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Multiscale simulation of the responses of discrete nanostructures to extreme loading conditions based on the material point method

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Abstract

A particle-based multiscale simulation procedure is being developed that includes a concurrent link between the Material Point Method (MPM) and Dissipative Particle Dynamics (DPD) and a hierarchical bridge from Molecular Dynamics (MD) to DPD. In this paper, an interfacial scheme is presented that can be used to effectively cast spatial discretization at different scales into a unified MPM framework. The advantage to the approach is that the interactions among discrete nanostructures under extreme loading conditions can be simulated without the need for master/slave nodes as required in the Finite Element Method and other similar mesh-based methods. The proposed multiscale simulation scheme is applied to representative cases: tensile extension of a single nanobar, isothermal compression of a cube-shaped nanoparticle in a high-pressure fluid, and the behavior of nanosphere pairs and nanosphere–nanorod assemblies in a confining fluid for different initial arrangements of the components. The concurrent DPD/MPM results are in good qualitative agreement with the predictions obtained using a DPD-only description and all-atom MD, but require much less computational time as compared to all-atom simulations.

Keywords: Coarse-grain; Nanoassemblies; High-pressure fluid; Interfacial treatment; Multiscale simulations

1. Introduction

The geometric (size and shape) effect [1–3] on the responses of discrete nanostructures to extreme loading conditions is of considerable interest due to the potential benefits in modern engineering applications such as nano/micro-electromechanical system (MEMS/NEMS) devices and nanothermite composites [4,5]. Such devices and nanostructured formulations are increasingly prevalent in both commercial and military applications that entail large stresses and accelerations and high ambient pressures [6–8]. Understanding the geometric effect requires knowing and understanding the fundamental mechanical properties, deformation mechanisms, and failure modes of discrete structures with different sizes and shapes. Deformation and failure evolution at the nanoscale are inherently multi-scale phenomena. As a specific example, composites of CuO nanorods and Al nanoparticles were synthesized by

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self-assembly. The result was a nanostructured thermite fuel and oxidizer assembly that yielded enhanced combustion propagation rates and pressure [9]. The dynamic response of such composites was simulated at the continuum level by formulating an equation of state (EoS) and coupling computational fluid dynamics and solid dynamics in a single domain [10]. The simulations in [10] were performed without explicit consideration of the nanostructural and atomic-scale features of the nanothermite. In reality, the behavior of nanothermite composites is affected by many factors, such as morphology and constituent particle sizes and shapes [9]. Therefore a high-fidelity, predictive simulation of nanothermite response would require a multiscale simulation capability.

Recently, the influences of impact velocity, sample size, and impactor/sample aspect ratio on the impact response of discrete metallic nanostructures were studied [2,11–13] by using molecular dynamics (MD) simulations. The results provided detailed atomic-scale information [11,14], but the length and time scales that could be studied were quite small such that direct comparison to experiments was not possible. The Material Point Method (MPM) [15] has been developed over the past two decades with an eye toward improved capabilities for simulating failure evolution [16], which generally requires the ability to treat multiple scales and interacting material phases [17]. The original MPM [15] was subsequently improved and specialized into several important forms such as the Generalized Interpolation Material Point (GIMP) method [18], the Convected Particle Domain Interpolation (CPDI) method [19] and the Dual Domain Material Point (DDMP) method [20]. These led to improved accuracy for predictions of the mechanical behavior of materials subjected to large deformations. Efforts have also been made to enable the study of multiscale problems using the MPM framework. A multi-level refinement scheme that couples MD to the GIMP method has been developed [21]. A hierarchical approach has been proposed in which material points at the fine level in the MPM are coupled directly with the atoms in an MD domain [22]. A sequential procedure has been developed to simulate high-speed impact phenomena by using the MPM with parameterized material properties obtained from MD [23]. However, little has been done to extend multiscale MPM simulations to cases involving interactions among discrete nano/micro structures with different sizes and shapes, such as spheres and rods as mentioned above for Al/CuO thermite.

We recently proposed a particle-based multiscale simulation procedure in which the Dissipative Particle Dynamics (DPD) method was linked hierarchically to MD and coupled concurrently with the MPM [24]. In that work it was shown that the DPD details could be effectively coarse-grained through the use of a MPM background grid. The resulting concurrent link between the MPM and DPD enabled a nearly seamless integration of constitutive modeling at the continuum level with DPD particle-based forcing functions. However, that study left open questions of how well the proposed method would work for more general cases involving multiple materials and phases, such as discrete nanostructures embedded in a confining fluid. In this paper, an effective interfacial scheme is described to cast spatial discretizations at different scales into a unified MPM framework. The approach enables simulations of interactions among discrete nanostructures under extreme loading conditions without invoking any master/slave nodes as would be required for analogous simulations within a finite element framework [25]. Representative examples, namely, the tensile extension of a nanobar, isothermal compression of a cube-shaped nanoparticle in a high-pressure fluid, and interactions between multiple discrete nanostructures embedded in a confining fluid are used to illustrate and validate the potential usefulness of the proposed concurrent DPD/MPM procedure.

2. A particle-based multiscale simulation procedure

The concurrent DPD/MPM scheme, with preliminary demonstration, was introduced in a recent publication [24]. The key equations and procedures from [24] are reproduced here for continuity of presentation in the present study. The essential features of the governing equations for MD, DPD, and the MPM are presented in Section 2.1. The proposed interfacial scheme for multiscale simulations is described in detail in Section 2.2. A systematic implementation of the multiscale simulation procedure is given in Section 2.3.

2.1. Governing equations at different scales

The classical Lagrangian equation of motion for a system of N particles can be written as

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\boldsymbol{q}}_{\boldsymbol{i}}}\right) - \left(\frac{\partial L}{\partial \boldsymbol{q}_{\boldsymbol{i}}}\right) = Q_i, \tag{1}$$