



SUBMIT AN ABSTRACT FOR THE FOLLOWING SYMPOSIUM

DATA-DRIVEN AND COMPUTATIONAL MATERIALS DESIGN

Algorithms Development in Materials Science and Engineering

A foundational aspect of Materials Science is to understand, characterize, and predict the underlying mechanisms and behaviors of materials. Computational modeling and simulation provide many critical insights in these efforts, but also require constant development, validation, and application of numerical techniques. This symposium invites abstracts on the development and application of novel algorithms for materials science and engineering. This year's symposium will especially focus on (but is not limited to) the following topical areas:

- Novel methodologies for data mining, machine learning, image processing, microstructure generation, high-throughput databases and experiments.
- Surrogate and reduced-order modeling, and extracting useful insights from large data sets of numerical and experimental results.
- Algorithm development to enhance or accelerate classical computational materials science tools including density functional theory, molecular dynamics, Monte Carlo simulation, dislocation dynamics, phase-field modeling, CALPHAD, crystal plasticity, and finite element analysis.
- Development of novel physics-based, multiscale, multi-physics materials modeling.
- Algorithm development for fusing and evaluating the quality of multimodal data and their incorporation into computational materials workflows.
- Algorithm development and accelerated simulations using next generation GPUs and quantum computing
- Data visualization of large datasets
- Uncertainty quantification, statistical metrics from image-based synthetic microstructure generation, model comparisons, and validation studies related to novel algorithms and/or methods in computational material science.
- Development of novel methodologies for the analysis and management of data, including best practices for 'FAIRization' of data (FAIR: Findable, Accessible, Interpretable, Reproducible), as well as best practices for research software development and dissemination.
- Development of benchmark for the verification and validation of novel materials-centric algorithms.

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