Georgios (Giorgos) Kementzidis

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EDUCATION

Stony Brook University — Stony Brook, NY
PhD in Applied Mathematics and Statistics | GPA: 4.00 — May 2027

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

PUBLICATIONS & CONFERENCES

- Zhang, Z., **Kementzidis, G.**, Zhang, P., Zhang, L., Kozloski, J., Hansen, A., Rafailovich, M., Simon, M., & Deng, Y. (2024). Learning coarse-grained force fields for fibrogenesis modeling. Computer Physics Communications, 295, 108964. https://doi.org/10.1016/j.cpc.2023.108964
- Hasegawa, K., Burzachiello, J., Connolly, L., **Kementzidis, G.,** Niu, Z., Papadopoulos, E., Aktas, B. H., & Deng, Y. (2024). Structural and dynamical analyses of Apo and Cap-binding eIF4E: An *in silico* study. bioRxiv. https://doi.org/10.1101/2024.05.18.594816
- Xie, E., Hasegawa, K., **Kementzidis, G.**, Papadopoulos, E., Aktas, B. H., & Deng, Y. (2024). An AI-driven framework for discovery of BACE1 inhibitors for Alzheimer's disease. bioRxiv. https://doi.org/10.1101/2024.05.15.594361
- **Kementzidis, G.** (2024, June). *In silico* Studies of Fibrinogen-PLA Interactions and Implications for Thrombosis. In 27th International Fibrinogen Research Society (IFRS) Workshop, Esbjerg, Denmark.

PROFESSIONAL WORK EXPERIENCE

Stony Brook University — February 2023 – Present
Graduate Research Assistant

- Use high-performance computing (HPC) clusters to run programs faster, on multiple CPUs and GPUs.
- Actively use the tools of the PyTorch and scikit-learn libraries to develop ML models to facilitate computational methods used in MD simulations and other applications.
- Lead a group of high-school and undergraduate students working on one of our research projects.
- Actively participate in a weekly journal club, where we read and present papers on ML models.

Stony Brook University — August 2022 – Present
Graduate Teaching Assistant

- Teach "Applied Calculus II" to a class of 70 students, assign homework and exams.
- Mentor 140-150 students in undergraduate classes: "Applied Linear Algebra", "Differential Equations".
- Teach recitations; maintain office hours; hold review sessions; develop and grade exams.

PROJECTS

Personal Project — July-August 2024

- Developed a PyTorch-based LSTM classification model for the detection of spam emails with a Kaggle dataset.
- Identified the strengths and weaknesses of the model and its potential application to other datasets.
- Post a tutorial with step-by-step instructions and comments on GitHub.

Stony Brook University, Department of Applied Mathematics and Statistics — January 2023 – Present
Graduate Research Assistant; multiple projects

- Use PIPL to develop coarse-grained force fields that speed up protein MD simulations by almost 10^5 times.
- Study the formation of the fibrin net and fibrinogen interactions through all-atomic and coarse-grained MD simulations.
- Explore the effects of temperature and pH on the behavior of proteins through MD simulations conducted in GROMACS.
- Improve current VAE-based methods to more accurately back-map coarse-grained structures (e.g., large proteins).
- Explore the use of generative AI & other models (GANs, AEs, RL, GA, GNN) for *de novo* drug design (ligand-based and pocket-based) and assess the generated molecules (binding energy calculation, docking, etc.).

Schonfeld Strategic Advisors — April 2024
Early Engagement (PhD) Summit - Datathon

- Participated in an invitational Datathon with other PhD students from the US.
- Explored the role of data analysis and feature engineering in the design of long-short portfolios.
- Collaborated with my four teammates to develop a trading strategy and won second place.

Stony Brook University, Department of Applied Mathematics and Statistics — October 2023 – December 2023
Student Researcher; course embedded research; AMS 530 Principles in Parallel Computing

- Built fast and efficient algorithms to parallelize large computations (e.g., matrix multiplication, linear system solver).
- Ran code on an HPC cluster and got familiar with the supercomputing architectures and how to use them efficiently.
- Used MPI, JIT, and CUDA to parallelize programs and operations and assessed their performance.

Grinnell College, Department of Mathematics and Statistics March 2022 – May 2022
Student Researcher; course embedded research; MAT 306 Mathematical Modeling
- Collaborated with another student to extract, clean, and analyze data using Python and R.
- Applied mathematical and statistical techniques to model a disease outbreak draw conclusions from real data.
- Wrote a report "Exploring the Correlation between Government Stringency and Disease Transmission based on SIR".

Grinnell College, Department of Mathematics and Statistics October 2021 – December 2021
Student Researcher; course embedded research; MAT 317 Complex Analysis
- Explored fields of complex analysis, dynamical systems, and fractal geometry, proved lemmas and theorems.
- Used numerical methods in Python to visualize fractals coming from dynamical systems.
- Completed a report "Montel's Theorem and its Application to the Common Boundary Condition".

Grinnell College, Department of Physics September 2021 – November 2021
Student Researcher; course embedded research; PHY 462 Advanced Laboratory
- Conducted an experiment to determine the lifetime of muons.
- Worked independently and responsibly with equipment (oscilloscope, PMT, CFD, TAC, MCA) to collect data.
- Applied the theory to analyze the results (pandas) and correctly identify the sources of error.

University of Connecticut, Department of Mathematics May 2021 – August 2021
Student Researcher, Research Experience for Undergraduates (REU)
- Studied measure theory, optimal transport, explored solutions to an original problem, used programing in Python.
- Presented "An Introduction to Optimal Transport on the Sierpinski Gasket" at the "REU Vir(tu)al Conference 2021".

Grinnell College, Department of Physics May 2020 – July 2020
Student Researcher, Mentored Advanced Project
- Learned material related to General Relativity and Differential Geometry.
- Produced a report focusing on Fiber Bundles and Generalized Geometry.

OTHER SKILLS

- **Programming languages**: Python (PyTorch, pandas, scikit-learn, scikit-image, OOP, DSA), C++, C, MATLAB, R
- **Other software skills**: Git, Linux, MPI, GPU, HPC, Docker, Ubuntu, GROMACS, LAMMPS, Excel, LaTeX, ImageJ
- **Languages**: Fluent: Greek and English; Advanced: German