Stability issues may appear in the expansion of the kernel, resulting in either extremely large or extremely tiny matrices. We showed that this can be easily fixed by diagonal scaling techniques. We would also like to briefly mention the proxy point method for kernel matrices compression, which does not require analytic kernel expansion. This is particularly useful when kernel expansion is too complicated. Theoretical justifications are shown for some special cases.

Marco Berghoff, Karlsruhe Institute of Technology, Germany

Design of high-performance computing applications:

In computational science, bigger and faster high-performance computing systems enable more complex models, larger domains, and finer resolutions. At the same time, however, it becomes more difficult to achieve peak-performance with the increasingly parallel systems on several levels. In this talk, I will show which computational challenges currently exist and how they can be tackled. It will be discussed how a good scalability, the omission of unnecessary calculations, and high node-level performance are related. It will also be shown how these three points have to be tackled together to get the best performance out of them and to increase the accomplishment for the computational science described at the beginning.

Computational PDE

Kevin Andrew Williamson, University of Maryland Baltimore County

Application of adaptive PCM-ANOVA and reduced basis methods to the stochastic Stokes-Brinkman problem:

The Stokes-Brinkman equations model flow through a highly heterogeneous porous medium by combining Stokes and Darcy into a single system of equations. In this talk, we will consider solutions to a stochastic Stokes-Brinkman problem in which the Darcy permeability is treated as a random field. An ANOVA decomposition will be employed to decompose the solution into terms according to the degree of interaction among the random variables, and each individual term will be solved by the probabilistic collocation method (PCM). By truncating the ANOVA decomposition, we greatly reduce the number of deterministic solves required while preserving high accuracy. However, the number of deterministic solves may still be prohibitive. We reduce the overall computational cost by building a reduced basis through a small number of deterministic solves and then approximating the remaining deterministic solves through projections onto the space spanned by this reduced basis. We also consider two levels of adaptivity in the ANOVA decomposition by adaptively selecting which terms are computed as well as the polynomial order for the collocation of each computed term. Numerical results demonstrating the effectiveness of these methods will be presented.

Shang-Huan Chiu, New Jersey Institute of Technology

Viscous transport in eroding porous media:

Erosion is a fluid-mechanical process that is present in many geological phenomena such as groundwater flow. We present a boundary integral equation formulation to simulate two-dimensional erosion in porous media. One numerical challenge is accurately resolving the interactions between nearly touching eroding bodies at low porosity. We present a Barycentric quadrature method to resolve these interactions and compare it with the standard trapezoid rule. To reduce the computational time, we use a hybrid method that combines the Barycentric quadrature rules and the trapezoid rule. We compute the velocity, vorticity, and tracer trajectories in the geometries that include dense packings of 20, 50, and 100 eroding bodies. Like in our previous work, we observe quick expending channels between close bodies, flat faces developing along the regions of near contact, and bodies eventually vanishing. Finally, having computed tracer trajectories, we characterize the transport inside of eroding geometries by computing and analyzing the tortuosity and anomalous dispersion rates. We present the validation of the tortuosities based on two different definitions and apply a reinsertion method on the implementation of anomalous dispersion rates.

Samuel Francis Potter, University of Maryland College Park

Computing the quasipotential for nongradient SDEs in 3D:

Nongradient stochastic differential equations frequently arise in contexts such as biology and ecology. To study the dynamics, it is useful to compare the stability of attractors, find the low-dimensional manifolds of the dynamics, determine transition rates between attractors, and compute maximum likelihood transition paths. Instead of addressing these questions using direct simulation, Friedlin and Wentzell's large deviation theory can be used to provide asymptotic answers in the vanishing noise limit. The key function here is the quasipotential, analogous to the potential function for gradient dynamics; computing it is central in the study of rare events.

Since the quasipotential is the solution of a particular static Hamilton-Jacobi equation, numerical methods for solving such equations can be adapted to its computation. Previous works have developed ordered line integral methods (OLIMs) for computing the quasipotential in 2D: these are semi-Lagrangian Dijkstra-like direct solvers, analogous to the fast marching method for solving the eikonal equation, which compute the quasipotential in a single pass by following characteristics.

In this work, we successfully promote the previous 2D OLIMs to 3D by employing several technical innovations: (i) a new hierarchical update strategy, (ii) a method of skipping updates based on constrained optimization theory, and (iii) pruning unnecessary updates by using a fast search. These improvements reduce runtimes on meshes with 600^3 nodes from days to hours. An extensive numerical study is conducted on examples where the quasipotential is available analytically or can be found otherwise. In particular, we apply the solver to Tao's examples in which transition states are hyperbolic periodic orbits, and to the genetic switch model of Lv et al.

Modelling, Simulation, and Data Science

RABIE RAMADAN, TEMPLE UNIVERSITY

A computational study of the stability of jamitons:

MING ZHONG, JOHNS HOPKINS UNIVERSITY

Moment limiters for the discontinuous Galerkin method on unstructured meshes:

Particle- and agent-based systems are ubiquitous across many disciplines. We consider the fundamental problem of inferring, in a nonparametric fashion, interaction kernels from observations of agent-based dynamical systems given observations of trajectories, in the case of large families of systems exhibiting complex, emergent dynamics, as well as of families of systems corresponding to an unknown parametrized family of kernels. We extend the estimators introduced in [1], based on suitably regularized least squares estimators, to these larger classes of systems. We provide extensive numerical evidence that the estimators provide a faithful approximation to the interaction kernels, and provide accurate predictions for trajectories started at new initial conditions, throughout the "training" time interval in which the observations were made. We demonstrate this on prototypical systems displaying collective dynamics, ranging from opinion dynamics, flocking dynamics, milling dynamics, synchronized oscillator dynamics. Our experiments also suggest that our estimated systems can display the same emergent behaviors of the original systems, that occur at larger timescales than those observed in training data. Finally, in the case of families of systems corresponding to a parameterized family of interaction kernels, we introduce novel estimators that estimate the parameterized family of kernels, splitting it into a common interaction kernel and the action of parameters. We demonstrate this in the case of gravity, by learning both mass and the "common component" $\frac{1}{r^2}$, from observations of planetary motions in our solar system.

[1]: F. Lu, M. Zhong, S. Tang, M. Maggioni, nonparametric inference of interaction laws in systems of agents from trajectory data, PNAS, 116 (3), 14424 - 14433, 2019.

Abstracts of Posters

Abhijit Biswas, Temple University

Optimal finite volume limiter functions:

Limiter functions are applied to finite volume methods to avoid oscillations near discontinuities and sharp transitions. Many limiter functions have been introduced in the literature, and the general approach is to design a limiter function and demonstrate that it performs well on some test problems. Here we wish to investigate the inverse problem instead: given a portfolio of representative test cases, and a cost functional, determine the optimal limiter function.

Xiaofeng Cai, University of Delaware

Eulerian-Lagrangian discontinuous Galerkin method for transport problems and its application to nonlinear Vlasov dynamics:

We propose a Eulerian-Lagrangian (EL) discontinuous Galerkin (DG) method. The method is designed as a generalization of the semi-Lagrangian (SL) DG method for linear advection problems proposed in [J. Sci. Comput. 73: 514-542, 2017], which is formulated based on an adjoint problem and tracing upstream cells by tracking characteristics curves highly accurately. Depending on the velocity field, the shape of upstream cells could be of arbitrary shape, for which a more sophisticated approximation is required to get high order approximation. For example, in the original SLDG algorithm, quadratic-curved (QC) quadrilaterals were proposed to approximate upstream cells in order to obtain third-order spatial accuracy in a swirling deformation example. In this poster, for linear advection problems, we propose a more general formulation, named the ELDG method, for which the scheme is based on a modified adjoint problem for which upstream cells are always quadrilaterals. This leads to a new formulation of the ELDG method, which avoids the need to use QC quadrilaterals to better approximate upstream cells in the original SLDG algorithm. The newly proposed ELDG method can be viewed as a new general framework, in which both the classical RK DG formulation and the SL DG formulation can fit in. Numerical results on linear advection problems, as well as the nonlinear Vlasov dynamics using the exponential RK framework, will be presented to demonstrate the effectiveness of the proposed approach.

Fayçal Chaouqui, Temple University

Asynchronous two-level optimized Schwarz method:

Current computational problems require the use of computer architecture with an increasing number of cores. This makes asynchronous communication more favorable than its synchronous variant since it avoids waiting for the idle time, i.e., time for which some processors are not being used but could be. We explore here such iterations for the Optimized Schwarz Method for the solution of large sparse linear systems arising from the discretization of PDEs. In particular, we treat the one- and two-level cases. The latter is required to ensure the weak scaling. Moreover, a particular coarse grid should be considered in order to ensure the convergence of the two-level method iteratively, and hence be more suitable in the asynchronous framework. We provide some numerical experiments that shows the proof of concept.

Kayla Diann Davie, University of Maryland College Park

Preconditioners for PDE-constrained optimization problems:

PDE-constrained optimization problems, or PDE-control problems, are optimization problems where the constraints themselves are partial differential equations (PDEs). Discretizing these problems results in large linear systems that are computationally expensive to solve. The goal of this research is to explore solution algorithms for parameter-dependent stochastic PDE-constrained optimization problems. We begin by reviewing methods for solving the deterministic problem. Recently, a great deal of research has gone into solving PDE-control problems using iterative Krylov subspace methods, which enjoy constant work per iteration and rigorous convergence bounds. When paired with strong preconditioners, these methods can achieve convergence rates independent of the dimensions of the discrete problem. We look specifically at two example problems: the Poisson control problem and the convection-diffusion control problem. We propose a way to extend the research done for the deterministic problem to analyze the parameter-dependent stochastic PDE-control problem where diffusion coefficients that are subject to uncertainty have been introduced. We will begin by considering Monte Carlo sampling and exploring the feasibility of computing solutions of low rank.

Joshua Finkelstein, Temple University

A new family of exact Langevin integration methods with application toward coarse-grained dynamics:

The Langevin equation is a stochastic differential equation frequently used in molecular dynamics (MD) for simulating molecular systems in a canonical ensemble. The increasingly broader uses of this equation for models at different levels of resolution, e.g. coarse-grained (CG) models, may necessitate parameter choices outside of the range for which many existing discretization methods were developed originally. Here, we illustrate how popular MD methods can fail and offer a new family of methods with more favorable properties in these regions of parameter space. A new scheme from this class is chosen and tested on atomistic and coarse-grained model systems representative of materials science and biological applications. Results show a significant improvement in accuracy and numerical stability for the model systems considered, suggesting that the new scheme is suitable for general use in a variety of applications.

Néstor Sánchez Goycochea, Universidad de Concepción, Chile

A priori and a posteriori error analyses of an unfitted HDG method for semi-linear elliptic problems in curved domains:

We present a priori and a posteriori error analyses of a Hybridizable discontinuous Galerkin (HDG) method applied to a semi-linear elliptic problem posed on a piecewise curved, non polygonal domain. We approximate the not polygonal domain by a polygonal subdomain and propose an HDG discretization, which is shown to be optimal under mild assumptions related to the non-linear surce term and the distance between the boundaries of the polygonal subdomain and the true domain. Moreover, a local non-linear post-processing of the scalar unknown is proposed and shown to provide an additional order of convergence. A reliable and efficient a posteriori local error estimator that takes into account the curved geometry is also provided.

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