# Aravind Chandrasekaran

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## Employment

**Postdoctoral Fellow** August, 2021-Present
Department of Mechanical and Aerospace Engineering
University of California, San Diego **Advisor**: Prof. Padmini Rangamani

## Education

**Ph.D.** *Chemistry*, University of Maryland, College Park July, 2021
**Thesis**: *Emergent network organizations in linear and dendritic actin networks revealed by mechanochemical simulations*
**Advisor**: Prof. Garegin Papoian

**M.Sc.** *Bioinformatics and Structural Biology*, National Tsing Hua University, Taiwan Spring, 2014
**Thesis**: *Protein dynamics and contact topology studies reveal characteristics of Protein-DNA binding and distribution of enzyme catalytic sites*
**Advisor**: Prof. Lee-Wei Yang

**B.Tech.** *Chemical Engineering*, Anna University, India Spring, 2011
**Thesis**: *Plant Design for Manufacture of Selegiline Hydrochloride*
**Advisor**: Prof. T.R. Kubendran

## Research Interests

- **Statistical physics** of active matter
- **Reaction-Diffusion modeling** to understand information transfer in biological signaling pathways
- **Molecular modeling and simulation** of biophysical systems: atomistic to mesoscale resolutions
- **Machine learning** guided design of green materials

## Publications

1. C Floyd, **Chandrasekaran, A.**, H Ni, Q Ni, GA Papoian (2021) Segmental Lennard-Jones interactions for semi-flexible polymer networks Molecular Physics, e1910358.
2. **Chandrasekaran, A.**, Upadhyaya, A., and Papoian, G. A. (2019) Remarkable structural transformations of actin bundles are driven by their initial polarity, motor activity, crosslinking, and filament treadmilling. *PLOS Comput. Biol.*, **15**(7) e1007156
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
5. **Chandrasekaran, A.** and Jain, S. R. (2012) Kac's ring: Entropy and Poincaré recurrence. *Phys. A Stat. Mech. and its Appl.*, **391**, 3702

***In Preparation***(* denotes equal contribution)

1. **Chandrasekaran, A.**, Papoian, G. A., and Giniger, E. Axonal remodeling by Abl signaling is dominated by branching mechanokinetics *(In Draft)*

2. **Chandrasekaran, A.***, Ni, H.*, Ni, Q., Floyd, C., and Papoian, G. A. Improving scalability and features of MEDYAN4.2 - towards simulating cell-scale active networks *(In Draft)*

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**Research Experience**

Sep., 2020-Present

**Devising an operator splitting scheme to accelerate simulation of reaction-diffusion networks**

- Formulated an operator splitting scheme to evolve reaction and diffusion events independently using Lie-Trotter scheme with limited loss in accuracy
- Devised additional algorithmic optimization in diffusion event sampling using Bernoulli trials

June, 2018-Present

**Modeling and simulation of multivalent linker dynamics**

- Co-developed coding/debugging modules to account for multivalent linker reactions in MEDYAN in collaboration with Cheung and Wolynes groups at Rice University's Center for Theoretical Biophysics

July, 2019-Dec., 2019

**Restart feature to improve timescales of simulations in home-built software, Mechano-chemical Dynamics of Active Matter (MEDYAN)**

- Enabled feature to periodically deposit relevant information of chemical species, reaction propensities, mechanochemical constants and necessary geometric constraints in a single file
- Wrote C++ classes to transform information in the file to exactly recreate an instance of the chemical reaction network thereby ensuring accurate trajectory restart

June, 2016-August, 2016

**Accelerating visualization of MEDYAN trajectories using VMD**

- Rendered MEDYAN trajectories to be VMD readable by translating information to a PDB model file
- Incorporated necessary changes to visualize a trajectory with dynamically varying degrees of freedom

Feb., 2012-Jan., 2014

**Examining dynamics features of binding residues in DNA binding proteins**

- Studied Entropic contribution of DNA binding proteins using Elastic Network Models (ENMs)
- Identified domain planes from ENM and calculated enrichment ratio of poses from docking studies

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**Presentations** ([O] - Oral, [P] - Poster)

P "Computational study of Abl guidance based axonal guidance", at Physics of Living Systems (iPoLS) Network, June, 2020.

O "To bundle or not - morphological transitions in actin bundles are determined by their initial polarity, myosin activity, crosslinking, and filament treadmilling" at Annual Meeting of American Institute of Chemical Engineers, Nov., 2019.

O "To bundle or not - morphological transitions in actin bundles are determined by their initial polarity, myosin activity, crosslinking, and filament treadmilling" at UMD Physics of Living Systems seminar, Oct., 2019.

O "Towards a computational model for actomyosin driven axonal guidnace" at *Drosophila* Neuroscience Club Seminar, National Institutes of Neurological Diseases and Stroke (NINDS) Sep., 2019.

P "Towards a computational model for Abl signaling", at NINDS Annual retreat, June 2019.

P "Towards a computational model for Abl signaling", at Annual meeting of the Biophysical Society, March, 2019.

O "Myosin and crosslinker mechanokinetics as well as actin filament treadmilling rate control actin bundle stability" at *Annual Meeting of the International Physics of Living Systems (iPoLS) Network*, May, 2018.

P "Filament polarity and myosin concentration determine untethered actomyosin bundle stability and contractility", at Annual Meeting of the International Physics of Living Systems (iPoLS) Network, May, 2017.

P "Filament polarity and myosin concentration determine untethered actomyosin bundle stability and contractility", at Biophysical Symposium, UMD, April, 2017.[P]

P "Stability and dynamics of unipolar bundles: $\alpha-$ actinin, NMII-A minifilament dependence", at Biophysical Society Pennsylvania Network Meeting, Oct., 2016.

P "Stability and dynamics of unipolar bundles: $\alpha-$ actinin, NMII-A minifilament dependence", at Annual Meeting of the International Physics of Living Systems (iPoLS) Network, July, 2016.

P "Dynamics features of binding residues in DNA binding proteins," at $18^{th}$ Biophysics Conference, Taiwan, July, 2013.

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**Awards and Fellowships**

- NIH Predoctoral Fellow, National Institutes of Neurological Diseases and Stroke (NINDS), NIH, July-Dec., 2018, 2019, and 2020
- Dean's Fellowship, University of Maryland, 2014-15, 2015-16, and 2019-2020
- International Student Scholarship, National Tsing Hua University, 2012-13, and 2013-14
- Summer Research Fellowship Programme-2010, Indian Academy of Sciences, Physics stream

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**Computational Skills**

Programming Languages: C++, Java, MATLAB, Python
Parallel Programming Libraries (C/C++ Based): MPI, OpenMP, Pthreads, CUDA, UMESIMD
Cloud Programming Framework: Hadoop

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**Teaching Experience**

***GTA for Laboratory courses***

CHEM483 Physical Chemistry Lab I - UMD Spring 2017, Fall 2017, Spring 2018, Spring 2020
CHEM232 Organic Chemistry Lab I -UMD Spring 2015
CHEM132 General Chemistry Lab - UMD Fall 2014

***GTA for Lecture courses***

CHEM131 General Chemistry I - UMD Spring 2021
CHEM684 Chemical Thermodynamics - UMD Fall 2016 (Graduate)
Computational Biology - NTHU Spring 2014 (Graduate)

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**Professional Service**

***Outreach***

Oct., 2020 - Prepared and faciliated a panel discussion on *Addressing impostor syndrome* as part of **Grow PoLS virtual workshop: Growing equity, inclusion and diversity for the Physics of Living Systems network**

April, 2016 - Volunteered at the *Biophysical Society* booth as part of **US science and engineering festival**

***Manuscript reviews***: Reviewer for PLOS One, Biophysical J., J. Chem. Inf. and Modeling.

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