Jack A. Logan

Website

Summary

Dynamic and detail-oriented theoretical and computational physicist with over 9 years of experience in computational modeling, data analysis, analytical methods, and high-performance computing. Proficient in programming languages such as Python and C++, with expertise in Molecular Dynamics, Monte Carlo simulations, and innovative solutions in physics, materials science, nanotechnology, and proteins. Proven leadership in managing multidisciplinary teams that include both theorists and experimentalists, delivering impactful research in soft matter physics, polymers and proteins, and nanomaterials.

Technical Skills

Programming: Python, C++, CUDA, Bash
Simulation Tools: Molecular Dynamics, Monte Carlo methods
Data Analysis: Statistical Analysis, Optimization, Machine Learning
High-Performance Computing: Parallel Computing, HPC Clusters
Machine Learning: Linear Regression | Support Vector Machines (SVMs) | Multilayer Perceptrons (MLPs) | PyTorch (Artificial Neural Networks) | PyTorch Geometric (Graph Neural Networks) | Physics-based Modeling using Neural Networks
Collaboration Tools: Git, GitHub

Professional Experience

Yale University, New Haven, CT *2022-2025*
Postdoctoral Fellow, Mechanical Engineering & Materials Science

- Led a team of researchers to develop a novel simulation framework for studying polymer dynamics as compared to proteins.
- Developed GPU-accelerated code using CuPy in Python to compute the packing fraction of particle clusters, achieving a 1500x performance increase.
- Designed and implemented an object-oriented C++ program to run over 20,000 simulations on high-performance computing (HPC) clusters to model collapsed polymers, analyzed data using Python, and derived insights that have been submitted to a leading scientific journal.
- Collaborated with a multidisciplinary team comprising diverse backgrounds across theory, computation, and experiment.
- Mentored undergraduate, and high school students in the successful development and deployment of a support vector regression model for protein docking analysis.

Brookhaven National Laboratory, Upton, NY *2016-2022*
Research Assistant, Center for Functional Nanomaterials

- Developed analytical and computational methods to characterize symmetry in nanoparticle assemblies, leading to the design of more efficient materials for many applications.
- Partnered with experimental teams to develop enhanced methodologies for material analysis and innovation.
- Developed novel Monte Carlo algorithm to enumerate configurations of constrained particle systems and implemented them in C++ for efficient computation using linear algebra libraries such as Eigen.
- Derived a compact formula that accurately describes van der Waals interactions between nanorods in arbitrary configurations that cuts simulation time.

- Published 5+ peer-reviewed papers and presented findings at international conferences and invited talks.

Education

Stony Brook University, Stony Brook, NY *2022*
PhD in Physics
Advisor: Alexei Tkachenko
Dissertation: *Geometric and Topological Aspects of Self-Assembly: from spheres and rods to designer particles*

Stony Brook University, Stony Brook, NY
Master of Arts in Physics

Long Island University, Brookville, NY
Master of Science in Applied Mathematics
Summa Cum Laude

Selected Publications

- Logan, J.A., et al. (2025) *The effect of stereochemical constraints on the structural properties of folded proteins*. Physical Review E.
- Grigas, A.T., Liu, Z., Logan, J.A., et al. (2025) *Protein folding as a jamming transition*. PRX Life.
- Logan, J.A., et al. (2023). *Symmetry-specific characterization of bond orientation order in DNA-assembled nanoparticle lattices*. Journal of Chemical Physics.
- Logan, J.A., Tkachenko, A.V., (2022). *Geometric and Topological Entropies of Sphere Packing*. Physical Review E.
- Mushnoori, S., Logan, J.A., et al. (2022). *Controlling morphology in hybrid isotropic/patchy particle assemblies*. Journal of Chemical Physics.
- Logan, J.A., et al. (2022). *Symmetry-specific orientational order parameters for complex structures*. Journal of Chemical Physics.
- Logan, J.A., Tkachenko, A.V., (2018). *Compact interaction potential for van der Waals nanorods*. Physical Review E.

Leadership & Awards

- Mentor, student Summer projects, Yale University (2024)
- GSNP Postdoctoral Speaker Award Finalist, APS March Meeting (2024)
- Team Leader, Protein Folding Simulation Project, Yale University (2022-2025)
- PEB Travel Fund Award, Yale University (2023)
- Postdoctoral Scholars Travel Fund Award (2023)
- Jonathan Kaufman Student Excellence Prize (2019)