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PHYSICS-BASED DATA-DRIVEN MODELING AND UNCERTAINTY QUANTIFICATION IN COMPUTATIONAL MATERIALS SCIENCE AND ENGINEERING

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Advances in physics-based modeling are responsible for the generation of massive datasets containing rich information about the physical systems they describe. Efforts in Uncertainty Quantification (UQ), once an emerging area but now a core discipline of computational mechanics, serve to further enrich these datasets by endowing the simulation results with probabilistic information describing the effects of parameter variations, uncertainties in model-form, and/or their connection to and validation against physical experiments.

This MS aims to:

- 1. Highlight novel efforts to (A) Harness the rich datasets afforded by potentially multi-scale, multiphysics simulations for the purposes of uncertainty quantification; and (B) Develop physics-based stochastic models, solvers, and methodologies for identification, forward propagation, and validation;
- 2. Address modeling problems at multiple length-scales, ranging from the atomistic level to the component level, for a broad class of materials (including metals, metallic alloys, composites, polymers, and ceramics).

This includes, but is not limited to, efforts that:

- Merge machine learning techniques with physics-based models;
- Develop physics-based stochastic models and low dimensional representations of very high dimensional systems for the purposes of uncertainty quantification;
- Extract usable/actionable information from large, complex datasets generated by physics-based simulations;
- Develop active learning algorithms that exploit simulation data to inform iterative/adaptive UQ efforts;
- Develop stochastic solvers and sampling algorithms;
- Interpolate high-dimensional data for high-fidelity surrogate model development;
- Learn the intrinsic structure of physics-based simulation data to better understand model-form and its sensitivity;

- Develop new methodologies for model identification;
- Assess similarities/differences/sensitivities of physics-based models and validate them against experimental data.

The MS aims to span across applications of mechanics, with an emphasis placed on methodological developments that can be applied to physical systems of all types.