

Abstract Submitted  
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**Grain Scale Modeling - Impact of Constitutive Models** COLE YARRINGTON, AIDAN P. THOMPSON, TZU-RAY SHAN, RYAN WIXOM, Sandia National Labs — There are many model considerations that are unique to the grain-scale continuum approach. Most of these considerations revolve around the treatment of continuum model parameters, now applied to the fully dense matrix of material with dispersed discrete heterogeneous features. An example of this is how the equation of state (EOS) for a grain scale material must be the fully dense EOS, as opposed to the bulk EOS measured at lower densities. This poses unique validation and parameterization challenges, as most experimental data is gathered for bulk materials. We show how different theoretical tools for smaller length scales (MD, DFT-MD) can be used to calibrate the necessary models to achieve accurate simulation results.

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