Vyas **Ramasubramani**

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Summary

I am a PhD candidate at the University of Michigan, Ann Arbor. I use molecular simulations (both MD and MC) and machine learning methods to study the self-assembly of proteins and nanoparticles into complex structures. I am most interested in using machine learning methods to inform and advance physics-based modeling of complex systems. I am the lead developer of a number of open-source projects (signac and freud are two of the largest) and contribute actively to a number of others, including the HOOMD-blue simulation engine. I have also contributed to the broader SciPy ecosystem of tools, including SciPy itself.

Education

Ph.D. in Chemical Engineering and Scientific Computing - University of Michigan *2015 - 2020*

B.S.E. in Chemical Engineering - Princeton University *2009 - 2013*

Research Experience

Research Assistant - University of Michigan - Glotzer Group *Oct 2015 - Present*

- Developed a mean-field simulation technique for the molecular dynamics of anisotropic particles and optimized it for modern GPUs.
- 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.

Thesis Researcher - Princeton University - Prud'homme Lab *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.

Undergraduate Researcher - Academy of Sciences of the Czech Republic - Ettrich Lab *Jul 2012 - Jun 2013*

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

Skills

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

Tools & Frameworks Data Science & ML: scikit-learn, TensorFlow, pandas, NumPy, data.table, dplyr Parallelism: MPI, OpenMP, TBB
Molecular Dynamics: LAMMPS, HOOMD-blue, GROMACS Simulation Analysis: freud, MDAnalysis, MDTraj

Selected Projects

Lead Developer - signac framework (github.com/glotzerlab/signac)

- 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.

Lead Developer - freud (github.com/glotzerlab/freud)

- 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 using more efficient algorithms and improved memory management as part of the 2.0 release.

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

- 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.

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. 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).
4. 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).
5. 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).