ML-driven Models for Microstructure Simulation and Multi-scaling

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Machine learning (ML) provides enormous opportunities to augment materials characterization data and to provide fast surrogates to enable multi-scale modeling of materials. After a brief introduction to the challenges of an integrated AI-driven materials approach, this talk will cover two themes: 1) digital generation of ensembles of microstructures that represent key features of the limited experimentally obtained microstructures; and 2) ML models that provide rapid representation of micro-scale behavior in two-phase materials. The first challenge of digitally generating microstructures requires that the simulation process captures all the salient features of the microstructure, which may or may not be addressed by simply considering 2- or even n-point correlations. Furthermore, extrapolating from two-dimensional images of experimentally obtained microstructure to digitally generated three-dimensional images is possible using this technique. Specifically, we us a transfer learning approach to rapidly generate three-dimensional microstructures describing different families of material microstructures. The second challenge of leveraging physics-based analyses makes use digitally generated microstructures, to create training data. ML models that connect microstructure to properties and/or contour plots of local stresses, strains and damage accelerate the analyses by orders of magnitude when compared to purely physics-based FEM models. These accelerated representations are particularly important in the context of materials design, in which rapid assessment of samples from a very high-dimensional design space is necessary for any realistic optimization approach. These representations also support real-time decisions in the context of high-throughput experimentation on materials.