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

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, Cuda, R, MySQL, MATLAB Intermediate: Java, PHP
Tools & Frameworks	Data Science & ML: scikit-learn, TensorFlow, pandas, NumPy, data.table, dplyr 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

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. http://dx.doi.org/10.1063/5.0019735 (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. 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., 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. http://www.sciencedirect.com/science/article/pii/S0927025618300429 (2018).
7. 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).
8. Ramasubramani, V. *Flocculation Depletion in a Dual Drug Delivery System for Lung Cancer* Bachelor's Thesis (Princeton University, 2013).
9. Ramasubramani, V. & Glotzer, S. C. rowan: A Python package for working with quaternions. *The Journal of Open Source Software* **3,** 787 (2018).
10. 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).

Presentations

1. Ramasubramani, V. *et al. Freud: Powerful particle simulation analysis in Python* in (Orlando, Florida, Nov. 2019).
2. Ramasubramani, V., Adorf, C. S., Anderson, J. A. & Glotzer, S. C. *How to Professionally Develop Reusable Scientific Software — And When Not To* in (Feb. 2019).
3. Dice, B. D., Adorf, C. S., Ramasubramani, V. & Glotzer, S. C. *Reproducible Computational Scientific Workflows with signac* in (Feb. 2019).
4. Dice, B. D. *et al. Freud: Powerful particle simulation analysis tools for machine learning and materials design* in (Boston, Massachusetts, Dec. 2019).
5. Ramasubramani, V. *et al. Applications of freud for nanoscale simulation analysis* in (Orlando, Florida, Nov. 2019).
6. Ramasubramani, V. *et al. freud: A Software Suite for High-Throughput Analysis of Nanoscale Simulation Data* in (Austin, Texas, July 2019).
7. Adorf, C. S., Ramasubramani, V., Dice, B. D. & Glotzer, S. C. *High-throughput analysis of large heterogeneous and dynamic data spaces with signac* in (Mar. 2019).
8. Dice, B. D., Adorf, C. S., Ramasubramani, V. & Glotzer, S. C. *Recent Developments in the Signac Data Management Framework* in (Orlando, Florida, Nov. 2019).
9. Adorf, C. S., Ramasubramani, V., Anderson, J. A. & Glotzer, S. C. *How to Professionally Develop Reusable Scientific Software — And When Not To* in (Orlando, Florida, Nov. 2019).
10. Glaser, J. *et al. Modeling the self-assembly of super-charged green fluorescent proteins* in (Pittsburgh, Pennyslvania, Oct. 2018).

11. Adorf, C. S., Dodd, P. M., Ramasubramani, V., Dice, B. D. & Glotzer, S. C. *Reproducible Computational Workflows with signac* in (Pittsburgh, Pennyslvania, Oct. 2018).

12. Ramasubramani, V., Adorf, C. S., Dodd, P. M., Dice, B. D. & Glotzer, S. C. *signac: A Python framework for data and workflow management* in (Austin, Texas, July 2018).

13. Ramasubramani, V., Adorf, C. S., Dodd, P. M. & Glotzer, S. C. *Simple data and workflow management with signac* in (Dec. 2017).

14. Dice, B. D., Adorf, C. S., Ramasubramani, V., Dodd, P. M. & Glotzer, S. C. *HPC Data Management and Visualization Workflows with the signac Framework* in (Ann Arbor, Michigan, Mar. 2018).

15. Ramasubramani, V., Karas, A., Glaser, J. & Glotzer, S. *The Effects of Depletion on the Stability and Assembly of Colloidal Crystals* in (915 E Washington St, Ann Arbor, MI 48109, Apr. 2017).

16. Ramasubramani, V., Karas, A., Glaser, J. & Glotzer, S. *The Effects of Depletion on the Stability and Assembly of Colloidal Crystals* in (1000 Beal Ave, Ann Arbor, MI 48109, May 2017).

17. Ramasubramani, V. *Flocculation Depletion in a Dual Drug Delivery System for Lung Cancer* in (Princeton University, Princeton, NJ, USA, May 2013).

18. Ramasubramani, V. & Lively, L. *Examining the Relative Efficacies of the 4ZEV, ZEV, GEV Artificial Transcription Factors* in (Princeton University, Princeton, NJ, USA, Mar. 2012).

19. Ramasubramani, V. *Computational Modeling of the Restriction-Modification System EcoR124* in. Won "Best Presentation Award" (Nove Hrady, CR, June 2012).

20. Baikova, T. *et al.* *Functional Coupling of Duplex Translocation to DNA Cleavage in a Type I Restriction Enzyme* in (Princeton University, Princeton, NJ, USA, Oct. 2012).

21. Baikova, T. *et al.* *Functional Coupling of Duplex Translocation to DNA Cleavage in a Type I Restriction Enzyme* in (Carbondale, IL, USA, Sept. 2012).