Georgios (Giorgos) Kementzidis

(641) 260 - 4187 | giorgoskement@gmail.com | LinkedIn | Google Scholar

EDUCATION

Stony Brook University Stony Brook, NY
PhD in Applied Mathematics and Statistics | GPA: 4.00 May 2027
Institute for Advanced Computational Science (IACS) Junior Researcher Award 2025

Grinnell College Grinnell, IA
B.A. in Mathematics and Physics with honors | GPA: 3.97 May 2022

EXPERIENCE

Simons Foundation, Scientific Computing Core May 2025 – August 2025
Software Engineering Intern
- Developed a C++ library to accelerate particle simulations, translating research papers into high-performance software.
- Improved performance through benchmarking, cache optimization, vectorization, multithreading, and parallelization.
- Leveraged HPC clusters at the Flatiron Institute, effectively utilizing multi-CPU and GPU architectures.

Stony Brook University, Institute of Advanced Computational Studies February 2023 – Present
Graduate Research Assistant
- Develop computational workflows and ML models to facilitate methods used in computational biophysics.
- Lead a group of undergraduate students working on research projects.

TECHNICAL SKILLS

- **Languages**: Python (PyTorch, pandas, scikit-learn, TensorFlow), C++, C, MATLAB, R, SQL
- **Other software skills**: Git, MPI, OpenMP, HPC, Slurm, Docker, Weights and Biases
- **Concepts**: Machine Learning, Data Structures, Numerical Algorithms, Parallelization, Simulations, Benchmarking

PROJECTS

Moving Targets: Detecting Shifts in Corporate Performance Narratives via LLMs September 2025
- Competed in the 2025 Alphathon, a quantitative finance competition hosted by the Society of Quantitative Analysts.
- Developed a pipeline comprising of open-source LLMs to extract, encode, and compare features from corporate filings.
- Designed and evaluated a trading strategy based on the above pipeline.

Multiscale Modeling of Proteins with Coarse Grained Force Fields February 2023 – Present
- Use physics-informed parameter learning to develop force fields that speed up protein simulations by up to 10^5 times.
- Study fiber formation and surface-induced polymerization of fibrinogen through coarse-grained simulations in LAMMPS & NAMD, and all-atom simulations in GROMACS.

Two-step Generative Backmapping of Proteins June 2024 – June 2025
- Improved methods to increase backmapping accuracy of proteins with large coarse-grained beads by up to ~80%.
- Used Graph Neural Networks and Variational Autoencoders, conducted hyperparameter search using Weights and Biases.

GENOVA: GenAI for Novel Ligand Discovery April 2024 – May 2025
- Contributed to the development of an AI-driven framework for the discovery of BACE1 inhibitors for Alzheimer's disease.
- Assessed and improved the Machine Learning and Generative AI aspects of the model (WGAN-GP, QSAR prediction evaluation, transfer learning, genetic algorithm), which led to novel inhibitors with low binding energies.

Designing Trading Strategies from Data (Schonfeld Strategic Advisors) April 2024
- Selected to participate in a competitive Datathon with ~30 other PhD students from the US.
- Analyzed data, conducted feature engineering, and evaluated tree-based models for the design of trading strategies.
- Collaborated with my four teammates to develop a trading strategy and won second place among eight teams.

SELECTED PUBLICATIONS & CONFERENCES

- **Kementzidis, G.** (2025). Multiscale modeling of the structure and dynamics of soluble fibrin. In 28th International Fibrinogen Research Society (IFRS) Workshop, Corfu, Greece.
- **Kementzidis, G.**, et. al. (2025). An iterative framework for generative backmapping of coarse-grained proteins. ICML 2025 Generative AI and Biology (GenBio) Workshop.
- Niu, Z., **Kementzidis, G.**, et. al. (2025). Simulations of pH and Thermal Effects on SARS-CoV-2 Spike Glycoprotein. Frontiers in Molecular Biosciences, 12.
- Zhang, Z., **Kementzidis, G.,** Zhang, P., Zhang, L., Kozloski, J., et al. (2024). Learning coarse-grained force fields for fibrogenesis modeling. Computer Physics Communications, 295, 108964.