Vyas Ramasubramani

(+1) 408-421-2162 | vyas.ramasubramani@gmail.com | vyasr.com | vyasr | vyasr | Vyas | vyas-ramasubramani | Vyas

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

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

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.

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.

rowan (github.com/glotzerlab/rowan)

Lead Developer

- Wrote a Python package for quaternion mathematics.
- Completely mirrored NumPy broadcasting syntax to enable high-performance operations on large arrays in pure Python.

coxeter (github.com/glotzerlab/coxeter)

Lead Developer

- Wrote a Python package for geometric calculations, particularly focusing on polytopes in 2D and 3D.
- Developed and implemented a unified API for generating families of shapes via arbitrary parameterization.

gsd (github.com/glotzerlab/gsd)

Contributor

- Contributed to the specification of a generic binary file format for particle simulation data and the implementing C code.
- Improved memory mapping usage to allow efficient read-only access to very large files.

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

June 2018 **Rackham Conference Travel Grant,** University of Michigan

Apr 2018 **Departmental Nominee,** Beyster Computational Innovation Fellowship

May 2017 **ChE Outstanding Service Award,** Department of Chemical Engineering

Service and Leadership

DEI Student Advisory Board

Board Member — *Oct 2018 - Present*

Chemical Engineering Graduate Society

GSAC Representative — *Dec 2017 - Dec 2018*

Student Engagement Advisory Council

Council Member — *Jan 2017 - Apr 2017*

Chemical Engineering Graduate Recruiting

Chair — *Sept 2016 - Apr 2017*

Chemical Engineering Graduate Symposium

Fundraising Chair — *Sept 2016 - May 2017*

Chemical Engineering Peer Mentoring Program

Peer Mentor — *Jun 2016 - May 2017*

UM Mentorship Program

Faculty/Staff Mentor — *Jul 2016 - Jul 2019*

Chemical Engineering Graduate Society

Representative — *Dec 2015 - Dec 2016*

Engineering Graduate Symposium

Judge Recruiter — *May 2016 - Nov 2016*

Engineering Graduate Symposium

Session Chair — *May 2016 - Nov 2016*

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., 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).
6. 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).
7. Ramasubramani, V. *Flocculation Depletion in a Dual Drug Delivery System for Lung Cancer* Bachelor's Thesis (Princeton University, 2013).
8. Ramasubramani, V. & Glotzer, S. C. rowan: A Python package for working with quaternions. *The Journal of Open Source Software* **3,** 787 (2018).
9. 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).