

Harry Winston Sullivan

Curriculum Vitae

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Professional Summary Statement

- Chemical Engineering masters student with a focus on computational science and engineering. My diverse background contains professional research in computer science, physics, chemical engineering, machine learning, and finance.
- Highly adept and creative researcher with a proven track record of swiftly conceptualizing, designing, and implementing innovative solutions to intricate engineering challenges. Possesses strong communication skills to effectively convey complex ideas..

Education

- 2019 – Present **Masters in Chemical Engineering**, *University of Utah*, Salt Lake City, UT.
Neutron scattering analysis, molecular simulation, classical and quantum statistical mechanics, thermodynamics, Bayesian and machine learning, continuum mechanics, catalysis, density functional theory.
- 2019 – 2023 **Bachelors of Science in Computational Physics**, *University of Utah*, Salt Lake City, Utah.
Classical mechanics, statistical mechanics, quantum mechanics, scientific computing, liquid state theory, classical and quantum molecular simulation, neutron scattering analysis.
- 2019 – 2023 **Minor in Computer Science**, *University of Utah*, Salt Lake City, Utah.
Bayesian machine learning, uncertainty quantification, model validation, data structures and algorithms, neural networks.

Research Experience

- 2023 – Present **Graduate Research assistant in neutron scattering analysis with quantum molecular simulation and machine learning**, *University of Utah*, Salt Lake City, UT, **Dr. Michael Hoepfner**, *Associate Professor* ([link](#)).
Utilized quantum statistical mechanics in tandem with variational optimization to determine interatomic forces from microstructure of soft matter.
- 2023 – 2023 **Analysis of cryptocurrency markets using machine learning and scientific computing**, *University of Utah*, Salt Lake City, UT, **Blank Page Studios** ([link](#)).
3 months of contracted research into the application of machine learning, scientific computing, and data analysis for algorithmically trading cryptocurrency and analyzing NFT sales data. Managed by Kenny Abitbol of Coinbase and Marcus Corbett.
- 2021 – 2023 **Undergraduate researcher in neutron scattering analysis with molecular simulation and machine learning**, *University of Utah*, Salt Lake City, UT, **Dr. Michael Hoepfner**, *Associate Professor* ([link](#)).
Application of classical statistical mechanics and Bayesian machine learning to determine interatomic forces from microstructure of soft matter.
- 2021 – 2021 **Research on laser interferometer gravitational-wave data analysis**, *University of Utah*, Salt Lake City, Utah, **Dr. Yue Zhao**, *Assistant Professor* ([link](#)).
Summer research opportunity refactoring LIGO Analysis software using Python and Fortran. Created a standard operating procedure for analysis for future use of the tool.

Industry Experience

- 2023 **Trading Data Analyst**, *Blank Page Studios*.
Utilized machine learning to analyze cryptocurrency market data and NFT sales data.

Publications

- Oct, 2023 B.L. Shanks, **H.W. Sullivan**, A. R. Shazed and M.P. Hoepfner, *Accelerated Bayesian Inference for Molecular Simulations using Local Gaussian Process Surrogate Models*, arXiv, arXiv:2310.19108 ([link](#)).
Abstract: While Bayesian inference is the gold standard for uncertainty quantification and propagation, its use within physical chemistry encounters formidable computational barriers. These bottlenecks are magnified for modeling data with many independent variables, such as X-ray/neutron scattering patterns and electromagnetic spectra. To address this challenge, we apply a Bayesian framework accelerated via local Gaussian process (LGP) surrogate models. We show that the time-complexity of LGPs scales linearly in the number of independent variables, in stark contrast to the computationally expensive cubic scaling of conventional Gaussian processes. To illustrate the method, we trained a LGP surrogate model on the experimental radial distribution function of liquid neon, and observed a remarkable 288,000-fold speed-up compared to molecular dynamics with insignificant loss in predictive accuracy. We conclude that LGPs are robust and efficient surrogate models, poised to expand the application of Bayesian inference in molecular simulations to a broad spectrum of ever-advancing experimental data.

Conference Presentations

Contributed Talks

- Nov, 2023 **Bayesian Inverse Quantum Theory**, *U of U Theoretical Chemistry Department*, Salt Lake City, Utah.
A guided paper review of J.C. Lemm's year 2000 paper on the application of Bayesian field theory to quantum mechanical force field prediction from generic quantum observation.
- Sept, 2023 **Learning Interatomic Forces from Fluid Structure with Machine Learning Accelerated Bayesian Optimization**, ACS, Laramie, WY.
Abstract: In the realm of liquid state physics, the complex phenomena of self-assembly and structural ordering have fascinated researchers, intimately connecting macroscopic and microscopic behavior. The pursuit of accurate predictions for material behavior from the atomic scale has been a central objective, but the absence of comprehensive theories and computational techniques has posed a challenge for diverse systems. By tackling the computational cost associated with evaluating model force field structures, this study introduces a groundbreaking solution. Through the development of a local Gaussian process surrogate model, we have successfully accelerated the estimation of structural ordering for arbitrary potential energy functions. This advancement enables the application of a Bayesian optimization approach to force field development, unlocking unprecedented computational efficiency. Our results showcase the viability of employing machine learning to expedite interatomic force reconstruction, utilizing experimental diffraction data. This transformative tool not only enables profound insights into structural analysis but also empowers the optimization of force fields.

Poster Presentations

- Mar, 2022 **Recent Advances in Machine Learning Accelerated Molecular Dynamics**, *Centre Européen de Calcul Atomique et Moléculaire*, Trieste, IT.
Bayesian optimized force fields enabled by a radial distribution function surrogate model. Presented with Brennon L. Shanks PhD Candidate.