Aravind Chandrasekaran, Ph. D

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Biophysicist with expertise in building novel algorithms to study protein dynamics. Currently working on structure-property relationships of liquid protein droplets using minimal physics (mesoscopic) and continuum models. Passionate about leveraging computational frameworks to accelerate research and development.

Technical Skills

Molecular dynamics, reaction network modeling, agent-based modeling (ABM), Markov models, machine learning (PCA, K-means clustering), optimization (gradient-descent, least-squares, SLSQP)

Key Accomplishments

- Authored **14** peer-reviewed publications (recognized in prestigious journals such as Nature Physics, Nature Communications, PNAS, and Developmental Cell)
- Lead Developer for a biophysical simulation codebase, guaranteeing consistent project updates (5 releases), optimizing performance, and enhancing user experience
- Delivered 20+ talks/posters highlighting research findings (audience size 50-300), including 5 platform presentations at leading international conferences

Research Highlights in Press

- Graham, Chandrasekaran et. al., Nat. Phys., 2023 featured in Physics Today
- Chandrasekaran et. al., Mol. Biol. of the Cell, 2022 recommended to H1 Connect (Faculty Opinions)

Research Experience

Molecular modeling of cellular signaling (Postdoc and Ph.D.)

- Developed software to study spatial signaling models under both **stochastic** and **continuum frameworks**. Predictions from simulations were experimentally validated
- Devised and delivered automatic actin structure classifier using graph theoretical models, Markov state models, PCA, and machine learning techniques (K-means clustering)
- Developed statistics-driven metrics of protein clustering to understand signaling biophysics through in silico digital twins of experimental systems

Self-assembly algorithm development (Postdoc and Ph.D.)

• Lead developer, MEDYAN (<u>Github repo</u>, C++, **30,000+ lines** over five releases) and contributor, Cytosim (<u>GitLab</u> repo C++, forked edits for <u>constant polymer copy number</u> and <u>multimerization</u>)

Protein structure-function relationship (Master's)

- 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** delivered **2.5-fold** increase in the probability of identifying the protein-DNA structure (tested through bootstrapping)

Computational Skills

Programming languages	C++, Python, Tcl/Tk, Java
Python Libraries	Scikit-learn, scipy, matplotlib, numpy, pandas, PyTorch
Software development	Jira, Git
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
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Education		
Ph. D. in Chemistry		Aug 2014 – July 2021
	University of Maryland, College Park	
M. Sc. Bioinformatics & Structural Biology		Feb 2012 – Jan 2014
	National Tsing Hua University, Hsinchu, Taiwan	
B. Tech. Chemical Engineering		July 2007 – May 2011
	Anna University, Chennai, India	

Leadership and Empowerment

- Led project updates within a multidisciplinary team consisting of over 20 stakeholders
- Mentored **20+** students in science communication and presentation techniques, convened 4 tutorial workshops to introduce new users to cutting-edge research tools (MEDYAN, CytoSim, LAMMPS)
- Led and trained junior developers in software best practices, statistical modeling, and protein simulations, engaged **10** active users
- Organized multi-lab (UC Berkeley, UCSD, and Allen Institute) seminar series to develop novel hypotheses to test through collaborations with experimentalists and computational scientists
- Classroom instruction, Department of Chemistry, UMD for undergraduate and graduate courses (9 courses, total students 550+)

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

Outreach

- 2020 Facilitated panel discussion on addressing imposter syndrome, Grow PoLS workshop
- 2016 US Science & Engineering Festival, Washington D.C.
- 2014 Organized community-building events for the oSTEM UMD chapter

Publications (selected, 155 citations, total 14, full list here)

- Walker, C., Chandrasekaran, A., Mansour, D., Graham, K., Torres, A., Wang, L., Lafer, E.M., Rangamani, P., Stachowiak, J.C. (2025). <u>Liquid-like condensates that bind actin drive filament polymerization and</u> bundling, *Developmental Cell (In Press)*
- 2. **Chandrasekaran, A.**, Graham, G., Stachowiak, J.C., Rangamani, P. (2024). <u>Kinetic trapping organizes</u> <u>actin filaments within liquid-like protein droplets</u>, *Nature Communications*, 15, 3139
- Graham, G., Chandrasekaran, A., Wang, L., Ladak, A., Lafer, E.M., Rangamani, P., Stachowiak, J.C. (2024). <u>Liquid-like condensates mediate competition between actin branching and bundling.</u>, *PNAS*, 121(3), e2309152121
- Chandrasekaran, A., Clarke, A., McQueen, P., Fang, H.Y., Papoian, G. A., and Giniger, E. (2022) <u>Computational simulations reveal that Abl activity controls cohesiveness of actin networks in growth</u> <u>cones.</u> *Mol. Biol. of the Cell*, 33:ar92, 1