

Alexander Aghili

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Education

University of California - Santa Cruz, Santa Cruz, CA June 2026

Bachelors of Science in Computer Science and Mathematics

GPA: 3.94 | Dean's Honors List

Thesis Advisor: Dr. Razvan Marinescu

Senior Thesis: *Efficient Distributed Data Generation and Training of Graph Neural Network-Based Molecular Dynamics using Weighted Ensemble Sampling* ([Viewable Link](#))

Skills

High Performance Computing (HPC), GPU/Parallel Programming (CUDA, PyTorch DDP), Distributed Systems, AI/ML Infrastructure (PyTorch), Deployment (Docker, Slurm), Linux Systems Engineering, Scientific & Numerical Computing (C/C++, Rust, Python, OpenMM, LAVA, LES), Cloud (AWS, GCP)

Research Experience

University of California - Santa Cruz, Santa Cruz, CA

Undergraduate Research on Molecular Dynamics using Machine Learning Sep 2024–Present

- Developed and optimized Graph Neural Network (GNN) and Transformer-based architectures to accelerate Coarse-Grained Machine-Learned Molecular Dynamics simulations, creating new model architectures (TICA Energy Matching, Harmonic Models, etc.), incorporating non-Boltzmann generation methods (WESTPA), and building visualization and analysis tools.
- Implemented Weighted Ensemble (WE) sampling frameworks and high-throughput parallel workflows on NCSA and NERSC supercomputers, enabling large-scale sampling and benchmarking (5000+ GPU Hours) across models, contributing to reproducible pipelines with automated job orchestration and multi-node parallelization.
- Designed and deployed public software libraries supporting end-to-end model training and evaluation, including build systems, containerized environments, and documentation.
- Created onboarding materials and led cross-functional coordination that facilitated new-member integration and contributed to first-author and collaborative publications.

University of California - Santa Cruz, Santa Cruz, CA

Twizzler Research Operating System - TWISTED DARPA Project Dec 2023–Feb 2025

- Conducted research on novel operating system architectures, focusing on the design and correctness of paging systems for shared-memory, multithreaded, and distributed environments.
- Implemented and profiled memory-management subsystems for latency, concurrency, and isolation requirements.
- Integrated Kani Rust Formal Verification into the OS development pipeline, creating verification harnesses, proof strategies, and model-checking workflows to test correctness of select OS components (paging, NVMe device driver).

Work Experience

NASA Ames Research Center - Advanced Supercomputing Division

Computational Fluid Dynamics Intern

Apr 2025–Present

(Under Analytical Mechanics Associate ASSESS Contract)

- Supported the *Launch, Ascent, and Vehicle Aerodynamics* (LAVA) CFD team by developing advanced VTK-based visualization and analysis tooling and building pre-processing/meshing workflows for Voronoi and Cartesian pipelines for LAVA UI. Implemented automated region labeling, geometry trimming/cleanup, boundary-condition mapping, and feature-extraction utilities that improved mesh quality, reduced manual setup effort, and enabled engineers to iterate on SLS and X-59 vehicle analysis.
- Researched and prototyped constrained mixed-integer quadrangulation algorithms for generating high-quality curvilinear meshes on complex geometries, exploring energy-minimization formulations, curvature-aligned parameterizations, and anisotropy-aware optimization schemes to improve CFD numerical stability and mesh robustness.
- Designed schema-driven input-configuration systems using JSON Schema and automated C++ code generation, reducing manual configuration overhead and improving consistency across simulation pipelines; implemented validation rules, error-detection workflows, and extensible metadata structures to streamline large-scale CFD run setup on NASA HPC (HEC) systems.

Netskope Inc

Data & Analytics Intern

Jun 2024 – Sep 2024

- Designed and scaled analytical pipelines using Fivetran, Snowflake, dbt, and Looker, integrating cohort-based forecasting models (retention curves, survival analysis, LTV via discounted cash-flow), trend decomposition (additive/multiplicative time-series decomposition, STL), and sensitivity analyses (partial-derivative-based sensitivity, scenario modeling, elasticity estimation) to produce projections for product and revenue planning.
- Built IPO-ready reporting infrastructure, including data-collection requirements, KPI definitions, and governance processes; developed executive dashboards to show ARR, unit economics, retention, and usage trends using time-series regression, variance decomposition, and growth-rate normalization to ensure metrics aligned with S-1 expectations and investor due-diligence standards.

Appreciate Inc

Software Engineering Intern

Jun 2023–Aug 2023

- Developed, optimized, and extended production REST API endpoints supporting key business workflows, implementing caching, pagination, and schema-validation logic that reduced request overhead and improved end-to-end system reliability.
- Designed a normalized relational database schema with optimized indexing strategies, query-planning improvements, and schema-level constraints, resulting in a 20% reduction in average query latency and more predictable performance under peak load.
- Built and maintained CI/CD pipelines using GitHub Actions for automated testing, integration validation, and deployment; coordinated feature releases and backlog management through Jira, ensuring rapid iteration cycles and traceable development processes.

Publications

1. **Aghili, A.**, Bruce, A., Sabo, D., Murdeshwar, S., Bachelor, K., Mistreanu, I., Lokapally, A., & Marinescu, R. *A Standardized Benchmark for Machine-Learned Molecular Dynamics using Weighted Ensemble Sampling*. *Journal of Physical Chemistry B: At the Cutting Edge of Theoretical and Computational Biophysics VSI Virtual Special Issue*. <https://doi.org/10.1021/acs.jpcc.5c05365>
2. **Aghili, A.***, Bruce, A.*, Sabo, D., & Marinescu, R. (2025). *TICA-Based Free Energy Matching for Machine-Learned Molecular Dynamics*. In *ICML 2025 Workshop on Multi-Modal Foundation Models and Large Language Models for Life Sciences*.
Bruce, A., **Aghili, A.**, Marinescu, R., & Sabo, D. *Latent Spaces for Langevin Dynamics*. In *Proceedings of the 39th Conference on Neural Information Processing Systems (NeurIPS 2025) Workshop: Frontiers in Probabilistic Inference: Sampling Meets Learning*.

In-Preparation Papers

1. Ashby, C., & **Aghili, A.** (in preparation). *Mixed-Integer Quadrangulation for Automated Curvilinear Overset Grid Generation*.
2. Nagaraj, A., Roberts, C., Lin, S., **Aghili, A.**, Gillispie, T., Lokapally, A., & Marinescu, R. (in preparation). *HelixNet: Coarse-Grained DNA Simulations With Graph Neural Networks*.
3. **Aghili, A.**, Bruce, A., Sabo, D., & Marinescu, R. (in preparation). *WESchNet: A Machine Learning Framework for Efficient Generation and Learning of Slow Collective Motions With WESTPA*.

Awards, Honors, and Certificates

SIAM Northern Central California (NCC) Best Poster Award	October 2025
2024/2025 NASA Honor Award—Group Achievement Award	August 2025
CITRIS Technical Excellence Award	May 2025
CITRIS Tech Development Grant: “Wildfire Management with Multi-UAV Systems” (\$5000)	Dec 2024
Carbon Fund Grant: “Wildfire Management with Multi-UAV Systems” (\$5000)	Dec 2024
Supernal Award for Most Innovative Design in Urban Air Mobility	Apr 2024
Quantitative Biosciences Institute Hackathon – 1st Place	Oct 2023
FAA Private Pilot Certificate	May 2022
Qubit×Qubit Quantum Computing Course Certificate	May 2021

Conferences, Workshops, and Presentations

SIAM Northern Central California (NCC) Section – Lightning Talk, Poster	October 2025
Scenic Workshop – Talk	Aug 2025
International Conference on Machine Learning – Poster	July 2025
CITRIS Aviation Prize – Talk	May 2025
ACMConf, UC Santa Cruz – Talk & Poster	May 2025
Bay Area Drone Fest, UC Berkeley – Short Talk	Apr 2025
DARPA TWISTED Demonstration – Slide Preparation	Feb 2025
NASA-UC Urban Air Mobility (UAM) Technical Summit – Talk	Apr 2024

Community Engagement and Teaching

Student Creativity, Empowerment, and Entrepreneurship Club Sep 2022–Present
Co-President, Executive Board Member

- Organized *Ideathon* (100+ students, weekend innovation event)
- Organized *Slug Tank* (pitch competition, 10 teams, 200+ audience, VC/local judges)
- Advised student-led companies with combined over \$100,000 in ARR

Slugbotics Sep 2023–Present
Unmanned Aerial Vehicles Subteam Lead

- Responsible for receiving grants, recruiting members, project management, and system integration.
- Lead and developer on simulation team utilizing Gazebo, NVIDIA IsaacSim and Pegasus Simulator to provide Software in the Loop (SITL) and Hardware in the Loop (HITL) capabilities for other teams to test software and hardware before deployment on drone.

Cruzhacks 2025 Sep 2024–Apr 2025
Deputy Director, Financial Organizer

- Organized the Largest Hackathon in Santa Cruz (400+ hackers, multiple corporate and academic sponsors)
- Managed sponsorships, purchases, and bank accounts.

CSE138 Distributed Systems Spring 2025
Student Tutor

- Held tutoring sessions to help students with assignments and course concepts.
- Assisted in the creation of the testing suite and grading system.

Supercomputing 2025 Nov 2025
Workshop, Conference Attendee