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**Multiscale Modeling of Plastic Bonded Explosives** GRANT SMITH, DMITRY BEDROV, University of Utah, OLEG BORODIN — We have developed a multiscale modeling paradigm for the prediction of the viscoelastic properties, equation of state and yielding behavior of plastic bonded explosives (PBXs). In our multiscale modeling approach the components of the explosive (e.g., energetic material, metal and binder) are explicitly resolved and the material point method (MPM) is utilized to predict the response of the composite material to loading (isentropic, shock, etc.). This data are then utilized to develop equation-of-state and constitutive models for the PBX. The properties of the components are determined either from atomistic simulations or are taken from the literature. Force fields for the atomistic simulations in turn have been developed based upon high-level electronic structure calculations of model compounds and molecular complexes. Hence, our multiscale simulation approach systematically bridges length scales from atomistic to macroscopic. Applications of this approach to PBX-9501 and other PBXs will be considered.

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