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

Shan Jiang,^{1,2} Zhen Chen,^{3,1*} Thomas D. Sewell,² and Yong Gan⁴

¹Department of Civil and Environmental Engineering, University of Missouri-Columbia, Columbia, MO 65211, USA

²Department of Chemistry, University of Missouri-Columbia, Columbia, MO 65211-7600, USA

³Department of Engineering Mechanics, Dalian University of Technology, Dalian 116024, China

⁴Department of Engineering Mechanics, Zhejiang University, Zhejiang 310027, China

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

* Authors to whom correspondence should be addressed. Email: chenzh@missouri.edu; jiangsha@missouri.edu

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 multiscale phenomena. As a specific example, composites of CuO nanorods and Al nanoparticles were synthesized by 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 a 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

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) - \left(\frac{\partial L}{\partial q_i} \right) = Q_i, \quad (1)$$

where q_i and $\dot{q}_i$ are generalized coordinates and velocities, respectively, and the Lagrangian function $L(\mathbf{q}, \dot{\mathbf{q}})$ is defined in terms of kinetic and potential energies (denoted as K and V) as follows:

$$L = K - V. \quad (2)$$

For the case of Cartesian coordinates Eq. (1) leads to Newton's equation of motion,

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = m_i \mathbf{a}_i = -\frac{\partial}{\partial \mathbf{r}_i} V(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) + \mathbf{F}_i \quad (3)$$

where m_i , $\mathbf{r}_i$, and $\mathbf{a}_i$ are, respectively, the mass, position, and acceleration vectors of particle i . The total potential energy V depends only on the relative particle positions, and $\mathbf{F}_i$ represents any external forces acting on the system (in which case the potential energy may depend on the particle positions in the lab frame). In most molecular dynamics (MD) simulations the particle trajectories are obtained by solving Newton's equations or, equivalently, Hamilton's equations.

The DPD method has been developed to capture physics at the mesoscale within a particle-based framework [26] by averaging over the conservative forces obtained from an all-atom description and including dissipation and random forces in the overall force expression. It is computationally more efficient than MD and, if applied with care, provides a path to incorporating salient mesoscale details that are otherwise inaccessible in continuum-level descriptions. The DPD governing equations for each coarse-grained particle i take the following form [27, 28]:

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = m_i \mathbf{a}_i = \mathbf{f}_i^C + \mathbf{f}_i^D + \mathbf{f}_i^R \quad (4)$$

$$\mathbf{f}_i^C = \sum_{i \neq j} -\nabla U(\mathbf{r}_{ij}) \mathbf{e}_{ij} \quad (5)$$

$$\mathbf{f}_i^D = \sum_{i \neq j} -\gamma_{ij} w^D(\mathbf{r}_{ij}) (\mathbf{v}_{ij} \cdot \mathbf{e}_{ij}) \mathbf{e}_{ij} \quad (6)$$

$$\mathbf{f}_i^R = \sum_{i \neq j} \sigma_{ij} w^R(r_{ij}) dW_{ij} \mathbf{e}_{ij} \quad (7)$$

where $\mathbf{f}_i^C$, $\mathbf{f}_i^D$, and $\mathbf{f}_i^R$ represent, respectively, the conservative force, dissipative force, and random force acting on particle i ; U is the inter-particle potential; and $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ and $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ are, respectively, the distance vector and relative velocity between particles i and j . The quantities γ_{ij} and σ_{ij} are coefficients that characterize the strengths of the non-conservative forces, w^D and w^R are distance-dependent weight functions for the dissipative and random forces, respectively, and W_{ij} describes independent one-dimensional Wiener processes. The quantity $\mathbf{e}_{ij} = \mathbf{r}_{ij} / |\mathbf{r}_{ij}|$ is the unit vector between particles i and j . The subscripts i and j run over all particles.

As a particle method based on a weak formulation similar to that used in the finite element method [15], the MPM discretizes a continuum body into a finite set of N_p material points (particles) that are tracked throughout the deformation process. The discretized equation for the MPM can be derived from the weak form of the equation of motion as follows:

$$\int_{\Omega} \rho \mathbf{w} \cdot \mathbf{a} d\Omega = - \int_{\Omega} \rho \mathbf{s}^s : \nabla \mathbf{w} d\Omega + \int_{S^c} \rho \mathbf{c}^s \cdot \mathbf{w} dS + \int_{\Omega} \rho \mathbf{w} \cdot \mathbf{b} d\Omega, \quad (8)$$

where $\mathbf{a}$ is the acceleration, $\mathbf{b}$ is the body force, ρ is the mass density, $\mathbf{w}$ is the test function, $\mathbf{s}^s$ is specific stress, Ω is the current configuration of the continuum body, and S^c is the part of the boundary subjected to a prescribed traction. A boundary layer can be used to enforce the moving traction boundary condition given by the prescribed traction vector $\mathbf{c}^s$. The final form of the discretized governing equation can be written as

$$m_i^t \mathbf{a}_i^t = (\mathbf{f}_i^t)^{int} + (\mathbf{f}_i^t)^{ext}, \quad (9)$$

where m_i^t and $\mathbf{a}_i^t$ are, respectively, the lumped mass and acceleration on the background mesh nodes i at a given time t . The quantities $(\mathbf{f}_i^t)^{int}$ and $(\mathbf{f}_i^t)^{ext}$ are, respectively, the internal nodal force and external nodal force on the background mesh.

2.2 Synopsis of the particle-based multiscale simulation procedure

It can be seen from Section 2.1 that Eqs. (3), (4), and (9) have similar forms although they are formulated at different scales and with different domains of influence (*e.g.*, cutoff radius or interpolation shape functions). Thus, it is numerically feasible to combine these different formulations within a single computational framework. The force expressions on the right-hand sides of these equations include the internal interactions among discrete particles (atoms, DPD particles, or material points) as well as external forces if present. The difference between the MPM and DPD or MD is that Eq. (9) is evaluated at the background grid nodes rather than at the material points (particles). As a result, the equation of motion in the MPM is solved on the background mesh. Instead of defining a representative domain (*i.e.*, a cutoff radius) as required in DPD and MD, the strain and stress fields in the MPM can be easily determined using, respectively, the gradient of nodal basis functions and the constitutive model. In the current work, a number of MD atoms are first coarse-grained into a single DPD particle, and then the DPD particles are combined with MPM particles in a single MPM background mesh. Ultimately, the DPD/MPM simulation is performed concurrently within the MPM framework. As illustrated in Fig. 1, the proposed multiscale simulation procedure consists of a hierarchical bridge from MD to DPD for nano- and submicron-scale phenomena and a concurrent link between the DPD and MPM particles to simulate micro- or macro-scale responses.

For the link between MD and DPD, a top-down procedure was used to derive the mesoparticle potential for the DPD particles. In the present study, face centered cubic (fcc) Cu is considered as a representative material. The Sutton-Chen [29] interatomic potential energy function for Cu was used for the MD simulations. The parameters in the DPD force expression were calibrated by using a genetic algorithm to optimize the fit between predictions from the Sutton-Chen atomic potential and an analogous coarse-grained form for the conservative part of the DPD force expression wherein one mesoparticle corresponds to eight copper atoms and the coarse-grained lattice parameter is twice the value for atomic Cu in the all-atom MD description [30]. Molecular dynamics simulations performed using only the coarse-grained conservative force (*i.e.*, Eq. (5), with Eqs. (6) and (7) defined to be zero) are hereafter referred to as coarse-grained MD (CG-MD), while simulations in which Eqs. (6) and (7) are included are referred to as DPD. The parameter γ in the DPD force expressions was set to 0.2 amu/ps. The coarse-grained conservative potential used here was obtained by fitting to the all-atom MD predictions for the 298 K isotherm. Additional details of the DPD parameterization are being published elsewhere [30].

A schematic depiction of the concurrent link between the DPD and MPM descriptions is shown in Fig. 2. The computational domain can be divided into two major regions, namely a DPD (mesoscale particle) region and an MPM (continuum-level particle) region. If it is needed, a third, intermediate region can be introduced in the neighborhood of the interface between the DPD and MPM regions. The treatment described here assumes that all three regions consist of the same substance (Cu). In the concurrent DPD and MPM computational domain, a particle is a DPD one if its force is defined by Eq. (4), which involves a cutoff distance. A particle is an MPM one if a constitutive model is used to calculate the internal force vector (see Eq. (9)).

Within the MPM framework, the DPD cutoff distance should be larger than the cell edge length. A single MPM cell can include both DPD and MPM particles at a given time such that the mapping and re-mapping procedure in the MPM algorithm yields a computational homogenization scheme over the cell domain.

After an entire structure is discretized into a finite set of material points (DPD or MPM) and all the state variables at these material points are initialized, the system of DPD/MPM particles should be equilibrated to minimize the stress in the initial system. After equilibration, but prior to subsequent simulations, an arbitrary background grid with appropriate spatial resolution needs to be defined. This grid is used to find the natural coordinates of any material point and to identify the grid cell that contains the material point. Each material point (whether DPD or MPM) carries its original material properties and is followed throughout the deformation process. The following section describes the specific solution steps required for a concurrent MPM and DPD simulation. Equations shown in Section 2.3 are numbered starting from Eq. (s-1) to describe the procedure for performing the concurrent multiscale time updates in a self-contained way. The presentation in Sec. 2.3 is modified slightly compared to [24] both for improved clarity and to correct minor typographical errors in the original presentation.

2.3 Numerical implementation of the concurrent DPD/MPM procedure

Step 1. For each material point (either DPD or MPM particle), perform the mapping operation from the material point to the cell nodes enclosing the material point,

$$m_i^t = \sum_{p=1}^{N_p} M_p N_i(\mathbf{x}_p^t), \quad (\text{s-1})$$

$$(\mathbf{mv})_i^t = \sum_{p=1}^{N_p} (\mathbf{Mv})_p^t N_i(\mathbf{x}_p^t), \quad (\text{s-2})$$

where m_i^t is the mass at node i at time t , M_p is the material point mass, N_i is the shape function associated with node i , $\mathbf{x}_p^t$ is the location of the material point at time t , $(m\mathbf{v})_i^t$ is the nodal momentum at node i at time t , and $(M\mathbf{v})_p^t$ is the material point momentum at that same time.

Step 2. Perform the calculations of the forces on the background nodes. For the MPM particles associated with the cell where they are located, the internal force vector at the cell nodes can be written as

$$(\mathbf{f}_i^t)^{int} = -\sum_{p=1}^{N_p} G_i(\mathbf{x}_p^t) \cdot \mathbf{s}_p^t \frac{M_p}{\rho_p^t}, \quad (\text{s-3})$$

in which $G_i(\mathbf{x}_p^t)$ is the gradient of the shape function associated with node i , evaluated at $\mathbf{x}_p^t$; $\mathbf{s}_p^t$ is the particle stress tensor at t ; and ρ_p^t is the particle mass density at t . For the DPD particles related to that cell, Eq. (s-3) is replaced with the following one:

$$(\mathbf{f}_i^t)^{int} = \sum_{p=1}^{N_p} (\mathbf{f}_{pj}^C + \mathbf{f}_{pj}^D + \mathbf{f}_{pj}^R) N_i(\mathbf{x}_p^t), \quad (\text{s-4})$$

where $\mathbf{f}_{pj}^C$, $\mathbf{f}_{pj}^D$, and $\mathbf{f}_{pj}^R$ represent, respectively, the conservative force, dissipative force, and random force acting on particle p by particle j ($j = 1, 2, \dots, N_p^j$, where N_p^j is the number of DPD particles within the cutoff radius of particle p).

For a single domain discretized using some combination of DPD and MPM particles, an interfacial treatment is necessary to interpolate the difference in the force descriptions for the two particle types. For the purpose of demonstration, the DPD and MPM particles are assumed here to have the same size (and to be composed of the same material, as noted above). If an

intermediate region is introduced then, instead of Eq. (s-3) and Eq. (s-4), the internal force in that region is calculated from the following equation:

$$\left(f_i^t\right)^{int} = \sum_{p=1}^{N_p^d} \left(f_{pj}^C + f_{pj}^D + f_{pj}^R\right) N_i\left(\mathbf{x}_p^t\right) - \sum_{p=N_p^d+1}^{N_p^d+N_p^m} \mathbf{G}_i\left(\mathbf{x}_p^t\right) \cdot \mathbf{s}_p^t \frac{M_p}{\rho_p^t}, \quad (\text{s-5})$$

where N_p^d and N_p^m are, respectively, the numbers of DPD and MPM particles within the interfacial region. The forces for DPD particles, that is, $\mathbf{f}_{pj}^C$, $\mathbf{f}_{pj}^D$, and $\mathbf{f}_{pj}^R$, and stress tensor $\mathbf{s}_p^t$ for MPM particles, are the same as those shown in Eqs. (s-3) and (s-4).

For DPD particles in the intermediate region (refer to Fig. 2) $\mathbf{f}_{pj}^C$, $\mathbf{f}_{pj}^D$, and $\mathbf{f}_{pj}^R$ are modified based on Eqs. (5)-(7) as follows:

$$\mathbf{f}_{pj}^C = \sum_{k=1, k \neq j}^{N_p^j} -\nabla U\left(\mathbf{r}_{jk}\right) \mathbf{e}_{jk} \quad (\text{s-6})$$

$$\mathbf{f}_{pj}^D = \sum_{k=1, k \neq j}^{N_p^j} -\gamma_{jk} w^D\left(\mathbf{r}_{jk}\right) \mathbf{v}_{jk} \quad (\text{s-7})$$

$$\mathbf{f}_{pj}^R = \sum_{k=1, k \neq j}^{N_p^j} \sigma_{jk} w^R\left(r_{jk}\right) dW_{jk} \mathbf{e}_j, \quad (\text{s-8})$$

where N_p^j is the total number of particles, including both DPD and MPM particles, within the cutoff radius of particle p . This treatment significantly reduces the force/displacement discontinuity at the interface between DPD and MPM regions, and yields a single nanostructure, composed of DPD and MPM sub-regions, that deforms as an integral body (demonstrated below in Section 4.1).

Step 3. Apply essential and natural boundary conditions to the cell nodes, compute the nodal force vector, and update the momenta at the cell nodes:

$$\mathbf{f}_i^t = (\mathbf{f}_i^t)^{int} + (\mathbf{f}_i^t)^{ext} \quad (\text{s-9})$$

$$(\mathbf{mv})_i^{t+\Delta t} = (\mathbf{mv})_i^t + \mathbf{f}_i^t \Delta t. \quad (\text{s-10})$$

Step 4. For each material point, perform the mapping operation from the nodes of the cell containing the material point to that point. Map the nodal accelerations and current nodal velocities back to the material point:

$$\mathbf{a}_p^t = \sum_{i=1}^{N_n} \frac{\mathbf{f}_i^t}{m_i^t} N_i(\mathbf{x}_p^t) \quad (\text{s-11})$$

$$\bar{\mathbf{v}}_p^{t+\Delta t} = \sum_{i=1}^{N_n} \frac{(\mathbf{mv})_i^{t+\Delta t}}{m_i^t} N_i(\mathbf{x}_p^t). \quad (\text{s-12})$$

Next, compute the current material point position and displacement:

$$\mathbf{x}_p^{t+\Delta t} = \mathbf{x}_p^t + \bar{\mathbf{v}}_p^{t+\Delta t} \Delta t \quad (\text{s-13})$$

$$\mathbf{u}_p^{t+\Delta t} = \mathbf{x}_p^{t+\Delta t} - \mathbf{x}_p^0. \quad (\text{s-14})$$

Step 5. Map the updated material point momenta back to the nodes of the cell containing the material points, and then find the updated nodal velocities:

$$(\mathbf{mv})_i^{t+\Delta t} = \sum_{p=1}^{N_p} (\mathbf{Mv})_p^{t+\Delta t} N_i(\mathbf{x}_p^t) \quad (\text{s-15})$$

$$\mathbf{v}_i^{t+\Delta t} = \frac{(\mathbf{mv})_i^{t+\Delta t}}{m_i^t}. \quad (\text{s-16})$$

Step 6. Apply the essential boundary conditions to the nodes of the cells containing the boundary points.

Step 7. For an MPM particle, find the current gradient of particle velocity and the particle strain increment so that the stress increment can be obtained from the constitutive model to update the stress tensor of the MPM particle:

$$\mathbf{s}_p^{t+\Delta t} = \mathbf{s}_p^t + \Delta \mathbf{s} . \quad (\text{s-17})$$

The stress tensor of the MPM particle (s-17) will be used in Eq. (s-3) in the next time step to evaluate the internal force on the nodes. For a DPD particle, go directly to the next step.

Step 8. Identify which grid cell each material point belongs to, and update the natural coordinates of the material point. This is the convective phase for the next time increment. If the required termination time has not been reached, go to **Step 1** to perform the next time increment.

The numerical procedure presented above and in [24] applies equally to DPD and MPM particles, meaning that both can be simulated concurrently within the overarching MPM framework. We note that for the interfacial treatment, Eqs. (s-6) to (s-8) above require that each DPD particle inside the interfacial region is subject to the interactions with all MPM particles within the cutoff radius of that DPD particle. Also, Eq. (s-5) includes the internal force contributions from particles of both types located within the interfacial region, so that each interfacial MPM particle is coupled with any neighboring DPD particles *via* the mapping and re-mapping process within the MPM framework.

The main application in [24] was a demonstration that, when the method is applied solely to DPD particles—the so-called “DPD/MPM-grid model” in [24], in which the MPM mapping/re-mapping algorithm is used to propagate the DPD particle motions—it closely, although not identically, reproduces the results obtained using standard energy-conserving DPD. We also showed some preliminary results pertaining to the DPD/MPM interfacial treatment. Below we present additional verification calculations and various applications that provide a systematic validation of the concurrent DPD/MPM procedure. We also characterize the computational efficiency of the procedure in comparison to other numerical methods.

3 Computational set-ups for example problems

Computational set-ups for several prototypical applications are presented in this section to illustrate the proposed multiscale simulation procedure and to demonstrate its capability for simulating assemblies of discrete nanostructures under extreme loading conditions. Results of the simulations are presented in Section 4. Examples studied include the tensile extension of a nanorod, isothermal compression of a single cube-shaped nanoparticle in a high-pressure fluid, and the behavior of discrete nanosphere-nanosphere and nanosphere-nanorod assemblies embedded in a confining fluid. The DPD force expression used in these simulations was summarized in Section 2.2 and further details will be provided in [30]. The force cutoff radius and reference temperature for DPD particles were set to 12 Å and 298 K, respectively. The time step for the concurrent DPD/MPM simulations was set to 10 fs.

3.1 Nanobar subjected to tensile strain

We consider a Cu nanobar with square cross section under tensile strain to demonstrate how DPD and MPM subdomains can be treated concurrently and nearly seamlessly in a single simulation domain. As discussed above, particular attention is focused on the development of an effective interfacial scheme for use in simulations of a single structure wherein different regions within the structure are described using different model representations. The concurrent DPD/MPM model for the finite-length nanorod was constructed with two “virtual” interfaces as shown in Fig. 3. The nanobar size is $578 \text{ Å} \times 72.3 \text{ Å} \times 72.3 \text{ Å}$ ($80a \times 10a \times 10a$, where $a = 7.23 \text{ Å}$). The bar is divided into three regions: one DPD region (with size $40a \times 10a \times 10a$) in the middle (green), with two identical MPM regions (each with size $20a \times 10a \times 10a$) symmetrically located at the two ends (red). The total numbers of DPD and MPM particles were 17861 and 17640, respectively. Small sub-regions, each of 15 Å thickness, at the ends of the MPM regions

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4 were treated as rigid bodies using MPM. These sub-regions were assigned a constant speed of
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6 1.0 Å/ps applied in opposite directions to impose tensile deformation on the nanobar.
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9 Prior to starting the tension test, the initial particle configuration of the entire system was
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11 equilibrated at 298 K for 1000 ps using the Berendsen thermostat [31]. All particles were
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13 temporarily treated as DPD-only particles during the equilibration. The final phase space point
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15 from the equilibration was used to define the starting point for concurrent DPD/MPM
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17 simulations, which were implemented as presented in Section 2.3. Specifically, at the end of the
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19 DPD-only equilibration, particles were defined either as DPD particles or MPM particles for the
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21 subsequent concurrent DPD/MPM simulations. In some cases identical DPD/MPM particle
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23 configurations were embedded into MPM background meshes of different sizes to enable
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25 convergence studies with respect to the MPM background mesh resolution.
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32 **3.2 Single cube-shaped nanoparticle in a high-pressure fluid**

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34 To demonstrate the feasibility of the concurrent DPD/MPM model to simulate discrete
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36 nanostructures under high-pressure confinement, a cube-shaped Cu nanoparticle described using
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38 DPD was embedded into a fluid medium represented by MPM particles contained in a cubic 3-D
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40 periodic simulation cell. Based on the discussions in previous work [24] and in Section 2.3, the
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42 standard MPM discretization procedure and numerical scheme should be valid for both solids
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44 and fluids because no constitutive equations are invoked in the development of the MPM weak
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46 formulation. The major distinction between fluid and solid material points is the continuum-level
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48 constitutive laws used to describe the two phases. For the solid-fluid interaction model studied
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50 here, the ideal gas equation of state is used for the MPM particles. It can be formulated as
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$$56 \quad P = (\gamma - 1) \rho I, \quad (10)$$

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where P is the pressure, ρ is the density, I is the internal energy of the gas, and γ is the ratio of specific heats at constant pressure and constant volume (taken to be constant, $\gamma = 1.4$). To investigate the influence of the hydrostatic pressure on the mechanical properties of the embedded inclusions, the pressure of the ideal gas was set to different values—0.01 GPa, 1 GPa, 3 GPa, and 5 GPa—corresponding to different values of the internal energy. The detailed MPM simulation procedure for the fluid domain can be found in previous work [10].

Figure 4 contains a snapshot taken at the beginning of a simulation for the 3-D concurrent DPD/MPM model for the nanoparticle in the fluid. The edge length of the periodic simulation cell is 144.6 Å and the size of the inclusion, which is located at the geometric center of the cell, is $10a \times 10a \times 10a$. The Cu nanoparticle and ideal gas fluid are represented by 4631 DPD particles and 7930 MPM particles, respectively. Prior to insertion into the fluid, the initial solid inclusion was equilibrated in vacuum at 298 K for 500 ps using the Berendsen thermostat [31]. The equilibrated inclusion was embedded into the MPM domain and the final phase space point from the equilibration was used as the initial condition for the concurrent DPD/MPM simulations. The coupled DPD/MPM model was then simulated at a prescribed pressure for 100 ps at 298 K.

Common Neighbor Analysis (CNA) [32] with the lattice constant a was used to identify the local arrangements of the DPD particles. In Figs. 4 and 5, as well as in the results in Section 4.3 for the particle configurations, fcc coarse-grained particles are shown as green, hexagonal close packed (hcp) particles are shown as red, and the remaining atoms (classified as disordered or surface particles) are shown as white. Ideal gas particles represented using MPM are shown as cyan. CNA was not applied to the MPM particles.

3.3 Sphere-sphere and sphere-rod assemblies in confining fluid

As mentioned in the Introduction, optimized self-assembled CuO nanorod and Al nanoparticle composites have been shown to yield improved performance in Al/CuO nanothermites [9, 10]. However, there have been few MD simulation studies of multi-component nanostructure assemblies [3, 33] and, to our knowledge, none for extreme pressure conditions. Here, mainly for demonstration purposes, we apply the concurrent DPD/MPM simulation procedure to study the behavior of various nano assemblies under high pressure. The study will show that the deformation patterns of the nanostructures under high pressure vary significantly depending on the initial arrangement of the components in the assembly.

Application of the coupled DPD/MPM model to nano assemblies in a confining ideal gas is similar to that described in Section 3.2 for the single inclusion. Two basic assembly types were constructed for the nanosphere-nanorod assemblies: *sphere-sphere assemblies* and *sphere-rod assemblies*, in which all components were represented by DPD particles and the confining fluid was represented by MPM particles. Each nanosphere has radius $4a$ and consists of 1048 DPD particles. Each nanorod has radius $4a$ and length $18a$ and consists of 3647 DPD particles. Because there was more than one discrete nanostructure inside the fluid, the simulation cell edge length was increased to $216.9 \text{ \AA}$. Prior to insertion of the nanostructures, the ideal gas consisted of 9261 MPM particles. All other parameters and basic numerical procedures are the same as those given in Section 3.2.

Schematics of the sphere-rod assemblies are provided in Fig. 5(a). Eight assemblies with different component arrangements, designated as Assembly 0, Assembly 1, ..., Assembly 7 were considered. Assembly 0 is the simplest and consists of a single sphere-sphere pair. This geometric arrangement is similar to those commonly used in MD simulations of nanoparticle

sintering [3, 33, 34]. The initial distance between the two spheres (surface to surface) is 7.23 Å. The remaining assemblies consisted of a nanorod, with one or more nanospheres, to yield sphere-rod assemblies. In Assemblies 1, 2, and 3 the two spheres are located on opposite sides of the nanorod, while in Assemblies 4 and 5 the two spheres are located on the same side of the nanorod. Assemblies 6 and 7 include four spheres, with two on each side of the nanorod. The distance between the rod and spheres (surface to surface) is 7.23 Å in all sphere-rod assemblies. The vertical distance between the spheres (surface to surface) is 7.23 Å in Assemblies 2, 4 and 6, and 72.3 Å in Assemblies 3, 5 and 7. Before the assembly was introduced into the fluid, the particle configuration of each component (that is, one nanosphere and one nanorod) was equilibrated separately for 400 ps in vacuum at 298 K using the Berendsen thermostat [31]. Following equilibration, replicates of these two components were inserted as necessary into the MPM fluid to yield the various assemblies shown in Fig. 5(a). Upon insertion of the nanostructure, if an MPM particle overlapped with the volume occupied by any component of the nanostructure, that MPM particle was removed. As a typical example, the initial 3-D configuration of Assembly 6 is shown in Fig. 5(b), wherein the expanded view to the right shows the configuration of the assembly in greater detail.

4. Results and Discussion

4.1 Nanobar subjected to tensile strain: deformation and stress-strain relationship

The concurrent DPD/MPM model and computational set-up described in Section 3.1 was used to simulate a nanobar under tensile deformation with and without the interface treatment between the DPD and MPM regions. As can be seen in the bottom panel of Fig. 6(a), there is a strong discontinuity on the interfaces between the two regions when the interface treatment is not

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4 included in the multiscale simulation procedure. This is the expected result because, without the
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6 interface treatment, the force on each DPD particle is calculated only from its neighboring DPD
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8 particles within the cutoff radius. The difference between the forces on DPD and MPM particles
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10 leads to the discontinuity of the deformation and makes the interface region the weakest part of
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12 the entire structure. Including the interface treatment in the intermediate regions between DPD
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14 and MPM parts leads to a consistent displacement field across the DPD/MPM boundaries. This
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16 is evident in the middle panel of Fig. 6(a), which shows a continuous tensile deformation of the
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18 nanobar as an integral structure. Necking of the bar is observed as the strain becomes large, in
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20 agreement with result obtained using the DPD-only model (Fig. 6(a), top panel).
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26 Figure 6(b) shows that the concurrent DPD/MPM model with the interface treatment
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28 predicts a physically reasonable stress-strain relationship within the elastic regime. The solid
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30 blue curve is the result for the DPD-only model and the dashed, dash-dotted, and dotted curves
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32 are the concurrent DPD/MPM predictions for successively coarser MPM grids. The stress and
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34 strain are obtained as the virial stress and engineering strain. Because the sample size is still
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36 within the nanometer range, the stress state in the sample can be suitably calculated based the
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38 definition of virial stress [35]. The results show that, for suitable MPM grid edge length, the
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40 concurrent DPD/MPM model yields the same elastic response as the DPD-only model—but with
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42 less computational cost, because particles in the MPM regions do not require any particle-
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44 neighbor searching algorithm for the force calculation. (This is similar to the result obtained in a
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46 previous study [24], using the so-called DPD/MPM-grid model wherein a collection of DPD
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48 particles is propagated in time by interpolating the inter-particle forces onto a background grid.
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50 Specifically, as the resolution of the grid is increased the peak stress approaches the value
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52 obtained from the DPD-only simulation.) Although the general deformations for the concurrent
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DPD/MPM model and DPD-only model are similar, the detailed defect patterns are not exactly the same for the two cases. This is because the mapping and re-mapping procedure inevitably leads to some smearing of the microscopic dynamics when the nodal accelerations and nodal velocities are mapped back to the particles, and is true whether a given cell of the MPM background mesh contains only DPD particles or a mixture of DPD and MPM particles. Note, however, that because of the single-value mapping, no overlaps between DPD and MPM particles will occur. Also, because the forces on the particles in the MPM regions are calculated using a constitutive law at the continuum level (albeit parameterized using basic mechanical properties obtained from the mesoscale level), some fine-scale information about material defects is also inevitably lost during coarse-graining. Thus, while it is unrealistic to expect to closely match the details obtained using MD [35] with an all-atom potential [36], as long as the MPM regions are able to predict the general dynamic response of the structure without losing the essential mechanical properties, one could use MPM in the areas that do not require highly resolved descriptions. Whereas, with an appropriate background mesh size, the DPD regions can be used in the areas where more detailed material deformation information is required, such as the necking region of a nanobar under tension or an impact surface where defects initially nucleate and evolve.

4.2 Single cube-shaped nanoparticle in a high-pressure fluid: 298 K isotherm

The 298 K isotherm was calculated for the Cu inclusion discussed in Section 3.2, to assess whether the particle-based concurrent DPD/MPM model predicts reasonable mechanical properties of the material. Following equilibration at a given pressure, the volume compression ratio V/V_0 of the Cu inclusion was calculated. Here, V is the volume of the Cu inclusion at the pressure of interest and V_0 is the volume at 1 atm. Inclusion volumes were estimated as the

product of the edge length of the nominally cube-shaped inclusion. The isotherm curve for a periodic sample with size $10a \times 10a \times 10a$, simulated using all-atom MD, is plotted in Fig. 7. Results for a periodic sample with the same cell size but consisting only of DPD particles, simulated using CG-MD with the mesoparticle potential [30] are also shown to provide an additional point of reference for the concurrent DPD/MPM simulations. As can be seen from Fig. 7, the result for the finite-size inclusion simulated using the concurrent DPD/MPM model is close to those obtained using MD and CG-MD. This implies that the bulk modulus of the Cu samples predicted using all three methods will be in close agreement.

It should be reiterated that the MPM particles are used to discretize the ideal gas in the concurrent DPD/MPM model. This provides a simplified approach for applying a hydrostatic load to an included solid. In conventional MD simulations of the hydrostatic compression of a finite-sized inclusion in a confining environment, a compliant medium (*e.g.*, Ar or Kr) needs to be introduced [37]. The MD simulation thus requires looping over numerous pairwise interactions between inclusion and medium atoms, and among medium atoms, during the force calculations. By contrast, using the concurrent DPD/MPM simulation procedure the stresses on MPM particles for the fluid medium are calculated from the constitutive law, which involves much less computational work. And by mapping onto the background mesh the hydrostatic loads can be applied indirectly to the DPD particles (*i.e.*, the inclusion), thereby also reducing the computational burden.

4.3 Sphere-sphere and sphere-rod assemblies in confining fluid: solid-state sintering and deformation patterns of many-body nanoassemblies

Discrete nanostructures (nanorod and nanospheres) such as those that were investigated in previous studies based on all-atom MD [3, 38] are studied here using the proposed particle-

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4 based multiscale simulation procedure. Simulations of solid-state sintering were performed for
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6 the prototypical assemblies defined in Section 3.3 in the presence of a confining fluid. The
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8 results shown below demonstrate that, within the limits of resolution available to the mesoscale
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10 descriptions, detailed deformation patterns can be obtained from the DPD sub-regions within the
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12 overall concurrent DPD/MPM simulation domain.
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16 17 ***4.3.1 Solid-state sintering of the sphere pair*** 18

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20 The sphere-sphere assembly (Assembly 0) was simulated to study the solid-state sintering
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22 process that commonly occurs spontaneously at the nanoscale. All-atom MD simulations of the
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24 same process are available for comparison [3, 33], albeit under vacuum conditions. The
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26 qualitative reliability of MD simulations has been proven for the case of sintering of metallic
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28 nanoparticles by comparing the simulated neck growth to the predictions from empirical
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30 theoretical relations [3]. As discussed in Sec. 4.2, the proposed DPD/MPM model provides a
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32 simple, practical approach for simulating nanostructures in prescribed ambient pressure
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34 environments.
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40 Figure 8(a) shows several snapshots during the solid-state sintering of two nanospheres at
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42 1 GPa and 298 K, predicted using the concurrent DPD/MPM model. The prediction is similar
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44 overall to what was obtained from MD simulations [3, 33] at 298 K in vacuum. The solid-state
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46 sintering of the sphere pair can also be predicted by using the concurrent DPD/MPM model.
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48 Although some of the MPM fluid particles initially occupy the gap between the spheres, those
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50 particles are extruded during sintering. From the snapshots it can be seen that the two
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52 nanospheres remain separated up to ~5 ps. Subsequently they move toward each other, make
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54 contact, and a neck rapidly forms between them. A dumbbell-shaped particle is formed at longer
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56 times (from 55 ps to 100 ps). Although the structure is relatively stable, it exhibits small rigid-
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body motions. This phenomenon of solid-state sintering at 298 K was observed for all cases studied in this work that involved initially separated discrete objects.

Figure 8(b) illustrates the formation of a stable neck as the solid-state sintering occurs. The neck width [3] is calculated as the smallest diameter of the circular plane in the neck region perpendicular to the line between the geometrical centers of the two spheres, as indicated in Fig. 8(b). Figure 8(c) shows the time history of the neck width during the solid-state sintering. For comparison, sphere pairs with the same particle size and initial configuration were also simulated using all-atom MD and the DPD-only model, at 298 K but under vacuum conditions. It should be pointed out that the instant of initial contact between the two spheres can differ somewhat for the same initial sample geometry but with different initial random seeds for velocity selection [33]. In Fig. 8(c), therefore, we focus on the long-time value of the neck width rather than the onset time for sintering in a given simulation. It can be seen that the DPD-only model and all-atom MD predict nearly the same value for the stable neck width. The neck widths predicted by the concurrent DPD/MPM model at 0.01 GPa and 1 GPa are also nearly the same as those predicted using all-atom MD and the DPD-only model. As the pressure is increased (from 0.01 GPa to 5 GPa), the neck widths predicted using the concurrent DPD/MPM model also increase. This suggests that more completely sintered structures can be obtained by using increased pressure.

4.3.2 Sphere-rod assemblies with different initial arrangements

Snapshots from concurrent DPD/MPM simulations for several initial arrangements of one rod and two spheres are shown in Figs. 9 and 10. Analogous results for the case of one rod and four spheres are shown in Figs. 11 and 12. Generically, as for the case of two spheres, the results for rod-sphere assemblies in Figs. 9-12 exhibit solid-state sintering. However, the results differ as functions of pressure and for different initial arrangements of the components.

Figure 9 shows snapshots taken at different times during the simulation of the symmetric “cross-like” Assembly 1 (298 K and 1 GPa). During the first 15 ps gas is extruded and the components approach, make contacts, and form necks. A relatively stable nanostructure is formed within 40 ps and, although it undergoes rigid-body motions in the fluid, it remains intact for the remainder of the simulation. At $t = 40$ ps stacking faults form near the contact surfaces between the rod and spheres; note the two layers of pink atoms in the figure. It was determined that the deformation in the rod is mainly accommodated by lattice slip on $\{111\}$ planes, similar to those obtained in MD simulations [39]. The slip events occur initially in the contact regions, and result in the emission of partial dislocations that eventually form a relatively stable pattern of parallel stacking faults on $\{111\}$ planes (see the snapshot at $t = 100$ ps).

Figure 10(a) shows snapshots for Assembly 2 at 1 GPa, which possesses rotational symmetry but non-centrosymmetry. The spheres contact the rod at $t = 15$ ps. This leads to a small rotation of the rod about the y-axis. The rod and spheres begin to rotate and reorient to achieve a relatively low-energy structure [3] (see the snapshot at $t = 45$ ps). Although a few are formed in the nanorod, most transient stacking faults are formed in the nanospheres. This might be due to the fact that the contact regions between the rod and spheres are near the “corners” of the rod, and therefore the space for the defects to expand is limited. A similar assembly (Assembly 3, also at the 1 GPa) but with a larger vertical offset distance between the spheres, was simulated, see Fig. 10(b). The deformation pattern is similar to that of Assembly 2. However, fewer lattice slip events occur, presumably because the contact regions between the rod and sphere are almost exactly at the “corners” of the rod, which provides little room for the stacking faults to form [40].

Figure 10(c) shows the snapshots of Assembly 4 at 1 GPa with two spheres on the same side of the rod. Contact between the spheres and the rod occurs, almost simultaneously for both spheres, at $t = 15$ ps. Shortly after, the spheres make contact and sintering between them begins (see the snapshot at $t = 20$ ps). The attraction between the two spheres leads to a bending deformation of the nanorod. Eventually (see the snapshot at $t = 75$ ps) the solid-state sintering among the three components is completed. The assembly becomes more stable with a reduced total surface area. One can see that deformation twins form in the rod due to its bending. This is in a good qualitative agreement with configurations obtained from MD simulations of nanowire bending [40]. Results for Assembly 5, which has the same starting geometry as Assembly 4 except that the vertical offset between the sphere is increased, are shown Fig. 10(d) for 1 GPa. In this case, while the distance between the spheres does decrease somewhat, they never contact each other. A slight bending deformation of the rod can be observed, leading to two sets of stacking faults on different types of $\{111\}$ planes; these eventually join up in the middle of the rod.

Figure 11(a) shows the assembly (Assembly 6) in which there are two closely spaced spheres on each side of the rod. The sphere-rod assembly remains quite symmetric during sintering 298 K and 0.01 GPa. The four spheres attach on the surface of the rod almost simultaneously (see the snapshot at $t = 15$ ps). Then, similar to Assembly 4, the sphere pair on each side begins to move toward the horizontal centerline (see the snapshot at $t = 25$ ps), reducing the “cavity” volume between them. Eventually, the sintering process results in a single nanoassembly without any remaining cavity space. While the “stable” assembly appears to be symmetric, the rod is actually somewhat bent, as can be seen in Fig. 11(b), which shows two

views of the assembly with the MPM fluid removed. These views show that the rod does not exhibit bending in the x-z plane, but that bending does occur in the y-z plane.

The components in Assembly 6 do not form a symmetric pattern when the pressure is increased to 1 GPa. The results for this case are shown in Fig. 12(a). As can be seen in the snapshot at $t = 15$ ps, the spheres do not attach onto the rod simultaneously, and the rod is tilted. The two spheres on the left-hand side reach the rod surface first, and those two spheres and the rod start to coalesce prior to complete attachment of the spheres on the right-hand side of the rod. This symmetry-breaking causes the ends of the rod to bend to the left (see the snapshot at $t = 60$ ps). This in turn leads to a much larger distance between the spheres on the right-hand side, which prevents those two spheres from coalescing, leading to a non-symmetric stable structure (at least on the time scale of the simulations).

Assembly 7 is similar to Assembly 6 but with a larger vertical offset distance between the two spheres on each side. Figure 12(b) shows snapshots for Assembly 7 at 298 K and 1 GPa. As for Assembly 6 at 1 GPa, the spheres on opposite sides of the rod do not contact it at the same time so the rod becomes tilted (see the snapshot at $t = 20$ ps in Fig. 12(b)). However, because the vertical gap between the spheres in Assembly 7 is large, no sintering occurs between the spheres. As a consequence, there is not a strong driving force to cause rod the rod to bend and the final structure is a symmetric “dog bone” assembly (see the snapshots at $t = 40$ ps and 100 ps).

4.4 Comparisons of the computing requirements for the various treatments

In this section the CPU and memory requirements for the proposed concurrent multiscale procedure are compared with those obtained from both serial and parallel all-atom MD simulations as well as **DPD-only simulations**. Obviously, the practical results will differ from one code to the next and for different levels of compiler optimization. The comparisons here are

based on purpose-written serial codes for the concurrent DPD/MPM and DPD-only simulations and the LAMMPS [41] code for the all-atom MD simulations with different numbers of cores (specifically, a single core for the serial case and 8 cores for the parallel case). The comparison simulations were performed using a 64-bit Intel Xeon Linux cluster with eight 2.67 GHz cores and 24 GB of shared memory per node. The parallel all-atom MD simulations were performed using all eight cores on a single node, so interbox communication is not a factor. The LAMMPS code was compiled using the Intel icc compiler whereas the concurrent DPD/MPM and DPD-only codes were compiled using the Intel Fortran90 compiler suite; basic (-O2) optimization options were used in all cases.

A nanobar with dimensions $578 \text{ \AA} \times 72.3 \text{ \AA} \times 72.3 \text{ \AA}$ (the same system considered in Sections 3.1 and 4.1) was chosen as a representative example for study. Table 1 contains a summary of system details and the timing and memory usage results. From the table, simulating the tension test for 1.0 ps using the concurrent DPD/MPM procedure requires 184 seconds of CPU time; that is, 1.84 CPU-seconds per time step. The corresponding DPD-only simulation requires 670 seconds of CPU time or 6.7 CPU-seconds per time step. By contrast, both MD simulations (serial and parallel) required more than 1000 seconds of CPU time for the same assembly (1.055 and 1.185 CPU-seconds per time step for the serial and parallel cases, respectively). The wall-clock time required to complete the concurrent DPD/MPM simulation is $\approx 73\%$ and $\approx 83\%$ less than those for the DPD-only and MD simulations, respectively, on a single processor ($100\% \times (t_{\text{MPM}} - t_{\text{DPD or MD}})/t_{\text{DPD or MD}}$). Compared to MD, the reduction is due to the reduced total number of particles and longer time steps in the concurrent DPD/MPM simulation; whereas compared to DPD the reduction is mainly due to the reduced number of iterations required for the particle neighbor search in the concurrent DPD/MPM method. It should also be

noted that whereas the LAMMPS code for the MD simulation is highly optimized, the code used for the concurrent DPD/MPM simulations is not. Thus, the comparison here provides an approximate lower bound of time efficiency for the concurrent DPD/MPM model. Future work should be performed to refine the concurrent DPD/MPM code, for example by using a cell linked-list instead of a simple loop algorithm to search for DPD neighbor particles, to further reduce the memory and time required for computation.

5 Conclusion and Future Work

A particle-based multiscale simulation procedure, with a concurrent link between the MPM and DPD and a hierarchical bridge from MD to DPD, has been presented and demonstrated. An interfacial scheme has been designed to effectively cast the spatial discretization at different scales into a unified MPM framework. The representative examples discussed in this paper provide qualitative validation for the overall procedure and suggest the suitability of the concurrent DPD/MPM procedure for the study of discrete nanostructures under extreme loading conditions. The major findings are as follows:

- The concurrent DPD/MPM model with interface treatment successfully reproduces the qualitative structural deformation of a nanobar under tension, including necking phenomena prior to fracture, obtained from DPD-only simulations. For a suitable choice of edge-length of the MPM background grid, the concurrent DPD/MPM model predicts both accurate elastic behavior and a reasonable stress-strain relationship for larger strains, in comparison to a corresponding model based on DPD-only simulations.
- The room temperature isotherm, calculated for pressures less than 15 GPa for a single cube-shaped Cu inclusion in a confining fluid, wherein the inclusion is described using

DPD particles and the fluid is treated using MPM, is in good agreement with those obtained using all-atom MD and DPD-only simulations.

- Predictions of solid-state sintering of two nanospheres in a confining fluid at 298 K, simulated using the concurrent DPD/MPM method, are qualitatively similar to what is obtained for the same pair of nanospheres in vacuum simulated using the DPD-only method, namely formation of a stable dumbbell-shaped configuration. Increasing pressure leads to increasing neck width in the sintered structures.
- Sphere-rod assemblies with different initial arrangements have been investigated at low (0.01 GPa) and high (1 GPa) pressure by using the concurrent DPD/MPM procedure. The results show that the shapes and detailed deformation patterns in the resulting nanostructures vary widely depending on initial geometry and ambient pressure. By tailoring the sintering pressure and the distance between the components, the discrete nanostructures can be assembled into particular shapes with a range of final surface areas.

Overall, the simulation results shown in this paper demonstrate that the proposed particle-based concurrent DPD/MPM procedure has the capability of predicting reasonable mechanical responses of the discrete nanostructures under extreme loading. Several steps could be taken to improve the method and make it more robust for simulation of more complicated objects:

- More accurate mesoscale potentials for DPD particles need to be developed. As discussed in Section 2, a model for the hierarchical bridge from MD to DPD is built by coarse-graining a certain number of atoms into a single mesoparticle. Based on the dissipative particle dynamics with conserved energy (DPDE), an internal energy variable is defined that allows energy exchange between the mesoparticle and its implicit internal degrees of

freedom. As can be seen from the simulation results for the DPD-only model, however, some basic mechanical properties, such as the yield stress and strain, are not exactly the same as those calculated from all-atom MD. Thus, additional work should be done to more accurately parameterize the DPD force expression. While the mesoscale particle potential used here has only been developed for Cu, the approach used to obtain it should be extendable together metals and metal-oxides, which would directly extend the range of applications accessible to the concurrent DPD/MPM model in its present form. Further efforts should also be made to develop DPD models that are accurate across wide temperature and density intervals to facilitate simulations of systems subject to strong driving forces such as shock waves or intense electromagnetic radiation, or to treat chemical reactions. These are challenging tasks [42, 43].

- Coupling DPD with other improved material point methods (*e.g.*, GIMP [18], CPDI [19], DDMP [20], and mesh-grading material point method (MGMPM) [44]) might yield better results, particularly for more complicated geometries and systems with large strain rates or strain rate gradients. In the original MPM [15], the numerical error can be huge if no special treatment is used when a material point crosses a boundary on the background mesh, due to the use of local, linear shape functions. Thus, nonlocal mapping procedures have been developed [19, 20] to avoid the cell-crossing error, and these could be implemented to improve the concurrent DPD/MPM method for general applications.

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Figures

Figure 1 Pictorial synopsis of the particle-based multiscale simulation procedure, which includes a hierarchical link from MD to DPD and a concurrent link between DPD and MPM.

Figure 2 Schematic of the concurrent DPD/MPM model. If needed, the computational domain can be divided into several regions with different types of particles. There are three distinct regions in the example shown: a mesoscale/DPD region, a classical MPM region, and an intermediate region between them.

Figure 3 Schematic of the concurrent DPD/MPM simulation of a Cu nanobar subjected to imposed tensile strain. The rod is divided into three regions: a DPD region in the middle (green), and MPM regions on either side of it (red). The blue boxes denote rigid platens composed of MPM particles and assigned constant velocities in opposite directions.

Figure 4 Snapshot from a simulation of a cube-shaped Cu inclusion embedded in an ideal gas fluid obtained using the concurrent DPD/MPM model at 298 K and 0.01 GPa. The inclusion and fluid were treated using DPD and MPM, respectively.

Figure 5 (a) Sketches of the sphere-rod assemblies with different arrangements of the components; structures are not shown exactly to scale. (b) Initial 3-D configuration of the DPD representation of Assembly 6 embedded in the MPM fluid.

Figure 6 (a) Deformation of a Cu nanobar under applied tensile strain using the DPD-only and concurrent DPD/MPM models with and without interface treatment. The strain rate is 0.0035/ps. (b) Stress-strain curves, simulated using the DPD-only model (solid curve) and the concurrent DPD/MPM model with interface treatment. Dashed, dot-dashed, and dotted curves denote different MPM grid edge lengths.

Figure 7 Pressure-volume relationships (298 K isothermal compression curve) for a cube-shaped inclusion simulated using the concurrent DPD/MPM model (yellow triangles), and bulk (3-D periodic) Cu crystals simulated using all-atom MD (red squares) and CG-MD (blue diamonds). The dotted curve is a fitting curve for data points from the all-atom MD simulations.

Figure 8 (a) Snapshots of the solid-state sintering of the sphere-sphere assembly (Assembly 0) at 298 K and 1 GPa. (b) The dumbbell-shaped sphere-sphere structure after the solid-state sintering. (c) Time history of the neck width of the sphere-sphere assembly, calculated using the concurrent DPD/MPM model at different pressures, and analogous results obtained using all-atom MD and DPD-only simulations at 298 K under vacuum.

Figure 9 Snapshots of the sphere-rod assembly (Assembly 1) at 298 K and 1 GPa.

Figure 10 Snapshots of sphere-rod assemblies at 298 K and 1 GPa: (a) Assembly 2; (b) Assembly 3; (c) Assembly 4; (d) Assembly 5.

Figure 11 (a) Snapshots of Assembly 6 at 298 K and 0.01 GPa. (b) Bending deformation of the nanorod induced by the sintering of the sphere pairs.

Figure 12 Snapshots of sphere-rod assemblies at 298 K and 1 GPa. (a) Assembly 6; (b) Assembly 7.

Table 1 Comparison of computing requirements for simulating a $578 \text{ \AA} \times 72.3 \text{ \AA} \times 72.3 \text{ \AA}$ nanobar with different simulation methods.

	MD simulation (serial)	MD simulation (parallel)	DPD-only simulation	DPD/MPM simulation
Total simulation time (ps)	1.0	1.0	1.0	1.0
Total number of time steps	1000	1000	100	100
Number of MD particles	269,801	269,801	N/A	N/A
Number of DPD particles	N/A	N/A	35,501	17,681
Number of MPM particles	N/A	N/A	N/A	17,640
Total number of particles	269,801	269,801	35,501	35,501
Number of processors used	1	8	1	1
Max. memory (Mbytes)	322	306	1390	718
Max. swap (Mbytes)	668	1799	1547	1547
Total CPU time (sec)	1055	1185	670	184
CPU-seconds per time step	1.055	1.185	6.7	1.84
Wall time (sec)	1055	148	670	184

fig.1.jpg

fig.2.jpg

fig.3.jpg

fig.4.jpg

fig.6.jpg

(a)

(b)

fig.7.jpg

fig.8.jpg

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fig.10.jpg

fig.11.jpg

(a)

(b)

fig.12.jpg