Justin M. Baker

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Appointments

Hedrick Assistant Adjunct Professor — Summer 2024 - Present
University of California, Los Angeles — *Computational and Applied Mathematics*

Graduate Research Summer Intern — Summer 2023
Oak Ridge National Laboratory

Education

University of Utah — June 2024
PhD, Applied Mathematics

University of Utah — May 2019
Honors Bachelor of Science, Applied Mathematics with Computational Emphasis

Professional Development

Argonne Training Program on Extreme-Scale Computing — Summer 2024
Argonne National Laboratory

Research Focus

AI for Science
Antibody and Antigen Therapeutic Design, Biomolecular Interactions

Mathematical Foundations of AI
Geometric Deep Learning, Projection Operator Formalism

Conference Proceedings

- **Justin M. Baker**, Harris Hardiman-Mostow, Yuer Tang, Andrea L. Bertozzi. "On the Dynamics of Coherent Memory Structures in Neural Fields." *Submitted to the International Conference on Learning Representations (ICLR)*. 2026.
- Shih-Hsin Wang, Yuhao Huang, Taos Transue, **Justin M. Baker**, Jonathan Forstater, Thomas Strohmer, Bao Wang. "Towards Multiscale Graph-based Protein Learning with Geometric Secondary Structural Motifs." *Advances in Neural Information Processing Systems (NeurIPS)*. 2025.
- Shih-Hsin Wang, Y Huang, **Justin M. Baker**, YE Sun, Q Tang, B Wang. "A Theoretically-Principled Sparse, Connected, and Rigid Graph Representation of Molecules." *The Thirteenth International Conference on Learning Representations (ICLR)*. 2025.
- **Justin M. Baker**, Shih-Hsin Wang, Thomasso de Fernex, Bao Wang. "An Explicit Frame Construction for Normalizing 3D Point Clouds". *International Conference on Machine Learning*. 2024.
- Shih-Hsin Wang, Yung-Chan Hsu, **Justin M. Baker**, Andrea L. Bertozzi, Jack Xin, Bao Wang. "Rethinking the Benefits of Steerable Features in 3D Equivariant Graph Neural Networks". *International Conference on Learning Representations*. 2024.

- **Justin M. Baker**, Qingsong Wang, Martin Berzins, Thomas Strohmer, Bao Wang. "Monotone Operator Theory-Inspired Message Passing for Learning Long-Range Interaction on Graphs". *International Conference on Artificial Intelligence and Statistics*. 2024.
- **Justin M. Baker**, Massimiliano Lupo Pasini, Cory Hauck. "Invariant Features for Accurate Predictions of Quantum Chemical UV-vis Spectra of Organic Molecules". *IEEE Southeast Conference*. 2024.
- **Justin M. Baker**, Qingsong Wang, Bao Wang, Cory Hauck. "Implicit Graph Neural Networks: A Monotone Operator Viewpoint". *International Conference on Machine Learning*. 2023.

Journal Publications

- **Justin M. Baker**, Elena Cherkaev, Vladimir Druskin, Shari Moskow, Mikhail Zaslavsky. "Regularized Lippmann-Schwinger-Lanczos Algorithm for Inverse Scattering Problems in the Frequency Domain". *Journal of Computational Physics* 525, 113725. 2025.
- **Justin M. Baker**, Elena Cherkaev, Akil Narayan, Bao Wang. "Learning POD of Complex Dynamics Using Heavy-ball Neural ODEs". *Journal of Scientific Computing* 95, 54. 2023.

Abstracts, Manuals, Workshops, and Technical Summaries

- Nemo Delignat, **Justin M. Baker**, Andrea L. Bertozzi. "Toward a General Graph Construction Method for Complete Invariant Graphs." *1st AAAI Workshop on SPARTA — Spatial Reasoning and Therapeutics with AI: From Omics to Imaging, 2026.*
- Tyler Headley, Narayanan Kannan, Anand Somajulya, **Justin M. Baker**, Adrien Weihs, P. Jeffrey Brantingham, Andrea L. Bertozzi. "Learning Intermittent Time Series with the Partial Autocorrelation Function Integral Transform (PACFIT)." *AAAI'25 Workshop — AI4TS: AI for Time Series Analysis: Theory, Algorithms, and Applications, 4 Mar. 2026.*
- Mia Adler, Shiyuan Liang, Tianzheng Peng, Oleg Presnyakov, **Justin M. Baker**, Jannelle Lauffer, Himani Sharma, Barry Merriman. "Conformational Rank Conditioned Committees for Machine Learning-Assisted Directed Evolution." *Machine Learning for Structural Biology (MLSB)*. 2025.
- Starlika Bauskar, Jade Jiao, Narayanan Kannan, Alexander Kimm, **Justin M. Baker**, Matthew J. Tyler, Andrea L. Bertozzi, Anne M. Andrews. "Boltzmann Graph Ensemble Embeddings for Aptamer Libraries." *IEEE International Conference on Data Mining (ICDM) Workshop on Graphs in Text, Audio, and Other Unstructured Data (GTA3).*
- **Justin M. Baker**, Jack Hirschman, Abhimanyu Borthakur, Harris Hardiman-Mostow, Sergio Carbajo, Andrea L. Bertozzi. "Photon Transport Neural Networks: A Digital Twin Approach." *Ultrafast Optics XIV (UFO XIV)*. 2025.
- Pasini, Massimiliano Lupo, Choi, Jong Youl, Zhang, Pei, **Baker, Justin**. "User Manual - HydraGNN: Distributed PyTorch Implementation of Multi-Headed Graph Convolutional Neural Networks". United States: N. p., 2023. Web. doi:10.2172/2224153.

Preprints

- **Justin M. Baker**, Shih-Hsin Wang, Andrea L. Bertozzi, Bao Wang. "Learning Symmetry Breaking via Symmetry-Adapted Neural Networks." *Preprint*. 2025.

- Shih-Hsin Wang, **Justin M. Baker**, Bao Wang, Cory Hauck. "Rethinking the Smoothness of Node Features Learned by Graph Convolutional Networks". *Preprint.* 2024.
- **Justin M. Baker**, Yuhao Huang, Shih-Hsin Wang, Massimiliano Lupo Pasini, Andrea L. Bertozzi, Bao Wang. "Stabilized E(n)-Equivariant Graph Neural Networks-assisted Generative Models". *Preprint.* 2024.
- **Justin M. Baker**, Hedi Xia, Yiwei Wang, Elena Cherkaev, Akil Narayan, Long Chen, Jack Xin, Andrea L. Bertozzi, Stanley J. Osher, Bao Wang. "Proximal Implicit ODE Solvers for Accelerating Learning Neural ODEs." *Preprint.* 2022.

Awards & Honors

Optimization and Inversion Research Training Grant Spring 2024
University of Utah, Department of Mathematics

Outstanding Graduate Student Award 2022
University of Utah, Department of Mathematics

Undergraduate Research Scholar 2019
University of Utah, Scholarship Designation

Selected Presentations

- Explainable Latent Representations for Digital Twins via Mori–Zwanzig Formalism. *Optimization and Machine Learning (OWL).* 2025.
- Explainable Neural Operators in Digital Twin Modeling for Ultra-fast Optics. *Symposium on Computational and Applied Mathematics for the Sciences (SOCAMS).* 2025.
- The Role of Traveling Waves in Neural Information Processing. *UCLA Level Set Meeting.* 2024.
- Message Passing Neural Networks for the Design of Atomic Structures. *UCLA Level Set Meeting.* 2023. University of California, Los Angeles
- Regularized Lippmann-Schwinger-Lanczos Algorithm for Inverse Scattering Problems in the Frequency Domain. *International Congress for Industrial and Applied Mathematics.* 2023. Tokyo, Japan
- Monotone Implicit Graph Neural Networks for Long-Range Dependency Learning. *SIAM Northern States Section Conference.* 2023. Logan, Utah
- Model Order Reduction Based on the Approximation of the Resolvent and Applications. *Fall Sectional of the American Mathematical Society.* 2022. SLC, UT
- Accelerating Learning Neural ODEs via Proximal Algorithms. *SIAM Conference on Mathematics of Data Science.* 2022. San Diego, California
- Survey of Kaczmarz Methods and Extension to Optimal Transport. *Topics in Advanced Optimization.* 2022. University of Utah
- Parallel-in-time methods for direct-adjoint studies. *Applied Mathematics Colloquium.* 2022. University of Utah
- Optimal Design in Monge-Kantorovich Optimal Transportation. *Texas-Louisiana Sectional of the Society of Industrial and Applied Mathematics.* 2021. South Padre Island, Texas
- Image Denoising Using the Alternating Direction Method of Multipliers. *Applied Mathematics Colloquium.* 2021. University of Utah
- Lyapunov Stability in Aerodynamics. *Graduate Student Colloquium.* 2019. University of Utah

Instruction

Machine Learning Winter 2026 (*Expected*)
University of California, Los Angeles

Numerical Analysis Fall 2025
University of California, Los Angeles

Mathematical Methods of Data Theory Fall 2024, Spring 2025, Winter 2026 (*Expected*)
University of California, Los Angeles

Precalculus (In Person, Virtual, Hybrid) Fall 2020, Spring 2021, Spring 2022
University of Utah

Teaching Assistance

Differential Equations and Linear Algebra Spring 2020
University of Utah

Accelerated Engineering Calculus II Fall 2019
University of Utah

Math for Elementary School Teachers Fall 2018, Spring 2019
University of Utah

Mentorship

How to Build an AI Biologist: In Silico Antibody Optimization Summer 2025
IPAM-RIPS & Avery Digital Systems

DNA Aptamer Design Summer 2025
UCLA - Computational and Applied Mathematics

Denver Crime Statistics Summer 2024
UCLA - Computational and Applied Mathematics

Efficient Eigensolvers Summer 2020
Brown University - Summer@ICERM

Random Projections and Dimension Reduction Summer 2020
Brown University - Summer@ICERM

Service

Conference Reviewer Fall 2024 - Present
NeurIPS, ICML, ICLR

Journal Reviewer Spring 2024
Neurocomputing

Conference Volunteer Summer 2023
International Conference on Machine Learning

First Year Graduate Student Mentoring Fall 2020 - Spring 2021
University of Utah

Professional Societies

Society for Industrial and Applied Mathematics
American Mathematical Society

Extracurricular: Instruction

Certified Flight Instructor 2019 - Present
Single Engine Land, Instrument Add-on

Policy Debate Coach 2017 - 2019
Skyline High School *Salt Lake City, Utah*

Extracurricular: Outreach

Organizer: Kids Cafe 2017
Supplemental Nutrition Assistance Program: After School At-Risk Meals *Kearns Library, Utah*
Volunteer: Allied 2017
A Gender and Sexuality Alliance for all teens in our community *Kearns Library, Utah*