Last update: October 5, 2022

Sept. 2019 - present

Appointment Graduate Research Assistant

Shields Uncertainty Research Group

Department of Civil and Systems Engineering

Johns Hopkins University

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in linkedin.com/in/katiana-kontolati (LinkedIn)

github.com/katiana22 (GitHub)

RESEARCH INTERESTS

Applied machine learning, uncertainty quantification, neural operators, transfer learning, generative modeling, manifold learning, surrogates, physics-based predictive modeling

EDUCATION

Johns Hopkins University, Baltimore MD, USA

Aug. 2019 - May 2023 (expected)

Ph.D. in Civil and Systems Engineering

• Research areas: Physics-informed machine learning, uncertainty quantification

• Advisor: Michael D. Shields, Associate Professor

• G.P.A.: 3.88/4.0

National Technical University of Athens, Athens, Greece

Sept. 2017 - July 2019

M.Sc. in Applied Mechanics, G.P.A.: 9.40/10.0

Major: Non-linear Dynamics

University of Thessaly, Volos, Greece

Sept. 2012 - July 2019

Diploma in Civil Engineering, (5-year curriculum), G.P.A.: 8.90/10.0

Major: Structural Engineering, Numerical Analysis

Experience

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

Shields Uncertainty Research Group

- Developing methodologies based on low-dimensional manifold learning and deep learning for surrogate modeling and uncertainty quantification in high-dimensional stochastic systems. Open-sourcing all codes on GitHub.
- Implemented proposed techniques for a variety of applications including parameterizing macroscopic models from atomistic simulation data and learning solutions 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 5 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

Aug. 2019 - present

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	National Science Foundation (NSF) Student Funding Society of Engineering Science (SES) 2022 Conference, Texas A&M University	Oct. 2022
	National Science Foundation (NSF) Fellowship MMLDT-CSET Conference, San Diego, California	Sept. 2021
	Teaching Assistant Award Department of Civil and Systems Engineering, Johns Hopkins University	May 2021
	Applied Machine Learning Summer Research Fellowship Los Alamos National Laboratory	Feb. 2021
	Joseph Meyerhoff Fellowship Whiting School of Engineering, Johns Hopkins University	Aug. 2019
	Graduate Research Fellowships Cornell University & ETH Zürich (declined)	Mar. 2019
	COST Travel Grant European Cooperation in Science & Technology, Action TU 1304	Apr. 2017
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

Publications

Journal Publications (* denotes equal contribution)

- 1. Goswami, S.*, **Kontolati, K.***, D. Shields, M., E. Karniadakis, G., (2022). Deep transfer learning for partial differential equations under conditional shift with DeepONet. https://doi.org/10.48550/arXiv.2204.09810 (provisionally accepted in *Nature Machine Intelligence*).
- 2. **Kontolati, K.***, Goswami, S.*, D. Shields, M., E. Karniadakis, G., (2022). On the influence of over-parameterization in manifold based surrogates and deep neural operators. https://doi.org/10.48550/arXiv.2203.05071 (under review in *Journal of Computational Physics*).

- 3. **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.
- 4. 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.
- 5. 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.
- 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.
- 7. 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

- 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.
- 2. 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.
- 3. **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].
- 4. 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.
- 5. **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.
- 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.
- 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.

Invited Talks

General Electric (GE) Research, Probabilistics Seminar, Niskayuna NY
Oct. 2021
CRUNCH Seminar, Division of Applied Math., Brown University, Providence RI
Sept. 2021
Dynamical Systems and Complexity, 26th Summer School, Athens Greece
Jul. 2019

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: Conference on Neural Information Processing Systems (NeurIPS) International Journal of Computational Fluid Dynamics (IJCFD) Journal of Computational Physics (JCP) 	2022 - present
	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 Volunteer, Columbia University	2020
Personal	Date of birth: November 4, 1994	
Information	Place of birth: Athens, Greece	
	Nationality: Greek	
Languages	English (fluent), Greek (native), Japanese (learner)	