Last update: December 6, 2022

Appointment Graduate Research Assistant

Sept. 2019 - present

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 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 - May 2023 (expected)

Ph.D. in Civil and Systems Engineering

• Research areas: Scientific machine learning, uncertainty quantification

• Advisor: Michael D. Shields, Associate Professor

• G.P.A.: 3.90/4.0

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

- 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

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

#### Publications

## **Journal Publications** (\* denotes equal contribution)

Teaching Assistant, Johns Hopkins University

- 1. Kontolati, K., Goswami, S., D. Shields, M., E. Karniadakis, G., (2022). Learning neural operators on latent spaces. (in preparation).
- 2. 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.
- 3. 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).

- 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-boxtype 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). 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.
- 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.
- 8. **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., Tsilifis, P., Ghosh, S., Andreoli, V., D. Shields, M., Wang, L. (2023). Multifidelity metamodeling in turbine blade airfoils via transfer learning on manifolds, AIAA SciTech Forum, National Harbor, Maryland, USA, January 23-27.
- 2. 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.
- 3. 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.
- 4. **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].
- 5. 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.
- 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.
- 8. **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<sup>th</sup> Summer School, Athens Greece Jul. 2019

TECHNICAL Languages: Python, FORTRAN, SQL SKILLS Software: PyTorch, Tensorflow, Mathematica, MSC Marc, AutoCAD 2D/3D Operating Systems: Microsoft Windows, Apple MacOS, Linux/Unix Software Development: UQpy (Uncertainty Quantification with Python) Reviewer for peer-reviewed journals: 2022 - present Service & Leadership • 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 Date of birth: November 4, 1994
Information Place of birth: Athens, Greece
Nationality: Greek

Languages English (fluent), Greek (native), Japanese (learner)