

Aditya Dendukuri

PhD Candidate

University of California, Santa Barbara

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adityadendukuri.github.io

Research Interests

Numerical analysis, mathematical modeling and scientific machine learning.

Education

University of California, Santa Barbara CA

Sept 2021 — Present

PhD in Computer Science

Advisor: Linda R. Petzold

University of Arkansas, Fayetteville AR

Aug 2018 — Jul 2020

MS in Computer Science

Advisors: David M. Ford and Matthew J. Patitz

Thesis: Nonlinear Dimensionality Reduction for the Thermodynamics of Small Clusters of Particles

University of Central Arkansas, Conway AR

Aug 2014 — May 2018

BS in Computer Science (Minor in Physics)

Advisor: Tansel Halic

Professional Experience

Lawrence Berkeley National Laboratory

Berkeley, CA

UC Graduate Student Researcher (GSR) Intern

July 2026 – present

- Develop efficient approximation methods for stochastic processes, particularly continuous-time Markov chains arising in chemical kinetics and reaction networks.
- Devise mathematical methods and implement computational programs for accurately simulating stochastic processes arising in physical science and artificial intelligence applications.
- Collaborate with scientists in the Applied Mathematics and Computational Research Division on computational methods in advanced mathematics and machine learning.

NSF National Center for Atmospheric Research (NCAR)

Boulder, CO

SIParCS Graduate Student Intern

May 2024 – July 2024

- Contributed to translating a radiative transfer codebase from Fortran to C++ and prepared documentation to support maintainability and future development.
- Implemented a custom solver for tridiagonal linear systems and benchmarked it against LAPACKE to evaluate numerical accuracy and performance.
- Extended testing coverage for critical linear algebra components using Google Test and added performance benchmarks with Google Benchmark.

University of Arkansas

Fayetteville, AR

Research Associate

Sept 2020 – June 2021

- Modeled nucleation and phase-transition processes using Monte Carlo simulations and implemented custom C code to analyze critical-cluster formation dynamics.

Research Assistantships

University of California, Santa Barbara

Santa Barbara, CA

Graduate Research Assistant

Sept 2021 – Present

- Develop structure-exploiting numerical algorithms for analyzing high-dimensional discrete stochastic systems, enabling efficient simulation and inference for complex reaction networks.
- Investigate surrogate modeling approaches for understanding activity in lab-grown neural tissues, using time-series analysis and dimensionality reduction to extract interpretable spatiotemporal dynamics.

University of Arkansas

Fayetteville, AR

Graduate Research Assistant

Aug 2018 – July 2020

- Explored the thermodynamic properties of colloidal clusters using data-driven methods, reconstructing energy landscapes and transition pathways from stochastic simulations.
- Simulated quantum circuits to investigate hybrid quantum-classical learning models and developed workflows for evaluating variational quantum algorithms.
- Published results on data-driven thermodynamics in *Computers & Chemical Engineering*.

University of Central Arkansas

Undergraduate Research Assistant

Conway, AR

Aug 2016 – May 2018

- Developed real-time surgical training simulations by coupling fluid-flow and heat-transfer models in a numerical solver.
- Conducted hierarchical task analysis using observational data from arthroscopic surgeries to inform system design and evaluation.
- Presented and published this work at the 23rd IEEE International Conference on Bioinformatics and Bioengineering.

Teaching Assistantships

University of California, Santa Barbara

Graduate Teaching Assistant

Santa Barbara, CA

Sept 2021 – Present

- Supported undergraduate instruction in scientific computing, data structures, and numerical methods, including programming in Python, C++, and MATLAB.

Preprints (Under Review/ In Press)

- A. Dendukuri, S. Chandrasekaran, and L. Petzold, *Flux-preserving adaptive finite state projection for multiscale stochastic reaction networks*, 2025. arXiv: 2512.17064 [cs.CE]. [Online]. Available: <https://arxiv.org/abs/2512.17064>
– Accepted for publication (in press) at *SIAM Multiscale Modeling and Simulation*.

Publications

- T. van der Molen, A. Spaeth, M. Chini, *et al.*, “Preconfigured neuronal firing sequences in human brain organoids,” *Nature Neuroscience*, vol. 29, no. 1, pp. 123–135, Jan. 2026, ISSN: 1546-1726. DOI: 10.1038/s41593-025-02111-0. [Online]. Available: <https://doi.org/10.1038/s41593-025-02111-0>
- A. Dendukuri, M. Tunc, D. Demirel, *et al.*, “Unified framework for real-time fluid simulation in virtual rotator cuff arthroscopic skill trainer (vircast),” in *Proceedings of the 23rd IEEE International Conference on Bioinformatics and BioEngineering*, In Press, IEEE Computer Society. DOI: 10.1109/BIBE60311.2023.00063
- D. M. Ford, A. Dendukuri, G. Kalyoncu, *et al.*, “Machine learning to identify variables in thermodynamically small systems,” *Computers & Chemical Engineering*, p. 106 989, 2020
- D. Demirel, A. Yu, S. Cooper-Baer, *et al.*, “A hierarchical task analysis of shoulder arthroscopy for a virtual arthroscopic tear diagnosis and evaluation platform (vatdep),” *The International Journal of Medical Robotics and Computer Assisted Surgery*, vol. 13, no. 3, e1799, 2017

Conference Presentations

- A. Dendukuri and L. Petzold, *Adaptive multigrid finite state projection for the reaction-diffusion master equation*, Colorado Conference for Iterative and Multigrid Methods, Boulder, CO, USA, June 26th, 2026
- A. Dendukuri, M. Tunc, D. Demirel, *et al.*, *Unified framework for real-time fluid simulation in virtual rotator cuff arthroscopic skill trainer (vircast)*, 23rd IEEE International Conference on Bioinformatics and BioEngineering (BiBE 2023). Presented by Doga Demirel, Oct 20-24, 2019
- A. Dendukuri, G. Kalyoncu, K. Luu, *et al.*, *Detecting subspaces for small lennard-jones clusters using spectral graph theory and machine learning*, 2021 SIAM Conference on Computational Science and Engineering, ., March 20-21, 2021
- D. M. Ford, A. Dendukuri, G. Kalyoncu, *et al.*, *Machine learning to identify variables in thermodynamically small systems*, Foundations of Process Analytics and Machine Learning., Aug 6-9, 2019
- A. Dendukuri, B. Keeling, A. Fereidouni, *et al.*, *Defining quantum neural networks via quantum time evolution*, Quantum Techniques in Machine Learning 2019, KAIST, Daejeon, South Korea. ., Oct 20-24, 2019
- A. Dendukuri, T. Mustafa, T. Halic, *et al.*, *Modeling fluid and heat flow in virtual arthroscopic tear diagnosis and evaluation platform (vatdep)*, Arkansas IDeA Network of Biomedical Research Excellence symposium. Fayetteville, AR., Oct 25-26, 2017
- A. Dendukuri, T. Halic, S. Kockara, *et al.*, *Modeling fluid flow in virtual arthroscopic tear diagnosis and evaluation platform (vatdep)*, Sixth Annual Central Arkansas Undergraduate Summer Research Symposium. University of Arkansas for Medical Sciences, Little Rock, AR., Jul 26, 2017

Honors

- Best paper award. IEEE Bioinformatics and Bioengineering (BIBE) Conference 2023.
- Masters thesis nominated for the *Conference of Southern Graduate Schools (CSGS)* outstanding master's thesis award.
- Graduate Student Council Travel Grant (\$500) for the Foundations of Process Analytics and Machine Learning Conference in Raleigh, North Carolina (Summer 2019).
- Advancement of Undergraduate Research in the Sciences (AURS) summer research fund (2016) (<http://www.aursfund.org>)
Award Amount: \$5000

Selected Courses

PhD Courses (UCSB)

- Matrix Analysis and Computation
- Level Set Methods
- Finite Element Methods
- Numerical Simulation
- Spectral Graph Theory

MS Courses (UofA)

- Deep Learning
- Natural Language Processing
- Computer Vision

Skills (2-3 Years of Full-Time Experience)

- **Programming:** Julia, Python, C/C++
- **Software:** Tensorflow and PyTorch (Python), Modelling Toolkit (Julia), SciML (Julia), Linux, CMAKE.

References

Dr. Linda R. Petzold (petzold@engineering.ucsb.edu)
 Mehrabian Distinguished Professor, Mechanical Engineering and Computer Science, University of California, Santa Barbara.

Jian Sun (sunjian@ucar.edu)
 Soft Eng/Prog II, NSF National Center for Atmospheric Research

Dr. David Ford (ford3dm@cmich.edu)
 Dean, Bagley College of Engineering, Mississippi State University.
 Past: Professor and Department Head. Ralph E. Martin Department of Chemical Engineering, University of Arkansas.

Dr. Tansel Halic (tanselhalic@gmail.com)
 Senior Software Engineer, Intuitive Surgical.