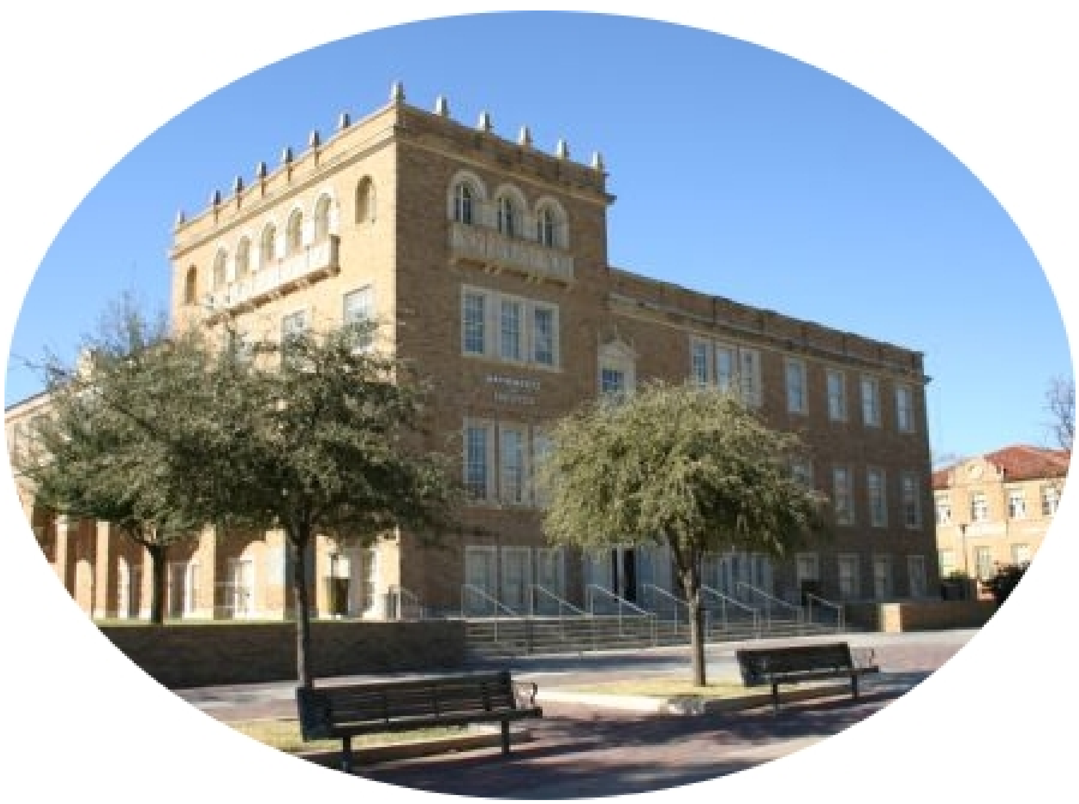
Current Trends in Numerical Analysis and Scientific Computing

Book of Abstracts

XVII Red Raider Mini-Symposium
Saturday, October 27, 2018



Department of Mathematics and Statistics
Texas Tech University

The Red Raider Mini-Symposium Series

This series was initiated in 2001 by *Prof. Frits Ruymgaart*, a Paul Whitfield Horn Professor, who generously used his professorship's endowment to partially fund the mini-symposium's activities. Since 2015, Horn Professor Linda Allen continues this line of funding with the same generosity.

Invited lecturers at the mini-symposium include distinguished scholars who made a great impacts in the field, as well as early career mathematicians and promising young scientists. The lectures expose the audience to current research problems, as well as their solutions and applications. The topics covered by the Red Raider mini-symposia span over broad areas of pure and applied mathematics and reflect the strengths of the scientific groups in the Department of Mathematics and Statistics at Texas Tech University. In chronological order, the previous symposia cover a large diversity of research interests:

2001 - *Control Theory in the Twenty-First Century*
2002 - *Contemporary Algebra and Algebraic Geometry*
2003 - *Mathematical and Computational Modeling of Biological Systems*
2004 - *Invariant Theory in Perspective*
2005 - *Geometry, Statistics and Image Analysis*
2006 - *Mathematical Modeling of Novel Material and Devices*
2007 - *Conformal Mapping, Circle Packing and Applications*
2008 - *The Topology and Geometry of Physics*
2009 - *Non-linear Analysis, PDEs and Applications*
2010 - *Mathematical Modeling in Population Biology and Epidemiology*
2011 - *High Level Mathematical Software for PDE's FEniCS'11*
2012 - *Computational and Theoretical Challenges in Interdisciplinary Predictive Modeling Over Random Fields*
2013 - *Aspects of Fluid Dynamics*
2014 - *Complex Analysis, Potential Theory, Special Functions and Applications*
2015 - *Spatial Inference on Manifolds Spatial Statistics, Statistics on Manifolds, Differential Geometry, and Computational Science*
2017 - *Structures on Free Resolutions*

Current Trends in Numerical Analysis and Scientific Computing

The XVII Red Raider Mini-Symposium is entitled *Current Trends in Numerical Analysis and Scientific Computing* and is featuring five distinguished speakers and five early-career speakers. The goal of the minisymposium is to bring together top scientists in the areas of Numerical Analysis and Scientific Computing to understand the most important lines of investigation in these fields. The minisymposium features an interplay of both theoretical and practical aspects that are at the forefront of current research efforts in the scientific community.

Organizers

- **Giorgio Bornia**, Texas Tech University
- **Wei Guo**, Texas Tech University

Sponsors

- **Horn Professor Linda Allen**, Texas Tech University
- **Department of Mathematics and Statistics**, Texas Tech University
- **SIAM Chapter**, Texas Tech University

Distinguished Speakers

WOLFGANG BANGERTH, ***Colorado State University***

Simulating complex flows in the Earth mantle

Good scientific computing is a two-way street: We use what we learn in numerical analysis to solve complex problems, and we learn about things that don't work yet and need to be further analyzed mathematically. In this talk, I will discuss what we have found applying modern numerical methods for complex flow in the Earth mantle: the region between the rigid plates at the surface and the liquid metal outer core at depth that behaves like a nonlinear fluid on long enough time scales.

While the Earth mantle moves only a few centimeters per year, the large length scales nevertheless lead to very large Rayleigh numbers and, consequently, very complex and expensive numerical simulations. The inaccessibility of the Earth mantle to direct experimental observation implies that numerical simulation is one of the few available tools to elucidate what exactly is going on in the mantle, how it affects the long-term evolution of Earth's thermal and chemical structure, as well as what drives and sustains plate motion.

I will here review the approach we have taken in building the state-of-the-art open source solver ASPECT (see aspect.geodynamics.org) to simulate realistic conditions in the Earth and other celestial bodies. I will focus on the choices we have made regarding the numerical methods used in ASPECT, and in particular on the interplay between higher order discretizations on adaptive meshes, linear and nonlinear solvers, optimal preconditioners, and approaches to scale to thousands of processor cores.

JEAN LUC GUERMOND, ***Texas A&M University***

Second-order invariant domain preserving approximation of the Euler equations using convex limiting

A second-order finite-element-based method for approximating the compressible Euler equations is introduced. The method preserves all the known invariant domains of the Euler system: positivity of the density, positivity of the internal energy and the local minimum principle on the specific entropy. The technique combines a first-order, invariant domain preserving, Guaranteed Maximum Speed method using a Graph Viscosity (GMS-GV1) with an invariant domain violating, but entropy consistent, high-order method. Invariant domain preserving auxiliary states, naturally produced by the GMS-GV1 method, are used to define local bounds for the high-order method which is then made invariant domain preserving via a convex limiting process. Numerical tests confirm the second-order accuracy of the new GMS-GV2 method in the maximum norm, where 2 stands for second-order. The proposed convex limiting is generic and can be applied to other approximation techniques and other hyperbolic systems.

MAX GUNZBURGER, *Florida State University*

A Localized Reduced-Order Modeling Approach for PDEs with Bifurcating Solutions

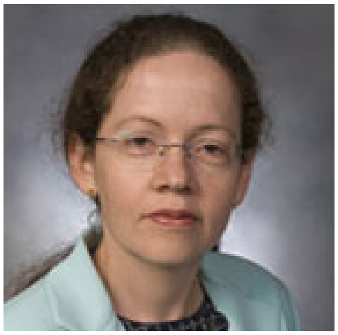
Reduced-order modeling (ROM) commonly refers to the construction, based on a few solutions (referred to as snapshots) of an expensive discretized partial differential equation (PDE), and the subsequent application of low-dimensional discretizations of partial differential equations (PDEs) that can be used to more efficiently treat problems in control and optimization, uncertainty quantification, and other settings that require multiple approximate PDE solutions. In this work, a ROM is developed and tested for the treatment of nonlinear PDEs whose solutions bifurcate as input parameter values change. In such cases, the parameter domain can be subdivided into subregions, each of which corresponds to a different branch of solutions. Popular ROM approaches, such as proper orthogonal decomposition (POD), results in a global low-dimensional basis that does not respect nor take advantage of the often large differences in the PDE solutions corresponding to different subregions. Instead, in the new method, the k-means algorithm is used to cluster snapshots so that within cluster snapshots are similar to each other and are dissimilar to those in other clusters. This is followed by the construction of local POD bases, one for each cluster. The method also can detect which cluster a new parameter point belongs to, after which the local basis corresponding to that cluster is used to determine a ROM approximation. Numerical experiments show the effectiveness of the method both for problems for which bifurcation cause continuous and discontinuous changes in the solution of the PDE. [Joint work with Alessandro Alla, Martin Hess, Gianluigi Rozza, Annalisa Quaini]

FENGYAN LI, *Rensselaer Polytechnic Institute*

Fully Discrete Energy Stable Methods for Maxwell's Equations in Nonlinear Media

The propagation of electromagnetic waves is modeled by time-dependent Maxwell's equations coupled with constitutive laws that describe the response of the media. In this work, we examine a nonlinear optics model that describes electromagnetic waves in linear Lorentz and nonlinear Kerr and Raman media. To design efficient, accurate, and stable computational methods, we apply high order discontinuous Galerkin discretizations and finite difference schemes in space. The challenge to achieve provable stability for fully-discrete methods lies in the temporal discretizations of the nonlinear terms. To overcome this, novel modifications are proposed for both the second-order leap-frog and implicit trapezoidal temporal schemes. The performance of the methods is demonstrated by numerical examples and also through numerical dispersion analysis of the methods applied to the linearlized model. This work was in collaboration with V. A. Bokil, Y. Cheng, Y. Jiang, and P. Sakkaplangkul.

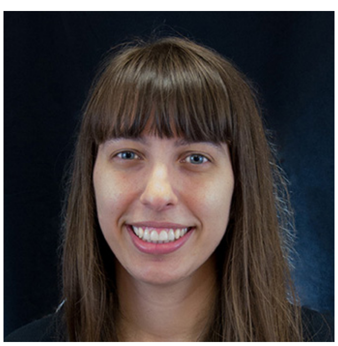
BEATRICE RIVIÈRE, ***Rice University***
Numerical solution of two-phase flow in porous media at the pore scale



Modeling multicomponent flows in porous media is important for many applications relevant to energy and environment. Advances in pore-scale imaging, increasing availability of computational resources, and developments in numerical algorithms have started rendering direct pore-scale numerical simulations of multiphase flow on pore structures feasible. I will present a pore-scale flow model based on the coupling of Cahn-Hilliard and incompressible Navier-Stokes equations. At the micro-meter scale, the rock structure is given and the fluid flows through the connected pores. The three-dimensional computational domain is the union of voxels, obtained from the micro-CT scanning of real rock samples. A priori error estimates show convergence of the scheme for sufficiently smooth solutions. Validation of the algorithm is obtained on a suite of benchmark problems.

Early Career Speakers

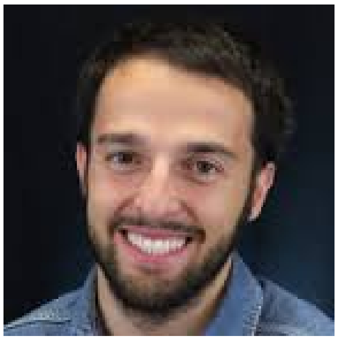
SARA CALANDRINI, ***Florida State University***
Exponential Time Differencing for the Tracer Equations Appearing in Primitive Equation Ocean Models



We consider the tracer equations that are part of the primitive equations used in ocean modeling. These equations describe the transport of tracers, such as temperature, salinity or chemicals, in the ocean. Depending on the number of tracers considered, several equations may be added to and coupled to the dynamics system. In many relevant situations, the time-step requirements of explicit methods caused by the transport and mixing in the vertical direction are more restrictive than the ones for the horizontal. We propose an exponential time differencing (ETD) solver where the vertical transport is treated with a matrix exponential, whereas the horizontal is dealt with in an explicit way. We investigate numerically the accuracy and computational speed-ups that can be obtained over an explicit or a fully exponential method. Results for the complete set of primitive equations are also shown, where a tracer system is coupled to the dynamics. Here, the tracer and dynamics equations are decoupled in each time-step, and a second-order ETD solver is employed for the dynamics system.

GIACOMO CAPODAGLIO, *Florida State University*

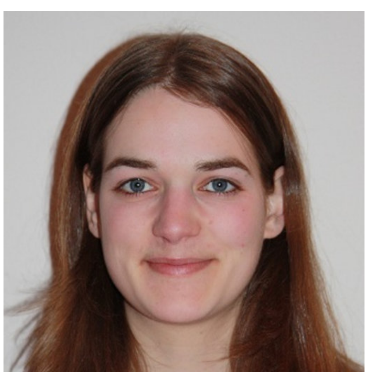
Approximation of probability density functions for SPDEs using truncated series expansions



The probability density function (PDF) of a random variable associated with the solution of a stochastic partial differential equation (SPDE) is approximated using a truncated series expansion. The SPDE is solved using two stochastic finite element (SFEM) methods, Monte Carlo sampling and the stochastic Galerkin method with global polynomials. The random variable is a functional of the solution of the SPDE, such as the average over the physical domain. The truncated series are obtained considering a finite number of terms in the Gram-Charlier (GC) or Edgeworth (ED) series expansions. These expansions approximate the PDF of a random variable in terms of another PDF, and involve coefficients that are functions of the known cumulants of the random variable. While the GC and ED series have been employed in a variety of fields such as chemistry, astrophysics and finance, their use in the framework of SPDEs has not yet been explored.

DIANE GUIGNARD, *Texas A&M University*

Error indicators for goal-oriented adaptive methods



When we are interested in computing a specific quantity of interest (QoI), for instance a linear functional of the solution of some partial differential equation, the energy norm is not a suitable measure of the error. Goaloriented error estimation has thus been introduced. Using an adjoint problem, with the QoI as right-hand side, the error in the QoI can be estimated through the error of both the primal and the dual solutions. In order to use an adaptive strategy, the error estimate need to be broken into local contributions and we can proceed in many different ways. Even though the various error decompositions yield the same result globally, i.e. when summing all the local contributions, the local error indicators vary from one representation to another. Therefore, adaptive algorithms will not perform the same using one or the other representations. The goal of this presentation is to introduce different local error indicators for an abstract problem and then to compare their performance, when used in an adaptive scheme, through numerical examples.

Alexander Mamonov, *University of Houston*

Imaging with waves and multiple removal via model order reduction

We introduce a novel framework for imaging and removal of multiples from waveform data based on model order reduction. The reduced order model (ROM) is an orthogonal projection of the wave equation propagator (Green's function) on the subspace of discretely sampled time domain wavefield snapshots. Even though neither the propagator nor the wavefields are known in the bulk, the projection can be computed just from the knowledge of the waveform data using the block Cholesky factorization. Once the ROM is computed, its use is twofold.

First, the projected propagator can be backprojected to directly obtain an image of reflectors, the discontinuities of the wave speed. ROM computation implicitly orthogonalizes the wavefield snapshots. This highly nonlinear procedure differentiates our approach from the conventional linear migration methods (Kirchhoff and reverse time migration - RTM). It allows to resolve the reflectors independently of the knowledge of the kinematics and to untangle the nonlinear interactions between the reflectors. As a consequence, the resulting images are almost completely free from the multiple reflection artifacts.

Second, the ROM computed from the original waveform data can be used to generate the Born data set, i.e. the data that the measurements would produce if the propagation of waves in the unknown medium obeyed Born approximation instead of the full wave equation. Obviously, such data only contains primary reflections and the multiples are removed. Consecutively, existing linear imaging and inversion techniques can be applied to Born data to obtain reconstructions in a direct, non-iterative manner. The method is purely linear-algebraic and is therefore equally applicable to acoustic, elastic and electromagnetic waveform data.

Lin Mu, *Oak Ridge National Laboratory*

A Fully Computable Posteriori Error Estimate for Polygonal Weak Galerkin Finite Element Methods of Stokes Equations

In this talk, we will present a simple posteriori error estimate for the weak Galerkin finite element method of the Stokes equations. This new estimator can be applied to general meshes such as polygonal mesh or mesh with hanging nodes. Because of the flexibility for applying on polygonal meshes, the adaptive mesh refinement will be more effective and has the feature for keeping local structures. The reliability and efficiency of the estimator will be provided and validated by several numerical examples.

Schedule

Saturday, October 27, 2018

08:15 am - Welcome and registration
08:40 am - Opening remarks by Dean **W. Brent Lindquist**

08:50 - 09:40 am - **Max Gunzburger**
A Localized Reduced-Order Modeling Approach for PDEs with Bifurcating Solutions
09:50 - 10:40 am - **Fengyan Li**
Fully Discrete Energy Stable Methods for Maxwell's Equations in Nonlinear Media

10:50 - 11:00 am - Coffee break

11:00 - 11:25 am - **Alexander Mamonov**
Imaging with waves and multiple removal via model order reduction
11:30 - 11:55 am - **Diane Guignard**
Error indicators for goal-oriented adaptive methods

12:00 - 1:30 pm - Lunch break

01:30 - 02:25 pm - **Wolfgang Bangerth**
Simulating complex flows in the Earth mantle
02:30 - 02:55 pm - **Sara Calandrini**
Exponential Time Differencing for the Tracer Equations Appearing in Primitive Equation Ocean Models
03:00 - 03:50 pm - **Beatrice Rivière**
Numerical solution of two-phase flow in porous media at the pore scale

04:00 - 04:30 pm - Coffee break

04:30 - 05:25 pm - **Jean-Luc Guermond**
Second-order invariant domain preserving approximation of the Euler equations using convex limiting
05:30 - 05:55 pm - **Giacomo Capodaglio**
Approximation of probability density functions for SPDEs using truncated series expansions
06:00 - 06:25 pm - **Lin Mu**
A Fully Computable Posteriori Error Estimate for Polygonal Weak Galerkin Finite Element Methods of Stokes Equations