Predictive modeling and simulation of High Energy Density (HED) dynamic response of materials

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We developed the Optimal Transportation Meshfree (OTM) method based on a combination of Optimal Transportation theory, material point sampling and Local Maximum Entropy interpolation to address the difficulties in the simulation of HED dynamic response of materials. A variational material point failure algorithm is presented for predicting the fracture and fragmentation and is mathematically provable to converge to the solution of Griffith fracture theory. In addition, to predict material behavior in extremely high pressure, temperature and strain rate, a thermomechanical concurrent multiscale computational framework is introduced that allows for direct numerical simulation of polycrystalline structures coupled with void growth, single crystal plasticity, phase transformation, physics-based hardening and rate sensitivity laws, and First principles calculations of the Equation of State and material properties. We take the model-based UQ analysis to determine the error and uncertainties of our model in the applications of terminal ballistics and hypervelocity impacts.

**Keywords:** HED, hypervelocity impact, OTM, material point failure, multiscale material modeling