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

TEMPLE UNIVERSITY®

Department of Mathematics

Friday, 4 November 2011 | 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

Schedule

9:20am-9:50am	Registration and coffee
9:50am-10:00am	Opening remarks
10:00am-11:00am	Presentations; *Eigenvalues and Other Spectral Properties of Matrices*
11:00am-11:10am	Questions and discussion
11:10am-11:25am	Mid-morning break
11:25am-12:40pm	Presentations; *Modeling and Numerical Methods*
12:40pm-12:50pm	Questions and discussion
12:50pm-2:00pm	Lunch
2:00pm-3:00pm	Keynote speaker: Lisa Fauci
3:00pm-3:15pm	Coffee break
3:15pm-4:30pm	Presentations; *Numerical Analysis for PDE*
4:30pm-4:40pm	Questions and discussion
4:40pm-4:55pm	Afternoon tea
4:55pm-5:55pm	Presentations; *Solution of Linear Systems*
5:55pm-6:05pm	Questions and discussion
6:05pm-6:15pm	Closing remarks
7:00pm-9:00pm	Dinner (optional)

Presentations

Keynote Speaker: Lisa Fauci (2:00pm-3:00pm)

Pendergraft Nola Lee Haynes Professor of Mathematics, Tulane University.

Waving rings and swimming in circles: some lessons learned in biofluiddynamics

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Eigenvalues and Other Spectral Properties of Matrices (10:00am-11:00am)

TIARA DANIELLE TURNER, Delaware State University.

A mixed finite element method for Helmholtz transmission eigenvalues

FEI XUE, Temple University.

Local convergence analysis of several inexact Newton-type methods for general nonlinear eigenvalue problems

MINGHAO WU, University of Maryland.

Lyapunov inverse iteration for identifying Hopf bifurcations in models of incompressible flow

MERT GURBUZBALABAN, New York University.

Fast algorithms for computing the stability radius of a matrix

Modeling and Numerical Methods (11:25am-12:40pm)

FEIYU CHEN, Delaware State University.

Partial volume simulation in software breast phantoms

PRINCE CHIDYAGWAI, Temple University.

Discontinuous Galerkin method for 2D moment closures for radiative transfer

QUAN DENG, University of Delaware.

Tear film with moving boundary condition

SHIMAO FAN, Temple University.

Traffic flow simulations on road networks

AZIZ TAKHIROV, University of Pittsburgh.

Improved accuracy in regularization models of incompressible flow via adaptive nonlinear filtering

Numerical Analysis for PDE (3:15pm-4:30pm)

QIFENG LIAO, University of Maryland.

Effective error estimators for low order elements

DUK-SOON OH, New York University.

Domain decomposition methods for Raviart-Thomas vector fields

CHRISTOPHER WILLIAM MILLER, University of Maryland.

Stochastic collocation with kernel density estimation

FANG ZENG, Delaware State University.

An inverse electromagnetic scattering problem for cavity

CHANGHUI TAN, University of Maryland.

Hierarchical construction of bounded solutions of divU=F in critical regularity spaces

Solution of Linear Systems (4:55pm-5:55pm)

EDWARD GEOFFREY PHILLIPS, University of Maryland.

Block preconditioners for an exact penalty viscoresistive MHD formulation

STEPHEN SHANK, Temple University.

Overlapping blocks by growing a partition with applications to preconditioning

CLAUDIO E. TORRES, University of Delaware.

Fast and accurate Stokes' approximation for hydrodynamic interactions

KIRK SOODHALTER, Temple University.

Block Krylov subspace recycling

Abstracts

LISA FAUCI. *Tulane University.*

*Waving rings and swimming in circles: some lessons learned in biofluiddynamics***:** Dinoflagellates swim due to the action of two flagella - a trailing, longitundinal flagellum that propagates planar waves, and a transverse flagellum that propagates helical waves. Motivated by the intriguing function of the transverse flagellum, we study the fundamental fluid dynamics of a helically-undulating ring in a viscous fluid. We contrast this biofluiddynamic study, where the kinematics of the waveform are taken as given, with a model of mammalian sperm hyperactivated motility. Here, our goal is to examine how the complex interplay of fluid dynamics, biochemistry, and elastic properties of the flagellum give rise to the swimming patterns observed. We will discuss the method of regularized Stokeslets, which is an easily-implemented and versatile computational method for examining fluid-structure interactions in very viscous flows.

FEIYU CHEN. *Delaware State University.*
Partial volume simulation in software breast phantoms: Computer models of breast anatomy have been used in preclinical validation of the breast cancer imaging systems. In this project, a modification to our simulation of breast anatomy is proposed by considering the partial volume of each voxel which contains two different materials (e.g., on the boundary between the skin and air or between Cooper's ligaments and tissue). For each voxel, a local planar approximation of the boundary surface is employed, then the partial volume is computed by decomposition into simple geometric shapes. Our results show that the partial volume simulation has improved the quality of simulated breast projections by reducing quantization artifacts.

PRINCE CHIDYAGWAI. *Temple University.*
Discontinuous Galerkin method for 2D moment closures for radiative transfer: Radiative transfer plays an important role in many engineering and physics applications. We consider the radiative transport equation applied to electron radiotherapy. In this case the transport equation describes the distribution of electrons in time and space assuming that the electrons do not interact with each other. The full radiative transfer equation is computationally expensive to solve because it is a high dimensional equation. We present high order Discontinuous Galerkin (DG) schemes to solve systems that approximate the full radiative transport equation. The approximating systems are obtained from moment methods.These methods start with a system of infinitely many moments that are equivalent to the radiative transfer equation. The truncation of this system is achieved using closure strategies results in both linear and non-linear hyperbolic systems. We show that the DG method is well suited to solve the approximating systems because it yields high order approximations and easily handles unstructured grids. We demonstrate that the method also scales very well on shared memory on a shared memory parallel implementation. We present numerical results verifying the high order of convergence of our numerical scheme on known smooth solutions as well as results form benchmark problems in radiative therapy test cases.

QUAN DENG. *University of Delaware.*
Tear film with moving boundary condition: The human tear film is studied to provide more insight into dry eyes, which can occur when the film breaks abnormally during a blinking cycle. Lubrication theory is used to develop nonlinear partial differential equations that govern the free surface of the human tear film during the complete blink cycle. A heat equation is coupled with the film equation, where temperature field and film domain share one same moving boundary, as a representation of eyelid movement. The first part of the talk is devoted to some background information about the relevant equations. I will then describe how spectral methods are used to solve the PDEs numerically. The talk will end with a discussion of the pros and cons of various spatial discretizations that can be used.

SHIMAO FAN. *Temple University*.
Traffic flow simulations on road networks: We model the traffic flow on networks based on conservation laws. As the fundamental diagram (FD) is essential for these conservation laws models. We determined the FD by fitting with the empirical data. We then formulate a new scalar model and apply it to simulate traffic flow on road networks. As a lot of researchers have pointed out, the scalar models are not enough to give a good reconstruction of traffic behavior. Then, we propose to give a new second order model which is a generalization of the famous Aw-Rascal model. This new model will allows us correct some main drawbacks of the original Aw-Rascal model, and we also expect it will give results that fit empirical data well.

MERT GURBUZBALABAN. *New York University.*
Fast algorithms for computing the stability radius of a matrix: The stability radius of an n x n square matrix A (or distance to instability) is a well-known measure of the stability of the linear dynamical system dx/dt = Ax. Existing techniques compute this quantity accurately but the cost is multiple SVDs of order n, which makes the method suitable to middle size problems. We present a novel approach based on a Newton iteration applied to the pseudospectral abscissa, whose implementation is obtained by a repeated computation of the spectral abscissa of a sequence of matrices. Such an approach turns out to be particularly well suited for large sparse matrices. We will also discuss the extensions of this approach to the more general problem of computing the H-infinity norm of a transfer matrix.

QIFENG LIAO. *University of Maryland*.
Effective error estimators for low order elements: This talk focuses on a posteriori error estimation for (bi-)linear and (bi-)quadratic elements. At first, the simple diffusion problem is tested for introducing the methodology we adopted for doing error estimation, which is based on solving local Poisson problems. Next, this methodology is applied to dealing with classical mixed approximations of incompressible flow problems. Computational results suggest that our error estimators are cost-effective, both from the perspective of accurate estimation of the global error and for the purpose of selecting elements for refinement within a contemporary self-adaptive refinement algorithm.

CHRISTOPHER WILLIAM MILLER. *University of Maryland.*
Stochastic collocation with kernel density estimation: The stochastic collocation method has recently received much attention for solving partial differential equations posed with uncertainty, i.e., where coefficients in the differential operator, boundary terms or right-hand sides

are random fields. Recent work has led to the formulation of an adaptive collocation method that is capable of accurately approximating functions with discontinuities and steep gradients. These methods, however, usually depend on an assumption that the random variables involved in expressing the uncertainty are independent with marginal probability distributions that are known explicitly. In this work we combine the adaptive collocation technique with kernel density estimation to approximate the statistics of the solution when the joint distribution of the random variables is unknown.

DUK-SOON OH. *New York University.*
Domain decomposition methods for Raviart-Thomas vector fields: Raviart-Thomas finite elements are very useful for problems posed in H(div) since they are H(div)-conforming. We introduce two domain decomposition methods for solving vector field problems posed in H(div) discretized by Raviart-Thomas finite elements. A two-level overlapping Schwarz method is developed. The coarse part of the preconditioner is based on energy-minimizing extensions and the local parts consist of traditional solvers on overlapping subdomains. We also consider a balancing domain decomposition by constraints (BDDC) method. The BDDC preconditioner consists of a coarse part involving primal constraints across the interface between subdomains and local parts related to the Schur complements corresponding to the local subdomain problems.

EDWARD GEOFFREY PHILLIPS. *University of Maryland.*
Block preconditioners for an exact penalty viscoresistive MHD formulation: We propose a block preconditioner for an exact penalty finite element formulation of the stationary viscoresistive magnetohydrodynamics equations, which implicitly enforces the divergence free condition on magnetics. Operators arising from a block decomposition of the discrete system are analyzed from a continuous perspective to develop approximations within the preconditioner. Approximate commutator arguments are also employed to further simplify computation. Numerical results indicate very good behavior of the preconditioner over a range of parameters on a variety of two-dimensional test problems.

STEPHEN SHANK. *Temple University.*
Overlapping blocks by growing a partition with applications to preconditioning: Given an arbitrary partition of an edge-weighted graph into subgraphs, we present a method for enlarging their associated sets of vertices, growing the partition into a decomposition with overlap. New vertices are added to a given set according to a criterion which measures the strength of connectivity of the candidate note with the remaining set. This method can be used on the associated digraph of a matrix to produce algebraic Schwarz preconditioners. Numerical results are given which demonstrate the effectiveness of the method in particular, for several test problems we show improvement of GMRES convergence with preconditioners based on non-overlapping partitions or ILU.

KIRK SOODHALTER. *Temple University.*
Block Krylov subspace recycling: The GCRODR algorithm (GMRES with subspace recycling) for linear systems, presented by Parks and et al [SIAM J. Sci. Comput., 2006] has been shown to offer significant acceleration of convergence over restarted GMRES. The method is particularly effective when solving a slowly-changing sequence of linear systems. We derive a version of this algorithm for use in the block Krylov setting. We call this method block GCRODR

(block GMRES with recycling). We demonstrate this method's effectiveness as a solver embedded in a Newton iteration arising in fluid density functional theory.

AZIZ TAKHIROV. *University of Pittsburgh.*
Improved accuracy in regularization models of incompressible flow via adaptive nonlinear filtering: Study of adaptive nonlinear filtering in the Leray regularization model for incompressible, viscous Newtonian flow. The filtering radius is locally adjusted so that resolved flow regions and coherent flow structures are not filtered-out', which is a common problem with these types of models. A numerical method is proposed that is unconditionally stable with respect to timestep, and decouples the problem so that the ltering becomes linear at each timestep and is decoupled from the system. Several numerical examples are given that demonstrate the effectiveness of the method.

CHANGHUI TAN. *University of Maryland.*
Hierarchical construction of bounded solutions of divU=F in critical regularity spaces: I will describe the problem of finding uniformly bounded solutions for the equation divU=F in the critical cases where f is an L^d function on a d-dimensional torus. J. Bourgain and H. Brezis have shown the existence of solutions for the problem. However, there exists no linear construction for the solutions. E. Tadmor constructed a solution using a nonlinear hierarchical decomposition. In 2-dimensional case, each hierarchical step is a minimization problem which involves both L^∞ norm and L^2 norm. I will present a duality argument and a variational approach to solve the minimization problem. Some numerical issues arise and should be treated carefully. This is a joint work with Professor Eitan Tadmor.

CLAUDIO E. TORRES. *University of Delaware.*
Fast and accurate Stokes' approximation for hydrodynamic interactions: The numerical simulation of tropical clouds is a challenging problem requiring the numerical solution of the Navier-Stokes equations. In this talk, we will discuss the hydrodynamic interaction among droplets in a turbulent cloud. The droplet interactions are modeled by a Stokes' approximation. The Stokes' approximation requires a solution of a linear system of equations for each time-step of the Navier-Stokes' solver. Using perturbation analysis, we will explore why the GMRes algorithm is particularly effective for this system. We will also discuss its implementation on massively parallel peta-scale machines.

TIARA DANIELLE TURNER. *Delaware State University.*
A mixed finite element method for Helmholtz transmission eigenvalues: The transmission eigenvalue problem has important applications in inverse scattering. Since the problem is non-self adjoint, the computation of transmission eigenvalues needs special treatment. Based on a fourth -order reformulation of the transmission eigenvalue problem, we choose a mixed finite element method. This method has two major advantages 1) the formulation leads to a generalized eigenvalue problem naturally, without the need to invert a related linear system and 2) the non-physical zero transmission eigenvalue, which has an infinitely dimensional eigenspace is eliminated. To solve the resulting non-Hermitian eigenvalue problem, we propose an iterative algorithm using the restarted Arnoldi method. To make the computation efficient, the search interval is decided using a Fabra-Khan type inequality for transmission eigenvalues and the interval is updated at each iteration. The algorithm is implemented using MATLAB. The code can be eas-

ily used in qualitative methods in inverse scattering and be modified to compute transmission eigenvalues for other models such as the elasticity problem.

MINGHAO WU. *University of Maryland.*
Lyapunov inverse iteration for identifying Hopf bifurcations in models of incompressible flow: The identication of instability in large-scale dynamical systems caused by Hopf bifurcation is difficult because of the problem of identifying the rightmost pair of complex eigenvalues of large sparse generalized eigenvalue problems. Lyapunov inverse iteration is a new method that avoids this computation, instead performing an inverse iteration for a certain set of real eigenvalues and that requires the solution of a large-scale Lyapunov equation at each iteration. In this talk, the speaker will discuss the theoretical basis of this method, and present numerical results for challenging test problems from fluid dynamics. Various implementation issues will be discussed as well, including the use of inexact inner iterations and the impact of the choice of iterative solution for the Lyapunov equations, and the effect of eigenvalue distribution on performance.

FEI XUE. *Temple University.*
Local convergence analysis of several inexact Newton-type methods for general nonlinear eigenvalue problems: We study the local convergence of several inexact numerical algorithms closely related to Newton's method for the solution of a siple eigenpair of the general nonlinear eigenvalue problem $T(\lambda)v=0$. We show that the inexact algorithms can achieve the same order of convergence as the exact methods if appropriate sequences of tolerances are applied to the inner solves. When the local symmetry of $T(\lambda)$ is present, the use of a nonlinear Rayleigh functional is shown to be fundamental in achieving higher order of convergence rates.

FANG ZENG. *Delaware State University.*
An inverse electromagnetic scattering problem for cavity: We consider the inverse electromagnetic scattering problem of determining the shape of a perfectly conducting cavity from measurement of scattered electric field due to electric dipole sources on a surface inside the cavity. We prove a reciprocity relation for the scattered electric field and a uniqueness theorem for the inverse problem. Then the near field linear sampling method is employed to reconstruct the shape of the cavity. Preliminary numerical examples are provided to show the viability of the method.

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* List complete as of 11/1/11

Notes