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] 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," Accepted: *Mechanics of Materials*, (2022).

[2] 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).

[3] 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).

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

[5] 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).

[6] 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).

[7] 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).

[8] 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] 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," Submitted: *ICLR 2022*, arXiv: 108.12515, (2021).

[2] 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).

[3] 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).

[4] 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).

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

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

[7] Li Z., <u>Kovachki N.B.</u>, 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

▪ Rough Paths Interest Group. *Talk* (Virtual).	Nov 2021
▪ 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) Minisymposium: *Operator Learning in PDEs, Inverse Problems, and UQ*	Apr 2022

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)	2022
	▪ 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
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▪ **Professor Animashree Anandkumar**
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▪ **Professor Thomas F. Miller III**
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