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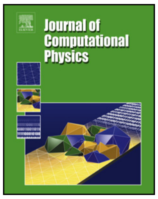

Shock waves simulated using the dual domain material point method combined with molecular dynamics

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ABSTRACT

In this work we combine the dual domain material point method with molecular dynamics in an attempt to create a multiscale numerical method to simulate materials undergoing large deformations with high strain rates. In these types of problems, the material is often in a thermodynamically nonequilibrium state, and conventional constitutive relations or equations of state are often not available. In this method, the closure quantities, such as stress, at each material point are calculated from a molecular dynamics simulation of a group of atoms surrounding the material point. Rather than restricting the multiscale simulation in a small spatial region, such as phase interfaces, or crack tips, this multiscale method can be used to consider nonequilibrium thermodynamic effects in a macroscopic domain.

This method takes the advantage that the material points only communicate with mesh nodes, not among themselves; therefore molecular dynamics simulations for material points can be performed independently in parallel. The dual domain material point method is chosen for this multiscale method because it can be used in history dependent problems with large deformation without generating numerical noise as material points move across cells, and also because of its convergence and conservation properties.

To demonstrate the feasibility and accuracy of this method, we compare the results of a shock wave propagation in a cerium crystal calculated using the direct molecular dynamics simulation with the results from this combined multiscale calculation.

1. Introduction

The equation of state or constitutive relation of a material is often obtained by assuming thermodynamic equilibrium. As a consequence of this assumption, the equation of state can only be applied to problems in which the time scale of the material deformation, defined by the inverse of the characteristic strain rate, is significantly larger than the time scale for the molecules in the material to relax to their thermodynamic equilibrium state after an external perturbation. For problems with a smaller ratio between the problem time scale and the relaxation time scale of the material, the equation of state cannot be used. These types of physical problems are the main focus of the present paper.

Since the time scale of the material deformation of concern here is comparable to or even smaller than the thermodynamic relaxation time, the material response at a given external disturbance depends on the microstructures of the material at that time, which depends on the history of the material. Therefore, the material behavior is generally history depen-

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dent for these types of problems. Furthermore, such high rates of material deformation often involve significant forces, for instance in hypervelocity impacts. Significant material deformations are common in these cases.

To numerically simulate these types of problems at the macroscopic level, on the theoretical front, one needs a set of continuum scale equations with a method to calculate the closure quantities accurately representing the microstructure and history effects. On the numerical front, one needs a numerical method capable of accurately tracking material deformation history in cases of large material deformation.

The continuum scale equations can be derived from the Liouville equation using ensemble average for fairly general cases [1,2]. The closure quantities, such as pressure, stress, and heat flux, are directly related to microscopic interactions among molecules and atoms. In this paper, we use these relations to calculate the necessary closure quantities directly from molecular dynamics (MD) simulations. Such closure quantities are used in continuum calculations to advance the macroscopic quantities. For thermodynamically equilibrium systems in the limit of Continuum Mechanics, we show that such calculated stress is consistent with the traditional concept. The method presented in the current paper is in the same philosophy of the heterogeneous multiscale method (HMM) [3–7]. For selected regions in a macroscopic domain, lower length scale simulations are performed in synchrony with the macroscopic continuum level calculation. These lower length scale simulations are constrained by the macroscopic information passed to them. Closure quantities, such as stress or heat flux, calculated from these lower length scale systems are passed to the continuum level calculation to advance the macroscopic state. In this work we emphasize the simulation method for history dependent systems undergoing large macroscopic deformations. Frequent reinitialization and time averaging are not allowed. While the non-linear terms are neglected in [3,5] and the work is limited to small material deformation, the Lagrangian coordinate system is capable of tracking material deformation history, which is an advantage of a Lagrangian method. The main disadvantage of a pure Lagrangian method, such as the Lagrangian finite element method, appears in problems involving large material deformation, where elements are often severely distorted and even entangled leading to loss of accuracy and eventual failure of the calculation. In the present paper, we use the dual domain material point (DDMP) method to avoid this numerical difficulty. For the fluid dynamics problems studied in [4], the simulated molecular dynamics systems are fixed in the spatial locations intended for history independent materials, such as Newtonian fluids, based on the pure Eulerian description. Unless special treatments, such as in [8,9], are used, Eulerian methods often lead to significant numerical diffusion of history dependent variables. Rather than proposing another multiscale computation philosophy or a method to perform MD simulations, the main purpose of this work is to show that the general strategy of HMM can be efficiently implemented with the dual domain material point (DDMP) method for thermodynamically nonequilibrium or history dependent systems undergoing large material deformation by taking advantage of the simultaneous use of Lagrangian particles and Eulerian meshes in the method.

The Lagrangian particles, also called material points, are used to track the history of the material deformation. These particles can be regarded as pieces of the material experiencing the history. The Eulerian mesh is used to perform numerical analysis, such as taking spatial derivatives. Since the information about material history is carried by the Lagrangian particles, numerical diffusion for the history dependent quantities is avoided. Furthermore, because the mesh is Eulerian, it remains unchanged in cases of large material deformations, thereby avoiding the mesh distortion difficulty suffered by a pure Lagrangian method. In the DDMP method, the closure quantities, such as the stress, are needed only at material points following the motion of the material. The numerical method does not require direct molecular dynamics simulation of the entire macroscopic computational domain. Direct molecular dynamics simulations are only performed in small representative domains around the material points. These simulations are driven by the continuum level DDMP calculation by imposing appropriate constraints to the molecular dynamics systems. The closure quantities calculated from these molecular systems are used to drive the macroscopic DDMP calculation. Such intimate communications between the macroscopic scale calculation and the microscopic scale simulations are unique for these types of multiscale calculations and need to be studied carefully to ensure physical consistency of the results.

In the DDMP method, material points only communicate with mesh nodes and not directly among themselves. Therefore, there is no need to form neighbor lists of the particles. This feature of the numerical method is very advantageous for parallel computation, especially for heterogeneous computers, such as CPU–GPU combined platforms. In the present paper, we take advantage of this feature to demonstrate the feasibility of such multiscale calculations.

2. Continuum scale equations and their solution method

2.1. Derivation of continuum scale equations

For a generic quantity g_α pertaining to atom α, the corresponding average $\overline{g}$ at time t and position $\boldsymbol{x}$ is defined using

$$n(\boldsymbol{x},t)\overline{g}(\boldsymbol{x},t)=\int\sum_{\alpha=1}^{N}\delta(\boldsymbol{x}_\alpha(t)-\boldsymbol{x})g_\alpha(\mathcal{C},t)P(\mathcal{C},t)d\mathcal{C}, \tag{1}$$

where n is the number density of the atoms which corresponds to $g_\alpha=\overline{g}=1$ in the above equation, N is the number of atoms in the system, $\mathcal{C}=\{\boldsymbol{x}_1,\cdots,\boldsymbol{x}_N;\boldsymbol{v}_1,\cdots,\boldsymbol{v}_N\}$ is a point in the position-velocity phase space for the system, and $P(\mathcal{C},t)$