

APPOINTMENT	Senior Machine Learning Researcher, Engineering & Data Science, Bayer R&D	May 2023 - present
CONTACT INFORMATION	 katiana.kontolati@bayer.com  katianakontolati.com (personal website)  linkedin.com/in/katiana-kontolati (LinkedIn)	
RESEARCH INTERESTS	Biologically-informed machine learning, uncertainty quantification, modeling & simulation, large language modeling, digital twins, transfer learning, computational genomics.	
EDUCATION	Johns Hopkins University , Baltimore MD, USA <i>Doctor of Philosophy</i> in Civil and Systems Engineering, G.P.A.: 3.90/4.0 Research areas: Physics-informed machine learning, uncertainty quantification	Aug. 2019 - April 2023
	National Technical University of Athens , Athens, Greece <i>Master of Science</i> in Applied Mechanics, G.P.A.: 9.40/10.0 Major: Non-linear Dynamics	Sept. 2017 - July 2019
	University of Thessaly , Volos, Greece <i>Bachelor of Science</i> in Civil Engineering, (5-year curriculum), G.P.A.: 8.90/10.0 Major: Structural Engineering, Numerical Analysis	Sept. 2012 - July 2017
EXPERIENCE	Bayer R&D , Crop Science Division, St. Louis, MO Sr. Machine Learning Researcher, Engineering & Data Science	May 2023 - present
	<ul style="list-style-type: none"> • Designing biologically-informed machine learning models to enhance predictive performance and interpretability across multiple crops and agronomic traits. • 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 industrial applications. 	
	General Electric (GE) Research , Niskayuna, NY Research Engineer Intern, Probabilistic Design & Optimization	May 2022 - Aug. 2022
	<ul style="list-style-type: none"> • 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 Applied Machine Learning Research Fellow, CCS-3	Jun. 2021 - Aug. 2021
	<ul style="list-style-type: none"> • 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
Shields Uncertainty Research Group

Aug. 2019 - Apr. 2023

- 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 six papers (five first-author) in top peer-reviewed journals and presented research at six 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
Construction Management Intern

June. 2016 - Sept. 2016

- 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

Miretta Flytzani-Stephanopoulos Doctoral Thesis Achievement Award	Nov. 2025
Presented by The Circle of Hellenic Academics in Boston [website]	
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] UT Austin , Oden Institute for Computational Engineering and Sciences, Austin TX Halliburton , Computational Sciences and Engineering for Energy, Houston TX General Electric (GE) Research , Probabilistics Seminar, Niskayuna NY Brown University , CRUNCH Seminar, Division of Applied Math., Providence RI Dynamical Systems and Complexity , 26 th Summer School, Athens Greece	May 2023 Apr. 2023 Dec. 2022 Oct. 2021 Sept. 2021 Jul. 2019
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- PUBLICATIONS **Journal Publications** (* denotes equal contribution)
1. **Kontolati, K.**, Gladstone, R. J., Davis, I., Pickering, E. (2025). Biology-informed neural networks learn nonlinear representations from omics data to improve genomic prediction and interpretability. *arXiv preprint*. <https://arxiv.org/abs/2510.14970>.
 2. Kumar, V., Goswami, S., **Kontolati, K.**, D. Shields, M., E. Karniadakis, G. (2025). Synergistic learning with multi-task DeepONet for efficient PDE problem solving. *Neural Networks*, 184, 107113. <https://doi.org/10.1016/j.neunet.2024.107113>.
 3. **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>.
 4. Tsapetis, D., Shields, M.D., Giovanis, D.G., Olivier, A., Novak, L., Chakraborty, P., Sharma, H., Chauhan, M., **Kontolati, K.**, VandanaP, 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>.
 5. **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>.
 6. 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>.
 7. **Kontolati, K.**, Loukrezis, D., Giovanis, D. G., VandanaP, 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>.
 8. 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>.
 9. **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>.
 10. **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>.
 11. **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). Non-linear 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)