Nikola B. Kovachki

3660 Monterosa Dr, Altadena, California 91001, USA
kovachki93@gmail.com • +1 (323) 423-6884 • https://kovachki.github.io/

EDUCATION

California Institute of Technology, Pasadena, CA, USA

- Ph.D. in Applied and Computational Mathematics — Oct 2016 – Jun 2022
  - Cumulative GPA: 4.0/4.0
  - Adviser: Prof. Andrew M. Stuart
  - Thesis: Machine Learning and Scientific Computing
- B. Sc. in Mathematics — Oct 2012 – Jun 2016
  - Cumulative GPA: 3.9 / 4.0
  - Adviser: Prof. Nikolai Makarov

RESEARCH

Development, analysis, and application of tools for scientific machine learning.

NVIDIA Corporation, Santa Clara, CA, USA — Aug 2022 – Present

- Research Scientist

Development and application of operator learning methods to large-scale engineering problems. Focus on fluid simulations with complex geometries, global scale weather and climate simulations, and generative modeling for Bayesian inverse problems. Continued work on the approximation theory of operator learning methods as well as methods for measure transport. Developed highly-parallelized software, running on NVIDIA's supercomputer Selene.

California Institute of Technology, Pasadena, CA, USA — Oct 2016 – Jun 2022

- Research Assistant

Interdisciplinary work at the intersection of scientific computing, machine learning, applied math, and engineering. Invented and analyzed the first operator learning methods. Applied them to problems in fluid mechanics, quantum chemistry, materials modeling, and inverse imaging. Developed and analyzed methods for conditional sampling using transport maps with applications to Bayesian inverse problems and experimental design. Analyzed methods for optimization and data assimilation and applied them machine learning problems.

Entos Inc., Los Angeles, CA, USA — May 2020 – Aug 2020

- Machine Learning Researcher (Intern)

Development of state-of-the-art graph neural network based methods for the approximation of ground state energies of complex molecules. Research of representation learning techniques to improve generalization and allow more efficient exploration of chemical space. Much of the work developed here has been part of two patents. Entos was recently acquired by Iambic Therapeutics.

TEACHING

Wide-ranging experience leading and assisting various courses in applied and computational mathematics.

California Institute of Technology, Pasadena, CA, USA — May 2016 – Present

INSTRUCTOR

- Approximation Theory and Neural Networks (ACM 270-1) — 2023
  - Co-taught with Samuel Lanthaler

TEACHING ASSISTANT

- Clustering and Classification on Graphs (ACM 270-2) — 2020
- Linear Analysis with Applications (CMS/ACM/IDS 107) — 2017 – 2019
- Introduction to Probability Models (ACM/EE 116) — 2016
- Technical Seminar Presentations (E 10) — 2015 – 2016

AWARDS

- Amazon AI4Science Fellowship — 2020 – 2021
- Computing and Mathematical Sciences Graduate Student Fellowship — 2016 – 2017

PUBLICATIONS

JOURNAL PUBLICATIONS

[1] Bhattacharya K., Kovachki N.B., Rajan A., Stuart A.M., Trautner M., "Learning Homogenization for Elliptic Operators," Accepted: *SIAM Journal on Numerical Analysis*, arXiv:2306.12006, (2023).

[2] Li Z., Zheng H., Kovachki N.B., Jin D., Chen H., Liu B., Azizzadenesheli K., and Anandkumar A., "Physics-Informed Neural Operator for Learning Partial Differential Equations," Accepted: *ACM/IMS Journal of Data Science*, arXiv:2111.03794, (2023).

[3] de Hoop M.V., Kovachki N.B., Nelsen N.H., and Stuart A.M., "Convergence Rates for Learning Linear Operators from Noisy Data," *SIAM Journal on Uncertainty Quantification*, vol. 11, no. 2, (2023).

[4] Kovachki N.B., Li Z., Liu B., Azizzadenesheli K., Bhattacharya K., Stuart A.M., and Anandkumar A., "Neural Operator: Learning Maps Between Function Spaces," *Journal of Machine Learning Research*, vol. 24, no. 89, (2023).

[5] Kovachki N. B., Liu B., Sun X., Zhou H., Bhattacharya K., Ortiz M., Stuart A. M., "Multiscale Modeling of Materials: Computing, Data Science, Uncertainty and Goal-oriented Optimization," *Mechanics of Materials*, 165, (2022).

[6] Liu B., Kovachki N.B., Li Z., Azizzadenesheli K., Stuart A.M., Bhattacharya K., Anandkumar A., "A Learning-based Multiscale Method and its Application to Inelastic Impact Problems," *Journal of the Mechanics and Physics of Solids*, vol. 158, (2022).

[7] Kovachki N.B., Lanthaler S., Mishra S., "On Universal Approximation and Error Bounds for Fourier Neural Operators," *Journal of Machine Learning Research*, vol. 22, no. 290, (2021).

[8] Bhattacharya K., Hosseini B., Kovachki N.B., Stuart A.M., "Model Reduction and Neural Networks for Parametric PDE(s)," *The SMAI journal of computational mathematics*, vol. 7, (2021).

[9] Kovachki N.B., Stuart A.M., "Continuous Time Analysis of Momentum Methods," *Journal of Machine Learning Research*, vol. 22, no. 17, (2021)

[10] Cheng L., Kovachki N.B., Welborn M., and Miller T.F. III, "Regression-clustering for improved accuracy and training cost with molecular-orbital-based machine learning," *Journal of Chemical Theory and Computation*, vol. 15, no. 6668, (2019).

[11] Kovachki N.B., Stuart A.M., "Ensemble Kalman Inversion: A Derivative-Free Technique For Machine Learning Tasks," *Inverse Problems*, vol. 35, no. 9, (2019).

REFEREED CONFERENCE PROCEEDINGS

[12] Li Z., Kovachki N.B., Choy C., Li B,, Kossaifi J., Otta S.P., Nabian M.A., Stadler M., Hundt C., Azizzadenesheli K., Anandkumar A., "Geometry-Informed Neural Operator for Large-Scale 3D PDEs" Accepted: *37th Conference on Neural Information Processing Systems (NeurIPS)*, arXiv: 2309.00583, (2023).

[13] Li Z., Liu-Schiaffini M., Kovachki N.B., Liu B., Azizzadenesheli K., Bhattacharya K., Stuart A., Anandkumar A., "Learning Dissipative Dynamics in Chaotic Systems," *36th Conference on Neural Information Processing Systems (NeurIPS)*, (2022).

[14] Li Z., Kovachki N.B., Azizzadenesheli K., Liu B., Stuart A.M., Bhattacharya K., Anandkumar A., "Fourier Neural Operator for Parametric Partial Differential Equations," *9th International Conference on Learning Representations (ICLR)*, (2021).

[15] Li Z., Kovachki N.B., Azizzadenesheli K., Liu B., Stuart A.M., Bhattacharya K., Anandkumar A., "Multipole graph neural operator for parametric partial differential equations," *Advances in Neural Information Processing Systems 33*, (2020).

PREPRINTS

[16] Azzizadenesheli K., Kovachki N.B., Li Z., Liu-Schiaffini M., Kossaifi J., Anandkumar A., "Neural Operators for Accelerating Scientific Simulations and Design" Submitted: *Nature Reviews*, arXiv: 2309.15325, (2023).

[17] Liu-Schiaffini M., Singer C.E., Kovachki N.B, Schneider T., Azizzadenesheli A., Anandkumar A., "Tipping Point Forecasting in Non-Stationary Dynamics on Function Spaces," Submitted: *Transactions on Machine Learning Research*, arXiv:2308.08794, (2023).

[18] Baptista R., Hosseini B., Kovachki N.B., Marzouk Y., Sagiv A., "An approximation theory framework for measure-transport sampling algorithms," Submitted: *Mathematics of Computation*, arXiv:2302.13965, (2023).

[19] Baptsita R., Hosseini B., Kovachki N.B., Marzouk Y., "Conditional Sampling with Monotone GANs: from Generative Models to Likelihood-Free Inference," Submitted: *SIAM Journal on Uncertainty Quantification*, arXiv:2006.06755, (2023).

[20] Lim J.H., Kovachki N.B., Baptista R., Beckham C., Azizzadenesheli K., Kossaifi J., Voleti V., Song J., Kreis K., Kautz J., Pal C., Vahdat A., Anandkumar A., "Score-based Diffusion Models in Function Space," Submitted: *Journal of Machine Learning Research*, arXiv:2302.07400, (2023).

[21] Kossaifi J., Kovachki N.B., Azizzadenesheli K., Anandkumar A., "Multi-Grid Tensorized Fourier Neural Operator for High-Resolution PDEs," Submitted: *Transactions on Machine Learning Research*, arXiv:2310.00120, (2023).

[22] Li Z., Kovachki N.B., Azizzadenesheli K., Liu B., Stuart A.M., Bhattacharya K., Anandkumar A., "Neural Operator: Graph Kernel Network for Partial Differential Equations," arXiv:2003.03485, (2020).

INVITED TALKS & PRESENTATIONS

Machine Learning for Scientific Computing

- Packaging and Integration of Electronic and Photonic Microsystems (InterPACK). *Panelist*. Oct 2023

Generative Models on Function Space

- Biennial Meeting of SIAM Pacific Northwest Section (PNW). *Talk*. Oct 2023
- International Congress on Industrial and Applied Mathematics (ICIAM23). *Talk*. Aug 2023

Deep Learning on Function Spaces

- IC on Scientific Computation and Differential Equations (SciCADE). *Talk*. Jul 2022
- Deep Learning and Inverse Problems (INI MDLW02). *Talk*. Sep 2021
- Computation and Learning in High Dimensions (MFO). *Talk*. Aug 2021
- Foundations of Bayesian Inference for Complex Statistical Models (MFO). *Talk* (Virtual). May 2021
- SIAM Conference on Mathematics of Data Science (MDS20). *Talk* (Virtual). Jun 2020

Conditional Sampling via Measure Transport

- Second Symposium on Machine Learning and Dynamical Systems. *Talk* (Virtual). Sep 2020
- SIAM Conference on Imaging Science (IS20). *Talk* (Virtual). Jul 2020

Understanding Momentum through Continuous Time Analysis

- International Congress on Industrial and Applied Mathematics (ICIAM19). *Talk*. Jul 2019
- Applied Inverse Problems (AIP). *Talks*. Jul 2019
- Inverse Problems and Machine Learning (IPML). *Talk*. May 2019
- SIAM Conference on Applications of Dynamical Systems (DS19). *Talk*. May 2019

Ensemble Kalman Inversion for Machine Learning

- International Congress on Industrial and Applied Mathematics (ICIAM19). *Talk*. Jul 2019
- Applied Inverse Problems (AIP). *Talks*. Jul 2019
- SIAM Conference on Computational Science and Engineering (CSE19). *Talk*. Feb 2019
- Southern California Applied Mathematics Symposium (SOCAMS). *Poster*. Apr 2018
- UQ for Inverse Problems in Complex Systems (INI UNQW04). *Poster*. Apr 2018
- Inverse Problems and Machine Learning (IPML). *Talk*. Feb 2018

ORGANIZING

- SIAM Conference on Uncertainty Quantification (UQ22) Apr 2022
  Minisymposium: *Operator Learning in PDEs, Inverse Problems, and UQ*

PATENTS

- U.S. Patent 16/817,489: "Systems and Methods for Determining Molecular Structures with Molecular-Orbital-Based Features," *Filled* September 17, 2020.
- U.S. Patent 62/817,344: "Harvesting, Databasing, And Regressing Molecular-Orbital-Based Features For Accelerating Quantum Chemistry," *Filled* March 12, 2019.

SOFTWARE

- Neural Operator Library
  - https://github.com/neuraloperator/
- Torch Harmonics
  - https://github.com/NVIDIA/torch-harmonics/
- Earth-2 MIP
  - https://github.com/NVIDIA/earth2mip

REVIEWING

JOURNALS

Foundations of Computational Mathematics	2022 – Present
Journal of Machine Learning Research	2022 – Present
Journal of Computational Physics	2021 – Present
Quantum	2021 – Present
Neural Networks	2021 – Present
Inverse Problems	2020 – Present
Constructive Approximation	2020 – Present
SIAM Journal on Scientific Computing	2020 – Present

CONFERENCES

Neural Information Processing Systems (NeurIPS)	2021 – Present
International Conference on Machine Learning (ICML)	2021 – Present
International Conference on Learning Representations (ICLR)	2020 – Present
Mathematical and Scientific Machine Learning (MSML)	2020 – 2021

PROGRAMMING

- Python, Linux/Unix, MATLAB, Mathematica, Julia, C/C++

LANGUAGES

- English (fluent), Bulgarian (native).

PRIMARY REFERENCES

- **Professor Andrew M. Stuart**
  Bren Professor of Computing and Mathematical Sciences
  California Institute of Technology
  1200 E California Blvd, Pasadena, CA 91125
  astuart@caltech.edu • +1 (626) 395 4076

- **Professor Animashree Anandkumar**
  Bren Professor of Computing and Mathematical Sciences
  Director of Machine Learning Research at NVIDIA
  California Institute of Technology
  1200 E California Blvd, Pasadena, CA 91125
  anima@caltech.edu

- **Professor Kaushik Bhattacharya**
  Howell N. Tyson, Sr. Professor of Mechanics
  California Institute of Technology
  1200 E California Blvd, Pasadena, CA 91125
  bhatta@caltech.edu • +1 (626) 395 8306

ADDITIONAL REFERENCES

- **Professor Youssef M. Marzouk**
  Professor of Aeronautics and Astronautics
  Co-director, MIT Center for Computational Science and Engineering
  Director, Aerospace Computational Design Laboratory
  Massachusetts Institute of Technology
  77 Massachusetts Ave, Cambridge, MA 02139
  ymarz@mit.edu • +1 (617) 253 1337

- **Professor Siddhartha Mishra**
  Chair Professor of Applied Mathematics
  Director of Computational Science Zürich
  Faculty at the ETH AI Center
  ETH Zürich
  Rämistrasse 101, 8092 Zürich, Switzerland
  siddhartha.mishra@sam.math.ethz.ch • +41 44 632 75 63
- **Professor Maarten de Hoop**
  Simons Chair and Professor of Computational and Applied Mathematics
  Rice University
  6100 Main St, Houston, TX 77005
  mdehoop@rice.edu • +1 (713) 348 5723