11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20–25, 2014, Barcelona, Spain

MULTISCALE COMPUTATION BASED ON THE DUAL DOMAIN MATERIAL POINT METHOD

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Key words: *Material Point Method, Multiscale*

In cases of rapid material deformation, many basic assumptions of traditional continuum mechanics and thermodynamics become questionable. To numerically simulate these material motions, one needs a numerical method that represents non-equilibrium thermodynamic effects under extreme and rapid deformation. In most of these cases, material behavior is history dependent because the time scale for the material to reach an equilibrium state is comparable to the time scale of the deformation [1]. To study this history dependency one needs to calculate lower (smaller) scale physics following the motion of the material. In other words, we need a Lagrangian capability in multiscale methods to numerically simulate material deformations under these extreme conditions. Most mesh based numerical methods suffer either numerical diffusion or mesh distortion, therefore cannot be used in history-dependent problems with large material deformations, while many meshless methods do not have enough accuracy in calculating spatial derivatives.

The dual domain material point method [2] is an advanced version of the material point method using both Lagrangian integration points to track material history and an Eulerian mesh to calculate spatial derivatives. Since the material points are Lagrangian points representing a piece of material, we can perform molecular dynamic simulations on the piece of the material to consider history dependency and to provide macroscopic closure quantities for the averaged equations considering the lower scale physics.

In this paper, we first introduce the dual domain material point method, its advantages over the traditional material point method, and then present a multiscale numerical scheme based on ensemble phase averaging method [3,4]. This scheme takes advantages of many multiscale algorithms and is capable of tracking histories of the material. In this scheme, a physical system is discretized into material points that are sub-systems and can be numerically simulated almost independently to consider the lower scale physics. These material points only communicate with upper (larger) scale physics. There is no need

for direct communication among the material points. In this method, material points still maintain needed communications among themselves, but these communications are through their information exchange with the upper scale physics, not directly among the material points. This numerical property allows us to setup a computer with a tree-like hierarchy of different processors, CPUs and GPUs, with difference computing and communication capabilities.

As an example, we study a numerical simulation of a one-dimensional shock propagation in monatomic gas. Each material point is a three-dimensional sub-molecular system. Molecular dynamic simulations are performed on these sub-system to calculate the closure quantities at the material points. Numerical results are compared to those obtained directly from the molecular dynamic simulation of the entire system and to those obtained from the traditional continuum mechanics based on the equation of state for thermodynamically equilibrated systems.

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