APPOINTMENT	Data Scientist, Genomics Modeling Crop Science Division Bayer R&D	May 2023 - present
CONTACT INFORMATION	800 N Lindbergh Blvd Creve Coeur, MO 63141 USA ✉ katiana.kontolati@gmail.com	
RESEARCH INTERESTS	Scientific machine learning, uncertainty quantification, modeling & simulation, digital twins, manifold learning, surrogate modeling, neural operators, transfer learning, generative modeling	

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, AI for Genome Modeling

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

- Conducting methodological research on predictive modeling based on latent representations using data-driven and physic-informed approaches. Open-sourcing all codes on GitHub.

- Implementing 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, 2 under review) in 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. Contributing 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	**Rising Stars in Computational and Data Sciences**	Feb. 2023

Rising Stars in Computational and Data Sciences   Feb. 2023
Organized by the UT Austin's Oden Institute for Computational Engineering Sciences, Sandia National Laboratories and Lawrence Livermore National Laboratory

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   **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, 26th Summer School, Athens Greece   Jul. 2019

PUBLICATIONS   **Journal Publications** (* denotes equal contribution)

1. **Kontolati, K.**, Goswami, S., E. Karniadakis, G., D. Shields, M. (2023). Learning in latent spaces improves the predictive accuracy of deep neural operators. (in preparation).

2. **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.

3. 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.

4. **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.

5. R. M. dos Santos, K., Giovanis D., Loukrezis, D., **Kontolati, K.**, D. Shields M. (2022). Grass-mannian diffusion maps based surrogate modeling via geometric harmonics. *International Journal for Numerical Methods in Engineering*, 1-23. https://doi.org/10.1002/nme.6977.

6. **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.

7. **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.

8. **Kontolati, K.** and Siettos, C. (2019). Numerical analysis of mesenchymal stem cell mechan-otransduction 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. **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.

2. **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.

3. **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.

4. **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.

5. **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].

6. **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.

7. **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.

8. **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.

9. **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.

Teaching Experience	**Gateway Computing: Python (EN.500.113)** Course Assistant, Johns Hopkins University	Fall 2021
	Introduction to Research (EN.560.511) Teaching Assistant, Johns Hopkins University	Spring 2021

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

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)