Nikola B. Kovachki

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EDUCATION

California Institute of Technology, Pasadena, CA, USA

- Ph.D. in Applied and Computational Mathematics — Oct 2016 – Present
  - Cumulative GPA: 4.0/4.0
  - Adviser: Prof. Andrew M. Stuart
- B. Sc. in Mathematics — Oct 2012 – Jun 2016
  - Cumulative GPA: 3.9 / 4.0

RESEARCH EXPERIENCE

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

- Research Assistant
- Teaching Assistant

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

- Machine Learning Researcher (Intern)

PUBLICATIONS

PUBLISHED

[1] 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).

[2] 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).

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

[4] 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).

[5] 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).

[6] 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," *J. Chem. Theory Comput.*, vol. 15, no. 6668, (2019).

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

PREPRINTS

[1] Hoop M.V., Kovachki N.B., Nelsen N.H., and Stuart A.M., "Convergence Rates for Learning Linear Operators from Noisy Data," Submitted: *SIAM JUQ*, arXiv: 108.12515, (2021).

[2] Kovachki N.B., Li Z., Liu B., Azizzadenesheli K., Bhattacharya K., Stuart A.M., and Anandkumar A., "Neural Operator: Learning Maps Between Function Spaces," Submitted: *JMLR*, arXiv: 2108.08481, (2021).

[3] Li Z., Kovachki N.B., Azizzadenesheli K., Liu B., Stuart A.M., Bhattacharya K., Anandkumar A., "Markov Neural Operators for Learning Chaotic Systems," arXiv: 2106.06898, (2021).

[4] Kovachki N.B., Lanthaler S., Mishra S., "On Universal Approximation and Error Bounds for Fourier Neural Operators," Submitted: *JMLR*, arXiv: 2107.07562, (2021).

[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," Submitted: *JMPS*, arXiv: 2104.05918, (2021).

[6] Kovachki N.B., Baptsita R., Hosseini B., Marzouk Y., "Conditional Sampling With Monotone GANs," arXiv:2006.06755, (2020).

[7] 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).

AWARDS

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

INVITED TALKS & PRESENTATIONS

Deep Learning on Function Spaces

- 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
- The Aerospace Corporation. *Talk* (Virtual). — Dec 2020
- SIAM Conference on Mathematics of Data Science (MDS20). *Talk* (Virtual). — Jun 2020
- MEDE-ARL Fall Meeting. *Poster*. — Oct 2019
- MEDE-ARL Fall Meeting. *Poster*. — Oct 2018

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 (ICIAM). *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

Regression Clustering for Molecular Predictions

- CMS 273 (Schmidt Futures). *Talk*. — Mar 2019

Ensemble Kalman Inversion for Machine Learning

- International Congress on Industrial and Applied Mathematics (ICIAM). *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*

TEACHING

TEACHING ASSISTANTSHIP

- Clustering and Classification on Graphs (ACM 270-2) — 2020
- Linear Analysis with Applications (CMS/ACM/IDS 107) — 2019
- Linear Analysis with Applications (CMS/ACM/IDS 107) — 2018
- Linear Analysis with Applications (CMS/ACM/IDS 107) — 2017
- Introduction to Probability Models (ACM/EE 116) — 2016
- Technical Seminar Presentations (E 10) — 2016

REVIEWING

JOURNALS

- 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

- International Conference on Learning Representations (ICLR) 2021
- Neural Information Processing Systems (NeurIPS) 2021
- Mathematical and Scientific Machine Learning (MSML2021) 2021
- International Conference on Machine Learning (ICML) 2021
- International Conference on Learning Representations (ICLR) 2020
- Mathematical and Scientific Machine Learning (MSML2020) 2020

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.

SKILLS

- Python (numpy, scipy, sklearn, pytorch, pytorch-geometric)
- MATLAB
- Mathematica
- Julia
- C/C++

LANGUAGES

English (fluent), Bulgarian (native).

REFERENCES

- **Professor Andrew M. Stuart**
  Bren Professor of Computing and Mathematical Sciences
  California Institute of Technology
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- **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
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- **Professor Thomas F. Miller III**
  Professor of Chemistry
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