Curriculum Vitae – Katiana Kontolati

Last update: December 8, 2024

Appointment

Data Scientist, May 2023 - present
Research & Data Science Hub,
Bayer R&D

Contact Information

katiana.kontolati@gmail.com

Research Interests

Scientific machine learning, uncertainty quantification, modeling & simulation, large language modeling, digital twins, transfer learning, generative modeling, computational genomics.

Education

Johns Hopkins University, Baltimore MD, USA Aug. 2019 - April 2023
Doctor of Philosophy in Civil and Systems Engineering, G.P.A.: 3.90/4.0
Research areas: Physics-informed machine learning, uncertainty quantification

National Technical University of Athens, Athens, Greece Sept. 2017 - July 2019
Master of Science in Applied Mechanics, G.P.A.: 9.40/10.0
Major: Non-linear Dynamics

University of Thessaly, Volos, Greece Sept. 2012 - July 2017
Bachelor of Science in Civil Engineering, (5-year curriculum), G.P.A.: 8.90/10.0
Major: Structural Engineering, Numerical Analysis

Experience

Bayer R&D, Crop Science Division, St. Louis, MO May 2023 - present
Data Scientist, Genome Design Science

- Designing, training, and evaluating deep learning models on genomic data, optimizing them for crop selection, design, and mining within the breeding pipeline.
- Developed an internal DNA sequence language model to predict and prescribe genetic edits for specific traits and desired outcomes in crops.
- Leading a team within the Research & Data Science Hub to establish and maintain high-quality coding standards, fostering a collaborative culture around clean, scalable, and efficient code development.
- Mentoring and guiding summer interns and graduate students through university collaborations focusing on hands-on research projects, bridging academic learning with real-world industrial applications.

General Electric (GE) Research, Niskayuna, NY May 2022 - Aug. 2022
Research Engineer Intern, Probabilistic Design & Optimization

- Designed and developed a transfer learning framework to leverage multi-fidelity CFD simulation data of industrial gas turbines (IGT) for efficient aerodynamic assessment based on the airfoil shape design of turbine blades.
- Developed a time series analysis framework as part of a BWRX-300 small modular reactor Digital Twin to predict mechanical failure and optimize operation and proactive maintenance.
- Performed surrogate modeling on low-dimensional manifolds and improved predictive accuracy of hydrogen flame propagation in zero-emission hydrogen internal combustion engines (ICE).

Los Alamos National Laboratory, Los Alamos, NM Jun. 2021 - Aug. 2021
Applied Machine Learning Research Fellow, CCS-3

- Developed a framework for constructing neural density estimators with normalizing flows on spectral latent spaces for regression and uncertainty quantification in very high-dimensional experimental spectral data.
- Applied proposed framework to laser-induced breakdown spectroscopy (LIBS) spectra generated by the Mars Curiosity rover to predict the elemental composition of Martian rocks and soil with associated uncertainties.

- Presented work at NeurIPS 2021 Workshop on Machine Learning and the Physical Sciences.

Johns Hopkins University, Baltimore, MD — Aug. 2019 - Apr. 2023
Shields Uncertainty Research Group

- Conducted methodological research on predictive modeling based on latent representations using data-driven and physic-informed approaches. Open-sourced all codes on GitHub.
- Implemented proposed techniques for a variety of applications including parameterizing macroscopic models from atomistic simulation data and learning operators of non-linear PDEs describing complex physico-chemical processes.
- Published 6 papers (5 first-author, 1 under review) in top peer-reviewed journals and presented in 6 International Conferences.
- Co-developer of **UQpy** (Uncertainty Quantification with python), a general purpose Python toolbox for modeling uncertainty in physical and mathematical systems. Contributed to the *Dimension Reduction* and *Surrogates* modules.

Aktor S.A., Athens, Greece — June. 2016 - Sept. 2016
Construction Management Intern

- Oversaw the entire planning and building process of the retrofitting of the Akron Ilion Krystal building and reported the quality of performance on site to all site construction managers.
- Developed CAD drawings, calculated final material quantities and costs and performed preliminary engineering reviews on the detailed construction and demolition plan drawings.
- Utilized structural and earthquake engineering software SAP2000, for preliminary numerical analysis of structural elements during the demolition process.

Honors & Awards

Mark O. Robbins Prize in High Performance Computing — July 2023
Advanced Research Computing at Hopkins, Johns Hopkins University
Grant of $3,000 for demonstrating outstanding achievement in HPC research [article]

Rising Stars in Computational and Data Sciences — Feb. 2023
UT Austin, Sandia National Labs and Lawrence Livermore National Lab [article]

Gerondelis Foundation Graduate Scholarship — Jan. 2023
Grant of $5,000 received for demonstrating outstanding academic performance [article]

Society for Industrial and Applied Mathematics (SIAM) Travel Award — Jan. 2023
Conference on Computational Science and Engineering, Amsterdam, The Netherlands

National Science Foundation (NSF) Student Funding — Oct. 2022
Society of Engineering Science (SES) 2022 Conference, Texas A&M University

National Science Foundation (NSF) Fellowship — Sept. 2021
MMLDT-CSET Conference, San Diego, California

Teaching Assistant Award — May 2021
Department of Civil and Systems Engineering, Johns Hopkins University

Applied Machine Learning Summer Research Fellowship — Feb. 2021
Los Alamos National Laboratory

Joseph Meyerhoff Fellowship — Aug. 2019
Whiting School of Engineering, Johns Hopkins University

Graduate Research Fellowships — Mar. 2019
Cornell University & ETH Zürich (declined)

COST Travel Grant — Apr. 2017
European Cooperation in Science & Technology, Action TU 1304

Invited Talks

Lawrence Livermore National Lab, Data Science Institute (DSI) Seminar [video] — May 2023
UT Austin, Oden Institute for Computational Engineering and Sciences, Austin TX — Apr. 2023
Halliburton, Computational Sciences and Engineering for Energy, Houston TX — Dec. 2022
General Electric (GE) Research, Probabilistics Seminar, Niskayuna NY — Oct. 2021

Brown University, CRUNCH Seminar, Division of Applied Math., Providence RI Sept. 2021
Dynamical Systems and Complexity, 26^{th} Summer School, Athens Greece Jul. 2019

Publications

Journal Publications (* denotes equal contribution)

1. **Kontolati, K.***, Goswami, S.*, E. Karniadakis, G., D. Shields, M. (2024). Learning nonlinear operators in latent spaces for real-time predictions of complex dynamics in physical systems. *Nature Communications*, 15(1), 5101. https://doi.org/10.1038/s41467-024-49411-w.
2. Tsapetis, D., Shields, M.D., Giovanis, D.G., Olivier, A., Novak, L., Chakroborty, P., Sharma, H., Chauhan, M., **Kontolati, K.**, Vandanapu, L. and Loukrezis, D., (2023). UQpy v4. 1: Uncertainty Quantification with Python. *SoftwareX*, Vol. 24, 101561. https://doi.org/10.1016/j.softx.2023.101561.
3. **Kontolati, K.***, Goswami, S.*, D. Shields, M., E. Karniadakis, G. (2023). On the influence of over-parameterization in manifold based surrogates and deep neural operators. *Journal of Computational Physics*, 112008. https://doi.org/10.1016/j.jcp.2023.112008.
4. Goswami, S.*, **Kontolati, K.***, D. Shields, M., E. Karniadakis, G. (2022). Deep transfer operator learning for partial differential equations under conditional shift. *Nature Machine Intelligence*, 1-10. https://doi.org/10.1038/s42256-022-00569-2.
5. **Kontolati, K.**, Loukrezis, D., Giovanis, D. G., Vandanapu, L., Shields, M. D. (2022). A survey of unsupervised learning methods for high-dimensional uncertainty quantification in black-box-type problems. *Journal of Computational Physics*, 111313. https://doi.org/10.1016/j.jcp.2022.111313.
6. R. M. dos Santos, K., Giovanis D., Loukrezis, D., **Kontolati, K.**, D. Shields M. (2022). Grassmannian diffusion maps based surrogate modeling via geometric harmonics. *International Journal for Numerical Methods in Engineering*, 1-23. https://doi.org/10.1002/nme.6977.
7. **Kontolati, K.**, Loukrezis, D., Giovanis, D., M. dos Santos, K., D. Shields, M. (2022). Manifold learning-based polynomial chaos expansions for high-dimensional surrogate models. *International Journal for Uncertainty Quantification*, 12(4): 39-64. https://doi.org/10.1615/Int.J.UncertaintyQuantification.2022039936.
8. **Kontolati, K.**, Alix-Williams, D., Boffi, N. M., Falk, M. L., Rycroft, C. H., and Shields, M. D. (2021). Manifold learning for coarse-graining atomistic simulations: Application to amorphous solids. *Acta Materialia*, 215, 117008. https://doi.org/10.1016/j.actamat.2021.117008.
9. **Kontolati, K.** and Siettos, C. (2019). Numerical analysis of mesenchymal stem cell mechanotransduction dynamics reveals homoclinic bifurcations. *International Journal of Non-Linear Mechanics*, 113, 146-157. https://doi.org/10.1016/j.ijnonlinmec.2019.04.001.

Conference Proceedings

1. Charalampopoulos A., T., Cryan E., **Kontolati, K.**, Pickering E. (2024). Advancing AI Genotype-Phenotype Modeling for Crop Science, *Plant and Animal Genome Conference*, San Diego, California, USA, January 12-17.
2. **Kontolati, K.**, Goswami, S., E. Karniadakis, G., D. Shields, M. (2023). Transfer and multi-task learning in physics-based applications with deep neural operators, *SIAM Conference on Computational Science and Engineering*, Amsterdam, The Netherlands, February 26-March 3.
3. **Kontolati, K.**, Tsilifis, P., Ghosh, S., Andreoli, V., D. Shields, M., Wang, L. (2023). Multi-fidelity metamodeling in turbine blade airfoils via transfer learning on manifolds, *AIAA SciTech Forum*, National Harbor, Maryland, USA, January 23-27.
4. **Kontolati, K.**, Goswami, S., E. Karniadakis, G., D. Shields, M. (2022). High-dimensional uncertainty quantification in overparameterized regimes, *Society of Engineering Science Annual Technical Meeting*, College Station, Texas, USA, October 16-19.
5. **Kontolati, K.**, Loukrezis, D., R. M. dos Santos, K., Giovanis, D., D. Shields, M. (2022). Manifold learning for forward and inverse UQ in high dimensions, *SIAM Conference on Uncertainty Quantification*, Atlanta, Georgia, USA, April 12-15.

6. **Kontolati, K.**, Klein, N., Panda, N., Oyen D. (2021). Neural density estimation and uncertainty quantification for laser-induced breakdown spectroscopy spectra, *NeurIPS 4th Workshop on Machine Learning and the Physical Sciences*. [paper], [poster].
7. **Kontolati, K.**, Loukrezis, D., Giovanis, D., R. M. dos Santos, K., D. Shields M. (2021). Nonlinear manifold-learning based dimensionality reduction for surrogate modeling and uncertainty quantification, *Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology*, San Diego, California, USA, September 26-29.
8. **Kontolati, K.**, L. Falk M., H. Rycroft C., D. Shields M. (2021). Atomistic-informed calibration of partial differential equations for material applications via machine learning. *SIAM Conference on Mathematical Aspects of Material Science*, Bilbao, Spain, May 17-28.
9. **Kontolati, K.**, Alix-Williams D., L. Falk M., H. Rycroft C., D. Shields M. (2021). Stochastic multi-scale material modeling via manifold learning. *4th International Conference on Uncertainty Quantification in Computational Sciences and Engineering*, Athens, Greece, June 27-30.
10. **Kontolati K.**, Koukouselis, A, Panagouli, O. (2017). Numerical investigation of weak-axis I profile connections, *9th Hellenic National Conference on Steel Structures*, Larissa, Thessaly, Greece, October 5-7.

Patents

Methods and Systems For Use in Trait Development in Agricultural Crops Oct. 2023
Inventors: Pickering E., Charalampopoulos A., **Kontolati K.**, Freitas Moreira F., Hahm K., Shi Z., Arp J., Ocheya S., Adhikari P., Fonseca J., Taramino G., Liu J., Gillespie M.
U.S. Patent (pending)

Teaching Experience

Gateway Computing: Python (EN.500.113) Fall 2021
Course Assistant, Johns Hopkins University

Introduction to Research (EN.560.511) Spring 2021
Teaching Assistant, Johns Hopkins University

Technical Skills

Languages: Python, FORTRAN, SQL
Software: PyTorch, Tensorflow, Mathematica, MSC Marc, AutoCAD 2D/3D
Operating Systems: Microsoft Windows, Apple MacOS, Linux/Unix
Cloud computing: Amazon Web Services (AWS), SageMaker
Software Development: UQpy (Uncertainty Quantification with Python)

Service & Leadership

Reviewer for peer-reviewed journals and conferences: 2022 - present
- International Conference on Machine Learning (ICML)
- Conference on Neural Information Processing Systems (NeurIPS)
- International Journal of Computational Fluid Dynamics (IJCFD)
- Journal of Computational Physics (JCP)

Graduate Representative Organization (GRO), Advocacy Chair, JHU 2020 - 2021
Homewood Council of Inclusive Excellence (HCIE), GS2F member, JHU 2020 - 2021
ISAH Ambassador @ Hopkins Education and Administration Committee, JHU 2020
Homewood Graduate Board (HGB) 2020
Representative Ph.D. student of Whiting School of Engineering, JHU
Machine Learning in Science & Engineering Conference 2020 2020
Volunteer, Columbia University

Personal Information

Date of birth: November 4, 1994
Place of birth: Athens, Greece
Nationality: Greek

Languages

English (fluent), **Greek** (native)