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, 2 November 2012 | 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 Dong Zhou, Jingmin Chen, Aziz Takhirov
11:00am-11:20am	Coffee break
11:20am-12:40pm	Presentations Jyoti Saraswat, Ana Maria Soane, Tim Mitchell, Stephen Shank
12:50pm-2:30pm	Lunch and poster session Prince Chidyagwai, Quan Deng, Shimao Fan, Sunnie Joshi, Geunseop Lee, Kathryn Lund, Bart Vandereycken
2:30pm-3:30pm	Keynote speaker: William Layton
3:30pm-3:45pm	Coffee break
3:45pm-4:45pm	Presentations Edward Phillips, Longfei Li, Ignacio Tomas
4:45pm-5:00pm	Coffee break
5:00pm-6:00pm	Presentations Qunhui Han, Kaveh Laksari, Abner Salgado
6:00pm-6:10pm	Closing remarks
6:45pm-8:30pm	Dinner (optional)

Presentations

Keynote Speaker: William Layton (2:30pm-3:30pm)

Professor of Mathematics, University of Pittsburgh.

Numerical Analysis of Turbulent Flow

Flows I (10:00am-11:00am)

DONG ZHOU, Temple University.

Jet Schemes for Hamilton-Jacobi Equations Using an Evolve-and-project Framework

JINGMIN CHEN, Drexel University.

Subdivision Surfaces and Willmore Flow Problem

AZIZ TAKHIROV, University of Pittsburgh.

Flow in Pebble Bed Geometries

Multigrid and More (11:20am-12:40pm)

JOYTI SARASWAT, University of Maryland Baltimore County

Multigrid Solution of a Distributed Optimal Control Problem Constrained by a Semilinear Elliptic PDE

ANA MARIA SOANE, University of Maryland Baltimore County.

Multigrid Preconditioners for Optimal Control Problems in Fluid Flow

TIM MITCHELL, Courant Institute of Mathematical Sciences, New York University.

State of the Art HIFOO: H-Infinity Controller Optimization for Large and Sparse Systems

STEPHEN DAVID SHANK, Temple University.

Krylov Subspace Methods for Large Scale Constrained Sylvester Equations

Posters (12:50pm-2:30pm)

PRINCE CHIDYAGWAI, Temple University.

Discontinuous Galerkin Method for Moment Closures for Radiative Transfer

QUAN DENG, University of Delaware.

Tear Film Evolution in 2-D Rectangular Domain

SHIMAO FAN, Temple University.

A Data-fitted Generalized Aw-Rascle-Zhang model

SUNNIE JOSHI, Temple University.

A Least-squares Formulation of an Inverse Sturm-Liouville Problem and its Finite Element Implementation

GEUNSEOP LEE, Pennsylvania State University.

Fast Algorithm for Total Least Squares Problems with Tikhonov Regularization

KATHRYN LUND, Temple University.

Five Dimensions of Traffic

BART VANDEREYCKEN, Princeton University.

The Geometry of Algorithms using Hierarchical Tucker Tensors

Flows II (3:45pm-4:45pm)

EDWARD GEOFFREY PHILLIPS, University of Maryland.

Approximate Commutator Preconditioners for Variable Viscosity Navier-Stokes Equations

LONGFEI LI, University of Delaware.

Tear Film Dynamics on an Eye-Shaped Domain

IGNACIO TOMAS, University of Maryland College Park.

Analysis of Fully Discretre Scheme for the Micropolar Navier Stokes Equations

<u>Accurate Methods for Evolution Equations (5:00pm-6:00pm)</u>

QUNHUI HAN, University of Delaware.

Reconstructing of the Flip Rate of a Broadwell Process Using the Project Method and Downward Continuation Method

KAVEH LAKSARI, Temple University.

Modeling Solid Mechanics using Discontinuous Galerkin Methods

ABNER J. SALGADO, University of Maryland.

A TV Diminishing Interpolation Operator and Applications

Abstracts

WILLIAM LAYTON. *University of Pittsburgh.*
Numerical Analysis of Turbulent Flow: One fundamental challenge in many phenomena is to do simulations that accurately predict turbulent flows. This is a challenge to physical understanding, analytic technique, models, computer capabilities and the complexity of a program that a human programmer can understand. One basic issue is that turbulence is a fully multiscale phenomena with a near continuum of scales and no scale separation. Another is that the unresolved scales [that which is unknowable] can determine the resolved scales [that which is observable]. This talk will review the basic theory of turbulence. Then consider the challenges of modeling. In contrast to most other work, modeling is considered an algorithmic challenge amenable to the tools of rigorous numerical analysis. A new approach of nonlinear filters will be shown and a few early, and positive, tests.

JINGMIN CHEN. *Drexel University.*
Subdivision Surfaces and Willmore Flow Problem: In this talk we introduce subdivision, one main method in geometric modeling. We explain how to compute geometric quantities and their gradients with respect to the control data of subdivision surfaces. Armed with these tools, we propose a new approach to solve the Willmore flow problem, which calculates the exact Willmore energy while others can only approximate the Willmore energy numerically. We then show numerical results of the simulation of vesicles consisting of bilayer membranes, which is known to illustrate a remarkable variety of shapes with different symmetries and topologies.

PRINCE CHIDYAGWAI. *Temple University.*
Discontinuous Galerkin method for 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 consider the method of moment approximations to the radiative transfer equation. We present a third order discontinuous Galerkin scheme as well as numerical results from benchmark test problems.

QUAN DENG. *University of Delaware.*
Tear film evolution in 2-D rectangular domain: Tear film is studied to provide more insight into dry eyes, which can occur when the film breaks abnormally during a blinking cycle. People use lubrication theory to develop nonlinear partial differential equation(s) that govern the free surface of the human tear film during the complete blink cycle. In current research, the polar lipid evolution is coupled with the film equation to model the possible Marangoni effect due to change of lipid concentration. The first part of the talk is devoted to some background information about the tear film equation, I will then introduce our approach with spectral method to solve the system. The talk will end with a discussion of numerical results.

SHIMAO FAN. *Temple University.*

A data-fitted generalized Aw-Rascle-Zhang model: The Aw-Rascle-Zhang (ARZ) model is a second order macroscopic traffic model that possesses a family of fundamental diagram curves, rather than a single one as in the first order Lighthill-Whitham-Richards (LWR) model. Hence, the ARZ model can agree better with historical fundamental diagram data, especially during congested traffic. However, the ARZ model also has some obvious shortcomings, e.g., it possesses various maximum traffic densities. To overcome these drawbacks, we consider a Generalized ARZ model (GARZ), fitted to historic traffic data. To investigate to which extent the GARZ model improves the prediction accuracy of models, we perform a comparison of data-fitted GARZ with two types of data-fitted LWR models and their second order ARZ generalizations, via a three-detector problem test. We consider two different kinds of traffic data during model construction and validation: detector data and vehicle trajectory data. Moreover, a relaxation term is added to the momentum equation of the GARZ model to overcome some unrealistic aspects of the homogeneous models. Computational results reveal on which time scales drivers actually adjust their driving behavior.

QUNHUI HAN. *University of Delaware.*

Reconstructing of the Flip Rate of a Broadwell Process Using the Project Method and Downward Continuation Method: We are interested in the inverse first passage time problem of the Broadwell process. A one-dimensional Broadwell process problem can be described as follows: given a fixed starting position x within an interval $[-L/2,L/2]$, a particle travels forward and backward within the interval with alternating constant velocity v and transition rate $F(x)$. The travel time is recorded once the particle exits from either endpoint. This travel time is called the first passage time of the particle. Thus, the inverse first passage time problem of the Broadwell process is to reconstruct the transition rate $F(x)$ given starting position x and velocity v. We develop a Monte-Carlo protocol to simulate the Broadwell process and generate the exit time distribution, which is the noisy data used in reconstruction. We also develop two different projection methods and a downward continuation method to reconstruct the transition rate. In the projection methods, we use Legendre polynomials as an expansion basis for $F(x)$, and try to reconstruct $F(x)$ by reconstructing the coefficients. In most cases, we can find first four coefficients to within $O(10^{-1})$ accuracy from $O(10^{4})$ exit times. We also explore the effectiveness of our algorithm for a fixed number of exit times under different speeds and find that optimal reconstruction occurs when $v=O(1)$. In the downward continuation method, we are able to reconstruct $F(x)$ with the boundary data only, and our reconstruction is accurate when F/v has small magnitude. More exploration and discussion related to the downward continuation method and the numerical results will be conducted in future research.

SUNNIE JOSHI, *Temple University.*

A least-squares formulation of an inverse Sturm-Liouville problem and its finite element implementation: In this work we present a finite element algorithm for the recovery of the potential in a classical Sturm-Liouville operator. For symmetric potentials, the given data are the first N eigenvalues, and for general potentials, the first N terminal velocities are provided in addition to the eigenvalues. An iterative method is constructed using a least-squares approach and numerical examples are presented for different boundary conditions to show the performance of the method.

KAVEH LAKSARI. *Temple University*.
Modeling Solid Mechanics using Discontinuous Galerkin Methods: The goal of this study is to model the equations of motion for solid materials using discontinuous galerkin (DG) methods. First an overview of different material models, i.e, hyperelastic and viscoelastic models, will be given and then the equations are simulated for the 1D case using DG. The advantage of such methods over finite element methods and are also discussed.

GEUNSEOP LEE, *Pennsylvania State University.*
Fast algorithm for total least squares problems with Tikhonov regularization: To solve an ill-conditioned total least squares (TLS) problem, an iterative algorithm with Tikhonov Regularization is considered. In particular, we present a Newton-based TLS solution that solves a system of nonlinear equations in the two regularization parameters derived from Golub et al. [SIMAX 21(1):185-194,1999]. Furthermore, we combine an orthogonal projection method with the proposed algorithm by employing generalized Krylov subspace expansion for the improvement of the execution speed. Experimental results show that our algorithm is very promising and produces a fast computation of the solution in various examples.

LONGFEI LI, *University of Delaware.*
Tear Film Dynamics on an Eye-Shaped Domain: We explore the human tear film dynamics on a 2D eye-shaped domain. We used Overture computational framework developed at LLNL, which employs overlapping grids and curvilinear finite difference methods, to conduct the numerical simulations. By including evaporation and Van der Waals force, we are able to reproduce results captured by experiments and existing 1D evaporation models. Time dependent flux boundary conditions that model the lacrimal gland tear supply and punctal drainage are imposed. Results show our model captures the hydraulic connectivity and other key physics of human tear film observed in vivo.

KATHRYN LUND, *Temple University.*
Five Dimensions of Traffic: Attempts to model vehicular traffic (mathematically and conversationally) have abounded for decades, but little work has been done to verify these conjectures with real traffic data. Though the present project is inspired by two "second-order" macroscopic models, namely the Payne-Whitham and Aw-Rascle-Zhang models, the main goal is not to verify any particular model but rather to determine data's dependency on five key variables. These variables include acceleration, velocity, density, and the derivatives with respect to displacement of the latter two. Before approaching the main problem, however, it is necessary to obtain a smooth function of these variables from the data, which is not a trivial task given the inherent noise of data and complexity of driving behaviors. What we present here are the methods used to create this function and progress thus far towards determining the data's dependency on each variable.

TIM MITCHELL. *Courant Institute of Mathematical Sciences, New York University .*
State of the Art HIFOO: H-Infinity Controller Optimization for Large and Sparse Systems: We present a new state of the art version of HIFOO, a Matlab package for optimizing H-Infinity and H-2 controllers for linear dynamical systems, supporting simultaneous multiple plant stabilization. Previous versions of HIFOO have generally been limited to smaller scale problems, due to the high asymptotic cost of computing the H-Infinity norm of the transfer matrix. How-

ever, new sparse methods for computing the H-Infinity norm allow HIFOO to extend efficiently to large and sparse systems.

EDWARD GEOFFREY PHILLIPS. *University of Maryland.*
Approximate Commutator Preconditioners for Variable Viscosity Navier-Stokes Equations: Variable viscosity problems arise in many complex fluid processes. When velocity is allowed to spatially vary, the linear systems resulting from discretizations of the Navier-Stokes equations become more difficult to solve, as compared to the constant viscosity case. For instance, commuting assumptions which hold for constant viscosity do not hold for variable viscosity. As a result, preconditioners based on approximate commutators, while very effective for constant viscosity Navier-Stokes, can be problematic in the current context. In this work, we consider strategies for extending such commutator-based preconditioners for variable-viscosity Navier-Stokes. We will study the performance of these preconditioners on systems arising from the Reynolds Averaged Navier-Stokes equations closed with the Spalart-Allmaras model for the turbulent viscosity. We will compare our methods with extensions of other block preconditioners developed for the variable viscosity Stokes equations as well as more general algebraic block preconditioners for saddle point systems

ABNER J. SALGADO. *University of Maryland.*
A TV diminishing interpolation operator and applications: We construct a finite element interpolation operator that does not increase the total variation. With the help of it we provide improved error estimates for discrete minimizers of the total variation denoising problem and for total variation flows.

JYOTI SARASWAT. *University of Maryland Baltimore County..*
Multigrid Solution of a Distributed Optimal Control Problem Constrained by a Semilinear Elliptic PDE: We study a multigrid solution strategy for a distributed optimal control problem constrained by a semilinear elliptic PDE. Working in the discretize-then-optimize framework, we solve the reduced optimal control problem using Newton's method. Further, adjoint methods are used to compute matrix-vector multiplications for the reduced Hessian. In this work we introduce and analyze a matrix-free multigrid preconditioner for the reduced Hessian which proves to be of optimal order with respect the discretization.

STEPHEN DAVID SHANK. *Temple University.*
Krylov subspace methods for large scale constrained Sylvester equations: Constrained Sylvester equations arise in various applications, in particular in control theory in the design of reduced-order observers. We show such a system of matrix equations may be recast as an unconstrained equation whose solutions automatically satisfy the constraint. Projection solvers for the resulting matrix equation are discussed, along with various properties of the reformulated equation. Numerical experiments are given to illustrate the new methodology.

ANA MARIA SOANE. *University of Maryland Baltimore County.*
Multigrid preconditioners for optimal control problems in fluid flow: We construct multigrid preconditioners to accelerate the solution process of optimal control problems constrained by the Stokes/Navier-Stokes equations. Our approach for the Stokes control problem is to eliminate the state and adjoint variables from the optimality system and to construct efficient multi-

grid preconditioners for the Schur-complement of the block associated with these variables. Similar preconditioners are constructed for the reduced Hessian in the Newton-PCG method for the optimal control of the stationary Navier-Stokes equations.

AZIZ TAKHIROV. *University of Pittsburgh.*
Flow in pebble bed geometries: Flow in complex geometries intermediate between free flows and porous media flows occurs in pebble bed reactors and in optimization of turbine placement in wind farms. The Brinkman models have consistently shown that for simplified settings accurate prediction of essential flow features depends on the impossible problem of meshing the pores. In this paper we investigate new model to understand the flow and its properties in these geometries.

IGNACIO TOMAS. *University of Maryland, College Park.*
Analysis of fully discretre scheme for the Micropolar Navier Stokes equations: The Micropolar-Navier-Stokes Equations (MNSE) is a system of coupled time-dependent PDEs: conservation of linear momentum, conservation of mass and conservation of angular momentum. This system constitutes a proper framework to describe the dynamics of an infinite number of interacting particles (subject to viscous forces) which have both translational and rotational degrees of freedom. Consequently, these equations are very attractive for the dynamic description of media subject to distributed couples and polar media in general. We propose and proceed to analyze the convergence properties of a fully-discrete semi-implicit time integration scheme for the MNSE, which decouples the equations for linear and angular momentum. The scheme turns out to be unconditionally stable, convergence rates are proved and verified numerically with classical validation problems which confirm the developed theory.

BART VANDEREYCKEN, *Princeton University.*
The geometry of algorithms using hierarchical Tucker tensors: Rank-structured tensors have become a popular computational tool to exploit the intrinsic low dimension of certain high-dimensional problems. In this poster, we present the differential geometry of the set of hierarchical Tucker tensors of fixed rank as introduced in [1]. After establishing a global smooth manifold structure and a scalable parametrization of the tangent space, we apply our derived geometry to two applications. First, we give a new convergence analysis of the nonlinear Gauss -Seidel iteration using low-rank tensors (including the minimization of the Rayleigh quotient) as used in [2,3]. Second, we present and analyze a generalization of the dynamical low-rank algorithm from [4] to approximate parameter-dependent hierarchical Tucker tensors. Parts of this is joint work with T. Rohwedder, R. Schneider, A. Uschmajew (T.U.Berlin) and C. Lubich (Universität Tübingen).

References
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DONG ZHOU. *Temple University.*
Jet Schemes for Hamilton-Jacobi Equations Using an Evolve-and-project Framework: Jet schemes are based on tracking characteristics and using suitable Hermite interpolations to achieve high order. For Hamilton-Jacobi equations, the characteristic equations are in general nonlinear, i.e. the characteristic curves may collide or emanate radially for local extrema. We demonstrate that in these situations, the use of explicit schemes for solving the characteristic equations can yield incorrect results. We therefore propose an implicit update rule that is based on solving a constrained polynomial optimization problem in each grid cell, and then reconstructing the solution from Hermite interpolations and evolving it in time. Numerical tests show that this implicit approach approximates entropy solutions correctly and achieves high order accuracy in the smooth part of the solution. Moreover, we demonstrate that this approach can be interpreted as an evolve-and-project process similar to the advect-and-project approach for linear advection equations.

List of Participants*

SOROUSH ASSARI (s.assari@temple.edu)

MAGGIE AVENER (avenerm@temple.edu)

JINGMIN CHEN (jc3227@drexel.edu)

PRINCE CHIDYAGWAI (chidyagp@temple.edu)

QUAN DENG (dengquan@udel.edu)

SHIMAO FAN (tub00072@temple.edu)

MONA HAJGHASSEM (mona4@umbc.edu)

QUNHUI HAN (qhan@udel.edu)

SUNNIE JOSHI (sjoshi@temple.edu)

SHELVEAN KAPITA (kapita@udel.edu)

ISAAC KLAPPER (klapper@temple.edu)

SCOTT LADENHEIM (saladenh@temple.edu)

KAVEH LAKSARI (kaveh.laksari@temple.edu)

GEUNSEOP LEE (gxl174@cse.psu.edu)

EDWARD LETZTER (letzter@temple.edu)

LONGFEI LI (longfei@math.udel.edu)

KATHRYN LUND (katlund@temple.edu)

TIM MITCHELL (tim.mitchell@cims.nyu.edu)

PETER MONK (monk@udel.edu)

MARINA MORAITI (mam328@pitt.edu)

EDWARD GEOFFREY PHILLIPS (egphillips@math.umd.edu)

ABNER SALGADO (abnersg@math.umd.edu)

JYOTI SARASWAT (jyo1@umbc.edu)

BENJAMIN SEIBOLD (seibold@temple.edu)

STEPHEN SHANK (sshank@temple.edu)

FAN SHIMAO (tub00072@temple.edu)

ANA MARIA SOANE (asoane@umbc.edu))

DANIEL B. SZYLD (szyld@temple.edu)

AZIZ TAKHIROV (azt7@pitt.edu)

IGNACIO TOMAS (ignaciotomas@math.umd.edu)

BART VANDEREYCKEN (bartv@math.princeton.edu)

MINGHAO WU (mwu@math.umd.edu)

DONG ZHOU (dong.zhou@temple.edu)

* List complete as of 10/31/12