JOHN M. ERICSON

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Overview: Computational scientist with training in chemistry, physics, and data science, combining hands-on research with practical software engineering. Published first-author research and developer of open-source tools professionally distributed on PyPI and Conda. Experienced in machine learning, biomolecular modeling, and molecular dynamics simulations, with a focus on reproducible, scalable workflows. Recognized for problem-solving, interdisciplinary collaboration, and delivering high-quality tools that advance healthcare and scientific discovery.

Technical Skills

- **Machine Learning & Data Science**: Predictive modeling, clustering, regression/classification; Python ML stack (NumPy, Pandas, SciPy, scikit-learn, TensorFlow; familiarity with PyTorch); model evaluation and workflow automation.
- **Visualization & Communication:** Data visualization, reproducible pipelines, scientific documentation, and cross-disciplinary communication.

- **Programming & Software Engineering:** Advanced Python; Git, Jupyter, REST APIs; professional open-source package development (vorpy3, foam_gen, coarsify).
- **Computational Biology & Biophysics:** Molecular dynamics (GROMACS), biomolecular and protein modeling, Voronoi-based spatial partitioning, coarse-graining, structural modeling workflows.

Work history

Research Fellow – *Georgia State University, Atlanta, GA*　　　　January 2025 - Current

- Published first-author paper on computational partitioning methods in biomolecular modeling.
- Released three open-source Python packages (vorpy3, foam_gen, coarsify) on PyPI and Conda, with emphasis on usability, reproducibility, and long-term support.
- Applied ML methods to predict statistical ensembles, analyze molecular dynamics outputs, and detect deviations in biomolecular workflows.
- Collaborated with cross-disciplinary teams and prepared manuscripts, presentations, and documentation for broad dissemination.

August 2021 – August 2023

Scientific Programmer – *Georgia State University, Atlanta GA*

- Designed and implemented algorithms and workflows for large-scale molecular simulations, improving efficiency and accuracy.
- Built, tested, and refined custom Python tools to analyze biomolecular datasets, laying the groundwork for later open-source releases.
- Developed visualization pipelines and reproducible reporting tools to communicate results clearly across research teams.
- Conducted extensive molecular dynamics simulations using established force fields and GPU/distributed workflows.

Software Developer / Lidar Engineer – *Levvel Consulting*   March 2021 - August 2021

- Created custom Python workflows to process and model 3D LIDAR point cloud data into architectural blueprints.
- Co-led a national team deploying LIDAR scanning systems in U.S. warehouses, ensuring data accuracy and efficiency.
- Applied computational geometry methods for real-world spatial modeling and optimization.

Physics Intern (Part Time) – *Physics.fm, Remote*   August 2020 - July 2021

- Developed Python-based simulations of canonical quantum experiments (Young's double slit, Stern–Gerlach).
- Translated theoretical physics models into computational workflows to assess feasibility and accuracy.
- Built visualization tools to communicate physical modeling results to non-specialist audiences.

Customer Service Coordinator – *Wahoo Fitness, Atlanta, GA*   Nov 2019 – March 2021

- Provided technical support for connected fitness products, resolving software and hardware issues with high customer satisfaction.
- Automated responses for common support queries, reducing resolution times.

Education

Chemistry, M.S. – *Georgia State University, Atlanta, GA*   December 2024

- Thesis: The Geometry of Spatial Decomposition: Evaluating Partitioning Schemes in Physical Chemical Systems — developed computational methods to compare and assess spatial partitioning approaches in molecular modeling.
- Research contributed to ongoing work that led to a first-author peer-reviewed publication in Physical Chemistry Chemical Physics (published post-graduation).
- Focus areas: computational chemistry, data science, software engineering for scientific applications.
- Achievements: Departmental research award for development of molecular partitioning and analysis software.
- GPA 3.93; Dean's List.

Physics, B.S. – *University of Georgia, Athens, GA*   August 2019

- Research in optics: conducted experiments on Faraday rotation of polarized light in dielectric materials under strong magnetic fields.
- Built strong foundations in computational physics, quantum mechanics, electromagnetism, thermodynamics, and advanced mathematical methods.
- Graduated early with an emphasis on theoretical and computational modeling.

Publications and Awards

- *Evaluation of Weighted Voronoi Decompositions of Physicochemical Ensembles. Physical Chemistry Chemical Physics* (First Author). DOI: 10.1039/D5CP00763A.
- (In progress) Manuscript integrating Voronoi decomposition approaches with molecular dynamics workflows, enabling software-driven analysis and coarse-graining of biomolecular systems.
- 2023 Georgia State University Chemistry Departmental Award for Research Excellence.