Honours Thesis Presentations

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Vahid Sheigani
Identifying local structures in colloid-polymer mixtures using machine learning

ABSTRACT: A colloid-polymer mixture with an applied electric field is subject to two categories of forces, the induced dipole-dipole interactions and depletion forces due to the polymer. The combination of these forces with different polymer concentrations and external electric fields results in the formation of various structures with different local order. To study these structures in more detail, the colloid-polymer system can be replicated computationally using the molecular dynamics method which enables us to calculate particle features such as bond order parameters computationally and further investigate these features using advanced methods such as machine learning. In this thesis, we apply a multi-step machine learning algorithm to dipolar-depletion systems and identify the local structure of atoms in the simulation box using the algorithm. The machine learning algorithm is a combination of multiple cutting-edge machine learning techniques including autoencoders, Gaussian mixture models, and a cluster merging technique. These algorithms are combined to create a multi step process that can identify different structures of matter in any molecular dynamics simulation output. This algorithm utilizes unsupervised machine learning which does not require labeled data and is applicable to known and unknown local structures.

Kayla Malcolm
Optical Conductivity: A Microscopic Perspective

ABSTRACT: Optical conductivity in a metal depends on electron-electron interactions in its 2-dimensional lattice. This research uses the Hubbard Model-the simplest theoretical model of interacting particles in a lattice and an extension of the "tight-binding" model to include short electron-electron interactions – to describe the subatomic process that facilitates optical conductivity. Dynamical Mean Field Theory (DMFT), as it relates to the Hubbard Model, considers the metal lattice as a system with a site (impurity) interacting with an electron "bath". Considering the probabilities of the site being occupied by a fermion, boson, both, or neither, the U-Energy coefficients and self energies of the system were calculated using Maxent, a code for

numerical analysis, assuming other factors are constant. These findings are key to the Hubbard Model Hamiltonian, and have led to the determination of the Joint Density of States, with respect to changes in frequency of the oscillations of the "impurity" in the metal lattice system. In this research, the Joint Density is related to the conductivity of the metal through Ohm's Law. The findings thus far support the notion that the optical conductivity is directly proportional to changes in Density of States, which is being further explored.

Shoumik Mugdho

Machine Learning of Chaotic Dynamical System

ABSTRACT: Chaotic dynamical systems exhibit sensitive dependence on initial conditions on a closed invariant set. This project focuses on a machine learning framework to discover chaotic dynamical systems from a given data snapshot. The methodology is based on the dynamic mode decomposition of chaotic systems to predict an operator that evolves an observed system state to a future state. The hypothesis has been tested against three data sets: the Lorenz dynamics, vortex shedding behind a cylinder and a NACA0015 airfoil. The results indicate that a single time signal of the Lorenz system is predicted reasonably accurately because the data was clustered through the time-delay embedding. However, the cylinder flow data is predicted relatively more accurately than the airfoil data. This is because the airfoil dynamics are more turbulent than the cylinder flow. The findings suggest dynamic mode decomposition is a potential data driven method that combines machine learning with first principle physics for the numerical modelling of chaotic systems. As the system becomes turbulent on a chaotic background, machine learning of turbulence becomes relatively challenging.

ALL ARE WELCOME!