



# KATIANA KONTOLATI

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## Education

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### Johns Hopkins University

Aug. 2019 – present

*Ph.D. in Civil and Systems Engineering*

*Baltimore, MD*

- Research areas: Scientific machine learning, uncertainty quantification, stochastic simulation
- Advisor: Dr. Michael Shields
- G.P.A.: 3.85/4.0

### National Technical University of Athens

Sept. 2017 – July 2019

*M.Sc. in Applied Mechanics*

*Athens, Greece*

- Thesis: Bifurcations and stability in mesenchymal stem cell differentiation dynamics
- Advisors: Dr. Constantinos Siettos & Dr. Yannis Kominis
- G.P.A.: 9.40/10.0 (ranked 1<sup>st</sup>)

### University of Thessaly

Sept. 2012 – July 2017

*B.Sc. in Structural Engineering*

*Volos, Greece*

- Thesis: Numerical investigation of weak-axis I profile connections (Advisor: Dr. Euripides Mistakidis)
- G.P.A.: 8.87/10.0 (ranked 2<sup>nd</sup>)

## Experience

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### Los Alamos National Laboratory

June 2021 – Aug. 2021

*Applied Machine Learning Research Fellow, CCS-3*

*Los Alamos, NM*

- Developed a framework for constructing neural density estimators with normalizing flows on spectral latent spaces for regression and uncertainty quantification on very high-dimensional 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.
- Collaborated with team members using version control systems (Git) to organize modifications and assign tasks.

### Johns Hopkins University

Aug. 2019 – present

*Graduate Research Assistant, SURG Group*

*Baltimore, MD*

- 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 3 papers (2 first-author) 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.

June 2016 – Sept. 2016

*Construction Management Intern*

*Athens, Greece*

- 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

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**National Science Foundation 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*

**April. 2021**

## Teaching Experience

- **Gateway Computing: Python (EN.500.113)**, Lead Course Assistant, Johns Hopkins University **Fall 2020**
- **Introduction to Research (EN.560.511)**, Teaching Assistant, Johns Hopkins University **Spring 2021**

## Publications

### Journal Publications

1. **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. *arXiv:2203.05071* (under review).
2. **Kontolati, K.**, Loukrezis, D., Giovanis, D., Vandanapu, L., D. Shields M. (2022). A survey of unsupervised learning methods for high-dimensional uncertainty quantification in black-box-type problems. *arXiv:2202.04648* (under review).
3. R. M. dos Santos, K., Giovanis D., Loukrezis, D., **Kontolati, K.**, D. Shields M. (2021). Grassmannian diffusion maps based surrogate modeling via geometric harmonics. *International Journal for Numerical Methods in Engineering* (accepted).
4. **Kontolati, K.**, Loukrezis, D., Giovanis, D., M. dos Santos, K., D. Shields, M. (2021). Manifold learning-based polynomial chaos expansions for high-dimensional surrogate models. *International Journal for Uncertainty Quantification* (accepted).
5. **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*, 117008.
6. **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.

### Conference Proceedings

1. **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*.
2. **Kontolati, K.**, Loukrezis, D., R. M. dos Santos, K., Giovanis, D., D. Shields M. (2021). Manifold learning for forward and inverse UQ in high dimensions, *SIAM Conference on Uncertainty Quantification*, Atlanta, Georgia, USA, April 12-15.
3. **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.
4. **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.
5. **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.
6. **Kontolati, K.**, Alix-Williams D., L. Falk M., H., D. Shields M. (2020). A manifold learning approach to coarse-graining atomistic simulations of plastic deformation in amorphous solids. *10th International Conference on Multiscale Materials Modeling*, Baltimore MD, USA (postponed for 2022).
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.

## Talks

- General Electric (GE) Research Probabilistics Seminar, Niskayuna NY **Oct. 2021**
- CRUNCH Seminar, Division of Applied Mathematics, Brown University, Providence RI **Sept. 2021**
- Dynamical Systems and Complexity, 26<sup>th</sup> Summer School, Athens Greece **July 2019**

## Technical Skills

- **Languages:** Python, Fortran, SQL
- **Software:** PyTorch, Tensorflow, Mathematica, MSC Marc, AutoCAD 2D/3D
- **Operating systems:** Microsoft Windows, Apple MacOS, Linux/Unix

## Service / Leadership

- **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)**, Representative Ph.D. student of Whiting School of Engineering, JHU **2020**
- **Machine Learning in Science & Engineering Conference 2020**, Volunteer, Columbia University **2020**

## Languages

Greek (native), English (fluent), German (basic)