Vyas **Ramasubramani**

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Education

University of Michigan

PH.D. IN CHEMICAL ENGINEERING AND SCIENTIFIC COMPUTING — *2015 - 2020*

M.S. IN CHEMICAL ENGINEERING — *2015 - 2017*

Princeton University

B.S.E. IN CHEMICAL ENGINEERING — *2009 - 2013*

Minors: Quantitative and Computational Biology, Applications of Computing

Research Experience

University of Michigan - Glotzer Group

RESEARCH ASSISTANT — *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.

Princeton University - Prud'homme Lab

THESIS RESEARCHER — *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.

Academy of Sciences of the Czech Republic - Ettrich Lab

UNDERGRADUATE RESEARCHER — *Jul 2012 - Jun 2013*

- Used all-atom molecular dynamics simulations to discover the physical origin of the functional transition in the EcoR124i transcription factor.

Work Experience

D.C. Energy LLC

SENIOR FINANCIAL ANALYST — *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.

Skills

Languages Python (expert), C++ (expert), C (advanced), R (advanced), MySQL (advanced), MATLAB (advanced), Java (intermediate), Cuda (intermediate), PHP (intermediate)

Toolkits scikit-learn, TensorFlow, Keras, pandas, NumPy, data.table, ggplot2, dplyr

Selected Projects

signac framework (github.com/glotzerlab/signac)

LEAD DEVELOPER

- 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.

freud (github.com/glotzerlab/freud)

Lead Developer

- Co-led development of a C++ tool with Cython-generated Python bindings for various fast, multithreaded analyses of molecular simulations using Intel TBB.
- 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 5-15x performance improvements across the package as part of the 2.0 release.

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

Core Developer

- 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

Service and Leadership

Oct 2018 - Present **Board Member,** DEI Student Advisory Board

Dec 2017 - Dec 2018 **GSAC Representative,** Chemical Engineering Graduate Society

Sept 2016 - Apr 2017 **Chair,** Chemical Engineering Graduate Recruiting

Sept 2016 - May 2017 **Fundraising Chair,** Chemical Engineering Graduate Symposium

Jun 2016 - May 2017 **Peer Mentor,** Chemical Engineering Peer Mentoring Program

Jul 2016 - Jul 2019 **Faculty/Staff Mentor,** UM Mentorship Program

Selected Publications

1. Ramasubramani, V. *et al.* freud: A software suite for high throughput analysis of particle simulation data. *Computer Physics Communications* **254,** 107275. ISSN: 0010-4655. http://www.sciencedirect.com/science/article/pii/S0010465520300916 (2020).
2. Dice, B. *et al.* Analyzing Particle Systems for Machine Learning and Data Visualization with freud. *Proceedings of the 18th Python in Science Conference.* http://dx.doi.org/10.25080/Majora-7ddc1dd1-004 (2019).
3. Simon, A. J. *et al.* Supercharging enables organized assembly of synthetic biomolecules. *Nature Chemistry* **11.** Worked featured on the cover of Nature Chemistry and the front page of XSEDE., 204–212. ISSN: 1755-4349. http://dx.doi.org/10.1038/s41557-018-0196-3 (Jan. 2019).
4. Ramasubramani, V., Adorf, C. S., Dodd, P. M., Dice, B. D. & Glotzer, S. C. *signac: A Python framework for data and workflow management* in *Proceedings of the 17th Python in Science Conference* (eds Akici, F., Lippa, D., Niederhut, D. & Pacer, M.) (2018), 91–98.
5. Adorf*, C. S., Ramasubramani*, V., Anderson, J. A. & Glotzer, S. C. How to Professionally Develop Reusable Scientific Software—And When Not To. *Computing in Science Engineering* **21.** (*these authors contributed equally to this work), 66–79. ISSN: 1521-9615 (Mar. 2019).
6. Adorf, C. S., Dodd, P. M., Ramasubramani, V. & Glotzer, S. C. Simple data and workflow management with the signac framework. *Computational Materials Science* **146,** 220–229. ISSN: 0927-0256. http://www.sciencedirect.com/science/article/pii/S0927025618300429 (2018).