SCALA 2024: SCIENTIFIC COMPUTING AROUND LOUISIANA

FRIDAY, JANUARY 19 – 20, 2024
LSU Campus, Digital Media Center Theatre

Friday, Jan. 19	
12:30	**Registration**
1:10	***Welcome***
1:15 – 2:00	***Keynote talk:*** *Maxim Olshanskii, Mathematics, University of Houston* **Numerical analysis of surface fluids and modeling of lipid membranes**
2:00 – 2:15	*Alex Nisbet, Mathematics, Tulane University* **Circle Methods for Regularizing Nearly Singular Boundary Integrals in 2D Pertaining to the Laplacian**
2:15 – 2:30	*Minh Vu, Louisiana State University* **Investigating Disentanglement in beta-VAE Framework within a Linear Gaussian Setting**
2:30 – 3:00	**Coffee Break**
3:00 – 3:15	*Jeremy Shahan, Mathematics, Louisiana State University* **Shape Optimization with an Unfitted Finite Element Method**
3:15 – 3:30	*Hongfei Chen, Tulane University* **Hydrodynamics of choanoflagellate colonies near a wall: a reduced model approach**
3:30 – 3:45	*Irene Erazo, Tulane University* **Rigid microspheres in a Stokes fluid: motion due to white noise**
3:45 – 4:00	Jon Loftin, MathWorks
4:00 – 4:30	**Coffee Break**
4:30 – 4:45	*Mayank Tyagi, Petroleum Engineering and Center for Computation & Technology, Louisiana State University* **Digital Twins for Oil Field Wellbores using Data-Driven Modeling (DDM) and Physics based Simulations**
4:45 – 5:00	*Zheng Wang, Mathematics, Tulane University* **A Modified Regularized Stokeslets Segments Approach with Piecewise Cubic Forces**

Saturday, Jan. 20	
9:00 – 9:45	***Keynote talk:*** *Katarzyna Rejniak, Integrated Mathematical Oncology, Moffitt Cancer Center* **Mathematical modeling of tumor microenvironment**
9:45 – 10:00	*Andrew Hicks, Louisiana State University* **Modeling and Numerical Analysis of the Cholesteric Landau--de Gennes model**
10:00 – 10:15	*Yangwen Zhang, University of Louisiana at Lafayette* **An Incremental SVD Method for Non-Fickian Flows in Porous Media: Addressing Storage and Computational Challenges**
10:15 – 10:45	**Coffee Break**
10:45 – 11:00	*Zequn Zheng, Louisiana State University* **Generating Polynomial Method for Non-symmetric Tensor Decomposition**
11:00 – 11:15	*Kendall Gibson, Tulane University* **A Flexible Hydrodynamic Model for a Choanoflagellate**
11:15 – 11:30	*Rubaiyat Bin Islam and Moselm Uddin, Mathematics, Tulane University* **Building an interactive modular app for the microscale pharmacokinetics/pharmacodynamics (microPKPD) model**
11:30 – 11:45	*Wen-Huai Tsao, Louisiana State University* **Multiscale analysis of fluid-structure interaction involving complex geometry**
11:45 – 12:00	*Gowri Priya Sunkara, Louisiana State University* **Frog Egg Quantification with Customized Stardist CNN: A Study in Precision and Real-World Application**
12:00 – 1:00	**Lunch**
1:00 – 1:45	***Keynote talk:*** *Michael Neilan, Mathematics, University of Pittsburgh* **Divergence-Free Finite Element Discretizations for Incompressible Flow on Split Meshes**
1:45 – 2:00	*Adnan Morshed, Tulane University* **Fluid-Elastic Coupled System for Modeling Filiform Insect Sperm Motion**
2:00 – 2:15	*Md Tanvir Emrose, Division of Electrical & Computer Engineering, Louisiana State University* **Broadband switchable infrared absorbers using phase-change materials**
2:15 – 2:30	**Coffee Break**
2:30 – 2:45	*Casey Cavanaugh, Louisiana State University* **A Hodge decomposition method for the 3D quad curl problem**
2:45 – 3:00	*Sang-Eun Lee, Tulane University* **Collective Dynamics of Self-avoidant, Secreting Particles**

Saturday, Jan. 20	
3:00	**Concluding Remarks**

ABSTRACTS

KEYNOTE SPEAKERS:

Title: Divergence-Free Finite Element Discretizations for Incompressible Flow on Split Meshes

Author: **Michael Neilan**

Abstract Text:

Using smooth piecewise polynomial spaces as a guide, we construct several stable divergence-free and pressure-robust finite element methods for the (Navier-)Stokes problem. These schemes utilize discrete spaces defined on Alfeld and Worsey-Farin splits of simplicial triangulations, which are well known in the field of multi-variate splines. These methods are uniformly stable and are supported in current finite element software libraries. Byproducts of this construction include characterizations of discrete divergence-free subspaces, commutative projections, and simple formulas for the dimensions of smooth polynomial spaces. We also briefly discuss how these results and tools can be extended to construct robust computational schemes for linear elasticity.

Title: Numerical analysis of surface fluids and modeling of lipid membranes

Author: **Maxim Olshanskii**

Abstract Text:

In this talk we focus on numerical analysis for systems of PDEs governing the motion of material viscous surfaces, the topic motivated by continuum-based modeling of lateral organization in plasma membranes. We shall consider several systems of fluid and phase-field equations defined on evolving surfaces and discuss some results about well-posedness of such problems. We further introduce a computational approach and numerical analysis for the resulting systems of PDEs. The methods are combined to deliver a computationally tractable and thermodynamically consistent model describing the dynamics of a two-phase viscous layer. The talk closes with an illustration of the model ability to predict lateral ordering in multicomponent vesicles of different lipid compositions.

Title: Mathematical modeling of tumor microenvironment

Author: **Katarzyna Rejniak**

Abstract Text:

Tumors develop in a complex microenvironment that includes other cells, the extracellular matrix, multiple chemical compounds, and the interstitial fluid. All these components interact with tumor cells, affect tumor behavior and its response to anti-cancer treatments. On the other hand, the microenvironment is also modified by the growing or invading tumor cells, as well as by the administered therapies. This complexity and reciprocal interactions are hard to reproduce experimentally in a controlled way. However, they can be simulated and analyzed by mathematical and computational models. I will present examples of tumor and microenvironment interactions using our data-based computational micropharamacology framework that combines off-lattice agent-based models and reaction-advection-diffusion PDEs.

OTHERS:

Title: A Hodge decomposition method for the 3D quad curl problem

Authors: S. C. Brenner, **C. Cavanaugh**, L.-Y. Sung

Abstract Text:

Using the Hodge decomposition for a divergence-free vector field, we develop a finite element method for the quad-curl equation in three dimensions. This approach allows the fourth-order problem to be reformulated as three second-order saddle point systems: two Maxwell systems and a Stokes system. Analysis and results are presented for a Nedelec-P1 discretization for Maxwell's equations, and a P2-P1 Taylor-Hood method for Stokes' equations.

Title: Hydrodynamics of choanoflagellate colonies near a wall: a reduced model approach

Authors: **Hongfei Chen**, Ricardo Cortez, Hoa Nguyen, Tom Hata, Mimi Koehl,Lisa Fauci

Abstract Text:

Many microbial eukaryotes, such as choanoflagellates, exist as unicellular organisms, while others form multicellular colonies. Nevertheless, the advantages or disadvantages in feeding performance or predator avoidance between singlecelled organisms and multicellular colonies are not yet well understood. Studying the hydrodynamics of colonies using detailed models of cells that represent flagella, microvilli, and cell bodies would be ideal. However, considering the presence of a hundred cells or more within a colony, this is not feasible. In our earlier research, we introduced a colony model comprised of reduced representations of individual cells. These reduced cell models were fine-tuned using the farfield velocities computed from a detailed model. Our results demonstrated a good agreement with the experimental data in free-swimming colonies. However, benthic flagella-in colonies that sit on the substrate are more commonly observed in lab environments, where the nearby wall changes the flow pattern. Building upon our previous work, we focus on colony hydrodynamics near a wall and compare the feeding efficiency between swimming and benthic colonies.

Title: Broadband switchable infrared absorbers using phase-change materials

Authors**: Md Tanvir Emrose**, Emily L. Payne, Chenglong You, and Georgios Veronis

Abstract Text:

We introduce multilayer structures with the phase-change material $Ge_2Sb_2Te_5$ (GST) for use as broadband switchable absorbers in the infrared wavelength range. We optimize both the material composition and the layer thicknesses of the multilayer structures, in order to maximize the difference between the absorption for GST in its crystalline phase and the absorption for GST in its amorphous phase in the wavelength range of interest. We show that in the optimized structures near perfect absorption can be switched to very low absorption in a broad wavelength range by switching GST from its crystalline to its amorphous phase. Our optimized lithography-free structures have better performance than harder-to-fabricate three-dimensional structures. Our results could pave the way to a new class of broadband switchable absorbers and thermal sources in the infrared wavelength range.

Title: Rigid microspheres in a Stokes fluid: motion due to white noise

Authors: **Irene M. Erazo**, Scott A. McKinley, Lisa J. Fauci

Abstract Text:

This study investigates the dynamic behavior of a small spherical particles subjected to externally applied random forces while immersed in a viscous fluid. Our computational approach uses a regularized Stokeslet formulation. In contrast to the stochastic immersed boundary method, which averages fluctuating random forces within the particle location, here, these forces are in the surrounding fluid, external to the particle surfaces. We assume the particles are spheres with rigid rotations and translations due to the applied transient forces. Moreover, the spheres interact through the fluid, and their trajectories and relative motion are investigated.

Title: A Flexible Hydrodynamic Model for a Choanoflagellate

Authors: **Kendall Gibson**, Ricardo Cortez, Lisa Fauci

Abstract Text:

A unicellular choanoflagellate has an ovoid cell body and a single flagellum surrounded by a collar of microvilli. By waving its flagellum, it swims and creates a water current that brings bacteria to its collar of microvilli. Detailed computational models of choanoflagellate hydrodynamics that capture body morphology typically assume rigid microvilli and prescribe the kinematics of the flagellum. However, the flagellum and microvilli are not rigid structures, but flexible filaments whose evolving shapes are coupled to their fluid environment. We present a model that treats the flagellum and the microvilli as elastic Kirchhoff rods whose shapes are not pre-set, but emerge from the coupled system. In addition to understanding the effect of compliance of these structures on the swimming of a single organism, we will study the hydrodynamic interaction of two choanoflagellates and how the collars might affect this interaction.

Title: Modeling and Numerical Analysis of the Cholesteric Landau--de Gennes model

Authors: **Andrew Hicks**

Abstract Text:

Liquid Crystals (LCs) are a key component of our life in the modern world, appearing in various technologies, such as LC displays and temperature sensors. We investigate the numerical analysis of the Landau--de Gennes (LdG) model, which utilizes a 3x3 symmetric tensor as the order parameter (the "Q-tensor"). This model is usually preferred over others, such as the Oseen-Frank model. We show how the standard LdG model can be extended to model cholesteric LCs, which have applications in droplet lasers, novel bio-sensors, and anti-counterfeiting markers. Next, we describe a finite element discretization of the model and an L^2 gradient flow scheme for computing local minimizers, and we discuss various time-step restrictions for the gradient flow scheme to be energy decreasing. Furthermore, we prove a mesh size restriction that is critical for avoiding spurious numerical artifacts in the numerical solutions, which is not well-known in the LC literature, particularly when simulating cholesteric LCs that exhibit "twist". Finally, we present various numerical simulations in 3-D, on both slab geometries and spherical shells, and connect these results with experiments.

Title: Collective Dynamics of Self-avoidant, Secreting Particles

Authors: **Sang-Eun Lee** (Tulane University), Ricardo Cortez (Tulane University), and Lisa Fauci (Tulane University)

Abstract Text:

Motivated by autophoretic droplet swimmers that move in response to a self-produced chemical gradient, here we examine the collective dynamics of individual motile agents using a simple reaction-diffusion system. The agents have an unlimited supply of a chemical, secrete it at a given rate, but are anti-chemotactic so move at a given speed in the direction of maximal decrease of this chemical. In both one- and two-dimensional periodic domains, we find intriguing long-time behavior of the system. Depending upon a non-dimensional parameter that involves secretion rate, agent velocity, domain size and diffusion, we find that the position of the agents either relax to regularly spaced arrays, approach these regular arrays with damped oscillation, or exhibit undamped, periodic trajectories. We examine the progression of particles that are initially seeded randomly, and we also examine the stability of the steady and periodic states.

Title: Fluid-Elastic Coupled System for Modeling Filiform Insect Sperm Motion

Authors: **Adnan Morshed**, Ricardo Cortez, Lisa Fauci

Abstract Text:

Across the taxonomic orders of insects, fascinating diversity is found in reproductive techniques and sperm morphology. We present a robust dynamical model of a filiform insect sperm, coupled with a viscous fluid, that encounters rigid obstacles while swimming. Characteristic insect sperm features such as lengthwise active and passive sections, and modulation of shape amplitude and frequency are preserved in the model. The swimming motion is achieved by prescribing the material properties of the filament as well as a traveling wave of preferred curvatures along the filament. The resultant waveform and motion of the sperm emerge through its interaction with the surrounding viscous fluid and the confining structures. We observe the effects of active length on swimming speed and investigate the power requirements and efficiencies of the swimming organisms. Swimmer-wall interactions and the interplay between geometric and elastohydrodynamic properties are also explored.

Title: "Circle Methods for Regularizing Nearly Singular Boundary Integrals in 2D Pertaining to the Laplacian"

Authors: **Alex Nisbet**, Ricardo Cortez

Abstract Text:

Solutions of Laplace’s equation play a central role in many physical phenomena, including Stokes flow, where the fundamental solution of Stokes equations is built from the fundamental solution of Laplace’s equation. Solutions to these PDEs can be represented by boundary integrals in terms of convolution with a weakly singular kernel, e.g. the Poisson kernel. However, computing these integrals for points near the boundary using a fixed set of quadrature nodes is problematic, and standard methods lead to large errors. For certain domains, e.g. spheres, specialized representations have been developed to compute these integrals accurately. In this talk I will discuss "Circle Method(s)" for regularizing such integrals, whereby the singularity is transferred to one or more circular domains and dealt with exactly using orthogonal polynomials.

Title: Shape Optimization with an Unfitted Finite Element Method

Authors**: Jeremy T. Shahan** and Shawn W. Walker

Abstract Text:

We present a formulation of a PDE-constrained shape optimization problem that uses an unfitted finite element method (FEM). The geometry is represented (and optimized) using a level set approach and we consider objective functionals that are defined over bulk domains. For a discrete objective functional (i.e. one defined in the unfitted FEM framework), we show that the exact shape derivative can be computed rather easily. In other words, one gains the benefits of both the optimize-then-discretize and discretize-then-optimize approaches. We illustrate the method on a simple model (geometric) problem with known exact solution, as well as shape optimization of structural designs. We also give some discussion on convergence of minimizers. This is joint work with Shawn W. Walker (walker@math.lsu.edu, LSU).

Title: "Frog Egg Quantification with Customized Stardist CNN: A Study in Precision and Real-World Application."

Authors: **Gowri Priya Sunkara**, Iswarya Sitiraju , and Peter Wolenski

Abstract Text:

Accurately quantifying the number of frog eggs in densely populated petri dishes has long presented a formidable challenge, necessitating the use of precise machine-learning tools. In response, we leveraged Stardist, a Convolutional Neural Network (CNN) algorithm developed by the team led by Schmidt et al. We tailored this algorithm to suit our specific dataset. Our approach entailed the creation of a meticulously curated dataset comprising 180 images of frog eggs within Petri dishes, each accompanied by detailed annotations for training. The customized Stardist model demonstrated an impressive average accuracy rate of 95% on both the training and testing sets. Notably, our team conducted extensive research to determine the optimal number of eggs and number of images required in the dataset for accurate results. To assess its real-world applicability, we subjected the model to a densely populated dataset featuring 2006 frog eggs, achieving a remarkable accuracy of 99.3%. This exceptional performance underscores the model's proficiency in accurately quantifying frog egg quantities within intricate environments, thereby providing valuable insights for scientific and ecological research.

Title: Multiscale analysis of fluid-structure interaction involving complex geometry

Authors: **Wen-Huai Tsao[1]**, Christopher E. Kees[2]

[1]IT Consultant, Louisiana State University. Email: whtsao@lsu.edu

[2]CSRS Distinguished Professor, Louisiana State University. Email: cekees@lsu.edu

Abstract Text:

The Cut Finite Element Method (CutFEM) is applied to carry out multiscale analysis of fluid-structure interaction involving complex geometry under wave and current effect based on the multi-phase Navier-Stokes model [1]. Instead of employing adaptive quadrature or local refinement for the cell meshes near the fluid-solid interface, CutFEM CutFEM utilizes Nitsche's method to directly enforce the no-slip condition on the cut cell while maintaining optimal accuracy in boundary-conforming meshes. This approach facilitates the use of 3D structure models obtained from pre-existing STL files or LiDAR scanners. In prototype-scale experiments [2], the study simulates wave propagation over mangrove forests, assessing hydrodynamic drag induced by prop root structures without the need for parameterization in physical experiments. The advantages of reducing meshing work for the wake are highlighted. The wave attenuation and force reduction are evaluated. Numerical results and experimental measurements are compared. This research highlights the potential of CutFEM and multiscale modeling techniques to enhance the design of coastal ecosystems and marine structures. By accurately simulating structural responses to waves and current effects, the approach provides valuable insights for the development of resilient and sustainable coastal infrastructure.

Keywords: CutFEM, Multi-phase Navier-Stokes flow, Fluid-structure interaction, Natural-based shoreline.

Reference

[1] Kees, C.E., Collins, J.H., Zhang, A. (2022). Simple, accurate, and efficient embedded finite element methods for fluid-solid interaction. Computer Methods in Applied Mechanics and Engineering, 389(1), 114404.
[2] Tsao, W.H. and Kees, C.E. (2023). Computational analysis of wave and current interactions with mangrove forests. American Geophysical Union Fall Meeting, San Francisco, USA.

Title: Digital Twins for Oil Field Wellbores using Data-Driven Modeling (DDM) and Physicsbased Simulations

Authors: **Mayank Tyagi** (LSU), Derek Stall (Cortec), Oscar Molina (Mathworks)

Abstract Text:

Multiphase flows dominate the dynamics inside typical oil field wellbores, pipelines, and risers. Detailed simulations using Computational Fluid Dynamics (CFD) tools are restricted to small domain sizes to keep the computational costs reasonable. Further, the uncertainties in the fluid properties as well as the operating conditions add to further challenges to the simulations. In this presentation, a data-driven modeling approach is taken to build a digital twin for the wellbores. It is imperative to include a physical setup along with its computational counterpart in the input data for machine learning (ML) models. Our past research works on bench-scale and pilot-scale wellbores for simple multiphase systems are shown as a promising approach for the digital twins of wellbores.

Title: Building an interactive modular app for the microscale pharmacokinetics/pharmacodynamics (microPKPD) model∗

Rubaiyat Bin Islam1,2, **Moslem Uddin1**,2, and Kasia A. Rejniak2

Abstract Text:

Research problems in the field of computational biology or mathematical oncology are very often quite complex and involve multiple cellular processes with a good number of parameters to work with. In such a situation, it's convenient to split a model into pieces (modules) and perform computational experiments withone module at a time[2, 5]. For instance, microPKPD model that has been reported in [3, 4, 5] incorporates interactions of tumor cells with interstitial fluid flow around them, and transported drugs or metabolites. This model explicitly takes into account structures on a patch of tumor tissue which include the positions and shapes of cells and vessels, physical properties of drugs and nutrients that are transported within the tissue via diffusion and advection. Fluid mechanics at a micro-scale (i.e. Stokes' equation) is used to model these transports and drugs or nutrients may be modeled as discrete molecules or continuous concentrations. To solve fluid equations, the method of regularized stokeslet[1] has been utilized. Cells can absorb what is present in the interstitium via receptors on cell membranes using different methods. In this project, we've created a graphical user interface (GUI) that has connected several modules of microPKPD model into an application. We've utilized the app designer platform of Mathworks' MATLAB to accomplish this goal[6]. The developed app will allow users to select dynamic tissue structures and show temporal advancements of individual molecules or continuous concentrations upon their choices of interstitial transport and mode of cellular uptake. In this talk, we'll review various microPKPD modules that have been incorporated into the app and we'll show a demonstration of the app which is currently in the primary stage of its development.

Title: Investigating Disentanglement in beta-VAE Framework within a Linear Gaussian Setting

Authors: **Minh Vu**, Xiaoliang Wan, Shuangqing Wei

Abstract Text:

This research investigates the disentanglement property within the beta-VAE framework, focusing on unraveling latent representations into semantically meaningful and independent factors. Disentanglement is characterized by variations in a single latent variable corresponding to variations in a specific generative parameter, yielding interpretable and transferable representations. The goal is to achieve a disentangled representation where each latent variable exclusively captures a distinct generative factor, elucidating the underlying factors of variation in the data. The study specifically explores disentanglement in a linear Gaussian setting using the gamma-lambda-VAE model, chosen for its controllability of reconstruction error. We introduce a mutual information-based metric, I_m, where m denotes the dimension of the latent variable, to assess disentanglement across three scenarios: no correlation, partial correlation, and full correlation among generative variables. Our investigation reveals that the proposed metric is most effective under full correlation, less efficient under partial correlation, and may not be effective when no correlation exists. Furthermore, we compare our I_m metric with contemporary metrics, such as the SAP metric, in the linear Gaussian framework across the three aforementioned scenarios. This comparative analysis aims to elucidate the strengths and limitations of each metric in evaluating disentanglement.

Title: A Modified Regularized Stokeslets Segments Approach with Piecewise Cubic Forces

Authors: **Zheng Wang**

Abstract Text:

The regularized stokeslets segments method is used to simulate the motion of a flagellum swimming in a viscous fluid. It is based on the exact solution of Stokes equation on a piecewise linear flagellum, derived by assuming a linear continuous distribution of regularized forces along each line segment. We present a variation of the Regularized Stokeslet segments method by adopting a piecewise cubic force distribution, enabling interpolation through cubic spline. Therefore, a general filament is approximated by a piecewise linear curve with C1 continuous external force spanning the entire filament. This modification enhances the flexibility and accuracy of the Regularized Stokeslets segments approach.

Title: An Incremental SVD Method for Non-Fickian Flows in Porous Media: Addressing Storage and ComputaBonal Challenges

Author: **Yangwen Zhang**

Abstract Text:

It is well known that the numerical solution of the Non-Fickian flows at the current stage depends on all previous time instances. Consequently, the storage requirement increases linearly, while the computational complexity grows quadratically with the number of time steps. This presents a significant challenge for numerical simulations. While numerous existing methods address this issue, our proposed approach stems from a data science perspective and maintains uniformity. Our method relies solely on the rank of the solution data, dissociating itself from dependency on any specific partial differential equation (PDE). In this paper, we make the assumption that the solution data exhibits approximate low rank. Here, we present a memory-free algorithm, based on the incremental SVD technique, that exhibits only linear growth in computational complexity as the number of time steps increases. We prove that the error between the solutions generated by the conventional algorithm and our innovative approach lies within the scope of machine error. Numerical experiments are showcased to affirm the accuracy and efficiency gains in terms of both memory usage and computational expenses.

Title: Generating Polynomial Method for Non-symmetric Tensor Decomposition

Authors: Jiawang Nie (University of California at San Diego), Zi Yang (University at Albany SUNY),

Hongchao Zhang (Louisiana State University), and **Zequn Zheng**{Louisiana State University}

Abstract Text:

Tensors or multidimensional arrays are higher order generalizations of matrices. They are natural structures for expressing data that have inherent higher order structures. Tensor decompositions play an important role in learning those hidden structures. In this talk, we present a novel algorithm to find the tensor decompositions utilizing generating polynomials. Under some conditions on the tensor's rank, we prove that the exact tensor decomposition can be found by our algorithm. Numerical examples successfully demonstrate the robustness and efficiency of our algorithm.