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Multi-scale modeling of the shock response of energetic materials: Comparing HMX and TATB ANAS NASSAR, NIRMAL KUMAR RAI, OISHIK SEN, H. S. UDAYKUMAR, University of Iowa, UNIVERSITY OF IOWA TEAM — Hot spots in heterogenous energetic materials (HEs) are localized sites where self-sustaining chemical reactions are initiated. Hotspots in HEs subjected to shock loading can result from the closure of voids, cracks, or defects within the micro-structure, i.e. at the meso-scale. Macro-scale quantities of interest (QoIs), such as shock to detonation transition (SDT), run-to-detonation distance, and criticality hinge on the rates of chemical reactions initiated at meso-scale hotspots. In previous work, we developed multi-scale models coupling the meso- and macro-scales for pressed HMX. The bridge between scales is provided by surrogate models (a.k.a. metamodels) that encapsulate energy localization phenomena at hotspots. The work presented here compares metamodels for two HEs, viz. HMX and TATB, along with their criticality criteria. High resolution meso-scale calculations supply the input data to construct metamodels which facilitate comparison of the behaviors of the two different materials. The physics underlying the differences in sensitivity of the two materials is elucidated by the calculations of void collapse and hotspot ignition and growth in the two materials. Metamodels for the materials and the way in which macro-scale sensitivity relates to meso-scale physics are also revealed by the results obtained from this work.

Anas Nassar
University of Iowa

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