Harry Winston Sullivan

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Education

University of Utah Salt Lake City, Utah
Bachelors of Science Anticipated Graduation: May 2023
Computational Physics Major, Computer Science Minor GPA: 3.84

Research Experience

Zhao Group May, 2021 - August, 2021

- Analyzed python code that combed raw LIGO detector data for future scientists and presented this analysis to the research group.
- Helped remake LIGO analysis python code to better comb the data as well as provide better documentation for future work.

Hoepfner Group June, 2021 - Present

- Utilized molecular dynamics simulations in tandem with machine learning to infer atomistic potential energy functions of simple liquids from experimental neutron scattering data of fluids.
- Modified the classic implementation of Bayesian optimization to better suit the large datasets involved in molecular dynamics simulation. This implementation decreased the time to simulate liquid benzene from hours to less than 0.1 seconds. Unlocking the ability to apply Bayesian potential energy inference on systems of molecules.
- Created an information theory based algorithm to quantify the uncertainty in structure to potential energy inversion schemes.

Publications

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1. B. Shanks, H.W. Sullivan, M. Hoepfner, *A Bayesian optimized structural force field for molecular fluids via modified Gaussian processes modeling* (In Internal Review)
2. H.W. Sullivan, B. Shanks, M. Hoepfner, *Calculating the limits of neutron diffraction to predict interatomic interactions with Bayesian experimental design and information quantification* (In Internal Review)

Conference Presentations

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1. B, Shanks, M. Hoepfner, H. W. Sullivan, S. Smith, P. Smith, J. Potoff, *A Bayesian optimized structural force field for noble gasses enabled by a radial distribution function surrogate model*, Centre Européen de Calcul Atomique et Moléculaire: Recent Advances in Machine Learning Accelerated Molecular Dynamics

Skills

- Classical and quantum molecular dynamics simulation in LAMMPS, HOOMD, and I-PI
- Proficient in: Python, Java, Matlab and LaTeX
- Probabilistic machine learning

Employment

Advanced Youth Climbing Coach May 2018 - May 2020

- Taught young climbers, ages 8-13, the fundamentals of climbing safely and effectively.

Undergraduate Researcher - Hoepfner Group January 2022 - Present

Extra Curricular

University of Utah Climbing Team August 2019 - October 2022