SCIENTIFIC COMPUTING AROUND

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A B S T R A C T S

INVITED SPEAKER ABSTRACTS:

Optimization-based modeling - an overview
<u>Pavel Bochev</u>, Sandia National Laboratories

Optimization-based modeling (OBM) is a "divide-and-conquer" strategy that decomposes multiphysics, multiscale operators into simpler constituent components and separates preservation of physical properties such as a discrete maximum principle, local bounds, or monotonicity from the discretization process. In so doing OBM relieves discretization from tasks that impose severe geometric constraints on the mesh, or tangle accuracy and resolution with the preservation of physical properties.

In a nutshell, our approach reformulates a given mathematical model into an equivalent *multi-objective constrained optimization problem*. The optimization objective is to minimize the discrepancy between a *target* approximate solution and a *state*, subject to constraints derived from the component physics operators and the condition that physical properties are preserved in the optimal solution. Three examples will illustrate the scope of our approach: (1) an optimization-based framework for the synthesis of robust, scalable solvers for multiphysics problems from fast solvers for their constituent physics components; (2) an optimization-based Atomistic-to-Continuum (AtC) coupling method; and (3) optimization-based methods for constrained interpolation (remap) and conservative, monotone transport.

This talk is based on joint work with Denis Ridzal, Kara Peterson, Mitch Luskin, Derek Olson, Alex Shapeev, and Misha Shashkov. This research is sup- ported by the Applied Mathematics Program within the Department of Energy (DOE) Office of Advanced Scientific Computing Research (ASCR). The work on AtC coupling methods is supported by the ASCR as part of the Collaboratory on Mathematics for Mesoscopic Modeling of Materials (CM4).

Modeling angiogenesis in the eye: the good and the bad
Yi Jiang, Georgia State University

Angiogenesis, or blood vessel growth from existing ones, is an important physiological process that occur during development, wound healing, as well as diseases such as cancer and diabetes. I will report our recent progress in modeling angiogenesis in the eye in two scenarios. The good refers to healthy blood vessel growth in the retina in mouse embryos, which is a perfect experimental model for understanding the molecular mechanism of normal angiogenesis. The bad is the pathological blood vessel growth in age related macular degeneration, which is the leading cause of vision loss in the elderly and a looming epidemic in our aging society. We develop cell-based, multiscale models that include intracellular, cellular, and extracellular scale dynamics, and show that biomechanics of cell-cell and cell-matrix interactions play crucial roll in determining the dynamics of blood vessel growth initiation as well as vascular network formation. Such models show great potential as in silico Petri-dishes for predictive modeling studies.

Many-core algorithms for high-order finite element methods: when time to solution matters
Tim Warburton, Department of Computational and Applied Mathematics, Rice University

The ultimate success of many modeling applications depends on time to solution. I will illustrate the critical nature of time to solution by describing a joint project between my group at Rice University and Dr. David Fuentes at the MD Anderson Cancer Center. The project goal is to evaluate the role and viability of using finite element modeling as part of the treatment planning process for MR Guided Laser Induced Thermal Therapy. The success of this project will depend in great part on the ability to model individual treatments with calculations that take mere seconds.

Modern many-core processing units, including graphics processing units (GPU), presage a new era in on-chip massively parallel computing. The advent of processors with O(1000) floating point units (FPU) raises new issues challenging conventional measures of "optimality" of numerical methods. The ramp up in FPU counts for each new generation of GPU over the past four years has been accompanied by a slower increase in the memory capacity of the GPU. For example, a few hundred US dollars currently buys a parallel computer that is capable of performing $O(4 \cdot 1012)$ floating point operations per second, but only of reading $O(5 \cdot 1010)$ values from memory per second. From the point of view of numerical analysis, this means that the traditional approach of comparing optimality of alternative numerical methods based on their floating point operation count per degree of freedom has become mostly irrelevant. Claims of optimality derived from this measure therefore need to be reevaluated and the formulation of numerical methods in general need to be revisited given the changing computational landscape. The presentation will touch on several important and inter-linked issues that impacted the development of high-order finite-element methods based solvers for many-core architectures that are rapidly evolving. We will discuss on-chip scalability, multi-GPU scalability, inter-generational GPU scaling, and specialization for element internal structure.

Finally, I will introduce the OCCA API that my team is developing as a thin portability layer to enable our simulation codes to be threaded using OpenMP, OpenCL, or CUDA as selected dynamically at runtime. This additional flexibility enables us to include the threading model as an additional search direction when we optimize the simulation codes for a given processor. I will give comparisons of the performance of the simulator using OCCA on multiple different vendor devices using different threading models.

TALK ABSTRACTS

Chemora: Dynamically generating complex stencil code for hybrid clusters
Marek Blazewicz, Ian Hinder, David Koppelman, Erik Schnetter, Steven R. Brandt, Peter Diener, Yue Hu, Frank Loeffler, Jian Tao; Louisiana State University

The Chemora project will build upon the Cactus Framework and provide the ability to automatically generate highly optimized code for high end computational resources. Chemora combines a set of partial differential equations (PDEs) describing a problem, with an automatically generated machine-specific performance profile, and will dynamically generate well-tuned stencil code for the particular hybrid CPU/GPU computing cluster it's running on. Chemora will improve programmability in this important domain by reducing the issues users need to understand; We have chosen the Einstein equations as our primary science driver and first example because these equations represent one of the more complex PDE systems, one with many hundreds of terms, and a problem scale that is challenging to optimize for most compilers.

Scientific computing in high school
Brad Burkman; Louisiana School for Math, Science, and the Arts

The scientific computing program at the Louisiana School for Math, Science, and the Arts continues to grow. New opportunities for students and faculty this year include Digital Humanities tools incorporated into an American History course, Perl implemented in the Genetics course, and more students interested in scientific visualization and data visualization. Many opportunities exist for university faculty to be part of the program and steer students into productive work in scientific computing.

A partition of unity method for the displacement obstacle problem of simply supported Kirchhoff
Susanne C. Brenner, Christopher B. Davis, and Li-yeng Sung; Louisiana State University

In this talk, we propose a partition of unity method for the displacement obstacle problem of simply supported Kirchhoff plates. Due to the simply supported boundary condition, under certain conditions, the regularity of the solution can become low causing problems for standard numerical methods. By constructing appropriate local approximation spaces, we are able to show that the partition of unity method converges optimally. Numerical results are given which show the optimal convergence of this method.

Using OpenACC to accelerate Loop Quantum Cosmology Computations
Peter Diener, Brajesh Gupt, Miguel Megevand, Parampreet Singh; Louisiana State University

I will report on the successful port of a CPU based Loop Quantum Cosmology code within the Cactus framework to run on GPU's using OpenACC. OpenACC is a compiler directive approach to GPU programming (similar to the OpenMP approach to shared memory parallelization). I will briefly describe the underlying physics problem, the structure of the equations and the OpenACC directives needed for the port. I will finally present some performance results.

Adaptive C^0 interior penalty method for biharmonic eigenvalue problems
Susanne C. Brenner, Joscha Gedicke and Li-Yeng Sung; Louisiana State University

This talk presents a residual based *a posteriori* error estimator for biharmonic eigenvalue problems and the C^0 interior penalty method. This method is nonconforming and avoids the use of complicated C^1 finite elements by using simple Lagrange basis functions. Biharmonic eigenvalue problems occur in the analysis of vibrations and buckling of plates. The *a posteriori* error estimator is proven to be reliable and efficient up to some additional term which is shown to be of higher order for sufficiently large penalty parameter and sufficiently small global mesh size. The reliability and efficiency of the *a posteriori* error estimator for the eigenvalue error is verified in numerical experiments for convex and non-convex domains. The numerical experiments show that uniform mesh refinement may result in sub optimal convergence, while adaptive mesh refinement leads to optimal convergence rates.

Forecasting epidemic progression using syndromic data
Kyle Hickmann; Tulane University

To forecast disease spread using a complex epidemic model one must estimate both the current state of the model and an optimal parametrization/initialization. These must be estimated from public health data sources that are both sparse and, perhaps, only indirectly related to actual infection levels. This talk will detail the application of the Ensemble Kalman Filter to iteratively update epidemic model predictions. With these methods an epidemic simulation has its parametrization, including perhaps its initialization, and current state adjusted as data becomes available. This allows an optimal model forecase to be derived that accounts for data and model error simultaneously. Since public health data does not give direct observations of infection levels in the population one also must determine an optimal map between data source and model. One method to determine this mapping, which can be applied to general epidemic models and syndromic data sources, will be presented.

Computing flow from cilia
Franz Hoffmann; Tulane University

Cilia are hair-like structures on surfaces of cells that through coordinated beating move the surrounding fluid. For example, cilia are responsible for transporting foreign particles from the human lung. We present a computational model for the flow created by cilia.

Undergraduate research in computational and theoretical physics at Southeastern
Hye-Young Kim; Southeastern Louisiana University

I will present the experience and outcomes gained from performing state-of-the-art research projects in computational and theoretical physics with undergraduate students only. Also presented will be the challenges I face to sustain the computational and theoretical research program at a primarily undergraduate institution.

An R&E network's perspective of a science
Lonnie Leger; Louisiana Optical Network/Louisiana State University

In an effort to eliminate "Big Data" flow problems, LSU and the LONI Network are in the midst of implementing a project that will connect specific research resources, people and machine, across the state of Louisiana's public universities to a common cyberinfrastructure known as a Science DMZ. The NSF funded projects, "CC-NIE Network Infrastructure: CADIS -- Cyberinfrastructure Advancing

Data-Interactive Sciences" and CC-NIE Network Infrastructure: BDoSDN -- Bridging, Transferring and Analyzing Big Data over Campus-Wide Software Defined Networks" coupled with funding from the Louisiana Board of Regents will build upon a NSF EPSCoR completed project, "Louisiana's Cyber Connectivity via LONI" to provide a network infrastructure which connects LSU's HPC resources and LONI's HPC resources to 5 research centers and 6 colleges on the campus of LSU. The Science DMZ will provide connectivity to the resources in 10 and 40-gigabit speeds with connectivity back to the LONI Network core and Internet2's AL2S at 100-gigabit. Our vision is to provide straightforward paths for upgrading laboratories and offices to higher bandwidth connectivity as the capabilities of LONI and I2 expand, create opportunities for diverse research community to more effectively interact with huge data sets that are generated on local (LSU), regional (LONI), and national (XSEDE) HPC resources, enabling new scientific and engineering discoveries, establish a Software Defined Network parallel model to our traditional campus approach, tune our network delivery for Big Data transmission with the assistance of perfSONAR, and develop Bid Data frameworks using Hadoop and MPI technologies over HPC resources.

Cactus: a thorny problem solver
<u>Frank Löffler</u>; Louisiana State University

A lot of physical problems can be described by hyperbolic (think wave-like) systems of equations. While coming from completely different fields solving these systems numerically is often similar enough so one can use existing computer codes, maybe with only slight changes. We will give a short overview of the Cactus code, providing guidance when to choose it, and when possibly not. The Cactus code is lead from, and partially developed at LSU.

Motion in viscoelastic media at the zero Reynolds number
<u>Sabrina Lynch</u>, Aaron Barrett, Jacek Wrobel; Tulane University

We present a simple model of a free microswimmer in a highly heterogeneous, viscoelastic medium. An effect of viscoelasticity is modeled by immersing viscoelastic elements into a highly viscous environment. Perturbed, due to a flow, elements generate forces that can affect a swimmer. Regions of high element concentrations can significantly change the swimming pattern of a microorganism. Several tests were performed in various elements configurations.

A mathematical model for the role of resident and migrant birds in West Nile virus outbreaks
Louis Bergsman, <u>Carrie Manore</u>, Mac Hyman; Tulane University

West Nile virus (WNV) is a mosquito-borne infectious disease that spreads primarily in birds, although humans are also susceptible and infection can lead to serious complications. We present a hybrid multi-host seasonal model for WNV spread in resident and migrant bird species. We explore differences in host competence and mosquito feeding preference between bird species. When the migrant bird species is a competent host with lower death from disease than the resident species, our analysis shows that the migratory birds play an important role in supplying susceptible hosts and driving the significant seasonal upswings in WNV, even if they don't arrive initially infected.

Dynamic multi-scale model of the lung
<u>Jason Ryans</u>, Hideki Fujioka, David Halpern, Donald P. Gaver III; Tulane University

Strategies to treat pulmonary diseases such as acute respiratory distress syndrome (ARDS) and infant respiratory distress syndrome (IRDS) involve mechanical ventilation; however, this may result in ventilator-induced lung injury (VILI) that can damage the respiratory system. To elucidate the interacting mechanisms governing these conditions, dynamic multi-scale models of the lung will be

developed to predict the complex interactions from the cellular to organ level. A key component of this modeling technique is the coupling of phenomena at each hierarchal level with the use of agent based modeling (ABM), which links lung airways (agents) viaa series of rules that direct their interactions.

In our study, the lung model was generated based on algorithms by Tawhai et al. (2000), with the boundary of the lung lobe walls represented preliminarily by a cube. Flow in each airway is assumed to follow Poiseuille flow driven by a sinusoidally varying pleural pressure. Additionally, airway resistance is governed by morphological data and a tube law described by Lambert et al. (1982) that represents the cross sectional area as a function of the transpulmonary pressure. Pressure-volume curves described in Venegas et al. (1998) and Fujioka et al. (2013) allowed for simulation of a variety of conditions including normal respiration and mechanically ventilated patients with acute respiratory distress syndrome. To define the Poiseuille flow throughout the bronchial tree, a hydraulic circuit analogy was implemented that relates pressure gradients, volumetric flow, airway resistance and transpulmonary pressure to determine flows and stresses throughout the bronchial tree. The formulation is specifically designed to account for nearest neighbor interactions that can affect the flow in the lung through parenchymal tethering effects.

The model has been used to simulate normal respiration and ventilation under normal and pathophysiological conditions at the acinar level, which resulted in heterogeneous ventilation. The sensitivity of the acini pressures on the bronchial flow distribution could yield knowledge of its affects on overall lung stability. With these relationships clarified, the incorporation of micro-scale phenomena can be introduced via ABM to investigate complex flow regimes such as those occurring with liquid occluded airways.

Accurate integration of high dimensional functions using polynomial detrending
James Macklin Hyman, Mu Tian; Tulane University

Abstract Text: I will present a robust method to improve the accuracy of numerical integration of high-dimensional functions defined at a sparse set of scattered points. Numerical quadrature built on a lattice of grid points can quickly suffer from the curse of dimensionality. Monte Carlo and Quasi Monte Carlo method have been widely adopted to overcome this problem by providing a convergence rate independent of dimensionality. Unfortunately, the errors of these Monte Carlo methods converge very slowly when there are large variations in the underlying integrand. I will describe the polynomial detrending approach, where the integrand is approximated by a moderate degree multivariate polynomial, and provide numerical examples demonstrating that it can be efficient way to increase the integration accuracy. The accuracy of the approximation depends upon identifying an effective set multivariate bases functions for the detrending polynomial. I will describe how to identify these basis functions using a sparse L1 regularization algorithm for the underlying least-squares approximating polynomial. The resulting methodology has the potential of being one of the most accurate and effective methods for the numerical integration of high-dimensional smooth functions.

Controlling the footprint of droplets
Antoine Laurain and Shawn W. Walker; Louisiana State University

Controlling droplet shape via surface tension has many technological applications, such as droplet lenses and lab-on-achip. This motivates a PDE-constrained shape optimization approach for controlling the shape of droplets on flat substrates by controlling the surface tension of the substrate. We use shape differential calculus to derive an L^2 gradient flow approach to compute equilibrium shapes for sessile droplets on substrates. We then develop a gradient based optimization method to find the substrate surface tension coefficient that yields an equilibrium droplet shape with a desired footprint (i.e. the liquid-solid interface has a desired shape). Well-posedness and differentiability of

the optimization problem are considered. Numerical results are also presented to showcase the method.

Model the nonlinear instability of wall-bounded shear flows as a rare event
Xiaoliang Wan; Louisiana State University

In this work, we study the nonlinear instability of two-dimensional wall-bounded shear flows from the large deviation point of view. The main idea is to consider the Navier-Stokes equations perturbed by small space-time white noise and then examine the noise-induced transitions between the two stable solutions due to the subcritical bifurcation. When the amplitude of the noise goes to zero, the Frendlin-Wentzell (F-W) large deviation theory provides the most probable transition path in the phase space, which characterizes the development of the nonlinear instability subject to small random perturbations. Such a path is given by the minimizer of the F-W action functional, based on which we define a critical Reynolds number for the nonlinear instability in the probabilistic sense. Then the stability theory based on action is applied to study two-dimensional Poiseuille flow in a short channel.

Preconditioned locally minimal residual methods for large-scale Hermitian eigenvalue problems
Eugene Vecharynski, Fei Xue; University of Louisiana at Lafayette

We study the preconditioned locally minimal residual (PLMR) methods for computing a large number of interior eigenvalues of Hermitian eigenproblems $Av=\lambda Bv$. PLMR is a newly developed eigensolver which does not require computation of shift-invert matrix-vector product to enhance the desired spectrum. We introduce the construction of PLMR and show that this algorithm exhibit robust convergence towards interior eigenvalues if good preconditioners are available. Using partial deflation of converged eigenvalues, PLMR's arithmetic and CPU cost increase linearly with the number of desired eigenvalues.

Modeling elastic fibers in viscoelastic fluid by immersed boundary method
Qiang Yang, Lisa Fauci; Tulane University

Many physical and biological systems involve inextensible fibers immersed in a fluid. In such systems, the dynamics of the immersed fibers may play a significant role in the observed macroscale fluid dynamics. In this presentation, I will use a continnum model to simulate the dynamics of fibers in a viscoelastic fluid based on the immersed boundary method.

Approximation Methods for Nonconvex Stochastic Composite Optimization
H. Zhang and S. Ghadimi and G. Lan; Louisiana State University

We consider a class of constrained stochastic composite optimization problems whose objective function is given by the summation of a differentiable (possibly nonconvex) component, together with a certain nondifferentiable (but convex) component. A randomized stochastic projected gradient (or gradient-free) algorithm will be introduced. In these algorithms, proper mini-batch of samples are taken at each iteration depending on the total budget of stochastic samples allowed. Complexity and some preliminary numerical results of these algorithms will be also discussed.