Vyas Ramasubramani

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Summary

I am a PhD candidate in Chemical Engineering and Scientific Computing at the University of Michigan, Ann Arbor, where I use molecular simulations and machine learning methods to study the self-assembly of proteins and nanoparticles into complex structures. In addition to this research, my prior work has included studies of the binding capabilities of zinc finger nucleases and the conformational changes in the EcoR124I transcription factor, as well as large-scale data analysis of genomic data to characterize evolutionary rates. In my role as a scientific software developer, I serve as the lead developer of a number of open-source projects in my research area, and I also contribute to other well-known tools like SciPy.

Education

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

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

Minors: Quantitative and Computational Biology, Applications of Computing

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.
- 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.

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 molecular dynamics 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

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.
- Standardized memory handling, revamped APIs and achieved a 5-15x performance increase across the package 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. 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., 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).
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).