Poster 1 - Alexander Havrilla: GLoRe: When, Where, and How to Improve LLM Reasoning via Global and Local Refinements

State-of-the-art language models can exhibit impressive reasoning refinement capabilities on math, science or coding tasks. However, recent work demonstrates that even the best models struggle to identify \textit{when and where to refine} without access to external feedback. We propose Stepwise ORMs (\textbf{SORMs}) which are trained, only on synthetic data, to approximate the expected future reward of the optimal policy or $V^{\star}$. More specifically, SORMs are trained to predict the correctness of the final answer when sampling the current policy many times. We then train \textit{global} refinement models, which take only the question and a draft solution as input and predict a corrected solution, and \textit{local} refinement models which also take as input a critique indicating the location of the first reasoning error. With this strategy we can improve the accuracy of a LLaMA-2 13B model (already fine-tuned with RL) on GSM8K from 53\% to 65\% when greedily sampled.

Poster 2 - Amy Sims: A simplified mathematical model for cell proliferation in a tissue-engineering scaffold

This work presents a comprehensive continuum model for cell proliferation within two-dimensional tissue-engineering scaffolds. The study reduces computational burdens and solves mathematical models for tissue growth within porous scaffolds. The model incorporates fluid dynamics of nutrient feed flow, nutrient transport, cell concentration, and tissue growth, considering the evolving scaffold porosity due to cell proliferation. The crux of the work establishes the ideal pore shape for channels within the scaffold to obtain maximum tissue growth. We investigate scaffolds with specific two-dimensional initial porosity profiles; our results show scaffolds which are uniformly graded in porosity throughout their depth promote more tissue growth.

Poster 3 - Biraj Dahal: Nonlinear Model Reduction with Autoencoders for Operator Learning

In light of the high dimensionality of data present in many problems involving learning physical processes from data, model reduction is a useful tool. Autoencoders use neural networks to learn low-dimensional representations of data, so they can be used for model reduction. We use AutoEncoder-based Neural Networks (AENet) to learn the latent variables of inputs and then transform the latent variables into the output. Using mathematical analysis and numerical experiments, we show that AENets can successfully learn the solution operator for PDEs, demonstrating their utility over other model reduction based methods such as PCA based methods.

Poster 4 - Christian Austin: Numerical Simulations of Certain Oldroyd Models for Non-Newtonian Fluids

Two of the most influential and historically significant models for viscoelastic non-Newtonian fluids include the Oldroyd models and the grade-two model. Recently, algorithms have been developed for solving the Oldroyd 3-parameter subset model with tangential boundary conditions, and the grade-two model with inflow and outflow. In this poster, we will discuss the history of and some problems with certain viscoelastic fluid models, some numerical results from a finite-element implementation of the Oldroyd 3-parameter algorithm, and future plans to exploit Tanner duality to extrapolate ideas from the grade-two algorithm to the Oldroyd 3-parameter algorithm to allow for inflow and outflow.

Poster 5 - Conlain Kelly: Hybrid Learning Models for Stochastic Materials Design

Most engineering systems exhibit spatial heterogeneity (both in structure and response) across a variety of length scales, and physical properties of interest (e.g. creep, fatigue, damage, and failure) are inherently driven by local motions. Mathematically, this necessitates the solution of PDEs with variable coefficients, where the coefficients (e.g. microstructures) are the result of an upstream manufacturing process and are generally high-dimensional, discontinuous, noisy fields. In this work we explore the utility of data-driven methods to accelerate the prediction of local deformations over heterogeneous materials microstructures. Furthermore, we employ existing numerical solvers to enhance and interpret our learned surrogate models.

Poster 6 - Ho Law: Image Vectorization with Depth: A Shape Layering and Convexifying Approach

Image vectorization, or image tracing, converts raster images into Scalable Vector Graphics (SVG) using mathematical formulas. We developed a method to enhance them with depth ordering and inpainting effect.

Poster 7 - Idowu E. Ijaodoro: Calculation of electrostatic free energy for the nonlinear Poisson-Boltzmann model based on the dimensionless potential

The Poisson-Boltzmann (PB) equation governing the electrostatic potential with a unit is often transformed to a normalized form for a dimensionless potential in numerical studies. To calculate the electrostatic free energy (EFE) of biological interests, a unit conversion has to be conducted, because the existing PB energy functionals are all described in terms of the original potential. To bypass this conversion, this paper proposes energy functionals in terms of the dimensionless potential for the first time in the literature, so that the normalized PB equation can be directly derived by using the Euler-Lagrange variational analysis. Moreover, alternative energy forms have been rigorously derived to avoid approximating the gradient of singular functions in the electrostatic stress term. A systematic study has been carried out to examine the surface integrals involved in alternative energy forms and their dependence on finite domain size and mesh step size, which leads to a recommendation on the EFE forms for efficient computation of protein systems. The calculation of the EFE in the regularization formulation, which is an analytical approach for treating singular charge sources of the PB equation, has also been studied. The proposed energy forms have been validated by considering smooth dielectric settings, such as diffuse interface and super-Gaussian, for which the EFE of the nonlinear PB model is found to be significantly different from that of the linearized PB model. All proposed energy functionals and EFE forms are designed such that the dimensionless potential can be simply plugged in to compute the EFE in the unit of kcal/mol, and they can also be applied in the classical sharp interface PB model.

Poster 8 - Jiahui Cheng: High Dimensional Binary Classification under Label Shift:Phase Transition and Regularization

Label Shift has been widely believed to be harmful to the generalization performance of machine learning models. Researchers have proposed many approaches to mitigate the impact of the label shift, e.g., balancing the training data. However, these methods often consider the underparametrized regime, where the sample size is much larger than the data dimension. The research under the overparametrized regime is very limited. To bridge this gap, we propose a new asymptotic analysis of the Fisher Linear Discriminant classifier for binary classification with label shift. Specifically, we prove that there exists a phase transition phenomenon: Under certain overparametrized regime, the classifier trained using imbalanced data outperforms the counterpart with reduced balanced data. Moreover, we investigate the impact of regularization to the label shift: The aforementioned phase transition vanishes as the regularization becomes strong.

Poster 9 - Michelle Baker: Applying Acceleration to Kyrlov subspace Eigenvalue Solvers

Many modern-day problems involve solving for the eigenvalues of significantly large matrices. In 2002, Golub and Ye introduced a competitive inverse-free Kyrlov subspace eigenvalue solver that focuses on large, sparse, symmetric matrices. In 2010, Quillen and Ye introduced a block generalization of the method. Recently, momentum-type acceleration has been shown effective at a low-cost to reduce the number of iterations in an iterative method, including methods for eigenvalue problems. In this poster, we will explore the effect of applying acceleration to Ye's implementations of the methods for single and block symmetric generalized eigenvalue problems.

Poster 10 - Nirjal Shrestha: An Active Set Method for a Neural Network

We provide a novel approach to increase the sparsity in a neural network aiming to obtain simpler networks with comparable performance to the original architectures. We delve into existing methods for inducing sparsity, such as L1 regularization and pruning techniques, while evaluating their impact on model complexity and accuracy. In particular, we solve the optimization problem of a neural network's objective function designed for image classification. We extend the initial optimization problem and create an algorithm to solve it. Furthermore, we demonstrate the success of our approach by proving its convergence, finding a stationary point for the generalized optimization problem.

Poster 11 - Nyambura Njenga-Benton: LaSDI: A Data Driven Framework for Identifying Dynamics in the Latent Space

This poster presents the data-driven framework for parametric latent space dynamics described in LaSDI: Parametric Latent Space Dynamics Identification, a paper by William D. Fries, et. al. The parametric model is created by building a set of local latent space models. Each local latent space dynamics model guarantees accuracy within the local region of the parameter space. By allowing the set of local regions to cover the whole parameter space, one can guarantee accuracy throughout the space. The LaSDI framework enables fast and accurate simulations, an increasingly important tool in computational physics and machine learning.

Poster 12 - Yijie Jin: Parametrized Wasserstein Gradient Flow with Application in Porous-Medium Equation

Wasserstein gradient flow (WGF) is a powerful tool for understanding and analyzing density evolution processes. In the seminal work by Jordan, Kinderlehrer and Otto, they showed that Fokker-Planck equation (FPE) is essentially the gradient flow of the relative entropy functional under the Wasserstein metric. Since then, WGFs have shown extensive applications in optimal transport theory, optimization problems, Fokker-Planck equation, porous medium equation, and more.

However, numerical computation of WGF remains a challenging problem, especially when the state space is of high dimension. Furthermore, it is often desirable to find a sampler that generates samples following the solution of WGF rather than the actual density function solving WGF in many real-world statistics and machine learning applications.

We develop a fast and scalable numerical approach to solve Wasserstein gradient flows (WGFs), which is particularly suitable for high-dimensional cases.

Poster 13 - Yiming Ren: A FFT-accelrated high order finite difference method for elliptic interface problems

A fourth order augmented matched interface and boundary (AMIB) method is proposed for solving a three-dimensional elliptic interface problem which involves a smooth material interface inside a cuboid domain. On the boundary of the cuboid domain, the fourth order AMIB method can handle different types of boundary conditions, including Dirichlet, Neumann, Robin and their mix combinations in fictitious value generation. Moreover, zero-padding solutions are introduced so that the fast Fourier transform (FFT) algorithm is still valid near the boundary. In dealing with the interior interface, a fourth order ray-casting matched interface and boundary (MIB) scheme is proposed, which enforces the jump conditions along the normal direction for calculating fictitious values. Comparing with the existing MIB scheme, the ray-casting scheme naturally bypasses the corner issue and becomes more robust in handling complex geometry. Based on fictitious values generated near interface and boundary, the fourth order central difference can be corrected at various irregular points including corner points, by introducing Cartesian derivative jumps as auxiliary variables. This gives rise to an enlarged linear system, which can be efficiently solved by the Schur complement procedure together with the FFT inversion of the discrete Laplacian. Extensive numerical experiments have been carried to test the proposed ray-casting AMIB method for numerical accuracy, efficiency, and robustness in corner treatment. The numerical results demonstrate that the ray-casting AMIB scheme not only maintains a fourth order of accuracy in treating various interfaces and boundaries for both solutions and solution gradients, but also attains an overall efficiency on the order of O(n3logn) for a n ×n ×n uniform grid.

Poster 14 - Yuan Qiu: Derivative-enhanced Deep Operator Network

Deep operator networks (DeepONets), a class of neural operators that learn mappings between function spaces, have recently been developed as surrogate models for parametric partial differential equations (PDEs). In this work we propose a derivative-enhanced deep operator network (DE-DeepONet), which leverages the derivative information to enhance the prediction accuracy, and provide a more accurate approximation of the derivatives, especially when the training data are limited. DE-DeepONet incorporates dimension reduction of input into DeepONet and includes two types of derivative labels in the loss function for training, that is, the directional derivatives of the output function with respect to the input function and the gradient of the output function with respect to the physical domain variables. We test DE-DeepONet on three different equations with increasing complexity to demonstrate its effectiveness compared to the vanilla DeepONet.