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Johns Hopkins University, Baltimore, MD
Shields Uncertainty Research Group

Aug. 2019 - present

- 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

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

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

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

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>.
6. **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

1. **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.
6. **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.
7. **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 , 26 th 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:	2022 - present
	• 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), Japanese (learner)	