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 mean-field 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 ML models and deep neural networks using scikit-learn and TensorFlow to identify 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

NVIDIA

SENIOR SOFTWARE ENGINEER — *Mar 2020 - Present*

- Implemented critical algorithms to ensure Spark GPU outperforms Spark CPU on industry standard benchmarks in all cases.
- Spearheaded push to release packages on PyPI, including (re)writing CMake build systems and architecting new DevOps processes.
- Redesigned Python package internals for improved performance, robustness, and flexibility.

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++, CUDA ADVANCED: C, R, MySQL, MATLAB INTERMEDIATE: Rust, Java, PHP

Tools & Frameworks DATA SCIENCE & ML: scikit-learn, TensorFlow, pandas, NumPy, data.table, dplyr PARALLELISM: MPI, OpenMP, TBB BUILD SYSTEMS CMake

Selected Projects

cuDF

DEVELOPER

- Launched redesign of the Python API and led team push to implement a more flexible and performant API.
- Built out new benchmarking frameworks and led associated effort to optimize Python, C++, and CUDA code.
- Rewrote build systems to support building wheels to make our package available to much wider audiences.
- Implemented crucial algorithms to support accelerating TPC-DS queries in the Spark GPU plugin.

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 defining complex workflows.

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.
- 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. *The Journal of Chemical Physics* **153,** 084106. ISSN: 1089-7690 (Aug. 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 (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* (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 (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.** Editor's choice., 220–229. ISSN: 0927-0256 (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 (2014).