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 EXPERT: Python, C++ ADVANCED: C, R, MySQL, MATLAB INTERMEDIATE: Java, Cuda, PHP

Tools & Frameworks PYTHON PACKAGES: scikit-learn, TensorFlow, Keras, pandas, NumPy, numba PARALLELISM: MPI, OpenMP, TBB

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 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 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., Vo, T., Anderson, J. A. & Glotzer, S. C. A Mean-Field Approach to Simulating Anisotropic Particles. *Journal of Chemical Physics, in review* (2020).
2. 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).
3. 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).
4. Simon, A. J. *et al.* Supercharging enables organized assembly of synthetic biomolecules. *Nature Chemistry* **11.** Work 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).
5. 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.
6. 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).
7. 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).
8. Sinha, D. *et al.* Interdomain communication in the endonuclease/motor subunit of type I restriction-modification enzyme EcoR124I. English. *Journal of Molecular Modeling* **20.** ISSN: 1610-2940. http://dx.doi.org/10.1007/s00894-014-2334-1 (2014).