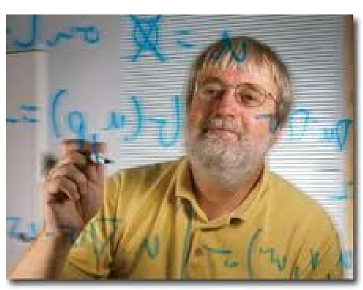
# Advances in Scientific Computing and Applied Mathematics

Welcome to the conference on "Advances in scientific computing and applied mathematics," October 9-12 in the Stratosphere Hotel in Las Vegas, Nevada. The conference is co-sponsored by the Oak Ridge National Laboratory, Sandia National Laboratories and The Office of Science, Advanced Simulation Research Computing (ASCR), at the Department of Energy.

The conference has been co-organized by Drs. Pavel Bochev, Qiang Du, Steve Hou, and Clayton Webster, and features original work by leading researchers in numerical analysis, mathematical modeling and computational science covering the following subject areas:

- Climate modeling and groundwater flows: including ocean and ice sheet modeling, numerical algorithms;
- Computational fluid dynamics;
- Computational geometry, mesh generation and image processing;
- Finite element methods: including Least-squares FEMs, Stabilized FEMs, Compatible FEMs, DG, and DPG;
- Flow control, theory, numerical methods and applications;
- Materials modeling: including multi-scale methods, quasi-continuum methods, atomistic to continuum coupling, peridynamics and nonlocal model, applications in superconductivity;
- Reduced order modeling, domain decomposition and multidisciplinary simulation and optimization, and;
- Uncertainty quantification and numerical methods for partial differential equations with random. inputs

There will be a special issue of the journal "Computers and Mathematics with Applications" to honor Prof. Max Gunzburger's 70th birthday. The papers will undergo rigorous peer review process managed by the guest editors (Bochev, Du, Hou and Webster) and supervised by the journal's Editor-in-Chief, Prof. Leszek Demkowicz.



Prof. Gunzburger is the Francis Eppes Distinguished Professor of Mathematics and the Robert O. Lawton Distinguished Professorship at Florida State University. He is currently the Chair of the the Department of Scientific Computing at Florida State University. Previously, he was the 2008 winner of the SIAM W.T. and Idalia Reid Prize in Mathematics. He is an extremely rare mathematician, in that, he is considered a worldwide leader in multiple disjoint disciplines, including flow control, finite element analysis, superconductivity and Voronoi tessellations, with impacts in a multitude of applications including aerodynamics, materials, acoustics, climate change, groundwater, image processing and risk assessment. On a personal level, Max is much more than a Ph.D. advisor or a colleague to us; he is one of our most trusted mentors and a closest friends.

**Invited speakers...**

- Bacim Alali
- Pavel Bochev
- Jeff Borggaard
- Giorgio Bornia
- John Burns
- Yanzhao Cao
- Qingshan Chen
- K. Chrysafinos
- Eugene Cliff
- Marta D'Elia
- Leszek Demkowicz
- Qiang Du
- Greg Forest
- Marc Gerritsma
- Steve Hou
- Douglas Jacobsen
- Lili Ju
- Angela Kunoth
- Hee-Dae Kwon
- Alexander Labovsky
- Bill Layton
- Jeehyun Lee
- Eunjung Lee
- Hyung-Chun Lee
- Hyesuk Lee
- Rich Lehoucq
- Sandro Manservisi
- Tom Manteuffel
- A. J. Meir
- Ju Ming
- Hoa Nguyen
- Mauro Perego
- Pablo Seleson
- Ralph Smith
- Miroslav Stoyanov
- Catalin Trenchea
- James Turner
- Hans-Werner van Wyk
- Xiaoming Wang
- Clayton Webster
- Geoff Womeldorff
- Guannan Zhang
- Yanzhi Zhang

**Organizers & Guest Editors:**
Pavel Bochev
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Steve Hou
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Clayton Webster
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# Schedule

**Saturday October 10, 2015**
**Sunrise Room on 104th Floor**
7:30-8:45 **Breakfast**
8:45-9:00 **Opening remarks**

9:00-9:15 Greg Forest
9:15-9:30 James Turner
9:30-9:45 Hoa Nguyen
9:45-10:00 Jeehyun Lee

10:00-10:30 **Coffee Break**

10:30-10:45 Tom Manteuffel
10:45-11:00 Eugene Cliff
11:00-11:15 Leszek Demkowicz
11:15-11:30 Qingshan Chen

11:30-13:00 **Lunch (on your own)**

13:00-13:15 John Burns
13:15-13:30 Angela Kunoth
13:30-13:45 Jeff Borggaard
13:45-14:00 Hee-Dae Kwon
14:00-14:15 Catalin Trenchea
14:15-14:30 K. Chrysafinos

14:30-15:00 **Coffee Break**

15:00-15:15 Eunjung Lee
15:15-15:30 Douglas Jacobsen
15:30-15:45 Mauro Perego
15:45-16:00 Hyung-Chun Lee
16:00-16:15 A. J. Meir
16:15-16:30 Ju Ming
16:30-16:45 Pavel Bochev
16:45-17:00 Steve Hou

18:00 -20:00 **Dinner (on your own)**

**Sunday October 11, 2015**
**Sunrise Room on 104th Floor**
7:30-8:45 **Breakfast**

9:00-9:15 Bill Layton
9:15-9:30 Xiaoming Wang
9:30-9:45 Hyesuk Lee
9:45-10:00 Sandro Manservisi

10:00-10:30 **Coffee Break**

10:30-10:45 Alexander Labovsky
10:45-11:00 Geoff Womeldorff
11:00-11:15 Marc Gerritsma
11:15-11:30 Giorgio Bornia

11:30-13:00 **Lunch (on your own)**

13:00-13:15 Rich Lehoucq
13:15-13:30 Guannan Zhang
13:30-13:45 Yanzhi Zhang
13:45-14:00 Marta D'Elia
14:00-14:15 Bacim Alali
14:15-14:30 Pablo Seleson

14:30-15:00 **Coffee Break**

15:00-15:15 Ralph Smith
15:15-15:30 Yanzhao Cao
15:30-15:45 Lili Ju
15:45-16:00 Miroslav Stoyanov
16:00-16:15 Hans-Werner van Wyk
16:15-16:30 Qiang Du
16:30-16:45 Clayton Webster

19:00 -22:00 **Banquet, Horizon Room**
Bochev, Forest, Manteuffel, Webster

**Monday October 12, 2015**, **Sunrise Room on 104th Floor**
7:30-8:45 **Breakfast**

9:00-9:45 Open discussions
10:00- **Closing statements and depart to airport**

# Abstracts

*(in alphabetical order by speaker surname)*

## Bacim Alali, Kansas State University

*Nonlocal Interface Conditions*

Abstract not available at time of publication.

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## Pavel Bochev, Sandia National Laboratories

*Coupling strategies for interface problems*

Numerical solution of problems with interfaces arises in importance science and engineering applications. In this talk we focus on partitioned solution approaches in which the governing equations are discretized and solved separately on the subdomains defined by the interface. The talk examines several strategies for exchanging information between the subdomain problems. Numerical examples illustrate numerical properties of different approaches, such as linear consistency and convergence rates.

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## Jeff Borggaard, Virginia Tech

*Rotational Stabilization of Cylinder Wakes Using Linear Feedback Control*

We demonstrate the feasibility of linear feedback control to stabilize vortex shedding behind several cylinders using cylinder rotations. Our approach is to linearize the flow about a desired steady-state flow, use interpolation-based model reduction on the resulting linear model to generate a low-dimensional model of the input-output system with input-independent error bounds, then use this reduced model to design the feedback control law. Closed-loop simulations of the nonlinear system show the success of this control strategy.

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## Giorgio Bornia, Texas Tech University

*Multigrid and domain decomposition methods for incompressible Fluid Structure Interaction problems*

We investigate the numerical performance of a monolithic Newton-multigrid solver with domain decomposition smoothers for the solution of incompressible FSI problems. A monolithic approach is considered with an Arbitrary Lagrangian Eulerian (ALE) scheme for the domain deformation. The implementation of the Jacobian matrix is a nontrivial task which can be achieved by using automatic differentiation tools. Numerical results of challenging incompressible steady-state benchmark tests are presented in order to highlight the robustness of the proposed approach.

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## John Burns, Virginia Tech

*Control of Thermal Fluid Systems*

In this this presentation we discuss several computational issues involved with designing feedback controllers for thermal-fluid systems. The problems are motivated by applications to the design and operation of aircraft environmental control systems and modern HVAC systems. These problems are typical of many of today's complex multi-physics, data-driven, uncertain physical systems and, although this presentation will focus on thermal fluid systems, the issues arise in a wide variety of modern engineered systems. A key observation is that even if one has an excellent numerical scheme for simulating the open-loop system, this scheme may not be suitable for controller design and may fail when applied to the closed-loop system. Examples are provided to illustrate the issues and to suggest areas for future research.

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## Yanzhao Cao, Auburn University

*Backward SDE method for nonlinear filtering problems*

It is well known that nonlinear filtering problems can be solved by solving stochastic partial differential equations (Zakai filter). The main challenge of Zakai filter is that it is very difficult to construct high order methods. In this talk we show that the nonlinear filtering problems can be solved by solving backward stochastic differential equations. One of the main advantages of the BSDE method is that high order methods can be constructed seamlessly.

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## Qingshan Chen, Clemson University

*Mimetic and convergent discretization of vector fields on unstructured meshes*

In this talk, we present a new theoretical framework for analyzing FD/FV schemes for a wide range of fluid problems. There are two essential ingredients to this framework. The first is the external approximation of function spaces, which seems particular adept in dealing with discontinuous functions. The second is the tracking of divergence and vorticity, instead of individual derivatives. This approach gets rid of the requirement for a Cartesian coordinate system, and makes this framework applicable to unstructured meshes. Once the framework has been presented, we will apply it to the classical incompressible Stokes problem, and prove that the discrete solutions converges to the solution of the continuous system, without assuming that one actually exists.

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## Konstantinos Chrysafinos, University of Athens

*Discontinuous time-stepping schemes for the Allen-Cahn equations and applications to optimal control*

We consider fully discrete schemes for the Allen-Cahn equation based on a discontinuous Galerkin (in time) approach, and we prove that these schemes are unconditionally stable under minimal regularity assumptions on the given data. Stability estimates in the natural energy norms are proved using an appropriate duality argument, combined with a boot-strap technique. Great care is exercised in order to quantify the dependence of various constants appearing in these estimates. The applicability of these estimates in a optimal control setting is also demonstrated.

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## Eugene Cliff, Virginia Tech

*On Time-Optimal Paths*

We survey time-optimal paths in several applications. Energy models in flight mechanics, which describe motions on intermediate time-scales, are useful approximations for real-time guidance. Next we consider energy/heading transients in an aircraft model with thrust-vectoring capability. There are two families of optimal paths separated by a locus of Darboux points. Lastly we discuss recent results on planar path planning with a variable-speed model; time-optimal paths are composed from a small number of candidate sub-arcs.

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## Marta D'Elia, Sandia National Laboratories

*An optimization-based coupling of local and nonlocal continuum models*

We present an optimization-based coupling of local and nonlocal continuum models. The coupling is formulated as a control problem where the states are the solutions of the nonlocal and local equations, the objective is to minimize their mismatch on the overlap of the local and nonlocal domains, and the controls are volume constraints and boundary conditions. We present numerical results illustrating the accuracy and efficacy of the method in the context of nonlocal diffusion and nonlocal elasticity.

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## Leszek Demkowicz, University of Texas, Austin

*Discontinuous Petrov Galerkin (DPG) method for Maxwell problems*

Due to their linear dependence, Maxwell equations present a challenge for both analysis and discretization. Standard conforming discretizations lead to the use of H(curl)-conforming elements and the exact sequence property. I will present a complete analysis for the discretization of time-harmonic Maxwell problems using two versions of the DPG method based on both classical and ultraweak variational formulations. We will see that the "old problems" leading to the exact sequence, do not disappear but emerge in somehow different form. I will discuss the benefits and drawbacks of the DPG method as compared with standard Galerkin and illustrate it with several numerical examples.

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## Qiang Du, Columbia University

*The search for optimal 3D tetrahedra*

Mesh optimization often involves the search for optimal shapes with elegant structures and nice approximation properties. While regular triangle is widely accepted as optimal in 2D, its 3D analog has been a subject of historical debate. Resolving the controversy concerning this seemingly elementary issue has fundamental significance in many applications. We argue that the second Sommerville tetrahedron is optimal in 3D. Such a tetrahedron is also dual to the optimal 3D centroidal Voronoi tessellation.

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## Greg Forest, UNC Chapel Hill

*Quantification of anomalous diffusion may be the miner's canary of human health*

Every organ in the human body is protected by a thin lining of "mucus". The defense mechanisms required in the nose, sinuses, eyes, reproductive tract, heart, gut, and lung are markedly different, so the body manufactures a range of different high molecular weight proteins, called mucins, and combines them in myriad ways with salt, water, and small molecular weight proteins to cook up barrier properties needed by that particular organ. I will discuss the discovery that diseases, both genetic and acquired, are associated with disruptions in normal mucus composition, and our mathematical tools to discern disease progression from the anomalous diffusion of tracers in mucus.

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## Marc Gerritsma, TU Delft

*A spectral mimetic least-squares method applied to the Stokes problem*

In June 2009 Bochev and Gunzburger presented the paper "*A locally conservative mimetic least-squares finite element method for the Stokes equations*" at the $7^{th}$ International Conference on Large Scale Scientific Computing in Sozopol, Bulgaria. In honor of Max's $70^{th}$ birthday, we apply the proposed mimetic least-squares formulation to the Stokes operator using mimetic spectral elements. Exact mass conservation will be shown independent of polynomial degree.

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## Steve Hou, Iowa State University

*TBD*

Abstract not available at time of publication.

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## Douglas Jacobsen, Los Alamos National Laboratory

*A global unstructured multi-resolution ocean model*

The Model for Prediction Across Scales (MPAS) is a flexible modeling framework that utilizes unstructured meshes. It is being developed jointly between the Los Alamos National Laboratory (LANL), and the National Center for Atmospheric Research (NCAR). Within the MPAS framework, LANL has been developing a global ocean model (MPAS-O) that is capable of simulating with variable horizontal resolution meshes. The MPAS-O model will be the ocean component of DOE's ACME Climate model.

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## Lili Ju
## University of South Carolina

*Centroidal Voronoi Tessellation Based Methods for Image Segmentation*

Centroidal Voronoi tesssellations (CVTs) are special Voronoi tessellations whose generators are also the centers of mass (centroids) of the Voronoi regions with respect to a given density function. CVT-based methodologies have been proven to be very useful in many diverse applications in science and engineering. In this talk, we will review recent advances of image segmentation methods based on the CVT and its variants, including the edge-weighted CVT (EWCVT), the multichannel EWCVT (MEWCVT), and the local variation and edge-weighted CVT (LVEWCVT) models. We will illustrate these interesting segmentation methods through extensive examples.

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## Angela Kunoth, University of Cologne

*Adaptive Approximations of Parametric PDE-Constrained Control Problems*

Optimization problems constrained by linear parabolic evolution PDEs are challenging from a computational point of view: one needs to solve a system of PDEs coupled globally in time and space. Conventional time-stepping methods require an enormous storage. In contrast, adaptive methods in both space and time which aim at distributing the available degrees of freedom in an a-posteriori-fashion to capture singularities are most promising. Employing wavelet schemes for full weak space-time formulations of the parabolic PDEs, we can prove convergence and optimal complexity. Yet another level of challenge are control problems constrained by evolution PDEs involving stochastic or countably many infinite parametric coefficients: for each instance of the parameters, this requires the solution of the complete control problem. Our method of attack is based on a new theoretical paradigm.

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## Hee-Dae Kwon, Inha University

*Feedback Control of Immune Response of Renal Transplant Recipients with Inequality Constraints*

We consider the increasingly important and highly complex immunological control problem: control of the dynamics of immunosuppression for organ transplant recipients. The goal in this problem is to maintain the delicate balance between over-suppression (where opportunistic latent viruses threaten the patient) and under-suppression (where rejection of the transplanted organ is probable). First, a mathematical model is formulated to describe the immune response to both viral infection and introduction of a donor kidney in a renal transplant recipient. In addition, we propose a feedback methodology based on Model Predictive Control (MPC) for designing optimal treatment regimes. We also address the problem of implementing MPC methodology and the Extended Kalman Filter(EKF) with inaccurate or incomplete observation data and long measurement time.

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## Alexander Labovsky
## Michigan Technological University

*Magnetohydrodynamic Flows: Boussinesq Conjecture*

The Boussinesq assumption that turbulent fluctuations have a dissipative effect on the mean flow is the basis for most turbulence models used in practical flow simulations.It has recently been proven to hold in a time averaged sense for the Navier-Stokes equations. In Magnetohydrodynamic (MHD) flows the dynamo effect suggests an inverse cascade of energy from small to large scales, but we will show that the Boussinesq assumption also holds for MHD turbulence.

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## Bill Layton, University of Pittsburgh

*Algorithms and Models for Turbulence not at Statistical Equilibrium*

This talk will present an analysis of the energy flow between means and fluctuations. Based on this analysis corrections to eddy viscosity models will be presented and analyzed.

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## Jeehyun Lee, Yonsei University

*Parameter estimation using Kalman Filter in epidemiology*

Mathematical models in epidemiology have been used to predict the course of an infectious disease and to compare the effects of different control strategies. Estimation of parameters is one of the most important issues because parameters play a crucial role to determine the disease dynamics. However, it is very challenging due to the properties of epidemiology including non-reproducible and incomplete epidemic data. In this research, to overcome difficulties in least square method (LSM), a standard approach for parameter estimations, we apply ideas and techniques of Kalman filter (KF). Numerical simulations show that KF is much more robust than LSM to the perturbation of initial states and the timing of sampling when the data is insufficient to represent complete dynamics. Therefore, Kalman filter has a great potential as a tool for real time parameter estimations and is applied to the national data of antiviral agent prescription in Korea for Pandemic Influenza.

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## Eunjung Lee, Yonsei University

*Least squares method for a nonlinear Stokes problem in glaciology*

In this paper, we analyze the nonlinear Stokes equations which is appeared in glaciology problems with least-squares finite element method. The modified Picard iteration is used to linearize the given nonlinear problem. We first establish minimization problem which finds minimizer of residual functional in corresponding Sobolev spaces and prove theoretical results. From numerical experiments, we find an approximation of weak solution and verify the error estimates.

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## Hyung-Chun Lee, Ajou University

*New finite element method to compute accurate solution for Poisson equation with domain singularities*

In this talk, we consider the Poisson equation with homogeneous Dirichlet boundary condition defined on a polygonal domain with one reentrant corner. The solution of this problem has singular behavior near that corner even when the source term is smooth enough. Such singular behavior affects the accuracy of the finite element method throughout the whole domain. The solution can be written as a sum of regular part and singular part, where the singular part is a multiple of a constant(called 'stress intensity factor') and well-known singular function. The stress intensity factor can be computed by extraction formula from the solution and input function $f$. Using this stress intensity factor, we propose new partial differential equation, whose solution belongs to $H^2$, from which we can compute the solution with optimal convergence rate. Some computational results are given for showing our theory is efficient and feasible.

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## Hyesuk Lee, Clemson University

*Numerical and analytical studies of fluid-structure interaction (FSI) problems*

Simulating fluid-structure interactions is challenging due to the tight coupling between the solid and fluid substructures in a moving domain. Explicit and implicit decoupling methods often either fail or require relaxation when densities of the two materials are close. In this talk both monolithic and decoupling approaches are considered for analytical and numerical studies of FSI problems where a fluid is governed by a Newtonian or non-Newtonian model. An optimization based method which allows FSI problems to be stably decoupled is discussed and numerical results are presented.

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## Rich Lehoucq, Sandia National Laboratories

*A novel class of strain measures for digital image correlation*

We propose a novel class strain measures for use with digital image correlation (DIC). Whereas the traditional notion of compatibility (strain as the derivative of the displacement field) is problematic when the displacement field varies substantially either because of measurement noise or material irregularity, the proposed measure remains robust, well-defined and invariant under rigid body motion. Moreover, when the displacement field is smooth, the classical and proposed strain measures are approximations of each other. We demonstrate, via several numerical examples, the potential of this new strain measure for problems with steep gradients. We also show how the nonlocal strain provides an intrinsic mechanism for filtering high frequency content from the strain profile and so has a high signal to noise ratio. This is a convenient feature considering image noise and its impact on strain calculations.

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## Sandro Manservisi, University of Bologna

*Optimal control problems for the Navier-Stokes system coupled with a two-equation turbulence model*

The optimal control problem for the kappa-omega two equation turbulence model coupled with the Navier-Stokes system is considered. The optimal solution is obtained by solving the full state-adjoint optimality system and some numerical examples are reported.

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## Tom Manteuffel, University of Colorado

*First-Order System Least Squares for a Two-Fluid Electromagnetic Plasma Model*

A two-fluid plasma (TFP) model is presented both as a stand-alone solver and as the preconditioner to a fully implicit, particle-in-cell (PIC) simulation. The model couples fluid conservation equations for ions and electrons to Maxwell's equations. A Darwin approximation of Maxwell is used to eliminate spurious light waves. After scaling and modification, the TFP-Darwin model yields a nonlinear, first-order system of equations whose Fréchet derivative is shown to be uniformly H1-elliptic. This system is addressed numerically by nested iteration (NI), a First-Order System Least Squares (FOSLS) discretization, adaptive local mesh refinement, and scaled AMG system solver. Numerical tests demonstrate the efficacy of this approach, yielding an approximate solution within discretization error in a relatively small number of computational work units (WU).

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## A. J. Meir, Auburn University

*Elliptic and Parabolic Problems with an Integral Constraint*

Chemical and isotopic diffusion gradients in minerals provide record of the temperature and duration for a vast range of geologic processes. When solving an inverse problem in geochronology we encounter an integral constrained parabolic equation. We discuss the existence and uniqueness of solutions of elliptic and parabolic problems with an integral constraint as well as the finite element approximation of solutions of these equations. This is joint work with Dmitry Glotov and Bertran Sedar Ngoma Koumba.

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## Ju Ming, Beijing Computational Science Research Center

*Stochastic Homogenization of Distributed Elliptic Optimal Control Problems*

In this talk, we investigate mathematically and numerically a class of distributed control problems in which the governed equations, given by second-order elliptic equations, have rapidly oscillation coefficients with stochastic perturbations. Without the assumption of periodicity or ergodicity, the existence of the optimal solutions in the framework of homogenization theory is discussed. Our results show that the stochastic optimization system will converge to a deterministic one in the sense of H-convergence. Some numerical experiments are performed to validate our theory.

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## Hoa Nguyen, Trinity University

*Coupled RapidCell and Lattice-Boltzmann Models to Simulate Hydrodynamics of Bacterial Transport in Response to Chemoattractant Gradients in Confined Domains*

The RapidCell model was developed to simulate E. coli chemotaxis with spatiotemporally varying chemoattractant gradients, which is suited for motility simulations in unbounded non-fluid environments. This limits its use in biomedical applications hinging on bacteria-fluid dynamics in microchannels. We couple the RapidCell model with the colloidal lattice-Boltzmann model to simulate trajectories of self-propelled chemotactic particles in initially stagnant fluids in bounded domains. The chemotactic particles reached the chemoattractant source with the success rates of 20-72%.

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## Mauro Perego, Sandia National Laboratories

*Implicit Coupling of Ice Sheet Momentum and Thickness Evolution Equations*

Ice sheet modeling is important for performing accurate predictions of sea level rise. Ice behaves as a shear-thinning fluid and can be modeled with Stokes equations coupled with an advection equation for the ice thickness evolution. Due to the shallow nature of the ice sheets, the Stokes equations and the advection equations are tightly coupled. In this talk we analyze the coupled problem and we propose a method to effectively solve the coupled system.

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## Pablo Seleson, Oak Ridge National Laboratory

*Analysis and Correction of Surface Effects in Peridynamics*

Peridynamics is a nonlocal reformulation of classical continuum mechanics, based on integro-differential equations, suitable for material failure and damage simulation. Peridynamic models have been originally formulated for points in the bulk of materials, i.e., far from domain boundaries. Consequently, a direct application of peridynamic models in engineering simulations with free surfaces commonly produces undesired surface effects. In this presentation, we will analyze the sources of those surface effects and propose appropriate corrections.

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## Ralph Smith, North Carolina State University

*Gradient-Free Active Subspace Construction Via Adaptive Morris Indices*

In this presentation, we present a gradient-free algorithm for constructing active subspaces for physical and biological applications having high-dimensional input spaces. The objective of this approach is two-fold: determine low-dimensional active input spaces for high-dimensional problems and construct surrogate models based on these reduced spaces. Whereas there exist a variety of algorithms to construct low-dimensional subspaces when gradients are available, a number of production codes do not provide gradient or adjoint capabilities. To accommodate these applications, we consider a gradient-free approach in which adaptive Morris indices are used to construct the reduced input space. In this approach, steps are adapted to dominant directions in the parameter space to improve the accuracy and efficiency of algorithms. Attributes of the method are demonstrated for examples arising in aerodynamics and nuclear power plant design.

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## Miroslav Stoyanov, Oak Ridge National Laboratory

*Anisotropic Dynamic Adaptivity for Multidimensional Approximation of Analytic Functions*

Abstract not available at time of publication.

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## Catalin Trenchea, University of Pittsburgh

*A generalized stochastic collocation approach to constrained optimization for random data*

We present a scalable, parallel mechanism for stochastic identification/control for problems constrained by PDEs with random input data. Several identification objectives are discussed that either minimize the expectation of a tracking cost functional or minimize the difference of desired statistical quantities in the appropriate $L^p$ norm. The stochastic parameter identification algorithm integrates an adjoint-based deterministic algorithm with the sparse grid stochastic collocation FEM approach. The proof of the error estimates uses a Fink-Rheinboldt theory.

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## James Turner, Virginia Tech

*A Finite Element Library for Predictive Medicine*

The current paradigm for surgery planning for the treatment of neurodegenerative and cardiovascular disease is dictated by a protocol that is a result of empirical clinical studies, where effects of different treatments are compared statistically in large groups of patients with similar pathology. With increased diagnostic detail, groups become less uniform, necessitating smaller and more numerous subgroups. Consequently, the characteristics of an individual undergoing therapy likely differ from the mean of the clinical study, thus the therapy may not benefit every patient, or worse, may even complicate the disease process. To address this issue, we describe our efforts in support of the emerging paradigm of predictive medicine whereby the physician utilizes computational tools to construct and evaluate a combined anatomic/physiologic model to predict the outcome of alternative treatment plans for an individual patient.

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## Xiaoming Wang, Florida State University

*An efficient and long-time accurate third-order scheme for the Stokes-Darcy system*

We discuss a novel third-order in time numerical algorithm for the Stokes-Darcy system for flows in fluid saturated karst aquifers. The scheme is efficient in the sense that one needs to solve, at each time step, decoupled Stokes and Darcy problems. Therefore, legacy Stokes and Darcy solvers can be applied in parallel. It is also unconditionally stable and, with a mild time-step restriction, long-time accurate in the sense that the error is bounded uniformly in time. Numerical experiments are used to illustrate the theoretical results.

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## Clayton Webster, Oak Ridge National Laboratory

*Best $s$-term and quasi-optimal polynomial approximations for high-dimensional parameterized PDEs*

In this talk, we present a generalized methodology for constructing and analyzing quasi-optimal polynomial approximations, applicable to a wide class of parameterized PDEs with both deterministic and stochastic inputs. Rigorous stability analysis, explicit cost bounds, and $\ell_1$ minimization estimates, of the various quasi-optimal techniques will also be explored. Computational evidence complements the theory and shows the advantage of our generalized methodology compared to previously developed estimates.

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## Geoff Womeldorff, Los Alamos National Laboratory

*A Communication Staging Technique for a Hierarchical Ocean Model*

We study a communications staging technique applied to an algorithmically accelerated, free-surface, z-level ocean model. The ocean model is implemented in a hierarchical high-order / low-order fashion, which allows both mapping to heterogeneous architectures and exploitation of advanced communication algorithms. We compare the benefit of communication staging between a current state of the art numerical method and a research method under development, within this high-order / low-order framework . We provide numerical examples to support our study and compare to traditional implementations.

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## Guannan Zhang, Oak Ridge National Laboratory

*A Stochastic Approach for a Class of Anomalous Diffusion Problems*

We propose a novel numerical approach for linear nonlocal diffusion equations with integrable kernels, based on the relationship between the backward Kolmogorov equation and a class of backward stochastic differential equations (BSDEs) driven by Levy processes with jumps. The nonlocal diffusion problem under consideration is converted into a BSDE, for which numerical schemes are developed and applied directly.

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## Yanzhi Zhang, Missouri University of Science and Technology

*Eigenvalues and eigenfunctions of the fractional Laplacian*

Recently, one debate in the literature is whether the fractional Schrodinger equation in an infinite potential well has the same eigenfunctions as those of its standard (non-fractional) counterpart. Due to the nonlocality of the fractional Laplacian, it is challenging to find the eigenvalues and eigenfunctions of the fractional Schrodinger equation analytically. In this talk, we numerically study the eigenvalues and eigenfuctions of the fractional Schrodinger equation.

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