

Abstract Submitted
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Hierarchical Multi-Scale Framework for Materials Modeling: Equation of State Implementation and Application to a Taylor Anvil Impact Test of RDX BRIAN BARNES, CARRIE SPEAR, KEN LEITER, RICHARD BECKER, JAROSLAW KNAP, US Army Research Laboratory, MARTIN LISAL, ICPF - Academy of Sciences of the Czech Republic, JOHN BRENNAN, US Army Research Laboratory — In order to progress towards a materials-by-design capability, we present work on a challenge in continuum-scale modeling: the direct incorporation of complex physical processes in the constitutive evaluation. In this work, we use an adaptive hierarchical multi-scale (HMS) framework running in parallel on a heterogeneous computational environment to couple a fine-scale, particle-based model computing the equation of state (EOS) to the constitutive response in a finite-element multi-physics simulation. The EOS is obtained from high-fidelity materials simulations performed via dissipative particle dynamics methods. This HMS framework is progress towards an innovation infrastructure that will be of great utility for systems in which essential aspects of the material response are too complex to capture by closed form material models. The design, implementation, and performance of the HMS framework are discussed. Also presented is a proof-of-concept Taylor anvil impact test of non-reacting 1,3,5-trinitroperhydro-1,3,5-triazine (RDX).

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