

Computing@PNNL SEMINAR

Data-Driven, Co-Designed Simulations and Experiments of Material Synthesis



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With concentrated efforts from the materials science community to develop new multifunctional materials using unique processing conditions, the need for modeling tools that accurately describe the physical phenomena at each length scale has only further been emphasized. To address challenges posed by these demands, Dr. Matouš will present an image-based (data-driven) multiscale framework for modeling the chemo-thermo-mechanical behavior of complex heterogeneous systems. This integrated computational approach combines macro- and micro-continuum representations with statistical techniques, nonlinear model reduction, and high-performance computing and exploits the instantaneous localization knowledge to decide where more advanced computations are required.

The hierarchically parallel HPC framework executes on hundreds of thousands of processing cores with exceptional scaling performance and features a strategy for constructing a complex computational domain. This work also includes an integrated verification and validation/uncertainty quantification program with co-designed simulations and experiments.



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