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NEW COMPUTATIONAL FRONTIERS IN MICROSTRUCTURE–SENSITIVE MATERIALS DESIGN 500,700,1200

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ABSTRACT

Due to recent advances in computational capabilities, there has been a great push towards the development of new algorithms and software to take advantage of state-of-the-art computing resources for materials design. These resources include high performance computing cluster/grid, cloud computing and emerging quantum computers. These new algorithms will be paramount in advancing the study of material science, specifically, concerning the new frontiers in microstructure sensitive materials design and advanced manufacturing [1]. Quantifying of shape, size, spatial distribution and microstructure textures and variation are central for determining the links between processing and microstructure, and between microstructure and properties.

This mini-symposium is devoted to new developments in computational materials science for modeling and designing materials with controlled microstructures. The main focus is on novel algorithms for large scale simulations involving multi-scale modeling, machine learning, optimization and uncertainty quantification to understand material behavior in length-scales ranging from microscale to the scale of engineering components. A non-exhaustive list of typical topics of interest for the mini-symposium are listed below:

1. Algorithms and software for multi-scale modeling of composites and polycrystalline materials taking into account location–specific microstructures.
2. New computational concepts for large-scale microstructure representation, quantification and model–building in spatial and temporal domains.
3. System identification techniques applied to material science, for instance, physics informed ma-

chine learning and deep learning for designing additive manufacturing processes.

4. Homogenization and localization model development, including the modifications of the current-state-of-the-art finite element models, fourier techniques, particle methods, one or multi-point probability descriptors for modeling conventional and additive manufacturing processes.
5. Computational algorithms for large scale inverse design problems developing computational process design solutions to tailor microstructures for prescribed material property distributions.
6. Computational/analytical techniques for uncertainty quantification and uncertainty propagation (modeling the propagation of the uncertainties across different length scales) [2], understanding the effects of the uncertainties in multi-scale materials design.
7. Multi-objective, multi-physics, and multi-disciplinary optimization for computational design of materials. Reduced and surrogate model development for material constitutive models, such as the application of crystal plasticity microstructural models for process optimization [3].
8. Emerging quantum algorithms for materials science including solvers for differential equations [4] and quantum artificial intelligence algorithms.

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