Aravind Chandrasekaran, Ph. D.

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Code repositories

Research Interests

Bioinformatics, pharmacodynamics, protein design, drug discovery, structure-function relationship, data-driven modeling, scientific computation

Technical Skills

Molecular dynamics, multiscale modeling and simulation, ODE, PDE, agent-based modeling (ABM), QSP, mechanism-based PK/PD, optimization (gradient-descent, least-squares, SLSQP), machine learning (PCA, K-means clustering), multi-objective optimization

Computational Skills

Software development	Jira, Git
Parallel computing	CUDA, MPI, OpenMP, Pthreads, UMESIMD
Programming languages	C++, Python, Tcl/Tk, Java
Python Libraries	Scikit-learn, scipy, matplotlib, numpy, pandas, PyTorch
Molecular modeling	LAMMPS, Cytosim, MEDYAN, VMD, FTDock
Other	MATLAB, LaTeX, VCell

Work Experience

Postdoctoral Researcher	University of California San Diego	*Aug 2021– Present*
Research Fellow	National Institutes of Health, Bethesda	*Aug 2018 – Dec 2019*
Teaching Assistant	University of Maryland College Park	*Jan 2017– May 2018*
Research Scientist	National Tsing Hua University, Hsinchu Taiwan	*Feb. 2014 – May 2014*

Research and Leadership Experience

Molecular modeling of cellular signaling

- Developed software to study spatial signaling models under both **stochastic** and **continuum frameworks**
- Devised and delivered automatic actin structure classifier using graph theoretical models, Markov state models, PCA, and K-means clustering

Protein structure-function relationship

- Established a non-redundant dataset of DNA-binding proteins incorporating multiple sequence alignment, EC number classification, CATH codes, and crystal structure analysis
- Developed a **docking pose filter** for DNA-protein through principal component analysis and normal model analysis – delivered 2.5 fold enrichment in near-native poses

Software application development

Lead developer, MEDYAN (Github repo, C++) **and contributor, Cytosim** (GitLab repo C++, forked edits for constant polymer copy number and multimerization)

- Contributed **30,000+ lines** over **five releases**, improving user-interface, additional features, and algorithmic optimizations to achieve **10x acceleration**
- Led and trained junior developers in software best practices, statistical modeling, and protein simulations, engaged 10 active users

Teaching

- *Instructor,* Department of Chemistry, UMD *for* **nine semesters, undergraduate** (General Chemistry, Organic Chemistry, Physical Chemistry) and **graduate** (Chemical Thermodynamics, Computational Biology) courses

Education

Ph. D. *in Chemistry*	University of Maryland, College Park	*Aug 2014 – July 2021*
M. Sc. *Bioinformatics & Structural Biology*	National Tsing Hua University, Hsinchu, Taiwan	*Feb 2012 – Jan 2014*
B. Tech. *Chemical Engineering*	Anna University, Chennai, India	*July 2007 – May 2011*

Honors and Awards

2024	Chosen for the Summer School 2024: Self-Organizing Matter: From Inanimate to the Animate, University of Colorado, Boulder
2023	Chosen for the Rising Stars in Soft and Biological Matter Symposium, University of Chicago
2019, 2015, & 2014	Dean's Fellowship, University of Maryland, College Park
2018	NIH-UMD Partnership Fellowship
2013 & 2012	International Student Scholarship, National Tsing Hua University, Taiwan
2010	Summer Research Fellowship Programme, Indian Academy of Sciences

Platform Presentations selected

2025	Biophysical Society Annual Meeting, Los Angeles, CA
2024	American Society of Cell Biology Annual Meeting, San Diego, CA
2023	Rising Stars in Soft and Biological Matter Symposium, Chicago, IL
2019	American Institute of Chemical Engineers Annual Meeting, Orlando, FL
2018	International Physics of Living Systems Annual Meeting, Houston, TX

Professional Services

- 2021 Co-organized multi-lab seminar series (Allen Institute of Cell Science, Drubin/Barnes Lab, UC Berkeley, and Rangamani Lab, UC San Diego)
- 2020 Facilitated panel discussion on addressing imposter syndrome, Grow PoLS workshop
- 2016 US Science & Engineering Festival, Washington D.C.
- Reviewer Journal of Chemical Information and Modeling, Journal of Computational and Theoretical Chemistry

Publications (selected, 138 citations, total 14, full list here)

1. Walker, C., **Chandrasekaran, A.**, Mansour, D., Graham, K., Torres, A., Wang, L., Lafer, E.M., Rangamani, P., Stachowiak, J.C. (2025). Liquid-like condensates that bind actin drive filament polymerization and bundling, *Developmental Cell (In Press)*
2. **Chandrasekaran, A.**, Graham, G., Stachowiak, J.C., Rangamani, P. (2024). Kinetic trapping organizes actin filaments within liquid-like protein droplets, *Nature Communications*, 15, 3139
3. **Chandrasekaran, A.**, Chan, J., Lim, C., and Yang, L. W. (2016) Protein Dynamics and Contact Topology Reveal Protein-DNA Binding Orientation. J. Chem. Theory Comput., **12**, 5269
4. Li, H., Sakuraba, S., **Chandrasekaran, A.**, and Yang, L. W. (2014) Molecular binding sites are located near the interface of intrinsic dynamics domains (IDDs). J. Chem. Inf. Model., **54**, 2275