

Luke Evans

Flatiron Institute, Center for Computational Mathematics
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Education

University of Maryland, College Park, MD
Ph.D in Applied Mathematics, Emphasis in Scientific Computation May 2023
Advisors: Maria Cameron and Pratyush Tiwary

San Francisco State University, San Francisco, CA
Master of Arts in Mathematics May 2017
Advisor: Chun-Kit Lai

Hendrix College, Conway, AR
Bachelor of Arts in Mathematics May 2015
Advisor: Lars Seme

Honors and Awards

University of Maryland, College Park, MD
Recipient of James C. Alexander Prize for Graduate Research May 2024

- Awarded to at most two recently graduated Ph.D. mathematics students per year for outstanding dissertation research.

Recipient of Ann G. Wylie Dissertation Fellowship April 2022
Recipient of Outstanding Research Assistant Award January 2022

San Francisco State University, San Francisco, CA
Recipient of Graduate Student Distinguished Achievement Award May 2017

- Nominated by math department for significant contributions in research
- Sole mathematics recipient among College of Science and Engineering

Recipient of Achievement Rewards for College Scientists Scholarship (ARCS) June 2016

Hendrix College, Conway, AR
Magna cum laude, graduation with distinction May 2015
Recipient of Philip E. Parker Undergraduate Research Award May 2015

Publications and Preprints

L. Dingeldein, D. Silva-Sanchez, L. Evans, E. D’Imprima, N. Grigorieff, R. Covino, P. Cossio. **Amortized template-matching of molecular conformations from cryo-electron microscopy images using simulation-based inference**, submitted, bioRxiv:2024.07.23.604154 (2024).

D. Wang, Y. Wang, L. Evans, P. Tiwary. **From latent dynamics to meaningful representations**, *Journal of Chemical Theory and Computation*, 1549-9168 (2024).

S. Sule, L. Evans, M. Cameron. **Sharp error estimates for target measure diffusion maps with applications to the committor problem**, submitted, arXiv:2312.14418 (2023).

L. Evans, M. Cameron, P. Tiwary. **Computing committors in collective variables via Mahalanobis diffusion maps**, *Applied and Computational Harmonic Analysis*, 64, 62-101 (2023).

L. Evans, M. Cameron, P. Tiwary. **Computing committors via Mahalanobis diffusion maps with enhanced sampling data**, *Journal of Chemical Physics*, 157, 214107 (2022).

L. Evans, C.K. Lai. **Conjugate phase retrieval on \mathbb{C}^M by real vectors**. *Journal of Linear Algebra and its Applications*, 587 (2019), 45 - 69.

C. Olson, L. Evans, N. Bayya, J. Edelberg. **A comparison of encoding methods for automated design of optical architectures**. *Proceedings of SPIE, Novel Optical Systems Design and Optimization XXI*, 107460J (2018).

Past Research Projects

University of Maryland, College Park, MD

Graduate Researcher, advised by Maria Cameron and Pratyush Tiwary January 2020 - May 2023

- Computing committor functions and reactive currents on collective variable (CV) molecular simulation data using the Mahalanobis diffusion map algorithm (MMAP)
- Rigorously proving that the MMAP output converges to the generator of overdamped Langevin dynamics with position-dependent diffusion tensor
- Extending MMAP to data from biased molecular simulations

AMSC 663-664: *Advanced Scientific Computing* Project, advised by Maria Cameron August 2018 - May 2019

- Combined manifold learning techniques with ensembles of local simulations to coarse-grain stochastic differential equations

Naval Research Laboratory, Washington, D.C.

Student Intern, Applied Optics, mentored by Colin Olson May - August 2018

- Developed evolutionary algorithms for design of optical systems

San Francisco State University, San Francisco, CA

Graduate Researcher, Dept. of Mathematics, advised by Chun-Kit Lai August 2016 - January 2018

- Developed the *conjugate phase retrieval problem*, proved results for complex vectors and Fourier phase retrieval of band-limited functions

Lawrence Livermore National Laboratory, Livermore, CA

Student Intern, Weapons and Complex Integration, mentored by Walt Nissen May - August 2016

- Applied locational optimization techniques to approximation of Voronoi tessellations for use in smoothed-particle hydrodynamics

Hendrix College, Conway, AR

Undergraduate Researcher, Dept. of Mathematics, advised by Lars Seme January - December 2014

- Created dynamical systems framework for the iterated Newton's method applied to complex-valued polynomials

Presentations

AMS Fall Eastern Sectional Meeting, Albany, NY

Invited Talk, "Computing Committors with Diffusion Maps: Rare Events, Importance Sampling and Sharp Error Estimates" October 2024

4th Annual NY Area Cryo-EM Meeting, New York, NY

Poster, "Amortized template-matching of molecular conformations from cryo-electron microscopy images using simulation-based inference" June 2024

IMSI Learning Collective Variables and Coarse Grained Models Workshop, Chicago, IL

Poster, "Amortized template-matching of molecular conformations from cryo-electron microscopy images using simulation-based inference" April 2024

Rare Events: Analysis, Numerics, and Applications, College Park, MD

Talk, "Computing committors in collective variables using Mahalanobis diffusion maps" February 2023

SIAM Washington-Baltimore Section Fall Meeting 2022, Ballston, VA

Poster, "Computing committors with Mahalanobis diffusion maps" November 2022

Mid-Atlantic Numerical Analysis Day , Temple University, Philadelphia, PA Talk, “Computing committors in collective variables using Mahalanobis diffusion maps”	October 2022
SIAM Annual Meeting , Virtual Talk, “Computing committors in collective variables using Mahalanobis diffusion maps”	July 2022
SIAM Conference on Uncertainty Quantification , Virtual Talk, “Computing committors in collective variables using Mahalanobis diffusion maps”	April 2022
American Physical Society March Meeting , Virtual Poster, “Data-driven committor approximation for anisotropic diffusions in collective variables”	March 2021
SFSU Graduate Student Research Showcase , San Francisco, CA Poster, “Phase and Conjugate Phase Retrieval”	April 2017
MAA Mathfest , Portland, Oregon Talk, “Newton’s Method in the complex plane”	July 2014

Academic Service

- Co-organizer for “Machine Learning Techniques for Quantifying Rare Events” minisymposium at 2022 SIAM Conference on Uncertainty Quantification, April 12-15, 2022
- Co-organizer for “Machine Learning For Rare Events” seminar at UMD Mathematics Department, Spring 2022, Website: <https://www.math.umd.edu/~evansal/rit.html>
- Co-organizer for “Norbert Wiener Center” seminar at UMD Mathematics Department, Fall 2018 - Spring 2019
- Co-president of SIAM Chapter and Applied Math Graduate Student Council, University of Maryland, Fall 2021 - Spring 2022
- Reviewer for Journal of Physical Chemistry, January-February 2024
- Reviewer for Journal of Physical Chemistry Letters, March 2023, May 2023
- Reviewer for Science China Mathematics, Spring 2020

Teaching, Mentoring and Administrative Experience

University of Maryland , College Park, MD REU Teaching Assistant, “Machine learning methods for the study of rare events in stochastic systems”	May 2022 - July 2022
<ul style="list-style-type: none"> • Mentored undergraduate researchers in conceptual understanding and python coding for stochastic simulation and rare event sampling 	
Teaching Assistant	August 2017 - May 2018
<ul style="list-style-type: none"> • T.A for calculus I, calculus II 	
San Francisco State University , San Francisco, CA Graduate Teaching Associate	August 2015 - May 2017
<ul style="list-style-type: none"> • Instructor for college algebra • T.A for calculus I 	
Hendrix College , Conway, AR Tutor, Teaching Assistant	August 2013 - May 2015
<ul style="list-style-type: none"> • Grader for calculus I • Tutor for pre-calculus through calculus II 	