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Mesoscopic description of hot spot phenomena: a route for hybrid multiscale simulations

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We describe large scale simulations of hot spot phenomena in single TATB crystals within the DPDE framework. The mesoscopic DPDE model is calibrated on all atom simulations, and particular attention is given to the rate of heat exchange between intramolecular and intermolecular degrees of freedom, which control the non-equilibrium behaviour of the system. Simulations of pore collapse at different shock speeds and for different pore sizes are performed, and a criterium for the quantification of the hot spot energy is proposed. These results are considered as reference data for subsequent comparison with top down simulations of similar processes. We present a reformulation of the (hydrodynamic) SDPD method allowing a direct coupling with the DPDE model, then opening the route for hybrid multiscale simulations.