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Addressing the gap between meso(grain) and continuum scales with stochastic burn models and probability density function theory[1]

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Within the energetics community, considerable effort is being directed to find a robust scale-bridging link between the unreacted material microstructures and the observed material responses, e.g. detonation and sub- detonative phenomena. One area of active research is mesoscale modeling of explosives initiation (MMEI); here, microstructures are imported directly or as statistical reconstructions into a hydrocode. While MMEI is attractive for simulating the ignition process with ever-increasing model fidelity, a large gap remains between the data being generated at the mesoscale and the calibration of burn model parameters. In this work, we begin to explore and apply scale-bridging techniques found in other fields. This includes particle methods from granular and droplet-laden flows, that use stochastic Langevin-type equations. Further parallels are drawn to turbulent combustion modeling, which leads to preliminary developments using probability density function (pdf) theory by Baer. In order to implement these new scale-bridging concepts, one example of a stochastic burn model is explained in greater detail. Results from the stochastic burn model and numerical method of particle-averaged characteristics (MOPAC) are given to illustrate the approach. Overall, if stochastic continuum-level models are adopted, then the pdf distributions from MMEI could function as the missing scale-bridging link. I.e., the stochastic (random, aleatoric) fluctuations would be sampled from a pdf distribution representative of the thermodynamic states found in an MMEI calculation. Ultimately, the execution of this scale-bridging work will be a community endeavor; to achieve such a capability, research efforts should focus on full-field data mining and pdf evolution in addition to new numerical techniques for hydrocodes.

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