Christopher A. Myers, PhD

LinkedIn | GitHub | Google Scholar
Email: Myers.Christopher@Proton.me | Phone: 518-258-0461

Scientific Computing Specialist

- Computational and data scientist with experience developing both data-informed and physics-based models to solve complex scientific and academic research problems.
- Highly skilled in building and optimizing software in Python and C++ within high-performance and distributed computing environments for training, validation, and visualizing model predictions.
- Experienced in leading applied computing efforts, managing multiple concurrent projects while mentoring colleagues across computational and technical domains.

Program Manager – Physical Scientist GS-14
U.S. Department of Energy (DOE), *Office of Science, ASCR Facilities Division, January – May 2025*

- Oversaw HPC resource allocations for national laboratory, industrial, and academic research projects for the ASCR Leadership Computing Challenge (ALCC), managing ~20M GPU and CPU node hours annually across DOE supercomputing facilities.
- Led proposal evaluations and stakeholder coordination across mission-specific program offices, contributing subject matter expertise in computational chemistry and AI during proposal review and program development.

Postdoctoral Researcher – HPC and Scientific Software Development
University of California, Merced, *Department of Chemistry & Biochemistry | Nov. 2022 - Present*

- Led the integration of machine learning algorithms and numerical methods using PyTorch, TensorFlow, SciPy, scikit-learn, and RDKit to improve the speed and accuracy of small-molecule simulations.
- Developed data cleansing, descriptor generation, and visualization dashboards for high-dimensional chemical data for the use in MLPs, CNNs, clustering, PCA, and kernel-regression models.
- Collaborated with academic research teams nationwide to develop PySCES, a quantum chemical software for high-performance computing environments. Achieved an 8x speedup through GPU acceleration, protobuf-based data serialization, MPI, and enhancements to commercial C++/CUDA software.
- Constructed Python-based simulations of small-molecule dynamics using Newtonian trajectories and parameter estimation against experimental and curated chemistry datasets – an approach conceptually similar to supervised learning techniques.
- Delivered technical presentations and hands-on workshops at conferences and funding agency meetings on cheminformatics, HPC optimization, and computational chemistry algorithms.

Graduate Researcher – Molecular Dynamics and Parameterized Simulations
University at Albany (SUNY), *Chemistry Dept. and The RNA Institute | June 2017 – October 2022*
Physics Dept. (Teaching) and The RNA Institute | June 2014 – June 2017

- Crafted physics-informed parameterized models and custom software tools to simulate biological and chemical dynamics, collaborating directly with experimental research teams in materials chemistry, organic synthesis, and structural biology laboratories.
- Conceptualized and trained a novel physics-based model with custom loss functions, high-dimensional regression, and optimization routines in Python/C++ to enhance predictive accuracy of RNA simulations.
- Created and optimized CoSIMS, a parallelized C++/OpenMP software designed to simulate ion-mobility experiments of large biomolecules using trajectory-based methods, (RNA, DNA, proteins), outperforming competing solutions by 10x and supporting experimental mass spectrometry workflows.
- Maintained laboratory hardware and computing-cluster software compilations while coordinating with Research IT to maintain and support HPC resources for our team and collaborating laboratories.
- Taught undergraduate physics lab and recitation sections, working independently with minimal oversight to deliver hands-on instruction and managing assessments for up to 70 students per semester.

Education History

PhD, Physics | September 2022
Master of Science, Physics | June 2017
University at Albany (SUNY), Albany, NY

- PhD Dissertation: developed energy loss functions and parameterization schemes through the lens of computational, theoretical, and experimental collaboration.

Bachelor of Science, Physics | May 2014
University at Albany (SUNY), Albany, NY

Skills and Technical Abilities

Data Science & Machine Learning: Experience with deep and convolutional neural network techniques, linear, nonlinear, and kernel-ridge regression, clustering algorithms, data curation procedures. Additionally experience with **PyTorch**, **Scikit-Learn**, **TensorFlow,** Numba (GIT), Matplotlib, Plotly, Pandas, RDKit.

Languages & Development Tools: Advanced fluency in Python and C++ (legacy & modern) in Linux environments, including functional and object-oriented programming techniques. Experience with C, C#, Java, Javascript, Matlab, Bash, Git and GitHub version control, and writing operating and diagnostic manuals.

Scientific Programming: MPI, OpenMP, BLAS, LaPACK, CuPy, NumPy, SciPy, Cython, threading and multiprocessing techniques. Familiar with CUDA, OpenCL, AWS, Singularity, and Docker containers.

Selected Presentations (out of 18)

- **Cavity Molecular Polaritons Annual MURI Review (2025):** Presentation on research progress and planned future directions to Department of Defense program officers in Washington D.C.
- **American Chemical Society National Meeting (2024):** Delivered a technical presentation on quantum chemistry and spectroscopy, designed for an audience with limited direct experience in these fields.
- **Chemistry Department, Physics Department, and RNA Institute, SUNY Albany (2022):** Delivered a multi-departmental talk on the synergy of computational, mathematical, and experimental research approaches in computational chemistry.
- **American Physical Society National Meeting (2021):** Presented on applying nonlinear regression techniques and optimizing energy loss functions to enhance predictive modeling in molecular dynamics.

Selected Publications (out of 8, first author)

- **PySCES: A GPU-Accelerated On-the-fly Nonadiabatic Dynamics Program (2024):** Developed a Python interface for the TeraChem electronic structure program, utilizing parallel computing, data processing, and performance optimization across distributed systems. *J. Chem. Phys. 161, 084114.*
- **MD and Optical Spectroscopy Simulations of Cresyl Violet in Methanol (2024):** Parameterized small molecule force fields using non-linear regression to reproduce UV-Vis and resonance Raman absorption spectra with various computational chemistry methods. *J. Phys. Chem. B, 128, 23, 5685.*
- **AmberFD: An Energy Mechanics Model for RNA Nucleobases (2023):** Devised and developed a Python library with a C++ backend that minimizes energy loss functions from nonlinear regression models. *ChemRxiv 10.26434/chemrxiv-2023-1rvh3.*
- **CoSIMS: A Collision Simulator for Ion Mobility Spectrometry (2019):** A self-written, OpenMP parallel C++ software for computing molecular structural properties. Designed for an experimental mass spectrometry laboratory *J. Phys. Chem. B, 123, 20, 4347.*

Awards and Acknowledgments

Excellence in Research

- Awarded by University at Albany Physics Department, Spring 2016, for exceptional research abilities.

Best Presentation at the PASCAL conference, Albany NY,

- Awarded by University at Albany Physics Department, Spring 2016.