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| APPOINTMENT            | Graduate Research Assistant<br>Shields Uncertainty Research Group<br>Department of Civil and Systems Engineering<br>Johns Hopkins University  | Sept. 2019 - present                                 |
| CONTACT<br>INFORMATION | 303 Latrobe Hall, 3400 N Charles St<br>Baltimore, MD 21218 USA<br>✉ <a href="mailto:kontolati@jhu.edu">kontolati@jhu.edu</a> (e-mail)<br>💻 <a href="http://katianakontolati.com">katianakontolati.com</a> (personal website)<br>in <a href="https://www.linkedin.com/in/katiana-kontolati">linkedin.com/in/katiana-kontolati</a> (LinkedIn)<br>📄 <a href="https://github.com/katiana22">github.com/katiana22</a> (GitHub)   |  |
| RESEARCH<br>INTERESTS  | Scientific machine learning, uncertainty quantification, modeling & simulation, digital twins, manifold learning, surrogate modeling, neural operators, transfer learning, generative modeling  |  |
| EDUCATION              | <b>Johns Hopkins University</b> , Baltimore MD, USA<br>Ph.D. in Civil and Systems Engineering <ul style="list-style-type: none"> <li>• Research areas: Physics-informed machine learning, uncertainty quantification</li> <li>• Advisor: Michael D. Shields, Associate Professor</li> <li>• G.P.A.: 3.90/4.0</li> </ul> <b>National Technical University of Athens</b> , Athens, Greece<br>M.Sc. in Applied Mechanics, G.P.A.: 9.40/10.0<br><b>Major:</b> Non-linear Dynamics   | Aug. 2019 - March 2023 (expected)                    |
|                        | <b>University of Thessaly</b> , Volos, Greece<br>Diploma in Civil Engineering, (5-year curriculum), G.P.A.: 8.90/10.0<br><b>Major:</b> Structural Engineering, Numerical Analysis   | Sept. 2017 - July 2019<br><br>Sept. 2012 - July 2019 |
| EXPERIENCE             | <b>General Electric (GE) Research</b> , Niskayuna, NY<br>Research Engineer Intern, Probabilistic Design & Optimization <ul style="list-style-type: none"> <li>• 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.</li> <li>• 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.</li> <li>• Performed surrogate modeling on low-dimensional manifolds and improved predictive accuracy of hydrogen flame propagation in zero-emission hydrogen internal combustion engines (ICE).</li> </ul> <b>Los Alamos National Laboratory</b> , Los Alamos, NM<br>Applied Machine Learning Research Fellow, CCS-3 <ul style="list-style-type: none"> <li>• 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.</li> <li>• 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.</li> <li>• Presented work at NeurIPS 2021 Workshop on Machine Learning and the Physical Sciences.</li> </ul> | May 2022 - Aug. 2022<br><br>Jun. 2021 - Aug. 2021    |

**Johns Hopkins University**, Baltimore, MD  
Shields Uncertainty Research Group

Aug. 2019 - present

- 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

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

**Rising Stars in Computational and Data Sciences** Feb. 2023  
Organized by the UT Austin's Oden Institute for Computational Engineering Sciences, Sandia National Laboratories and Lawrence Livermore National Laboratory

**Gerondelis Foundation Graduate Scholarship** Jan. 2023  
Grant of \$5,000 received for demonstrating outstanding academic performance

**Society for Industrial and Applied Mathematics (SIAM) Travel Award** Jan. 2023  
Conference on Computational Science and Engineering, Amsterdam, The Netherlands

**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., E. Karniadakis, G., D. Shields, M. (2022). Learning in latent spaces improves the predictive accuracy of deep neural operators. (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. *Journal of Computational Physics*, 112008. <https://doi.org/10.1016/j.jcp.2023.112008>.
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.**, Tsilifis, P., Ghosh, S., Andreoli, V., D. Shields, M., Wang, L. (2023). Multi-fidelity 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.
6. **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.
7. **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.

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| INVITED TALKS        | <b>General Electric (GE) Research</b> , Probabilistics Seminar, Niskayuna NY            | Oct. 2021      |
|                      | <b>CRUNCH Seminar</b> , Division of Applied Math., Brown University, Providence RI      | Sept. 2021     |
|                      | <b>Dynamical Systems and Complexity</b> , 26 <sup>th</sup> Summer School, Athens Greece | Jul. 2019      |
| TECHNICAL SKILLS     | <b>Languages:</b> Python, FORTRAN, SQL  |                |
|                      | <b>Software:</b> PyTorch, Tensorflow, Mathematica, MSC Marc, AutoCAD 2D/3D              |                |
|                      | <b>Operating Systems:</b> Microsoft Windows, Apple MacOS, Linux/Unix                    |                |
|                      | <b>Software Development:</b> UQpy (Uncertainty Quantification with Python)              |                |
| SERVICE & LEADERSHIP | <b>Reviewer for peer-reviewed journals:</b>   | 2022 - present |
|                      | • Conference on Neural Information Processing Systems (NeurIPS)                         |                |
|                      | • International Journal of Computational Fluid Dynamics (IJCFD)                         |                |
|                      | • Journal of Computational Physics (JCP)  |                |
|                      | <b>Graduate Representative Organization (GRO)</b> , Advocacy Chair, JHU                 | 2020 - 2021    |
|                      | <b>Homewood Council of Inclusive Excellence (HCIE)</b> , GS2F member, JHU               | 2020 - 2021    |
|                      | <b>ISAH Ambassador @ Hopkins</b> Education and Administration Committee, JHU            | 2020           |
|                      | <b>Homewood Graduate Board (HGB)</b>  | 2020           |
|                      | Representative Ph.D. student of Whiting School of Engineering, JHU                      |                |
|                      | <b>Machine Learning in Science &amp; Engineering Conference 2020</b>                    | 2020           |
| PERSONAL INFORMATION | <b>Date of birth:</b> November 4, 1994  |                |
|                      | <b>Place of birth:</b> Athens, Greece   |                |
|                      | <b>Nationality:</b> Greek   |                |
| LANGUAGES            | <b>English</b> (fluent), <b>Greek</b> (native), <b>Japanese</b> (learner)               |                |