

APPOINTMENT	Senior Machine Learning Researcher, Engineering & Data Science, Bayer R&D	May 2023 - present
CONTACT INFORMATION	 <a href="mailto:katiana.kontolati@bayer.com">katiana.kontolati@bayer.com</a>  <a href="http://katianakontolati.com">katianakontolati.com</a> (personal website)  <a href="https://www.linkedin.com/in/katiana-kontolati">linkedin.com/in/katiana-kontolati</a> (LinkedIn)	
RESEARCH INTERESTS	Biologically-informed machine learning, uncertainty quantification, modeling & simulation, large language modeling, digital twins, transfer learning, computational genomics.	
EDUCATION	<p><b>Johns Hopkins University</b>, Baltimore MD, USA Aug. 2019 - April 2023  <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</p> <p><b>National Technical University of Athens</b>, Athens, Greece Sept. 2017 - July 2019  <i>Master of Science</i> in Applied Mechanics, G.P.A.: 9.40/10.0  Major: Non-linear Dynamics</p> <p><b>University of Thessaly</b>, Volos, Greece Sept. 2012 - July 2017  <i>Bachelor of Science</i> in Civil Engineering, (5-year curriculum), G.P.A.: 8.90/10.0  Major: Structural Engineering, Numerical Analysis</p>	
EXPERIENCE	<p><b>Bayer R&amp;D</b>, Crop Science Division, St. Louis, MO May 2023 - present  Sr. Machine Learning Researcher, Engineering &amp; Data Science</p> <ul style="list-style-type: none"> <li>• Designing biologically-informed machine learning models to enhance predictive performance and interpretability across multiple crops and agronomic traits.</li> <li>• Developed an internal DNA sequence language model to predict and prescribe genetic edits for specific traits and desired outcomes in crops.</li> <li>• Leading a team within the Research &amp; Data Science Hub to establish and maintain high-quality coding standards, fostering a collaborative culture around clean, scalable, and efficient code development.</li> <li>• Mentoring and guiding summer interns and graduate students through university collaborations focusing on hands-on research projects, bridging academic learning with industrial applications.</li> </ul> <p><b>General Electric (GE) Research</b>, Niskayuna, NY May 2022 - Aug. 2022  Research Engineer Intern, Probabilistic Design &amp; Optimization</p> <ul style="list-style-type: none"> <li>• 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.</li> <li>• 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.</li> <li>• Performed surrogate modeling on low-dimensional manifolds and improved predictive accuracy of hydrogen flame propagation in zero-emission hydrogen internal combustion engines (ICE).</li> </ul> <p><b>Los Alamos National Laboratory</b>, Los Alamos, NM Jun. 2021 - Aug. 2021  Applied Machine Learning Research Fellow, CCS-3</p> <ul style="list-style-type: none"> <li>• 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.</li> </ul>	

- 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	<b>Lawrence Livermore National Lab</b> , Data Science Institute (DSI) Seminar <a href="#">[video]</a>	May 2023
	<b>UT Austin</b> , Oden Institute for Computational Engineering and Sciences, Austin TX	Apr. 2023
	<b>Halliburton</b> , Computational Sciences and Engineering for Energy, Houston TX	Dec. 2022
	<b>General Electric (GE) Research</b> , Probabilistics Seminar, Niskayuna NY	Oct. 2021
	<b>Brown University</b> , CRUNCH Seminar, Division of Applied Math., Providence RI	Sept. 2021
	<b>Dynamical Systems and Complexity</b> , 26 <sup>th</sup> Summer School, Athens Greece	Jul. 2019

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., 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>.
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., 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>.
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	<b>Methods and Systems For Use in Trait Development in Agricultural Crops</b> Oct. 2023 Inventors: Pickering E., Charalampopoulos A., <b>Kontolati K.</b> , 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	<b>Gateway Computing: Python (EN.500.113)</b> Fall 2021 Course Assistant, Johns Hopkins University <b>Introduction to Research (EN.560.511)</b> Spring 2021 Teaching Assistant, Johns Hopkins University
TECHNICAL SKILLS	<b>Languages:</b> Python, FORTRAN, SQL <b>Software:</b> PyTorch, Tensorflow, Mathematica, MSC Marc, AutoCAD 2D/3D <b>Operating Systems:</b> Microsoft Windows, Apple MacOS, Linux/Unix <b>Cloud computing:</b> Amazon Web Services (AWS), SageMaker <b>Software Development:</b> <a href="#">UQpy</a> (Uncertainty Quantification with Python)
SERVICE & LEADERSHIP	<b>Reviewer for peer-reviewed journals and conferences:</b> 2022 - present <ul style="list-style-type: none"> <li>• International Conference on Machine Learning (ICML)</li> <li>• Conference on Neural Information Processing Systems (NeurIPS)</li> <li>• International Journal of Computational Fluid Dynamics (IJCFD)</li> <li>• Journal of Computational Physics (JCP)</li> </ul>

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

PERSONAL INFORMATION	<b>Date of birth:</b> November 4, 1994
	<b>Place of birth:</b> Athens, Greece
	<b>Nationality:</b> Greek

LANGUAGES	<b>English</b> (fluent), <b>Greek</b> (native)
-----------	------------------------------------------------