Yonatan Kurniawan

Postdoctoral Fellow · Materials Science & Engineering

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Education

PhD Physics *Provo, UT*

Brigham Young University *Jan 2022 - Aug 2025*

- Advisor: Mark K. Transtrum
- Dissertation: "Information-based uncertainty quantification and experimental design for sloppy models: foundation, theory, and application for interatomic potentials and beyond"
  I developed an information-matching method for optimal experimental design and active learning to strategically and efficiently identify training data that contain important information to achieve some predefined target precision of the target predictions that we want to make using the model.

MS Physics *Provo, UT*

Brigham Young University *Sep 2018 - Dec 2021*

- Advisor: Mark K. Transtrum
- Thesis: "Bayesian, Frequentist, and Information Geometry approaches to parametric uncertainty quantification of classical empirical interatomic potentials"
  I explored the effect of having sloppy, unidentifiable parameters in the interatomic potentials in uncertainty quantification (UQ) process, both in Bayesian and frequentist approaches. I found that the existence of sloppy, unidentifiable parameters in the model makes the UQ results to be very sensitive to the details of the calculation, such as the choice of prior and confidence level in Bayesian and frequentist methods.

BS Mathematics, BS Physics Education *Laie, HI*

Brigham Young University – Hawaii *Apr 2014 - Dec 2017*

Professional Experience

Oct. 2025 - Current	**Postdoctoral Fellow**, Dept. of Materials Science and Engineering, University of Toronto
Sept. 2018 - Aug. 2025	**Graduate Research Assistant**, Dept. of Physics and Astronomy, Brigham Young University
Sept. 2018 - Dec. 2023	**Graduate Teaching Assistant**, Dept. of Physics and Astronomy, Brigham Young University
Dec. 2017 - July 2018	**Private Tutor**, Yogyakarta, Indonesia
July 2017 - Nov. 2017	**Physics Student Teacher**, Sedes Sapientiae High School, Indonesia
Aug. 2016 - June 2017	**Undergraduate Teaching Assistant**, Faculty of Science, Brigham Young University – Hawaii

Teaching Experience

Teaching Assistant

Brigham Young University

- **PHSCS 580: Theory of Predictive Modeling**
  Fall 2023, Fall 2021, Fall 2018
- **PHSCS 641: Mathematical Theory of Electricity and Magnetism**
  Fall 2022

Teaching Assistant

Brigham Young University–Hawaii

- **PHYS 110: Conceptual Physics**
  Winter 2016/2017
- **PHYS 121/L: Introduction to Newtonian Mechanics & Lab**
  Spring 2017, Fall 2016
- **PHYS 220/L: Introduction to Electricity and Magnetism & Lab**
  Spring 2017, Fall 2016
- **PHYS 221/L: Introduction to Waves, Optics, and Modern Physics & Lab**
  Winter 2016/2017

Mentoring

2026 **Zhecheng Yin**, Undergraduate research assistant, University of Toronto
2021-2022 **Dylan Bailey**, Undergraduate research assistant, Brigham Young University
2019-2021 **Kinamo Jahali Williams Jr.**, Undergraduate research assistant, Brigham Young University

Computational Experience

Languages: Python, Mathematica, Julia, MATLAB, R
Materials science: KLIFF, KIM-API, ASE, LAMMPS, Quantum Espresso, VASP
Machine learning: Emcee, CVXPY, Scikit-Learn, JAX, Pytorch, TensorFlow
Other: Git, TeX, OpenMP, MPI
Operating Systems: Windows, Linux

Open Source Projects

** Owner; † Contributor*

Autonomous Reinforcement ECM Composer†

Github: https://github.com/AUTODIAL/AutoREC

- A platform for developing and deploying reinforcement learning agent for generating equivalent circuit models for electrochemical impedance spectroscopy.

Information-matching*

Gitlab: https://github.com/yonatank93/information-matching

- Codes and examples for information-matching method for optimal experimental design and active learning.

Profile Likelihood*

Gitlab: https://gitlab.com/yonatank93/profile_likelihood

- A Python package to compute profile likelihoods of a parameterized model.

Orchestrator†

Github: https://github.com/LLNL/orchestrator

- Integrate the Fisher information matrix and information-matching score modules.

ASE†

Gitlab: https://gitlab.com/ase/ase

- Implement utility functions to allow updating parameters in OpenKIM models.

KLIFF†

Github: https://github.com/openkim/kliff

- Integrate Bayesian MCMC and bootstrap sampling methods for uncertainty quantification.

MBAM†

Github: https://github.com/mktranstrum/MBAM

- Convert the existing code for Manifold Boundary Approximation Method to a Python package.

Professional Development

Uncertainty Quantification for Active Learning in Atomistic Modeling, Organized and chaired a session at the SIAM conference on Uncertainty Quantification 2024.

Using Uncertainty Quantification to Improve Learning in Atomistic Modeling, Organized and chaired a session at the SIAM conference on Mathematical Aspects of Materials Science 2024.

Publications

Published

Kurniawan, Y., Neilsen, T. B., Francis, B. L., Stankovic, A. M., Wen, M., Nikiforov, I., Tadmor, E. B., Bulatov, V. V., Lordi, V., & Transtrum, M. K. (2026). An information-matching approach to optimal experimental design and active learning. Applied Physics Letters, 128(6), 064104. https://doi.org/10.1063/5.0296026

Glatt-Holtz, N. E., Harris, R. A., Holbrook, A. J., Krometis, J., **Kurniawan, Y.**, Ringer, H., & Whitehead, J. P. (2025). Embracing Uncertainty in "Small Data" Problems: Estimating Earthquakes From Historical Anecdotes. *Journal of Geophysical Research: Machine Learning and Computation, 2(3)*, e2025JH000667. https://doi.org/10.1029/2025JH000667

Kurniawan, Y., Petrie, C. L., Transtrum, M. K., Tadmor, E. B., Elliott, R. S., Karls, D. S., & Wen, M. (2022). Extending OpenKIM with an Uncertainty Quantification Toolkit for Molecular Modeling. *2022 IEEE 18th International Conference on E-Science (e-Science)*, 367–377. https://doi.org/10.1109/eScience55777.2022.00050

Kurniawan, Y., Petrie, C. L., Williams, K. J., Transtrum, M. K., Tadmor, E. B., Elliott, R. S., Karls, D. S., & Wen, M. (2022). Bayesian, frequentist, and information geometric approaches to parametric uncertainty quantification of classical empirical interatomic potentials. *The Journal of Chemical Physics*, 156(21), 214103. https://doi.org/10.1063/5.0084988

Preprints

Jaberi, A., **Kurniawan, Y.**, Black, R., M, S. M., Verma, K., Sadighi, Z., Miret, S., & Hattrick-Simpers, J. (2026). AutoREC: A software platform for developing reinforcement learning agents for equivalent circuit model generation from electrochemical impedance spectroscopy data (arXiv:2604.27266). arXiv. https://doi.org/10.48550/arXiv.2604.27266

Kurniawan, Y., Wen, M., Tadmor, E. B., & Transtrum, M. K. (2025). Comparative study of ensemble-based uncertainty quantification methods for neural network interatomic potentials (No. arXiv:2508.06456). arXiv. https://doi.org/10.48550/arXiv.2508.06456

In Preparation

Yonatan Kurniawan, Logan Williams, Ilia Nikiforov, Amit Samanta, Ellad Tadmor, Vincenzo Lordi, Mark Transtrum, Vasily Bulatov. Inverse design of bespoke interatomic potentials via active learning by information-matching.

Presentations

** presenting author; + mentored undergraduate*

Invited Talks

Yonatan Kurniawan*, Mark Transtrum. 2024. Application of information geometry to uncertainty quantification: Insights and challenges. SIAM conference on Uncertainty Quantification. Trieste, Italy.

Yonatan Kurniawan*, Mark Transtrum. 2023. An information-matching method for efficient data selection in interatomic potential training. BYU Condensed Matter Seminar. Provo, UT.

Yonatan Kurniawan*, Mark Transtrum. 2023. An information-matching method for efficient data selection in interatomic potential training. BYU Discussion in Theoretical Physics. Provo, UT.

Yonatan Kurniawan*, Mark Transtrum. 2023. An information-matching method for efficient data selection in interatomic potential training. BYU Applied Math Seminar. Provo, UT.

Yonatan Kurniawan*, Mark Transtrum. 2023. Application of information geometry in studying the effect of sloppiness on uncertainty quantification. SIAM Northern states section conference. Logan, UT.

Yonatan Kurniawan*, Mark Transtrum. 2023. Bayesian, frequentist, and information geometric approaches to parametric uncertainty quantification of classical empirical interatomic potentials. BYU Discussion in Theoretical Physics. Provo, UT.