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Particle-Based Multiscale Simulation within the MPM Framework

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The need for formulating the equation of state (EoS) of nano energetic composites necessitates the development of an effective multiscale procedure for simulating the discrete nano and sub-micron structural responses to impact loading. To effectively discretize the multiphase interactions involving multiscale failure evolution, a particle-based simulation procedure is being developed with a concurrent link between the Material Point Method (MPM) and Dissipative Particle Dynamics (DPD), and a hierarchical bridge from Molecular Dynamics (MD) to DPD [1].

The motivation for developing the MPM was for better simulating multi-phase interactions in processes that involve failure evolution, such as impact, penetration, perforation and blast-fragment interaction [2]. As reviewed by Chen *et al.* [3], the MPM is an extension to solid mechanics of the hydrodynamics method called FLIP which, in turn, evolved from the Particle-in-Cell Method. The essential idea of the MPM is to take advantage of the strengths of both the Eulerian and Lagrangian methods while avoiding the shortcomings of each. In comparison with other meshless methods, the MPM is less complex and has a cost factor of at most twice that associated with the use of corresponding finite elements. In addition, the MPM can be easily interfaced with the Finite Element Method (FEM) codes due to the use of the same weak formulation for both methods. In the original MPM [2], however, there exists a cell-crossing issue due to the use of local mapping functions; and in addition, special care is required to deal with a moving boundary condition. Much effort has been expended, especially over the past decade, to improve the original MPM through the use of nonlocal treatments (which would increase the computational expense), as illustrated in the representative references [4-6].

As can be found from the open literature, there are three particular advances in the MPM that are relevant for multiscale modeling and simulation. A multi-level refinement scheme has been designed for the Generalized Interpolation Material Point (GIMP) Method [7]; a hierarchical approach has been proposed and demonstrated in which material points at the fine level in the MPM are coupled directly with the atoms in MD simulations [8]; and a sequential procedure has been recently developed to formulate the EoS, based on MD results, for use in macroscopic MPM simulations [9]. However, each of the hierarchical/sequential or multi-level refinement approaches just mentioned requires a transition region between different spatial scales, which limits their usefulness for the study of physical situations where discrete nano/micro structures (for example, nano/micro rods and beams in energetic composites) interact with each other. Recently, a particle-based multiscale procedure has been proposed wherein Cluster Dynamics (CD) is linked hierarchically with MD for sub-micron scale domains and concurrently with the MPM for simulations on larger scales [10]. The method was used to explore the longitudinal impact response between two metallic microrods with different nanostructures. However, the CD method used in [10] relies on certain assumptions that limit the range of applicability, and much work remains to be done to generalize the method to more realistic situations.

In this presentation, we present the improved particle-based multiscale simulation procedure as described in [1]. Focusing on the link between DPD and the MPM, we first demonstrate that the dynamics of DPD particles, which interact via pairwise particle-particle forces, can be effectively coarse-grained using a straightforward adaptation of the standard MPM algorithm. Using this capability we then demonstrate how DPD and MPM subdomains can be treated concurrently, and nearly seamlessly, in a single computational domain. Particular attention is devoted to the development of an effective interfacial scheme for use in the concurrent simulations. Representative examples are considered to illustrate and verify the proposed simulation procedure. Although the elastic responses predicted by the proposed procedure are reasonable, further investigations are required to improve the current DPD forcing functions, understand the size effect on the inelastic and failure responses, and simulate the impact responses of discrete nano structures with various shapes and compositions.

Keywords: Material Point Method, Particle Methods, Multiscale Simulation, Energetic Composites

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