Curriculum Vitae – Katiana Kontolati

Last update: October 10, 2022

Appointment

Graduate Research Assistant — Sept. 2019 - present
Shields Uncertainty Research Group
Department of Civil and Systems Engineering
Johns Hopkins University

Contact Information

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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 — Aug. 2019 - present
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.
- Implementing 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 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

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. **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 learning for partial differential equations under conditional shift with DeepONet. https://doi.org/10.48550/arXiv.2204.09810 (provisionally accepted in *Nature Machine Intelligence*).
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*).

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). 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.
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 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). Nonlinear 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)