

# 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

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## 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

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## 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: molecular to mesoscale resolutions
  - **Machine learning** guided design of green materials
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## Publications

1. **Chandrasekaran, A.**, Clarke, A., McQueen, P., Fang, H.Y., Papoian, G. A., and Giniger, E. (2022). Computational simulations reveal that Abl activity controls cohesiveness of actin networks in growth cones. *Mol. Biol. of the Cell*, **33**
2. **Chandrasekaran, A.**, Papoian, G. A., and Giniger, E. (2022). Nucleation causes an actin network to fragment into multiple high-density domains. *Biophys. J. (In Press)*
3. Ciocanel, M.-V., **Chandrasekaran, A.**, Mager, C., Ni, Q., Papoian, G. A., Dawes, A. (2022). Simulated actin reorganization mediated by motor proteins. *PLOS Comput. Biol.*, **18**(4), e1010026
4. Floyd, C, **Chandrasekaran, A.**, H Ni, Q Ni, GA Papoian (2021) Segmental Lennard-Jones interactions for semi-flexible polymer networks. *Molecular Physics*, e1910358.
5. **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
6. **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

7. 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
8. **Chandrasekaran, A.** and Jain, S. R. (2012) Kac's ring: Entropy and Poincaré recurrence. *Phys. A Stat. Mech. and its Appl.*, **391**, 3702

### **Preprints**

1. Graham, G., **Chandrasekaran, A.**, Wang, L., Ladak, A., Lafer, E.M., Rangamani, P., Stachowiak, J.C. Liquid-like VASP condensates drive actin polymerization and dynamic bundling bioRxiv doi: <https://doi.org/10.1101/2022.05.09.491236>

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### **Research Experience**

Sep., 2020-July, 2021

#### **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 "Abl tunes actin networks between cohesive and weakly-coupled states primarily through changes to actin nucleation", at Annual Meeting of Biophysical Society, 2022.
- 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 guidance” 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<sup>th</sup> 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 facilitated 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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