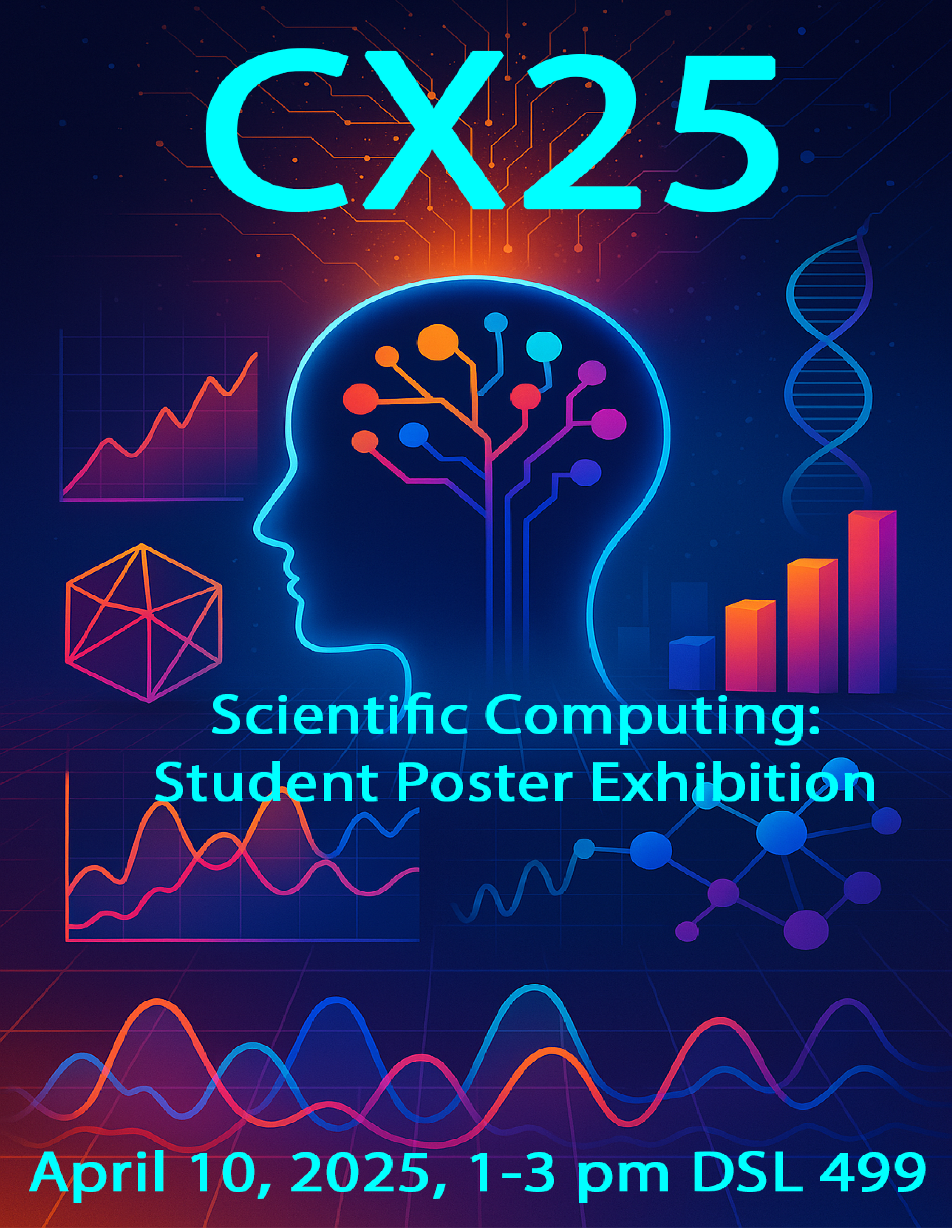


CX25

Scientific Computing: Student Poster Exhibition

April 10, 2025, 1-3 pm DSL 499

Chair's Welcome

Welcome to CX25, the annual Computational Xposition hosted by the Department of Scientific Computing (DSC) at Florida State University. This event celebrates the research of our undergraduate and graduate students, whose work spans the full spectrum of computational science.

This year's posters highlight our department's diversity and depth of research. From cutting-edge machine learning applications and high-performance simulations to innovative models in biology, physics, and beyond, the range of topics reflects technical excellence and a bold curiosity to explore and solve complex problems.

CX25 showcases what makes the DSC community so dynamic: a shared commitment to interdisciplinary thinking, rigorous analysis, and impactful science. These students represent the future of computational science, and many already contribute to real-world research and development efforts.

As our program continues to develop, it's encouraging to see students contributing to the direction of computational science. Their work reflects the solid academic environment and collaborative nature of our department.

Explore the posters and engage with the presenters. Thank you for supporting our students and joining us in celebrating their achievements.

Peter Beerli
Chair, Department of Scientific Computing
Florida State University

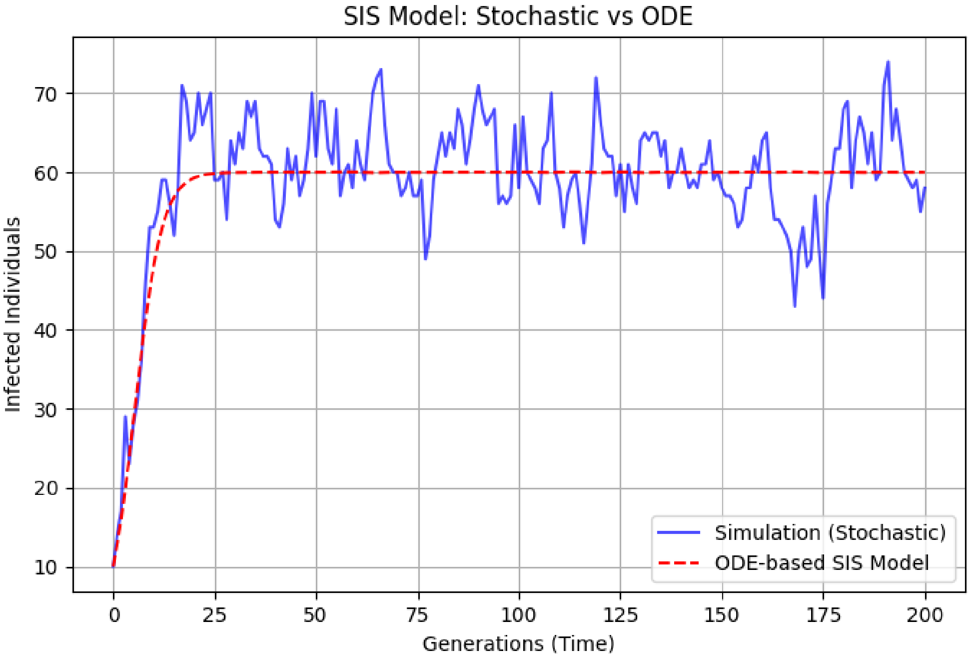
Contents

Epidemiology model inference and machine learning

Mahi Agrawal[1] and Peter Beerli[2]

[1] *Department of Computer Science and* [2] *Department of Scientific Computing, Florida State University, Tallahassee, FL*

Abstract: Epidemiology plays an important role in the prognosis of epidemics of diseases. Using one of the simplest epidemiological models, the SIS (Susceptible-Infected-Susceptible) model, we simulated the spread of infectious diseases where individuals can get infected, recover, and become susceptible to infection again. We have developed a SIS model using a stochastic approach, which tracks infections over multiple generations. Using this model, we have trained a neural network using PyTorch to estimate the infection rate (β) and the recovery rate (γ) based on the number of generations, the sample size, and the number of infected individuals at two time points. This model is tested against an SIS ODE, which verifies that this machine-learning approach accurately infers SIS model parameters. This model can be used for forecasting infection rates for future, real-world diseases, which can help improve epidemic preparedness and response.



Design and Implementation of Specialized Acoustic Chambers for High-Fidelity Capture of *Pseudacris* Advertisement Calls

Jessica Bellaire and Alan Lemmon

Department of Scientific Computing, Florida State University, Tallahassee, FL

Abstract: Bioacoustic research on amphibians faces significant challenges in isolating individual vocalizations from interfering noise. The recording environment must be adapted to meet the specialized habitat requirements of study organisms for accurate data collection. This research presents the development of a recording system designed specifically for capturing high-fidelity advertisement calls of upland chorus frogs (Pseudacris feriarum) in a controlled laboratory environment. From Fall 2024 to Spring 2025, we designed and constructed a specialized recording array featuring custom-built wooden acoustic chambers with specialized sound-dampening insulation. These chambers were engineered to isolate individual male frog vocalizations without environmental interference or acoustic distortion while maintaining appropriate temperature and humidity conditions critical for amphibian welfare. Each chamber incorporates directional microphones positioned for optimal sound capture, enabling the collection of clean, isolated calls free from external and playback noise contamination.

The chamber design underwent multiple iterative refinements based on acoustic testing and analysis to ensure optimal sound isolation properties and cost while maintaining appropriate environmental conditions for amphibian subjects. Key design considerations included: (1) selection of materials that balance acoustic isolation with moisture resistance, (2) chamber dimensions that minimize internal sound reflections while providing adequate space for natural calling behavior, (3) directional microphone positioning to maximize signal-to-noise ratio, and (4) implementation of a modular design allowing for efficient deployment and maintenance. The resulting recording system has been successfully deployed in ongoing research investigating geographical and genetic variation in Pseudacris advertisement calls across multiple populations. Preliminary analyses indicate that the acoustic chambers have significantly improved recording quality compared to traditional field recording methods, enabling more precise measurement of temporal and spectral call parameters. The high-fidelity recordings obtained through this system are facilitating analyses of correlations between genotypical acoustic features and genetic markers across populations, contributing to our understanding of the evolutionary processes shaping communication systems in these amphibians.

This project demonstrates an innovative application of acoustic engineering principles to solve a significant methodological challenge in bioacoustic research. The modular, cost-effective design of these recording chambers provides a template for similar applications across various species and research contexts, potentially expanding the toolkit available to researchers in bioacoustics, behavioral ecology, and conservation biology.

Fully installed Pseudacris recording chambers in laboratory.

Magnetized Turbulent Combustion

Kisalay Ghosh, Adam Mathews, Tomasz Plewa

Department of Scientific Computing, Florida State University, Tallahassee, FL

Abstract: The deflagration-to-detonation transition (DDT) is a critical mechanism in Type Ia supernovae (SNe Ia), enabling the transition from subsonic burning to a detonation wave in a turbulent white dwarf environment. While existing models, such as the data-driven subgrid-scale approach by Gusto (2022), focus on the role of turbulence in plasma preconditioning within the Zel'dovich gradient mechanism, the precise energy sources that facilitate this transition remain an open question.

A growing body of evidence suggests that localized ignition clusters regions of hot plasma with short ignition times play a crucial role in triggering detonation. The survival of these clusters depends on their ability to remain isolated from turbulence and avoid rapid mixing, allowing nuclear burning to accelerate and eventually lead to full ignition. However, the mechanisms that sustain these ignition kernels and supply the necessary energy remain unclear.

In this study, we investigate magnetic reconnection as a potential source of energy release that could influence DDT conditions. Magnetic reconnection, a fundamental process in high-energy plasmas, facilitates the rapid conversion of magnetic field energy into plasma thermal energy, leading to localized heating and turbulence. This process may significantly impact hotspot formation and thermonuclear runaway in the pre detonation phase.

To explore this hypothesis, we use the FLASH code to perform a series of computational experiments simulating reconnection driven energy release in burning dense stellar plasmas. Our approach builds on the reconnection analysis techniques of Servidio et al. (2009), which utilize magnetic field topology to identify reconnection regions, and we compare these results with the recently proposed method by Wang et al. (2024). The Wang approach, which avoids a potentially sensitive to numerical errors eigen analysis of the magnetic field Hessian.

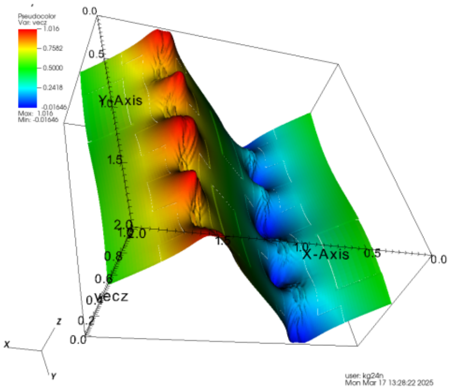


Figure 1: FLASH simulation of the 2D current sheet problem, showing localized reconnection zones. The evolution of magnetic field lines results in merging magnetic islands, altering the global topology.

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[1] Gusto, B. L. 2022, Florida State University, https://arxiv.org/abs/2401.16674;
[2] Servidio, S., Matthaeus, W. H., Shay, M. A., et al. 2009, PRL, 102, 115003;
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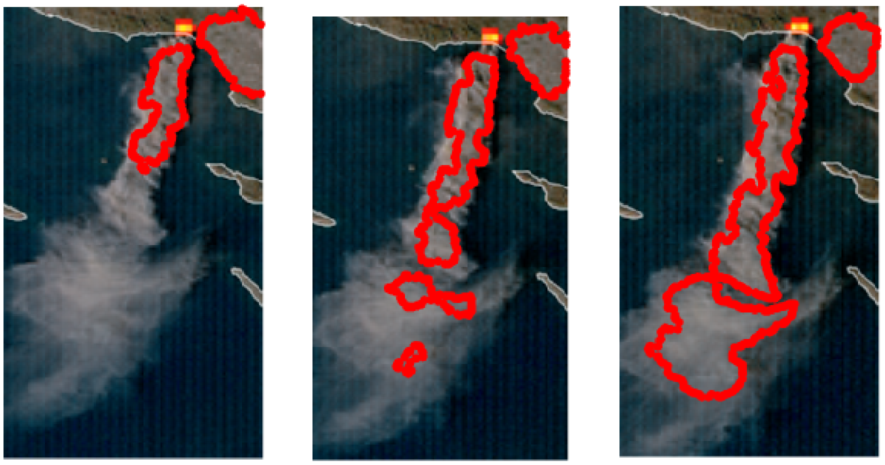
Discovering Governing Equations of Wildfire Smoke Dispersion via Weak SINDy: A Case Study of the Palisades Fire

Jhamieka Greenwood and Bryan Quaife

Department of Scientific Computing, Florida State University, Tallahassee, FL

Abstract: Modeling wildfire plume dynamics is challenging due to large amounts of uncertainty and turbulence. However, understanding these dynamics is critical to mitigate their environmental and public health impacts. One way to interpret the dynamics is to consider the motions of the plume boundary, thus creating a moving interface problem. Interfaces moving through a fluid show up in a variety of contexts, with a classical non-linear example being motion by mean curvature. Using Weak Sparse Identification of Nonlinear Dynamics (WSINDy), equations that govern moving interfaces will be learned. WSINDy is applied to simulated data generated by solving the motion by mean curvature and satellite data of the recent Palisades fire in Los Angeles, CA. WSINDy is an especially powerful method for the wildfire plume because of its ability to learn equations from data that have high noise-to-signal ratios and spatio-temporal inconsistencies. These learned equations reveal physics such as the spread and dispersion rates of the wildfire plume, and require much less data than is typically required to train data-driven models.



(a) 1/7/2025 4:34 pm (b) 1/7/2025 4:47 pm (c) 1/7/2025 4:59 pm

Calculated boundaries of the wildfire smoke plume from the Palisades fire satellite imagery.

Survey on Suspension of Particles in Viscous Stokesian Fluids

Lasitha Gunasekara, Bryan Quaife

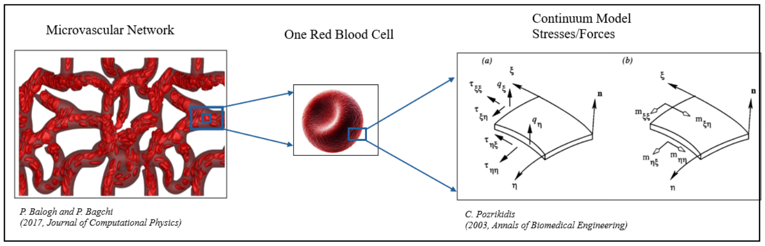
Department of Scientific Computing, Florida State University, Tallahassee, FL

Abstract: This study focuses on the dynamics of membranes suspended in small-scale, slow-moving fluids (Stokes flow). We consider both deformable membranes (red blood cells, vesicles, drops, and bubbles) and rigid bodies in flows where the fluid's viscous forces are much larger than its inertial forces. Understanding how these membranes move and change shape in such fluids is key to modeling biological and synthetic systems and has applications in biomedical engineering and microfluidics.

The shape of deformable membranes are determined by balancing forces such as bending, repulsion, adhesion, stretching, and tension. These forces induce a stress on the fluid thereby affecting the flow and creating a two-way coupling between the capsule shape and the fluid dynamics. For deformable membranes like red blood cells and vesicles, a Helfrich bending energy model describes the bending forces. For drops and bubbles, surface tension (described by the Young-Laplace equation) keeps their shape from rupturing, especially in tight spaces. Repulsion forces are also important in crowded systems to prevent membranes from overlapping.

Simulating these systems is not without challenging. One major issue is addressing membranes that are close to each other or close to solid walls, which we solve using techniques like high-order adaptive integration and smoothing; repulsion is another option. Another challenge is developing appropriate time stepping methods that minimize the numerical stiffness that arises from simulating deformable of membranes, particularly when dealing with large deformations. Finally, simulating large systems with many membranes requires powerful computers and advanced techniques like parallel computing, GPU acceleration, and fast algorithms like the Fast Multipole Method.

Different mathematical and computational methods have been developed to simulate these suspensions. Boundary Integral Equation methods take advantage of the Stokes flow assumption to reduce the dimension of the problem by placing all unknowns on the surface of the membranes. The Phase-Field Model can be applied to other fluid models by distributing membrane forces into the fluid and avoids it explicit tracking of the membrane. Finite Element Methods can be used to solve nonlinear equations for the stretching and bending forces balance. Finally, the Lattice Boltzmann Methods treat the membranes as collections of small particles that interact through particle distribution functions and collision rules. Each method has its own strengths and weaknesses in terms of accuracy, speed, and stability.This study provides a summary of the key methods, challenges, and strategies for simulating suspensions of deformable membranes and rigid bodies in slow-moving, small-scale fluids. By comparing different approaches, it helps researchers choose the best methods for their specific problems, balancing accuracy and computational efficiency.



P. Balogh and P. Bagchi (2017, Journal of Computational Physics)

C. Pozrikidis (2003, Annals of Biomedical Engineering)

Neural Circuit Model for Chorus Frog Mating Behavior

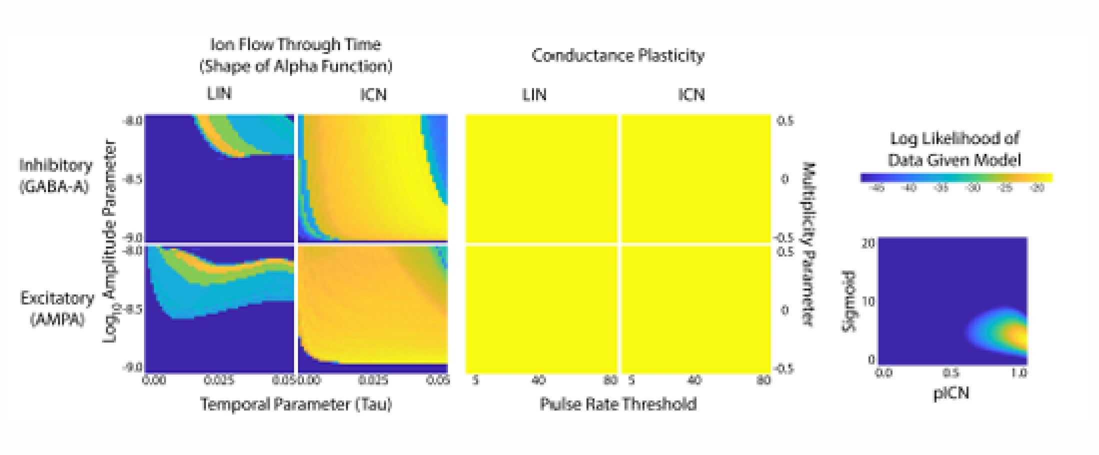
Skylar Haas[1] and Alan Lemmon[2]

[1]*Department of Computer Science, Florida State University, Tallahassee, FL*
[2]*Department of Scientific Computing, Florida State University, Tallahassee, FL*

Abstract: We currently know very little about how alterations in neural circuits translate to changes in behavior. The upland chorus frog (*Pseudacris feriarum*) is a prime subject for advancing our knowledge in this realm because their mating behaviors (consisting of male advertisement calls and female preferences for those calls) vary across populations.

We seek to identify the connection between neural circuits and mating behavior, focusing on the variables that are most likely to result in evolution. To do so, we fit neural circuit models to the behavioral data gathered from presenting alternative mating calls to female frogs testing and noting which calls attract the most females. This study was conducted in two populations that are known to differ substantially in their behaviors, an Alabama population and a Florida population.

In the end, my project hopes to find the evolutionary trajectory in neural circuit parameter space that allowed divergent evolution between these two populations. Specifically, I want to determine which neural circuits components have evolved. Additionally, I also hope to predict how female hybrids between these populations would behave when mating.

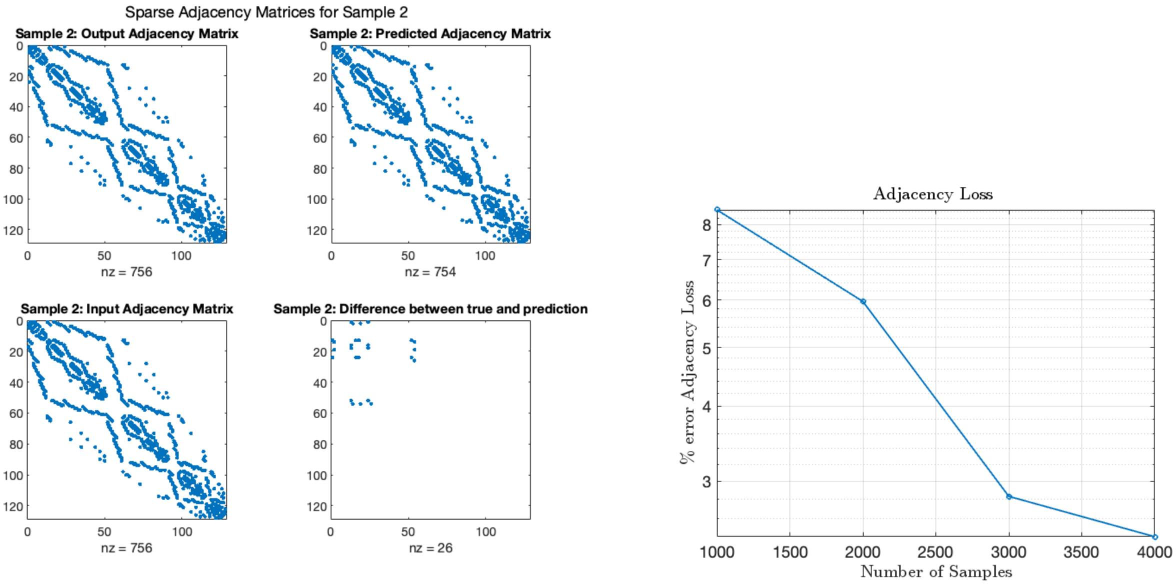


Approximation of Structural Topology Optimization through Graph Neural Network Techniques

Kunal C. Kanawade and Nick Dexter

Department of Scientific Computing, Florida State University, Tallahassee, FL

Abstract: In additive manufacturing engineering, graph and constraint-based representations have become instrumental for modeling micro-structures under various loading conditions. While these representations facilitate topological exploration, the resulting combinatorial optimization problems remain computationally prohibitive, necessitating efficient surrogate models. This research investigates Graph Neural Networks (GNNs) based architecture as surrogate models to learn the mapping from initial undirected graphs with edge attributes to their optimized topological configurations. Our approach leverages the GNNs to capture the intrinsic relationships and physical constraints inherent in structural designs. By training on data generated from a black-box topology optimizer, the model predicts optimized structures that satisfy design requirements and loading conditions, potentially offering significant computational acceleration while maintaining solution fidelity.



(a) (b)

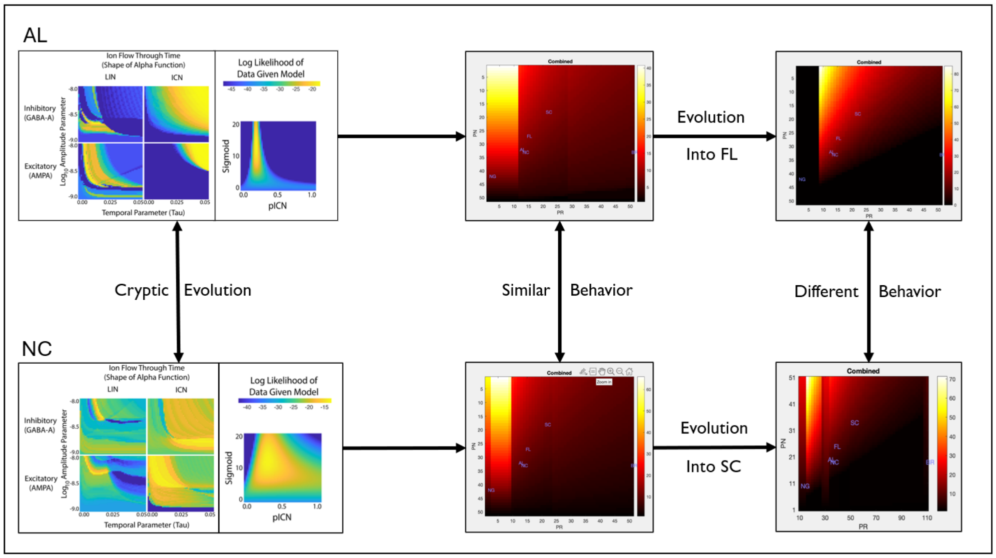
(a) Difference between the predicted and Output(truth) adjacency matrix, and (b) % loss in Adjacency prediction for different number of samples

Cryptic Evolution in the Neural Circuits of *Pseudacris feriarum*

Colin Lewis and Alan Lemmon

Department of Scientific Computing, Florida State University, Tallahassee, FL

Abstract: Little is known about the relationship between the evolution of the brain and behavior. Looking specifically at mating behavior, an examination of Pseudacris feriarum, a species of chorus frog, can shine a light on this relationship. Previous research has shown that relatively recently in its evolutionary history, populations of P. feriarum have become allopatrically separated from one another, with some populations overlapping with populations of other members of the genus Pseudacris. The resulting interaction has led to the evolution of mating behaviors to avoid hybridization. Using a particle swarm optimization technique, we identify neural circuit models that fit previously collected female preference data from female P. feriarum. One compelling question is: can two or more neural circuits with different configurations produce the same mating behavior? Examining allopatric populations in North Carolina and Alabama with this method allows us to see if there is any evidence of cryptic evolution (The process by which neural evolution could occur with no observable change in behavior.)



Model 1. Depicts different results of ion flow through time of inhibitory GABA-A and excitatory AMPA for LIN and ICN between AL and NC populations, leading to no outward difference in call response behavior between the populations. Also shows how their evolutionarily derived populations that live in sympatry with *P. Nigrita* have evolved different behaviors to avoid *P. Nigrita* calls.

Machine Learning for Ocean State Prediction: Enhancing Subsurface Field Estimation and Forecast Initialization at Different Scales.

Jose Roberto Miranda and Olmo Zavala-Romero

Department of Scientific Computing, Florida State University, Tallahassee, FL

Abstract: Understanding the ocean's subsurface dynamics is crucial for climate science and oceanography, yet it remains one of Earth's least observed domains due to logistical and financial constraints of direct measurements. Our broader research objective is to develop machine learning frameworks that improve data assimilation and initialization conditions for ocean forecast models, enhancing the forecast capabilities in critical regions like the Gulf of Mexico.

As a first step toward this goal, we developed Neural Synthetic Profiles from Remote Sensing and Observations (NeSPReSO) to accurately predict subsurface fields from surface data, which can later serve as improved initial conditions for operational ocean models. The model, trained and evaluated in the Gulf of Mexico using Argo profiles and glider data, over-performed other traditional synthetic data generation methods, such as the Gravest Empirical Modes (GEM), Multiple Linear Regression (MLR) and Improved Synthetic Ocean Profile (ISOP). We're currently working in a new iteration of NeSPReSO at a global scale with several improvements: use of spatial and temporal surface data, an improved modular neural network architecture, incorporation physical constraints into the loss function, transfer learning, fine-tuning, and uncertainty quantification.

This framework has broad implications for the oceanographic community, providing accessible and accurate ocean state estimation and enabling enhanced weather prediction capabilities, improved climate modeling, and data-driven marine resource management strategies. Future work will focus on fine-tuning NeSPReSO for regional applications, validation of forecast improvements with data assimilation experiments, and integration with operational forecast systems.

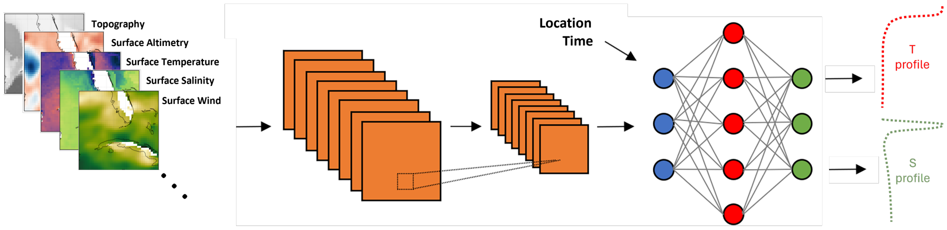


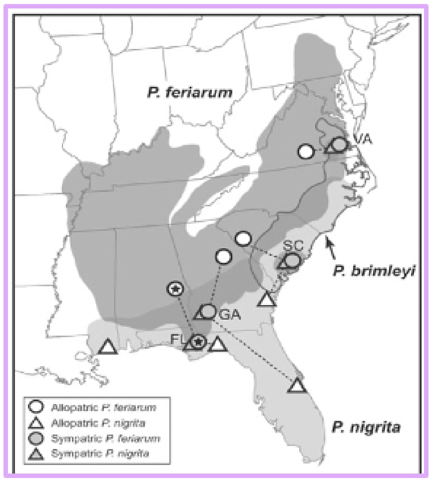
Diagram of the current iteration of NeSPReSO for predicting temperature (T) and salinity (S) profiles. Spatial and temporal multi-sensor environmental data is processed through convolutional layers for feature extraction. It is then passed to a fully connected neural network along with location and time metadata, generating temperature and salinity profiles as outputs.

Testing the Effects of Reproductive Character Displacement on Breeding Ecology of Upland Chorus Frogs (*Pseudacris feriarum*)

Ruby Moore and Emily Lemmon

Department of Biological Science, Florida State University

Abstract: Within the southeastern United States are two species of the genus Pseudacris found to hybridize: *Pseudacris feriarum* and *P. nigrita*. Hybrids of these species are less fit, and hybrid males are partially sterile. Because hybridization is maladaptive, females have evolved to prefer calls of conspecific males that are more different from that of the heterospecifics. The divergent preferences of *P. feriarum* females have caused males to evolve more energetically costly calls. Considering that mating signals for male anurans is their most energetically costly activity performed, I predict that greater energetic costs to *P. feriarum* male signaling could potentially lead to a decrease in the nightly duration of male signaling time, a shortening of the length of the annual breeding season, and/or increased intensity of breeding on the active nights (i.e., more dense choruses). To test these predictions, we are passively monitoring acoustic signaling behavior of frog choruses in six natural populations in Florida and Georgia. We are using AI to efficiently extract and analyze frog call data form large data files generated over five months of recordings in the field.

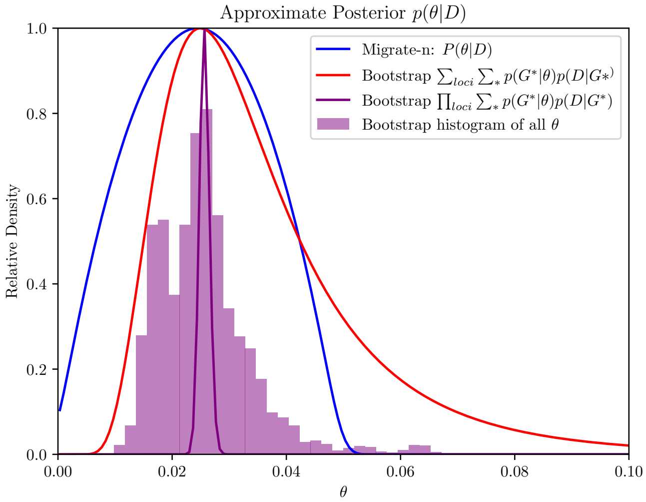


Is the inference of population size using the bootstrap biased?

Eesha Mukherjee and Peter Beerli

Department of Scientific Computing, Florida State University, Tallahassee, FL

Abstract: Estimating evolutionary parameters such as effective population size (N_e) and mutation rates from genetic data is a central challenge in population genetics. Several methods exist to infer these parameters, each with different assumptions and computational trade-offs. We compare three approaches: a method based on Bootstrap Monte Carlo Integration [1], Bayesian inference using Markov chain Monte Carlo Integration [2], and a Summary Statistics approach [3]. The bootstrap approach estimates likelihoods by resampling DNA sites; the Bayesian inference uses a biased random walk in genealogy space to evaluate the compatibility of the DNA data and population sizes drawn from a prior distribution; and the summary method uses the number of variable sites in the DNA data and expectations of coalescence theory. Using genealogies created using coalescent simulations and synthetic sequence data evolved on these genealogies; we evaluate how these methods perform under different conditions, such as small sample sizes and low mutation rates. Our analysis examines whether bootstrap resampling introduces biases, particularly in how it weights different genealogical configurations. We compare the three approaches in terms of bias, support intervals, and evaluation speed. Our findings provide insights into the reliability of bootstrap-based inference and the alternative strategies.



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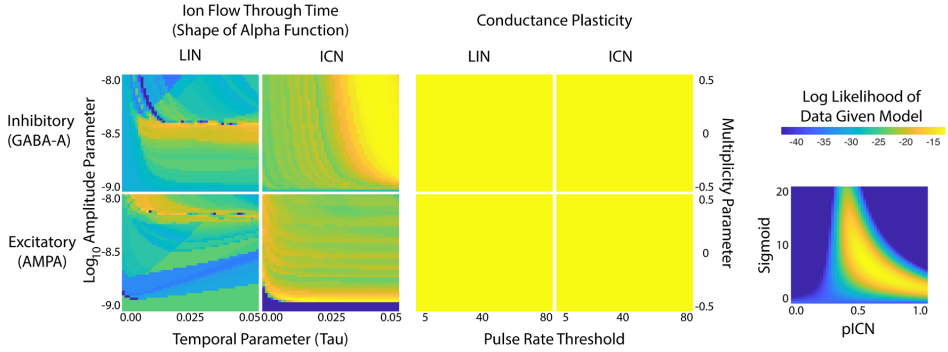
Does Sympatry Reinforce the Behavioral Divergence of *Pseudacris feriarum* in South Carolina?

Bryan Pineda[1], Emily Lemmon[2] and Alan Lemmon[3]

[1]*Department of Psychology, Florida State University, Tallahassee, FL*
[2]*Department of Biological Science, Florida State University, Tallahassee, FL*
[3]*Department of Scientific Computing, Florida State University, Tallahassee, FL*

Abstract: *Pseudacris feriarum* (*P. feriarum*), *Pseudacris nigrita* (*P. nigrita*), and *Pseudacris brimleyi* (*P. brimleyi*) are three species of chorus frogs found in the Southeastern United States (North and South Carolina [NC and SC, respectively]). *P. feriarum* exists in isolation in NC but coexists with the other species in SC. The purpose of this study is to determine how the neural circuits of *P. feriarum* evolved as a result of sympatry, and how the divergence of the neural circuit and general brain structures contribute to the variance in behavioral phenotypes. By analyzing the neurological changes that arise as a result of this species divergence, it would be possible to determine whether sympatric populations of *P. feriarum* in SC can be considered an early stage of speciation. Females from each population were presented with pairs of stimuli and those chosen by the females were recorded. The data collected from these calls will then be inputted into a program coded on MATLAB, allowing us to quantify, visualize, and analyze the divergence of the females' preferences through neural circuit modeling. This would also provide an improved understanding of how degrees of sympatry can affect a species. Once final results are obtained, it can be determined whether the calls and mating preferences of allopatric populations of *P. feriarum* can be considered an early stage of speciation. Because of this, some potential contributions to the field of evolutionary biology would be further knowledge of local ecologies, as well as a better understanding of how populations undergo speciation.

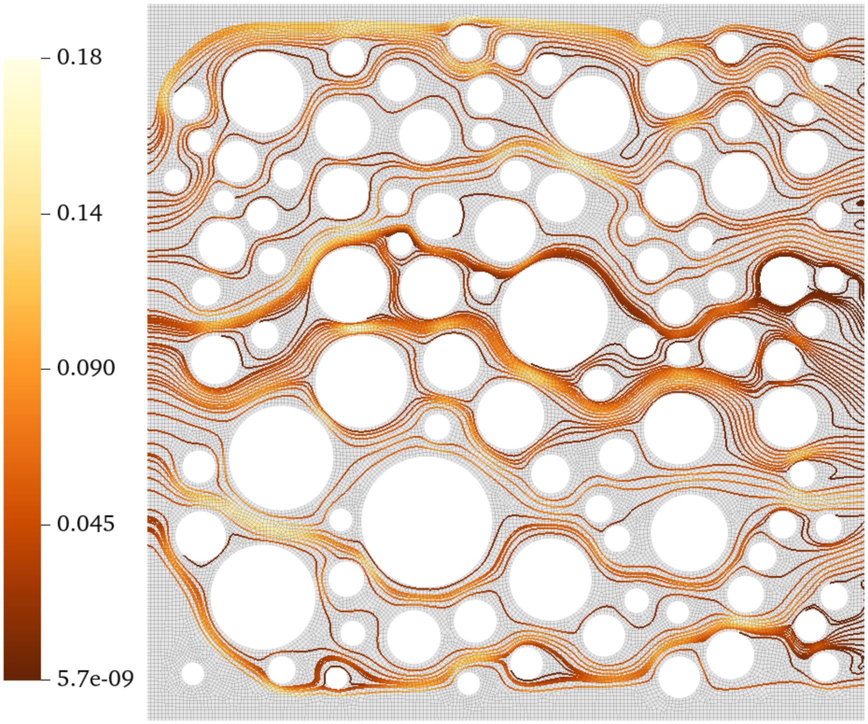


An enriched Galerkin method for the Navier-Stokes equations coupled with heat dynamics

Sanjeeb Poudel[1], Sanghyun Lee[2], and Lin Mu[3]

[1] *Department of Scientific Computing, Florida State University, Tallahassee, 32306, FL, USA*
[2] *Department of Mathematics, Florida State University, Tallahassee, 32306, FL, USA*
[3] *Department of Mathematics, University of Georgia, Athens, 30602, GA, USA*

Abstract: The coupling of fluid dynamics and heat flow presents a range of interesting scientific and engineering applications. This coupled system encompasses many challenges, like the inf-sup stability of finite element spaces. In this study, we implement the Enriched Galerkin (EG) finite element method, which provides an inf-sup stable scheme for solving the Navier-Stokes equations while having fewer degrees of freedom. However, in the standard formulation of the EG method, the velocity error depends on the pressure and viscosity. To address this, we study the pressure-robust EG scheme that resolves the issue through a velocity reconstruction operator. Additionally, we explore various stabilization techniques for advection-dominated flows and discuss various iterative methods to solve the coupled nonlinear system efficiently.



Quantifying Acoustic Signal Divergence During Speciation by Reinforcement in *Pseudacris feriarum*

Jack Rothbaum, Lia Garibay, Emily Lemmon[1] and Alan Lemmon[2]

[1] *Department of Biological Science, Florida State University, Tallahassee, FL*
[2] *Department of Scientific Computing, Florida State University, Tallahassee, FL*

Abstract: Speciation is the origin of new species through evolutionary divergence. Reinforcement, the evolution of behavioral reproductive isolation between species due to selection against hybridization, is one evolutionary force that can drive speciation. Prior studies have suggested that reinforcement between two chorus frog species, the Upland chorus frog (*Pseudacris feriarum*) and the Southern chorus frog (*P. nigrita*), can indirectly cause shifts in the male mating calls of *P. feriarum* populations. No studies to date, however, have examined these shifts in call structure across fine spatial scales. Here, we studied a transect of twenty *P. feriarum* populations spanning the Piedmont and Coastal Plain geographic regions near Macon, Georgia. Populations south of Macon have undergone reinforcement from interactions with *P. nigrita*, whereas populations north of Macon have not. By measuring and comparing call characteristics – such as wavelength, amplitude, pulse number, pulse rate, and frequency – across populations in the transect, this study provides valuable insights into the evolution of phenotypic variation and the divergence of mating behaviors during speciation.

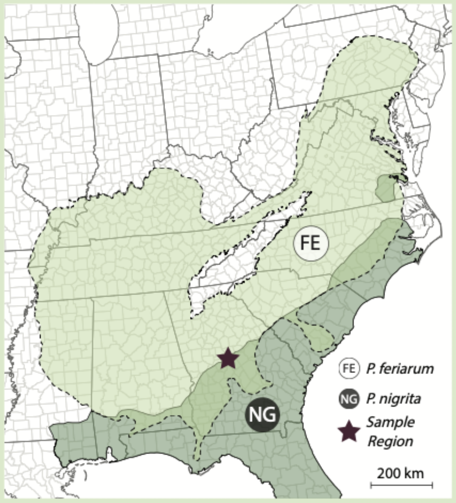

Map of *P. feriarum* and *P. nigrita* Populations

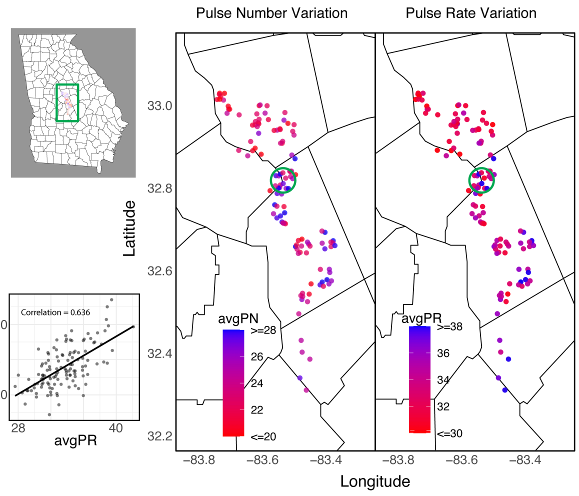
Figure 1. Map with the distribution of *P. feriarum* and *P. nigrita* populations and highlighted sampling region.

Comparing Within versus Between Individual Mating Call Variation in Upland Chorus Frog (*Pseudacris feriarum*) Population

Grzegorz Rusin, Isabella Merchan and Emily Lemmon

Department of Biological science, Florida State University, Tallahassee, FL

Abstract: A primary goal of evolutionary biology is to understand the forces driving the generation of Earth's biodiversity through speciation. Reinforcement—the evolution of behavioral reproductive isolation between species due to selection against hybridization—is one evolutionary force that can drive speciation by reducing the likelihood of interbreeding between incipient species. Reinforcement can also indirectly cause mating behaviors to diverge within a species, which can lead to reproductive isolation among populations of the same species. Chorus frogs (genus *Pseudacris*) are one group that shows evidence of speciation via reinforcement of male acoustic signals (calls) and female mating preferences in areas of overlap between species. One species, the Upland chorus frog (*P. feriarum*), also exhibits call divergence between its populations that do vs. do not overlap with another species, the Southern chorus frog (P. nigrita). What is unknown is whether *P. feriarum* with these extreme phenotypes recognize each other as the same species or whether they have become behaviorally isolated, thus representing incipient new species? Here, we investigated this question in a population of *P. feriarum* near Macon, Georgia, which contains individuals spanning a broad range of call phenotypes, including extremes. Specifically, we asked whether the call characters pulse rate (PR) and pulse number (PN) are more variable among different frogs than among calls of a single individual. We predicted that if individuals with very different call phenotypes from each other have evolved reproductive isolation, their call characters will be more variable among than within individuals. If, however, extreme individuals are not reproductively isolated, call variation among individuals is expected to be similar to the variation within individuals. To test this idea, we extracted and analyzed calls of 400 frogs from the Macon site, including twenty calls per frog: ten each from the beginning and end of a call bout across two recording sessions. Understanding the extent of individual variation in these call parameters will offer insight into how reproductive behaviors evolve and diversify during speciation by reinforcement.

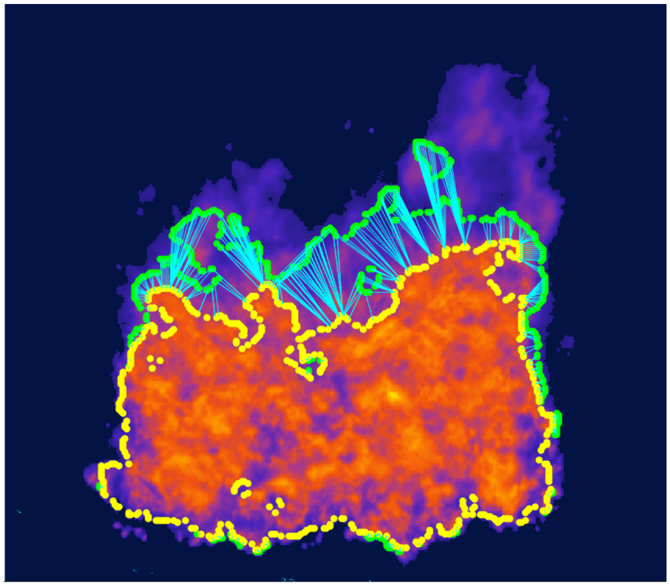


Watching Things Burn (with Fire Dynamic Vision)

Daryn Sagel and Bryan Quaife

Department of Scientific Computing, Florida State University, Tallahassee, FL

Abstract: The increasing frequency and severity of wildfires highlights the need for accurate fire and plume spread models. Traditional measurement methods often provide limited data, whereas computer vision techniques extract rich information from visual and infrared imagery. Fire Dynamic Vision (FDV) is a novel framework that tracks fire and plume dynamics across a wide range of spatial and temporal scales. FDV combines image segmentation and graph theory to delineate fire fronts and plume boundaries, effectively distinguishing them from visually similar objects in the scene. Its versatility is demonstrated through successful application to various image sources, ranging from synoptic-scale satellite images to sub-microscale images captured close to the fire environment. FDV also supports physics-based calculations, statistical analyses, and the generation of spatio-temporal datasets for machine learning applications.



Adaptive Sampling for Graph Neural Networks: A Christoffel-Based Analysis Framework

MJ Shooshtari and Nick Dexter

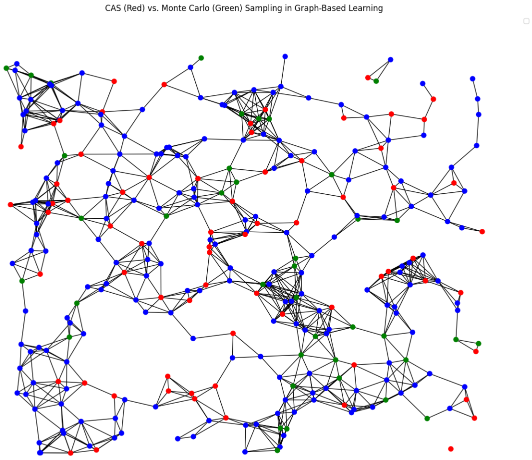
Department of Scientific Computing, Florida State University, Tallahassee, FL

Abstract: Graph Neural Networks (GNNs) have emerged as powerful models for learning from graph-structured data, yet their performance is significantly influenced by the quality of labeled samples. In many real-world scenarios, acquiring labeled data is expensive, motivating the need for intelligent sampling strategies. This research investigates the application of Christoffel Adaptive Sampling (CAS) for efficiently selecting informative samples in GNN-based learning tasks. Unlike conventional Monte Carlo-based sampling approaches, CAS leverages the spectral properties of the data representation to iteratively refine the selection of labeled points.

CAS4GNN adapts the CAS framework, originally developed for deep learning models, to the domain of graph-based learning. The method constructs a sampling distribution using the Christoffel function, computed via the singular value decomposition (SVD) of the penultimate layer representations of the GNN. This approach ensures that new samples are chosen in a way that maximizes diversity and informativeness, leading to improved learning efficiency. The project will compare CAS against Monte Carlo-based sampling techniques, assessing performance across various spatial graph datasets.

We will evaluate CAS4GNN on real-world spatial datasets, where graph-structured data plays a crucial role in predictive modeling. The study will focus on node-level regression tasks, such as predicting flight delays or traffic volume. Performance will be measured in terms of predictive accuracy, sample efficiency, and robustness to label scarcity.

This research contributes to the broader field of probabilistic modeling and computational learning by demonstrating the advantages of structured sampling techniques in GNN training. The anticipated results will provide insights into how adaptive sampling strategies can reduce labeling costs while maintaining model performance. This study also lays the groundwork for future extensions of CAS in other graph-based applications, including semi-supervised learning and knowledge graph construction.



Using Machine Learning to Quantify Complex Behavior in a Tropical Bird

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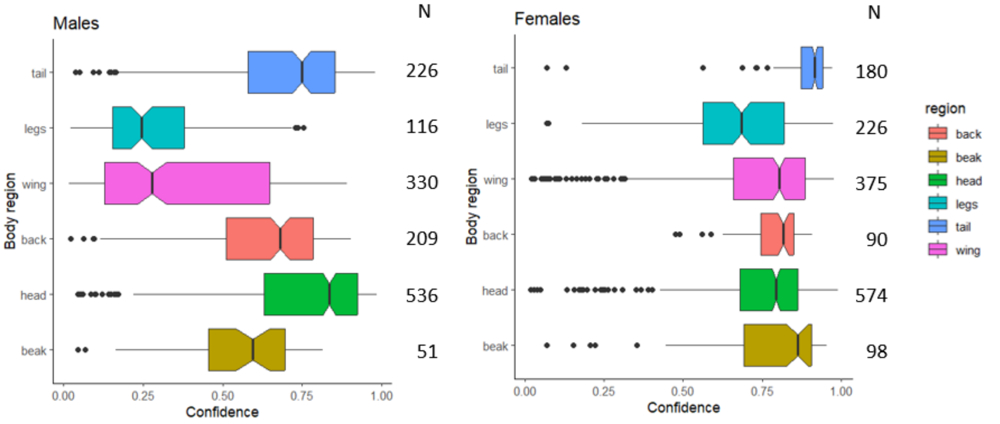
Abstract: Complex interactions are difficult to analyze, but are a key part of animal behavior. Lance-tailed Manakins (Chiroxiphia lanceolata) participate in complicated multi-male courtship displays that can be difficult and incredibly time consuming to analyze manually, as the complexity of these interactions makes it challenging to understand variation among competing groups, and details in patterns can be overlooked by the naked eye. However, the computational approaches of machine learning can be used to analyze and quantify these behaviors, offering a potential solution to these problems. Here we assess the ability of machine learning software to accurately quantify complex behavior. We first used a broad literature review to identify the best fit program for our model, then trained the program and analyzed results to assess accuracy. We chose DeepLabCut because of its capabilities for unsupervised, multi-animal identification and tracking. We then trained the program through extensive frame-labeling of displays and evaluated its accuracy in predicting body parts. Our results found that the confidence levels for identifying different body parts varied greatly within and across sexes. Within males, there was low confidence for identifying points on the wings and legs, and greatest confidence for points on the head. Females had greater confidence overall, with the tail being the greatest and legs being the weakest. Following this initial test, we plan to return to labeling to generate more data to increase the accuracy of the program so it can be used to better interpret this complex behavioral repertoire.

Figure 1.



Clustering-based Model Reduction for Glioma Graph Networks

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Abstract: We analyze structural and functional connectivity graphs for both healthy and glioma subjects by clustering-based model reduction to obtain a detailed understanding of these complex graphs. The reduced-order network is obtained by dividing the connected brain regions or nodes into disjoint clusters. Further, each cluster is replaced by a single new node in a reduced-size graph network. Several partitions are analyzed and evaluated based on model reduction errors.

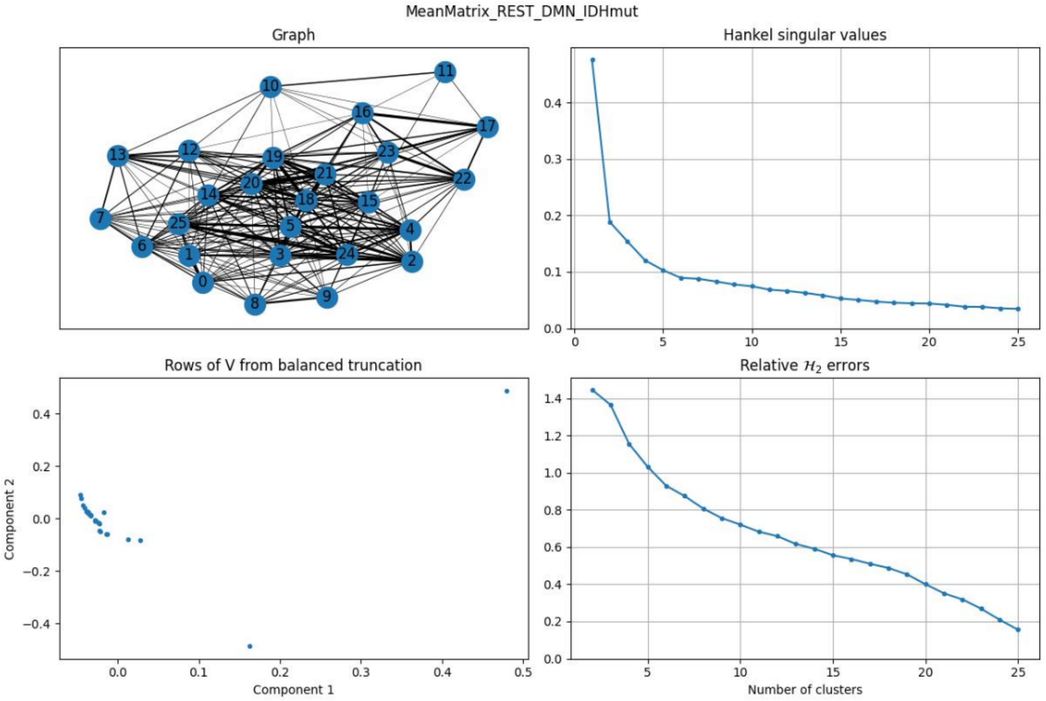

Figure 2. Clustering-based model order reduction for Functional Data, rsfMRI for IDHmut

Data-Driven Modeling of Critical Phenomena in Turbulent Combustion

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Abstract: The deflagration-to-detonation transition (DDT) is a fundamental process in both astrophysical and terrestrial combustion phenomena. In Type la supernovae (SNe la), DDT is believed to play a critical role in the explosive release of energy, yet the exact conditions under which it occurs remain poorly understood. Modeling this transition is particularly challenging due to the vast range of spatial and temporal scales involved (Fig. 1), making direct numerical simulation (DNS) of integrated systems infeasible. This work extends previous one-dimensional subgrid-scale (SGS) model development [2] by accounting for multidimensional effects in the Khokhlov equation [3], which parameterizes different combustion regimes. To this end, we introduce two new elements. First, we improve the SGS training process by using realistic distributions of input parameters based on DNS models of turbulent combustion. Second, we extend the existing ID SGS model to multidimensional applications (Fig.2). This multidimensional parametrization uses information about geometry of turbulent perturbations expressed in terms of curvature of relevant physical quantities, such as ignition time field (Fig. 3). Note that the limit of zero-curvature corresponds to the original one-dimensional SGS model. The new model'sintegration into the FLASH/Proteus code [1] will improve realism of large-scale simulations of SNe la explosions, and may also apply to select problems in terrestrial combustion.

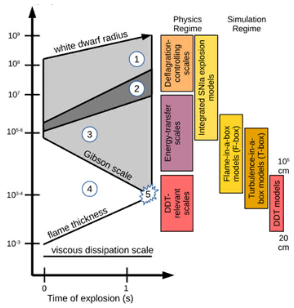

Fig. 1

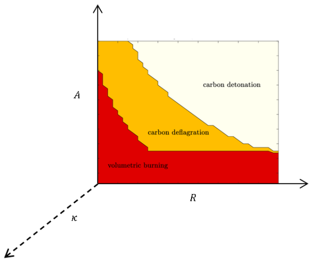

Fig. 2

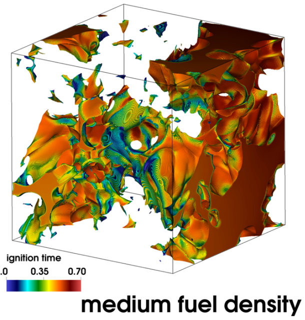

Fig. 3

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Embedded atom Approximation for Strongly Correlated Systems

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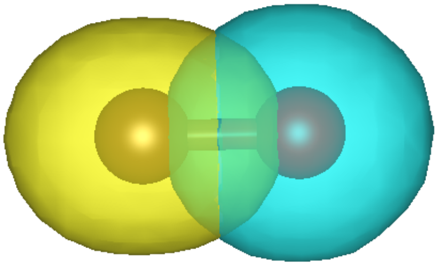
Abstract: Density Functional Theory (DFT) has been instrumental in understanding the electronic structure of materials, but accurately modelling the exchange-correlation (XC) energy in strongly correlated systems remains challenging. In this study, we propose a novel method to treat the on-site XC energies in strongly correlated systems. Our method involves partitioning a system's electron density onto individual atoms to enable a more accurate treatment of on-site correlations, such as the correlation between d and f electrons in transition metals and rare earth elements. This allows us to better capture the complex on-site correlations essential for understanding strongly correlated materials, such as transition metals oxides. Our method presents a potential solution to the limitations of existing methods like the local density approximation (LDA) + U method and the exact exchange for correlated electrons (EECE) method, which are two major methods for treating on-site correlations. One limitation of these two methods is that they rely on the choice of local projectors for defining local correlated orbitals, while our density partitioning scheme is first-principle and unique. Another more prominent limitation with LDA+U and EECE is that they cannot treat on-site correlation by using advanced orbital-based correlation energy functionals, since they only have access to occupied orbitals from the projection. Our method is able to employ any advanced correlation functional, such as the random phase approximation correlation energy functional, since each embedded atom is a complete Kohn-Sham system. With our method, it is possible to fully calculate the on-site correlation energy without any empirical parameter. In this poster, we demonstrate some preliminary results of this new method by performing non-self-consistent calculations on CO and N_2 molecules. To treat the on-site XC energies, a range-separated hybrid functional is used as the high-level XC functional. The binding energy curves and bond lengths agree with the benchmarks very well. The development of a fully self-consistent version of this new method is in progress in our group.



Atomic electron densities on carbon and oxygen from density partitioning.

Comparing Forward and Backward in Time Simulation: Structural Similarities and Differences

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Abstract: Studies of population dynamics, such as in fields like population genetics, ancestry reconstruction, or epidemiology, often depend on simulations of large populations. Forward Simulation (FE) models individual-level processes such as birth, death, and mutation in a forward-time manner, capturing stochastic variations due to environmental and demographic factors. In contrast, backward-in-time or Coalescent Simulation, traces lineages backward in time, offering computational efficiency but simplifying some biological complexities. This study aims to compare the structural similarities and differences between trees generated by these two models. We conducted simulations using both Forward and Coalescent models, generating phylogenetic trees under similar conditions. Key structural metrics were evaluated, including tree depth, total size, leaf count, branch count, and the cumulative distribution of branch lengths to explore the differences in tree topology. Forward Simulation trees were slightly shallower compared to Coalescent Simulation trees. Both models produced trees with similar sizes and leaf counts, indicating comparable topological properties. Coalescent trees exhibited a more uniform structure, while Forward trees showed higher variability due to individual-level randomness. Forward Simulation trees had more dispersed branch lengths, reflecting greater stochastic variation. Our findings suggest that while Coalescent models can approximate Forward models under stable conditions, they diverge in scenarios with dynamic population changes. The higher variability in Forward Simulation trees highlights the importance of individual-level stochasticity in modeling real-world populations. Coalescent models, with their computational efficiency, are suitable for large-scale studies but may oversimplify complex biological processes. The choice of model should depend on the specific research question, balancing biological realism against computational efficiency. Future work could extend this comparison to selection-driven populations and real-world genomic data to further highlight the differences and applications of these models.