Abstract Submitted for the SHOCK11 Meeting of The American Physical Society

Dynamical coupling atomistic and continuum simulations GUOWU REN, Institute of Fluid Physics, China Academy of Engineering Physics, Mianyang, Sichuan, China, DIER ZHANG, XINGAO GONG, Key Laboratory for Computational Physical Sciences (MOE), Fudan University, Shanghai, China — Multiscale modeling makes simulations at large length and time scales feasible because of limiting capability of massively parallel computers. Here a dynamical multiscale method is implemented which couples the molecular dynamics method for atomistic region and atomic-based finite element method for continuum region, matching much better than conventional finite element method originating from linear elastic mechanics. As for spurious reflection induced by the coupled interface, a new damping method theoretically derived from filter principle is proposed, which dampens the reflection of high-frequency phonons while keeping the low-frequency phonons traveling. A serial of numerical simulations validate these schemes.

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Date submitted: 17 Feb 2011

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