Katiana Kontolati

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Education

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^{st})

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^{nd})

Experience

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 5 papers (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. **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

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. 2017**

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 (* 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 (under review).
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).
3. **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. https://doi.org/10.48550/arXiv.2202.04648 (accepted for publication in the *Journal of Computational Physics*).
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.**, 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.
2. **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]
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.**, 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 Mathematics, Brown University, Providence RI **Sept. 2021**
- Dynamical Systems and Complexity, 26^{th} 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
- **Software development**: UQpy (Uncertainty Quantification with Python)

Service / Leadership

- **Reviewer for peer-reviewed journals,** Journal of Computational Physics **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),** 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), **Japanese** (learner)