Akashnathan Aranganathan

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RESEARCH INTERESTS

Statistical Mechanics; Biomolecular (Protein) Conformational Ensemble; Enhanced Sampling; Machine learning.

BRIEF OVERVIEW

Interested in understanding biomolecular interactions such as protein-protein, protein-RNA, etc., and quantifying their effects on a cellular-level length scale. I aim to achieve this in a principled manner, using principles of statistical mechanics and the laws of thermodynamics while augmenting them with machine-learning-based approaches.

EDUCATION

- **University of Maryland, College Park** *Aug 2021 - 2026**
  PhD Candidate in Biophysics MD, USA
  Advisor: Prof. Pratyush Tiwary & Co-Advisor: Dr. Grégoire Altan-Bonnet
  Thesis: Bridging Artificial Intelligence (AI) and Thermodynamics for Advancing Cancer Immunotherapy and Drug Discovery via AlphaFold2RAVE*

- **Indian Institute of Technology Madras** *Aug 2016 - Jun 2021*
  B.S. and M.S. TN, India
  Advisor: Prof. Athi N. Naganathan
  Major in Biological Sciences (Stream - Computational Biology)
  Minor in Physics
  Thesis : Conformational Landscape of Chaperone DnaK

PUBLICATIONS [SCHOLAR = 8] [ORCID = iD] (* - EQUAL CONTRIBUTION)

Under revisions or submissions:

[1] **Akashnathan Aranganathan***, Justin M. Mirazze*, Xiang Chen*, Dongya Jia, Makoto Ando, Sooraj R. Achar, Christopher D. Chien, Marie Pouzolles, Jienyu Ding, Kniya DéDé, Philippe Youkharibache, Naoko Mizuno, Raul Cachau, Kylie J. Walters, Grégoire Altan-Bonnet, Naomi Taylor and Pratyush Tiwary. **CAR-BOOSTing T-Cell Responsiveness through Synaptic Cleft Engineering**. *Nature Chemical Biology*.(under revision)

[2] **Akashnathan Aranganathan*** and Eric Beyerle*. (2025). **Applied causality to infer protein dynamics and kinetics**. *arχiv*. DOI: 10.48550/arXiv.2508.12060 (under submission)

Published:

[1] Xinyu Gu*, Venkata Sai Sreyas Adury*, **Akashnathan Aranganathan**, Xinhao Zhuang, Kristen Varney, David Weber and Pratyush Tiwary. (2025). **Hierarchical AF2RAVE for multi-conformation virtual screening**. *Journal of Chemical Theory and Computation*, Vol. 21, Issue 18, pp. 9214–9225. DOI: 10.1021/acs.jctc.5c01093

[2] Da Teng*, Vanessa J. Meraz*, **Akashnathan Aranganathan**, Xinyu Gu, and Pratyush Tiwary. (2025). **af2rave: protein ensemble generation with physics-based sampling**. *Digital Discovery*. Vol. 4, Issue 8, pp. 2052-2061. DOI: 10.1039/D5DD00201J

[3] **Akashnathan Aranganathan***, Xinyu Gu*, Dedi Wang, Bodhi P. Vani and Pratyush Tiwary. (2025). **Modeling Boltzmann weighted structural ensembles of proteins using AI based methods**. *Current Opinion in Structural Biology*. Vol. 91, ISSN 0959-440X, pp. 103000. DOI: 10.1016/j.sbi.2025.103000

[4] Xinyu Gu, **Akashnathan Aranganathan** and Pratyush Tiwary. (2024). **Empowering AlphaFold2 for protein conformation selective drug discovery with AlphaFold2-RAVE**. *eLife*. Vol. 13, pp RP99702. DOI: 10.7554/eLife.99702.1

[5] Bodhi P. Vani, **Akashnathan Aranganathan** and Pratyush Tiwary. (2023). **Exploring kinase DFG loop conformational stability with AlphaFold2-RAVE**. *Journal of Chemical Information and Modeling*. Vol. 64, Issue 7, pp. 2789–2797. DOI: 10.1021/acs.jcim.3c01436

[6] **Akashnathan Aranganathan***, Bodhi P. Vani*, Dedi Wang and Pratyush Tiwary. (2023). **AlphaFold2-RAVE: From Sequence to Boltzmann Ranking**. *Journal of Chemical Theory and Computation*. Vol. 19, Issue 14, pp. 4351–4354. DOI: 10.1021/acs.jctc.3c00290

[7] Athi N. Naganathan, Rahul Dani, Soundhararajan Gopi, **Akashnathan Aranganathan** and Abhishek Narayan. (2021). **Folding Intermediates, Heterogeneous Native Ensembles and Protein Function**. *Journal of Molecular Biology*. Vol. 433, ISSN 0022-2836, pp. 167325. DOI: 10.1016/j.jmb.2021.167325

[8] Soundhararajan Gopi, **Akashnathan Aranganathan**, Athi N. Naganathan. (2019). **Thermodynamics and folding landscapes of large proteins from a statistical mechanical model**. *Current Research in Structural Biology*. Vol. 1, ISSN 2665-928X, pp. 6-12. DOI: 10.1016/j.crstbi.2019.10.002

PATENTS

- **Enhancing Chimeric Antigen Receptors (CAR) T Cell Therapy By Modification of Hinge Sequence** *Feb 2025*
  Provisional Patent filed App. No.: 63/755,920
  - ◦ Method: CAR-Biophysically Oriented Optimization of Synaptic Topology (CAR-BOOST)
  - ◦ Developed a method to enhance CAR T Cell therapy from atomistic level information by inferring to evolutionary constraints.

PRESENTATIONS

- **Summer RosettaCon 2025 - Protein Dynamics Panel** *Aug 2025*
  Talk title: Predicting Druggable Multi-Conformational Targets using Boltzmann Ranking with AF2RAVE
- **Center for Integrative Biology and Systems MedicinE - Talk series** *May 2024*
  Talk title: AlphaFold2RAVE (AF2RAVE): From sequence to Boltzmann ranking
- **Biophysical Society - Annual meeting 2024** *Feb 2024*
  Poster title: Enhancing CAR T-Cell therapy through in-silico modeling of hinge sequence length based on epitope location
- **Gordon Research Conference - Protein folding and dynamics** *Jan 2024*
  Poster title: Enhancing CAR T-Cell therapy through in-silico modeling of hinge sequence length based on epitope location
- **NCI-UMD mini symposium** *Dec 2023*
  Talk title: Enhancing CAR T-Cell therapy through in-silico modeling of hinge sequence length based on epitope location
- **International Physics of Living Systems (iPoLS)** *Aug 2023*
  Poster title: Predicting cytotoxicity of Chimeric Antigen Receptors(CARs) with Artificial Intelligence
- **The Molecular Sciences Software Institute (MOLSSI Workshop** *Jun 2023*
  Poster title: AlphaFold2-RAVE: From Sequence to Boltzmann Ranking
- **NCI-UMD mini symposium** *Jan 2023*
  Talk title: Predicting cytotoxicity of Chimeric Antigen Receptors(CARs) with Artificial Intelligence
- **NCI-UMD talk series** *Dec 2022*
  Talk title: Reduced MSA AlphaFold2: AF2-RAVE and predicting cytotoxicity of CARs

MASTERS THESIS

- **Conformational Landscapes of Chaperone DnaK** *Jan 2020 - July 2021*
  Advisor: Prof. Athi N. Naganathan Indian Institute of Technology(IIT) - Madras
  - ◦ Generated conformational landscapes for DnaK, a heat shock protein, by developing the bWSME model.

ACHIEVEMENTS

- Awarded the UMD Graduate School's Ann G. Wylie Dissertation fellowship *2025*
- Awarded the NCI-UMD fellowship to work on cancer research *2022-2025*
- Secured 99.01 percentile with an All India Rank of 102 in Graduate Aptitude Test in Engineering (GATE) for Biotechnology profile *2020*
- Selected for the annual Bioengineering Summer Training (BEST) Fellowship programme at Indian Institute of Science (IISc), Bangalore *2019*
- Awarded the INSPIRE-SHE (Scholarship for Higher Education) scholarship which is given to support academically excelling undergraduate science students. *2016-2021*
- Secured 98.3 percentile in the Joint Entrance examination (JEE) among 1.5 million candidates across the nation *2016*

TEACHING AND MENTORING EXPERIENCE

- **Mentoring junior graduate students** *2023 - 2026**
  - ◦ Taught junior students in using packages like OpenMM, torch, and Prof. Tiwary's group methods such as SPIB.
  - ◦ Closely metnored a student along with Prof. Tiwary in designing their PhD projects, conferences, etc.
  - ◦ Lead multiple machine learning journal clubs and taught some complicated networks including transformers, AF2.
- **Teaching Assistant for MATH course** *Fall 2021 and Spring 2022*
  - ◦ MATH135 Discrete Mathematics for Life Sciences at University of Maryland College Park.
- **Teaching Assistant for Biology course** *Spring 2021*
  - ◦ BT4240 Food Biotechnology at Indian Institute of Technology, Madras.

PEER REVIEWER FOR JOURNALS

- **Computational Biology and Chemistry**
- **Current Opinion in Structural Biology**
- **Journal of Chemical Theory and Computation**
- **The Journal of Physical Chemistry**

SKILLS

- **Programming Languages:** C++, Python, MATLAB
- **Toolsets:** GROMACS, Pymol, VMD, PyTorch, OpenMM, Plumed, LaTeX.
  - ◦ **ML Toolsets:** AlphaFold2, ColabFold, OpenFold, Transformers, Variational Auto-Encoders.
- **Language:** English, Tamil