Vyas **Ramasubramani**

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Summary

I am a PhD candidate at the University of Michigan, Ann Arbor. I use molecular simulations and machine learning methods to study the self-assembly of proteins and nanoparticles into complex structures. I both lead and contribute to a number of open-source Python and C/C++ projects in my research area, including freud, HOOMD-blue, and signac, and have contributed to other tools in the SciPy stack. I have experience optimizing code in various languages and on both CPU and GPU architectures, and I have made use of tools like CuPy, cuDF, and numba to do so in Python. I also have worked in containerized environments for HPC resources and continuous integration, and I help maintain containers for ongoing research use.

Education

Ph.D. in Chemical Engineering and Scientific Computing - University of Michigan *2015 - 2020*

M.S. in Chemical Engineering - University of Michigan *2015 - 2017*

B.S.E. in Chemical Engineering - Princeton University *2009 - 2013*

Minors: Quantitative and Computational Biology, Applications of Computing

Work and Research Experience

Research Assistant - University of Michigan - Glotzer Group *Oct 2015 - Present*

- Developed a new simulation technique for the molecular dynamics of anisotropic particles and optimized it for modern GPUs.
- Employed a novel coarse-graining approach to explain the assembly of supercharged protein oligomers.
- Built machine learning models to identify key drivers of protein crystallization.
- Developed and implemented models of implicit solvation including parallelization via MPI and OpenMP.

Senior Financial Analyst - D.C. Energy LLC *Sep 2013 - Jul 2015*

- Increased trade profitability by combining powerflow analysis and various financial metrics to enhance automated trade optimization.
- Modernized the company's data infrastructure by improving web scraping frameworks, database design, and analytical algorithms.
- Built web tools using R, PHP, JavaScript, and MySQL to aid technical and fundamental market analysis.

Thesis Researcher - Princeton University - Prud'homme Lab *Sep 2012 - Jun 2013*

- Characterized phase separation in specific polymer blends to ameliorate effects of depletion flocculation.
- Developed nanoparticles and gel microparticles for incorporation into a targeted drug delivery system for lung cancer.

Skills

Languages expert: Python, C++ advanced: C, R, MySQL, MATLAB intermediate: Java, Cuda, PHP, JavaScript

Tools & Frameworks Python packages: scikit-learn, TensorFlow, Keras, pandas, NumPy, numba Parallelism: MPI, OpenMP, TBB

Selected Projects

Lead Developer - signac framework (github.com/glotzerlab/signac)

- Co-led development of a NumFOCUS-affiliated project for data and workflow management in Python.
- Enabled flexible, easy-to-use storage mechanism for research data in computational science and machine learning.
- Drove development of a new, compact API for workflow definition.

Lead Developer - freud (github.com/glotzerlab/freud)

- Co-led development of a C++ tool with Cython-generated Python bindings for fast, TBB-multithreaded analysis of molecular simulations.
- Spearheaded the creation of a standardized API achieving a high degree of flexibility and consistency.
- Standardized memory handling to simplify the user interface and minimize data copying.
- Achieved 3-15x performance improvements across the package as part of the 2.0 release.

Core Developer - HOOMD-blue (github.com/glotzerlab/hoomd-blue)

- Made various contributions to a general purpose, high-performance particle simulation toolkit for GPU-accelerated molecular dynamics and Monte Carlo simulations that is currently one of NVIDIA's official HPC benchmarks.
- Enabled bidirectional MPI communication to enable multi-body force fields in MPI simulations.
- Implemented the Gilbert-Johnson-Keerthi algorithm on CPUs and GPUs as part of an anisotropic pair potential.

Honors & Awards

Jul 2019 **Beyster Computational Innovation Fellow,** University of Michigan

Apr 2019 **2nd Place,** MICDE Symposium Poster Competition

Sep 2018 **Fellow,** Michigan Institute for Computational Discovery & Engineering