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A B S T R A C T S

INVITED SPEAKER ABSTRACTS:

Nick Cogan, Florida State University
Using Computations to Study Biological Processes
There is a long history of using mathematical models to provide insight into biological processes. As more details become available for specific biological applications, such as bacterial biofilms, the models become increasingly complicated -encouraging the use of computational methods. In many ways the mathematical treatment of biological processes has been expanded, supported by, and in some sense led by, numerical studies. In this talk, I will discuss several applications where numerical/computational methods are brought to bear on specific aspects of the scientific problem. These include extending our understanding of the model beyond the linear regime, providing transparency in the model predictions, and efficient sampling techniques to study the propagation of uncertainty through the model and parameter sensitivities.

James Nagy, Emory University
SVD Approximations for Large Scale Imaging Problems

A fundamental tool for analyzing and solving ill-posed inverse problems is the singular value decomposition (SVD). However, in imaging applications the matrices are often too large to be able to efficiently compute the SVD. In this talk we present a general approach to describe how an approximate SVD can be used to efficiently compute approximate solutions for large-scale ill-posed problems, which can then be used either as an initial guess in a nonlinear iterative scheme, or as a preconditioner for linear iterative methods. We show more specifically how to efficiently compute the SVD approximation for certain applications in image processing.

Carol Woodward, Lawrence Livermore National Laboratory
A Reconsideration of Fixed Point Methods for Nonlinear Systems

Newton-Krylov methods have proven to be very effective for solution of large-scale, nonlinear systems of equations resulting from discretizations of PDEs. However, increasing complexities and newer models are giving rise to nonlinear systems with characteristics that challenge this commonly used method. In particular, for many problems, Jacobian information may not be available or it may be too costly to compute. Moreover, linear system solves required to update the linear model within each Newton iteration may be too costly on newer machine architectures.

Fixed point iteration methods have not been as commonly used for PDE systems due to their slow convergence rate. However, these methods do not require Jacobian information nor do they require a linear system solve. In addition, recent work has employed Anderson acceleration as a way to speed up fixed point iterations.

In this presentation, we will discuss reasons for success of Newton's method as well as its weaknesses. Fixed point and Anderson acceleration will be presented along with a summary of known convergence results for this accelerated method. Results will show benefits from this method for a number of applications. In addition, the impacts of these methods will be discussed for large-scale problems on next generation architectures.

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TALK ABSTRACTS

Modeling the impact of screening and partner notification on chlamydia intervention in New Orleans
Asma Azizi, Jeremy Dewar, Patricia Kissinger, Mac Hyman

We created and analyzed an individual network-based model for the spread of the sexually transmitted infection, chlamydia trachomatis, in New Orleans. Chlamydia is the most common sexually transmitted infection in the United States with over 1.8 million cases each year. This includes approximately 12% of African American women and 8% of men between 15-25 years old currently infected in New Orleans. Chlamydia is the major cause of infertility, pelvic inflammatory diseases and ectopic pregnancy among women and been associated with increased HIV acquisition. We created a weighted bipartite sexual partnership network for men and women that captures biased heterosexual mixing between the risk groups. We then use a stochastic agent-based Markovian epidemic model to quantify the effectiveness of mitigation methods, such as screening and partner notification, in controlling the epidemic. Our simulations were used to optimize a mitigation program based on partner notification and screening both men and women. The model verified the existence of a threshold value for stopping the epidemic based on the fraction of an infected person's partners who are tested, and treated, for infection. We are collaborating with the Tulane School of Public Health and Tropical Medicine to use this model in helping public health officials implement effective policies in allocating resources to control the current chlamydia epidemic in New Orleans.

Flow Induced by Bacterial Carpets and Transport of Microscale Loads
Amy Buchmann (Tulane University) Lisa Fauci (Tulane University) Karin Leiderman (University of California Merced) Eva Strawbridge (James Madison University) Longhua Zhao (Case Western Reserve University)

Microfluidic devices carry very small volumes of liquid though channels and may be used to gain insight into many biological applications including drug delivery and development. In many microfluidic experiments, it would be useful to mix the fluid within the chamber. However, the traditional methods of mixing and pumping at large length scales don't work at small length scales. Experimental work has suggested that the flagella of bacteria may be used as motors in microfluidic devices by creating a bacterial carpet. Mathematical modeling can be used to investigate this idea and to quantify flow induced by bacterial carpets. We simulate flow induced by bacterial carpets using the method of regularized Stokeslets, and also examine the transport of vesicles of finite size by arrays of rotating flagella.

Shape optimization for drag minimization using the Navier-Stokes equation
Chukwudi Chukwudozie

This work computes the shape of a stationary 2D object of a given size that minimizes fluid drag at different Reynolds numbers. We solve the problem in the context of shape optimization, making use of shape sensitivity analysis. The state variables are fluid pressure and velocity modeled by the Navier-Stokes equation with cost function given by the fluid drag which depends on the state variables. Our optimization routine uses a variational form of the sequential quadratic programming (SQP) method with the Hessian replaced by a variational form for the shape gradient. The numerical implementation is done in Python while the open source finite element package, FEniCS, is used to solve all the partial differential equations. Remeshing of the computational domain to improve mesh quality is carried out with the open source 2D mesh generator, Triangle. Final shapes for low Reynolds numbers resemble an american football while shapes for moderate to high Reynolds numbers are more streamlined in the tail end of the object than at the front.

A Few Numerical Schemes for Two-Phase-Fluid-Flow Equations
Amanda Diegel, Steve Wise

In this talk, we investigate some numerical schemes which may be used to describe two-phase fluid flows. Due to the vastness in applicability, two-phase flow models have drawn the attention of a number of researchers in recent years. One of the biggest challenges to modeling these systems lies in the difficulties regarding the moving interfaces (or boundaries) between the various phases. The traditional sharp interface models usually lead to almost unsolvable theoretical problems, not to mention the hardships found while attempting to derive stable and convergent computational schemes for these problems. To overcome these hardships, a phase field approach is taken such that the Cahn-Hilliard equation is coupled with the fluid flow equations, thus creating a diffuse interface and eliminating the need to explicitly track a sharp interface. In this talk, we will discuss some numerical schemes which mimic the energy dissipation laws which are inherent to models using a phase field approach. Creating numerical schemes in this way makes it possible to rigorously prove three key properties: unconditional stability, unconditional unique solvability, and optimal convergence. Convergence results provide valuable feedback concerning the approximation properties of a numerical scheme and unconditional stability leads to enhanced convergence estimations which leads to high confidence that the numerical schemes accurately estimate solutions to the equations upon which they are designed.

Vector Based Parallel Branch and Bound Algorithm
<u>Jared Guilbeau</u>
Keywords: Interval analysis, Branch and Bound, global optimization, parallel computing

Global optimization problems sometimes attain their extrema on infinite subsets of the search space, forcing mathematically rigorous programs to require large amounts of data to describe these sets. This makes these programs natural candidates for vectorized arithmetic operations and parallel computing. Here we present a MATLAB implementation of a Branch and Bound algorithm that incorporates interval arithmetic as well as these techniques, make some observations about how sub-problem distribution can affect the reported solution, and present some preliminary numerical results.

Magneto-optical switches in metal-dielectric-metal plasmonic waveguides
<u>Ali Haddadpour</u>, Vahid Foroughi Nezhad, Zongfu Yu, and Georgios Veronis

The magneto-optical effect has been used to control the propagation of surface plasmon polaritons in plasmonic waveguides. Here we investigate single-interface metal-dielectric and metal-dielectric-metal plasmonic waveguides in which either the dielectric or the metal is a magneto-optical material. We derive the dispersion relation of these waveguides, and investigate the effect of an externally applied static magnetic field. We find that in metal-dielectric-metal waveguide structures in which the dielectric is a magneto-optical material, the symmetry of the structure prohibits any non-reciprocal propagation in the system. Moreover, the induced change in the propagation constant of the supported modes in the presence of an externally applied static magnetic field is relatively small. In addition, we find that using a magneto-optical metal in a single-interface metal-dielectric plasmonic waveguide results in non-reciprocal propagation of the plasmonic modes along the interface. We also find that in metal-dielectric-metal plasmonic waveguides in which the metal is a magneto-optical material, the propagation constant of the supported modes is dependent on the relative direction of the applied magnetic fields to the upper and lower metal regions. If the applied magnetic fields to the two metal regions are equal and in the same direction, the induced changes in the propagation constants of the modes propagating in the positive and negative directions are the same. On the other hand, if the directions of the applied external magnetic fields are opposite, the propagation constants of the modes propagating in the positive and negative directions are different. We finally investigate Fabry-Perot cavity magneto-optical switches.

A model of computational swimming lamprey driven by a central pattern generator with proprioceptive feedback
<u>Christina Hamlet</u>, Lisa Fauci, Kathleen Hoffman, Eric Tytell

The swimming of a simple vertebrate, the lamprey, can shed light on how a flexible body can couple with a fluid environment to swim rapidly and efficiently. Animals use stretch-receptor information to sense how their bodies are bending (proprioception), and then adjust the neural signals to their muscles to improve performance. We will present recent progress in the development of a computational model of a lamprey swimming in a viscous, incompressible fluid where a simple central pattern generator model, based on phase oscillators, is coupled to the evolving body dynamics of the swimmer through curvature and curvature derivative feedback. The system is numerically solved using the immersed boundary method. We will examine how the emergent swimming behavior and cost of transport depends upon these functional forms of proprioceptive feedback chosen in the model.

Quantifying performance in the medusan mechanospace with an actively swimming three-dimensional jellyfish model
Alexander Hoover, Boyce Griffith, Laura Miller

In many swimming and flying animals, propulsion emerges from the interplay of active muscle contraction, passive body elasticity, and fluid-body interaction. Changes in the active and passive body properties can influence performance and cost of transport across a broad range of scales; they specifically affect the vortex generation that is crucial for effective swimming at higher Reynolds numbers. Theoretical models that account for both active contraction and passive elasticity are needed to understand how animals tune both their active and passive properties to move efficiently through fluids. In this work, we develop an actively deforming model of a jellyfish immersed in a viscous fluid and use numerical simulations to describe the interplay between active muscle contraction, passive body elasticity, and fluid forces in the medusan mechanospace. By varying the strength of contraction and the flexibility of the bell margin, we quantify how these active and passive properties affect swimming performance and cost of transport. We find that for fixed bell elasticity, swimming speed increases with the strength of contraction. For fixed contracility, swimming speed increases as margin elasticity decreases. Varying the strength of activation in proportion to the elasticity of the bell margin yields similar swimming speeds, with a cost of transport is substantially reduced for more flexible margins. A scaling study reveals that performance declines as the Reynolds number decreases. This work yields a framework for a quantitative understanding of the roles of active and passive body properties in swimming.

A Factorized Sparse Approximate Inverse Preconditioner for Symmetric Indefinite Linear Systems
Sam Karbet
We propose a factorized sparse approximate inverse preconditioner for large real symmetric and indefinite linear systems. Factorized approximate inverse preconditioners have been developed and used successfully for symmetric positive definite and nonsymmetric linear systems, but it remains challenging to construct effective preconditioners of this type in the symmetric and indefinite setting.

We first demonstrate that the level of diagonal dominance of the coefficient matrix tends to have a greater impact on the sparsity of the preconditioner versus its inertia. This serves as a guiding property in the construction of our preconditioner.

Construction involves three stages: We first begin with a diagonal dominance enhancing preprocessing phase; this is implemented through HSL's symmetric MC64 subroutine, which scales and relocates large entries to super- and sub-diagonals near the diagonal. Second, our main incomplete conjugation algorithm uses the Bunch-Kauffman partial pivoting technique in order to control the growth of elements in our factorization. Lastly, we perform a sparest-columns-first dynamic reordering procedure for maintaining the sparsity of the factorized preconditioners.

Numerical results are provided to illustrate the effectiveness of the new preconditioner and its potential to be a competitive alternative to incomplete LDL^T preconditioners.

A numerical investigation of a simplified human birth model
Roseanna Pealatere, Alexa Baumer, Lisa Fauci, Megan C. Leftwich

This work uses a simplified model and numerical computations to explore the effects of both the fetal velocity and the viscosity of the surrounding fluid on the forces associated with human birth. The numerical model mimics an experimental model representing the fetus moving through the birth canal using a rigid cylinder (fetus) that moves at a constant velocity through the center of a passive elastic tube (birth canal). The entire system is immersed in highly viscous fluid. Due to low Reynolds number, the Stokes equations can be used to describe the linear relationship between velocity and forces in the system. The mathematical model uses the method of regularized Stokeslets to estimate the pulling force necessary to move the rigid inner cylinder at a constant velocity through the tube. The elastic tube through which the rigid cylinder passes is constructed by a discrete network of Hookean springs, with macroscopic elasticity matched to the tube used in the physical experiment. The pressure drop inside the tube induced by the movement of the inner cylinder results in non-axisymmetric buckling of the elastic. The physical contributors to this asymmetric buckling can be explored further through alternative elastic models coupled with the Stokes equations.

Finite Element Methods for an Elliptic Optimal Control Problem with Control Constraints
Susanne C. Brenner, Li-yeng Sung and Kamana Porwal

We analyze the conforming and the nonconforming finite element methods for the distributed elliptic optimal control problem with control constraints. Unlike the existing results, here we study the state-control minimization problem by reducing it to a minimization problem involving only the state variable, which can be reduced further to a fourth order variational inequality. This approach allows us to analyze the convergence of the state variable in H^2 type norm. The theoretical results are confirmed by the numerical examples.

Domain Decomposition and Multi-Scale Preconditioners for Heterogeneous Media Using Optimal Local Basis Functions
Robert Lipton, Paul Sinz

We describe a new class of multiscale preconditioners using the recently developed optimal local approximation spaces developed for GFEM [1,2]. The domain decomposition employs overlapping domains within the Partition of Unity Method. We provide explicit theoretical convergence rates for the iterative method.

References. [1]. Babuska, I. and Lipton, R. "Optimal local approximation spaces for generalized finite element methods with application to multiscale problems," Multiscale Modeling and Simulation, SIAM 9 2011, pp. 373–406. [2.] Babuska, I., Huang, X., and Lipton, R., "Machine computation using the exponentially convergent multiscale spectral generalized finite element method," ESAIM: Mathematical Modeling and Numerical Analysis 48 2014, pp. 493-515.

Shape Optimization Of Self-Avoiding Curves
Shawn W. Walker

We present a softened notion of proximity (or self-avoidance) for curves. We then give a shape sensitivity result for the proximity and combine it with a gradient-based optimization approach to compute three-dimensional, parameterized curves that minimize the sum of an elastic (bending) energy and a proximity energy that maintains self-avoidance by a penalization technique.

We demonstrate the method by simulating adsorbed polymer strands that are constrained to be bound to a surface and be (locally) inextensible. This is a basic model of semi-flexible polymers adsorbed onto a surface (a current topic in material science). Several examples of minimizing curve shapes on a variety of surfaces are shown. An advantage of the method is that it can be much faster than using molecular dynamics for simulating polymer strands on surfaces.