

Uncertainty-aware Machine Learning Surrogates for Scientific Applications

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Computational science and engineering applications have benefited from surrogate modeling brought by significant advances in machine learning (ML). By design, these flexible and high-capacity models are able to capture nonlinear and multiscale behavior present in complex physical phenomena. However, training ML-based surrogates for scientific applications often faces the challenges of limited, noisy, or biased data, whether from experiments or high-fidelity simulations. Thus, uncertainty quantification (UQ) becomes a necessary component in both training these models and generating trustworthy predictions, e.g. in digital twin frameworks and decision-making under uncertainty. To tackle these challenges we welcome submissions that include topics related to:

- Surrogate construction in and discovery of low-dimensional latent spaces and low-rank approximations,
- Hierarchical surrogate models, e.g. mixture of experts,
- Surrogate models equipped with UQ via Bayesian approximations,
- Generative or stochastic surrogate models, both supervised and unsupervised,
- Forward propagation of surrogate uncertainties into quantities of interest, e.g. via optimal transport or normalizing flows,
- Uncertainty attribution and sensitivity analysis with respect to input uncertainties and surrogate errors,
- Probabilistic models for AI agents.