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A New Method for Large Scale Molecular Dynamics Simulations of Shock-Induced Ejecta Production on Petaflopic Computer OLIVIER DURAND, LAURENT SOULARD, CEA, DAM, DIF, F-91297 Arpajon, France — We propose a new method for modelling large scale shock-induced ejecta production using petaflopic molecular dynamics (MD) simulations. A copper crystal with a sinusoidal surface finish representative of the roughness arising from a machine polishing is divided into a bulk and a surface part. The bulk part is simulated using the Hugoniostat technique, which allows a very large number of particles to reach a Hugoniot equilibrium state in a short physical time by the mean of a quasi-equilibrium MD simulation. The surface part is simulated with the NVE ensemble in order to account for the non-equilibrium character of the ejection process. With this method, the particle size distribution generated by a system with 5×10^8 to 10^9 atoms and different depths of defect is studied. Our MD results show that the particle size distributions exhibit a power law scaling in good agreement with the percolation theory. This theory suggests that the production of ejecta clusters is due to large-scale fluctuations present near a critical point, where there is no dominant characteristic scale.

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