Coupling Finite Element Method with Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) for Hierarchical Multiscale Simulations

Modeling and simulation of amorphous polymeric materials

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Received: date / Revised version: date

Abstract. In this work, we have developed a multiscale computational algorithm to couple finite element method with an open source molecular dynamics code — the Large scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) — to perform hierarchical multiscale simulations in highly scalable parallel computations. The algorithm was firstly verified by performing simulations of single crystal copper deformation, and a good agreement with the well-established method was confirmed. Then, we applied the multiscale method to simulate mechanical responses of a polymeric material composed of multi-million fine scale atoms inside the representative unit cells (r-cell) against uniaxial loading. It was observed that the method can successfully capture plastic deformation in the polymer at macroscale, and reproduces strain localization and necking deformation after the elastic limit. In addition, parallel scalability of the multiscale algorithm was examined up to around 100 thousand processors with 10 million particles, and an almost ideal strong scaling was achieved thanks to LAMMPS parallel architecture.

Key words. CG-PR method, QR decomposition, multiscale coupling algorithm, parallel computing

PACS. XX.XX.XX No PACS code given

1 Introduction

Multiscale simulation methods, which couple atomistic models and continuum models, are advanced computational technologies aimed to understand various properties of materials under specific conditions without using any empirical or experimental information. This is because almost all physical events in nature are inherently multiscale phenomena with different time and length scales. In past two decades, a variety of multiscale techniques have been proposed and developed [1,2,3,4], and the multiscale methods in condensed matters may be categorized into two major classes: the concurrent multiscale modeling and the hierarchical multiscale modeling.

The con-current multiscale approach directly connects continuum and atomistic models by communicating displacement or force of atoms to nodes, particles or quadrature points of continuum body on-the-fly to link microscale and macroscale. Since the latter half of the 1990s, several pioneering studies on coupling atomistics to finite elements have extensively investigated. Broughton et al. have demonstrated fracture simulation of silicon by coupling finite element method (FEM), molecular dynamics (MD) simulation and tight binding quantum calculation though a handshake Hamiltonian [5,6]. The bridging scale method uses a projection operator to decompose the displacement field into orthogonal coarse and fine scales, enables one to derive a coupled equations of motion in the MD and FEM models [7,8]. Recently, Li et al. have proposed a novel decomposition method of MD simulation, namely multiscale micromorphic molecular dynamics (MMMD), to model transition zone between microscale and macroscale through mesoscale region [9]. The method allows us to couple MD simulations and FEM [10] or Peridynamics [11], which usually models continuum region using particle discretization.

The other category of multiscale modelings is hierarchical coupling method, which locally embeds fine scale models into coarse scale models. A conventional procedure to build a hierarchical modeling is adopting micromechanics homogenization scheme by employing representative volume elements (RVE) e.g. [12]. One of the most successful hierarchical multiscale approaches is quasicontinuum (QC) method proposed by Tadmor et al.,
in which the finite element mesh covers the entire simulation system, and the mesh may be scaled-down to atomic dimensions, in which the fine scale modeling is in terms of molecular statics or energy minimization or optimization \cite{15,16,17}. A similar but much simpler hierarchical approach is the Cauchy-Born rule (CBR) method, which assumes affine deformation in continuum region, and it thus allows us to couple atomistic and continuum models directly through constant deformation gradient. CBR is mainly applicable to crystalline materials under uniform deformation because it is based on lattice statics; however, the idea can be extended to nonuniform deformation in crystalline solids by considering higher order deformation gradients \cite{18,19}. For instance, higher order CBR has been combined with crystal defect dynamics \cite{20,21} and cohesive zone model \cite{22} to investigate more complicated dislocation pattern dynamics and fracture mechanics of crystals.

Recently, the present authors have extended the idea of the lattice statics-based Cauchy-Born rule to amorphous solids to conduct hierarchical multiscale modeling of inelastic deformation in an amorphous solid \cite{23}. The method was called as the coarse-grained (CG) Parrinello-Rahman (PR) method, since the molecular statics in the representative unit cell of the fine scale model is used analogous to PR-MD simulation \cite{24}. The CG-PR method was systematically validated by comparing its numerical simulation results with that of MD simulations, and the CG-PR method was applied to study the mechanical responses of a Lennard-Jones (LJ) binary glass model \cite{25}. It has been shown that the CG-PR method can successfully reproduce shear band formation in a single-notched amorphous solids using relatively coarse mesh FEM models at macroscale \cite{23}. The advantage of CG-PR method is its independence of the constitutive empiricism, or in other words, it does not need any ad hoc empirical modeling of complicated constitutive relation of amorphous solids. However, a critical drawback of the method is its expensive computation cost, because a representative unit cell (r-cell) composed of many atoms is needed for each and every quadrature points of a FEM model, thus it requires running an enormous number of atomistic simulations all together. It is thus an effective parallel computation algorithm is crucial for practical applications of such method.

In this work, to improve computational efficiency of our in-house CG-PR code, the CG-PR algorithm was coupled with the large scale parallel MD code, namely the large scale atomic/molecular massively parallel simulator (LAMMPS) \cite{26}. To do so, we first develop a coupling algorithm for a single MD cell, whose shape is represented by an upper triangular stretch matrix of six components, instead of general non-symmetric r-cell mentioned in section \cite{2}. In section \cite{5} we first discuss the validation of the multiscale algorithm and multiscale code, which were first validated by performing a numerical simulation of deformation of crystalline copper. Then, we conducted a large-scale parallel computation for simulation of inelastic deformation of a polymeric material to demonstrate applicability of the method, which is implemented in a massively parallel supercomputer. Finally, Section \cite{4} summarizes and concludes the work.

2 Computational Methods

We first discuss coupling between molecular dynamics (MD) with finite element method (FEM).

2.1 Coupling MD and FEM

To start, we first prepare a representative unit cell (r-cell) whose shape is represented by a second order tensor or a matrix $H$. Atom position in the r-cell can be represented by a scaled atom position vector ($S_i(t)$) for atom $i$, and then the current position of the atom $i$ at time $t$ can be written as,

$$r_i(t) = H(t) \cdot S_i(t). \quad (1)$$

Employing CBR, we couple the deformation of an r-cell within an element in a continuum model, we may express the cell shape tensor as,

$$H_c(t) = F_c(t) \cdot H_c(0), \quad (2)$$

where $F_c$ is deformation gradient tensor of an element $c$, and $H_c(0)$ is an initial shape of the r-cell. Thus, the current position of an atom in an r-cell of the given $c$-th element is expressed as,

$$r_c^i(t) = F_c^i(t) \cdot S_c^i(t) = F_c(t) \cdot H_c(0) \cdot S_i(0). \quad (3)$$

To apply a general MD code for hierarchical multiscale modeling, the shape tensor $H_c(t)$ should correspond to shape of an MD unit cell. However, the shape tensor $H_c(t)$ is not symmetric and composed of independent nine components, while MD unit cell in LAMMPS should be upper triangular matrix with six components. In our algorithm, we therefore decompose the deformation gradient tensor $F_c$ into an orthogonal rotation matrix $Q_c$ and an upper triangular stretch matrix $R_c$ as follows.

$$F_c(t) = Q_c(t) \cdot R_c(t). \quad (4)$$

This process is conventional QR decomposition, which is calculated by the Gram-Schmidt orthogonalization. Note that the triangular stretch matrix $R_c$ should be positive definite. Otherwise, the stretch matrix $R$ will introduce wrong axial inversion.

Instead of $F_c(t)$, the upper triangular stretch matrix $R_c$ can be used as a deformation matrix of the MD unit cell as,

$$H_{MD}(t) = R_c(0) \cdot H_c(0). \quad (5)$$

where $H_{MD}(t)$ represents shape of the MD unit cell at time $t$. It is therefore, in a MD code, atomic coordinate should be

$$r_c^{MD}(t) = R_c(t) \cdot H_c(0) \cdot S_i(0). \quad (6)$$

Once we know the current atom coordinate, $r_c^{MD}(t)$, a MD code can calculate the stress of the MD unit cell.
In an r-cell as follows,

\[ \sigma_{\text{MD}}(t) \]  

The stress in MD coordinate system is transferred to the real coordinate system of FEM by using the rotation matrix \( Q_e \) as follows,

\[ \sigma_{\text{FEM}}(t) = Q_e(t) \cdot \sigma_{\text{MD}}(t) \cdot Q_e^T(t). \]  

(7)

In FEM code, the first Piola-Kirchhoff stress is used to evaluate a force acting on each node.

\[ \mathbf{P}_{\text{FEM}}(t) = J \sigma_{\text{FEM}}(t) \cdot \mathbf{F}^e_{\text{FEM}}(t), \]

where \( J \) is the Jacobian of the deformation gradient tensor \( \mathbf{F} \).

In our multiscale code, we used LAMMPS as the MD engine. Because LAMMPS memorizes previous deformation matrix, \( \mathbf{R}(t-1) \), our FEM code provides the following differentiation between current and previous upper triangular stretch matrices to LAMMPS,

\[ \Delta \mathbf{R}_i(t) = \mathbf{R}_i(t) \cdot \mathbf{R}_i^{-1}(t-1). \]  

(9)

The flow chart of the proposed multiscale computation algorithm is schematically depicted in Fig. 1, and its validation will be examined in Sec. 3.4.

### 2.2 Hierarchical coupling method for amorphous solids

Here we briefly introduce the algorithm of CG-PR method, which has been developed as a hierarchical multiscale modeling tool for amorphous solids [23,25].

In the framework of finite element method, the discrete equations of motion for node displacements can be evaluated form the following equation as,

\[ \mathbf{M} \cdot \ddot{\mathbf{d}} + \mathbf{f}^{\text{int}}(\mathbf{d}) = \mathbf{f}^{\text{ext}}, \]

where \( \mathbf{d} \) is node displacement vector, and \( \mathbf{M}, \mathbf{f}^{\text{int}} \) and \( \mathbf{f}^{\text{ext}} \) are the mass matrix, force vectors, and external force, respectively. These quantities are defined as follows,

\[ \mathbf{M} = \sum_{e=1}^{n_e} \rho_0 \mathbf{N}_e^T \cdot \mathbf{N}_e dV, \]

\[ \mathbf{f}^{\text{int}} = \sum_{e=1}^{n_e} \mathbf{B}_e^T \cdot \mathbf{P}_e(\mathbf{d}) dV, \]

\[ \mathbf{f}^{\text{ext}} = \sum_{e=1}^{n_e} \left\{ \int_{\Omega_e} \mathbf{N}_e^T \cdot \mathbf{B}_e dV + \int_{\partial \Gamma_e} \mathbf{N}_e \cdot \mathbf{T}_e dS \right\}, \]

where \( \mathbf{A} \) is the element assembly operator over all elements, \( \rho_0 \) is material density, \( \mathbf{N}_e \) is the element shape function matrix, \( \mathbf{T}_e \) is the traction vector on the surface, and \( \mathbf{B}_e \) is the element strain-displacement matrix as,

\[ \mathbf{B}_e = \left[ \frac{\partial \mathbf{N}_e}{\partial \mathbf{X}} \right]. \]

(14)

In Eq. (12), \( \mathbf{P}_e \) is the first Piola-Kirchhoff stress, which can be evaluated using interatomic interaction among atoms in an r-cell as follows,

\[ \mathbf{P} = \frac{1}{2 \Omega_0} \frac{\partial W}{\partial \mathbf{F}} = \frac{1}{2 \Omega_0} \sum_{i,j} \frac{\partial V(r_{ij})}{\partial r_{ij}} r_{ij} \otimes r_{ij}. \]

(15)

where \( \mathbf{r}_{ij} = \mathbf{H}(0) \cdot \mathbf{S}_{ij} \) is the distance vector between initial positions of atom \( i \) and \( j \), and \( \mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i \) is the vector between current positions of atom \( i \) and \( j \). \( V \) is interatomic potential as a function of distance \( r_{ij} \), and \( \Omega_0 \) is the volume of r-cell. In the case of single crystal, atom position \( r \) is unique, but it is not the case of amorphous solids. Optimizing the potential energy respect to distance \( r \), we can get the optimized position vector \( \mathbf{r}_{ij}^{\text{opt}} \) as,

\[ \mathbf{r}_{ij}^{\text{opt}}(t) = \arg\min_{r_{ij}} V(r_{ij}^{\text{opt}}), \]

where argmin stands for argument of the minimum, \( \mathbf{r}_{ij}^{\text{opt}}(t) \) is the position guessed from previous configuration at time \( t-1 \),

\[ \mathbf{r}_{ij}^{\text{opt}}(t) = \mathbf{F}(t)e \cdot \mathbf{H}(0)e \cdot \mathbf{S}_{ij}(t-1). \]

(17)

This equation is essentially the Cauchy-Born rule, because the guessed atom coordinates are uniformly deformed following the deformation gradient in an element.

Once we have found \( \mathbf{r}_{ij}^{\text{opt}} \), the following coordinates can be obtained,

\[ \mathbf{S}_{ij}^{\text{opt}} = (\mathbf{F}(t)e \cdot \mathbf{H}(0)e)^{-1} \cdot \mathbf{r}_{ij}^{\text{opt}}, \]

\[ \mathbf{R}_{ij}^{\text{opt}} = \mathbf{H}(0)e \cdot \mathbf{S}_{ij}^{\text{opt}}. \]

Then, the correct 1st Piola-Kirchhoff stress is eventually defined as follows,

\[ \mathbf{P} = \frac{1}{2 \Omega_0} \frac{\partial W}{\partial \mathbf{F}} = \frac{1}{2 \Omega_0} \sum_{i,j} \frac{\partial V(r_{ij}^{\text{opt}})}{\partial r_{ij}^{\text{opt}}} r_{ij}^{\text{opt}} \otimes r_{ij}^{\text{opt}}. \]

(20)

If we use a general MD code, the 1st Piola-Kirchhoff stress is calculated using Eq. (13) with the optimized coordinate \( \mathbf{r}_{ij}^{\text{opt}} \). The flowchart of the above algorithm is shown in Fig. 2.

### 2.3 Implementation of parallel MD systems in LAMMPS

Each element in FEM model has its own MD system at a quadrature point, in our hierarchical algorithm. LAMMPS can divide a MD system to multiple systems so that these systems are independent from others by splitting a message passing interface (MPI) communicator to multiple communicators assigned to each MD systems. These MD systems are independent at the MD simulation level, while exchanging the energy and momentum among them through FEM. Since the size of FEM is small in the present work, FEM is computed on a parent node, and LAMMPS is computed on full nodes. To communicate FEM and LAMMPS, simple scatter and gather algorithm has been implemented. The cost of the MPI communication is much small, which is discussed in Sec. 3.2.

### 3 Results

#### 3.1 Numerical validation

First of all, to test our multiscale code that couples the open-source MD code LAMMPS with FEM method, we
Fig. 1. Flowchart of the multiscale computation algorithm that couples a continuum finite element simulation with a general MD simulation code.

Fig. 2. Flowchart of the Coarse-grained Parrinello-Rahman (CG-PR) method. \[ \text{[A] Continuum simulation} \]

Fig. 3. Deformation patterns used for validation tests.

compare the stresses evaluated by the two independent algorithms mentioned above, i.e. the one that uses Eqs. (16)–(20) and the other one that uses LAMMPS with Eqs. (1)–(9). A crystalline copper model, which is composed of \( 10 \times 10 \times 10 \) FCC primitive cells, is used for the validation test. The supercell includes 4,000 atoms and the side length is 36.15 \( \AA \). Mashin’s EAM potential was employed to evaluate interatomic interaction.

Uniaxial stretching/compression and two kinds of asymmetric deformations were examined as schematically illustrated in Fig. 3. In the first case, the unit cell was simply elongated and compressed along z-axis with maintaining the cell length of the other two sides. The stresses in every components evaluated using two methods are compared in a scatter diagram in Fig. 4. confirms that the stresses
calculated by the two codes agree well for the symmetric deformation.

Next, we examined how the multiscale algorithm works when applied to simulate asymmetric deformations, in order to verify the multiscale algorithm ability to use QR decomposition to couple with a MD engine, which is LAMMPS in this case. In Case (B), one edge is displaced from -0.3 to +0.3 strain along y-axis, whereas the edge is moved within the same range of strain for all directions at the same time. In Table 1, we summarize the deformation gradients in this case. In Case (B), one edge is displaced from -0.3 to +0.3 strain along y-axis, whereas the edge is moved within the same range of strain for all directions at the same time. In Table 1, we summarize the deformation gradient tensor $F$, the orthogonal rotation tensor $Q$, and the upper triangular stretch tensor $R$ in addition to all stress components in both coordinate systems of LAMMPS and FEM. One may find that all stresses calculated by using QR decomposition (Eqs. (11)–(20)), $\sigma_{\text{FEM}}$, agree to those of the in-house CG-PR code with Eqs. (10)–(20), $\sigma_{\text{IH}}$. It is therefore reasonable to expect that the proposed multiscale coupling algorithm may be able to simulate even more complicated asymmetric deformations, which may not be feasible to simulate by using the Parrinello-Rahman method [24] with the periodic boundary condition.

In the next section, we shall demonstrate a large scale multiscale simulation of inelastic deformation of a polymeric material.

3.2 Large-scale parallel multiscale computation for polymer deformation

Here we report the results of using the coupled FEM-LAMMPS code to investigate inelastic deformation of a macroscale cubic polymeric specimen composed of many mono-disperse linear polymers. A schematic illustration of the numerical model is shown in Fig. 5. The coarse-grained polymer model, namely, the bead-spring model [28], was used to describe the polymer chains in r-cells. The polymer chain is composed of LJ particles linearly connected by finite extensively nonlinear elastic bonds. The potential parameters were set to the standard Kremer-Grest model [25]. The cubic specimen is composed of 100 tetrahedron finite elements, and each element has an r-cell that contains 100 polymer chains, and each of them is composed of 100 beads. In FEM calculation, each quadrature point is represented by an r-cell. Because of the linear four-node tetrahedron element is used in FEM modeling, each element has only one quadrature point. Thus, the total number of beads in fine scale model of the system is $100 \times 100 \times 100 = 10^6$, i.e. one million atomistic freedoms.

Initial states of polymers were prepared by using OCTA-COGNAC [29], where the polymers were equilibrated in melt condition. To impose the uniaxial stretch boundary condition to the polymeric material, the constant velocities were prescribed at both top and bottom surfaces of the cubic specimen along vertical direction. The sides of the material were free to move. The magnitude of the prescribed velocity was chosen sufficiently large so that one can observe nonlinear behaviors of the polymeric material. When the deformation rate is higher than a characteristic value $1/\tau_R$, where $\tau_R$ is the Rouse relaxation time of polymer chains, the polymeric material is expected to show a nonlinear behavior in an extensional deformation. In the case of polymer melt with 100 beads per a chain, $\tau_R \approx 10,000[\tau]$, where $\tau$ is the unit of time of LJ particle [30]. The results are summarized in Fig. 4.

Figure 4(a) shows the tensile stress versus the tensile ratio, where the tensile stress and the tensile ratio defined here are the magnitude of the largest eigenvalue of the stress tensor $\sigma_{\text{FEM}}$ and the deformation gradient tensor $F$, respectively, averaged over the whole system. The unit of the stress is $[\epsilon/\sigma^3]$, where $\epsilon$ and $\sigma$ are the units of the energy and the length of LJ coarse-grained polymer chain, respectively. Figures 4(b) to (f) show the appearances of the material at the characteristic tensile ratios, 1.0 (initial state) (b), 1.08 (c), 3.14 (d), 4.0 (e), 5.0 (f). The tensile stress increases monotonically from (b) to (c) and from (c) to (d). The former region is the elastic deformation region and the latter region is the plastic deformation region. The shape of the material is a rectangular parallelepiped in these small strain regions. Beyond the yield point (d), the tensile stress decreases and the material show necking.
### Table 1. Comparison of stresses [GPa] evaluated using in-house code $\sigma_{\text{IH}}$ and the coupling method with LAMMPS $\sigma_{\text{FEM}}$ for deformation drawn in Fig. 3 (B). Deformation gradient tensor $\mathbf{F}$ and the decomposition to the orthogonal rotation matrix $\mathbf{Q}$ and the upper triangular stretch matrix $\mathbf{R}$ are also displayed.

|        | $(0, 0.3, 0)$ | $(0, -0.3, 0)$ | $(0.3, 0.3, 0)$ | $(-0.3, -0.3, -0.3)$ |
|--------|---------------|---------------|----------------|---------------------|
| $\mathbf{F}$ | 1.000 -0.075 0.000 | 1.000 -0.075 0.000 | 0.975 0.075 0.075 | 0.925 -0.075 -0.075 |
|        | 0.000 1.075 0.000 | 0.000 0.975 0.000 | 0.075 1.075 0.075 | 0.075 0.925 -0.075 |
|        | 0.000 0.075 1.000 | 0.000 -0.075 1.000 | 0.075 0.075 1.075 | -0.075 -0.075 0.925 |
| $\mathbf{Q}$ | 0.997 0.075 0.000 | 0.997 -0.075 0.000 | 0.995 -0.074 -0.065 | 0.993 0.073 0.088 |
|        | -0.075 0.997 0.000 | 0.075 0.997 0.000 | 0.069 0.995 -0.065 | -0.081 0.993 0.088 |
|        | 0.000 0.000 1.000 | 0.000 0.000 1.000 | 0.069 0.060 0.996 | -0.081 -0.094 0.992 |
| $\mathbf{R}$ | 0.000 1.000 -0.006 | 0.000 0.922 0.000 | 0.000 1.069 0.134 | 0.000 0.920 -0.167 |
|        | 0.000 0.075 1.000 | 0.000 -0.075 1.000 | 0.000 1.061 0.061 | 0.000 0.000 0.905 |
| $\sigma_{\text{MD}}$ | 3.844 -9.429 -3.615 | -8.959 18.757 9.232 | -5.232 -13.891 -3.995 | 17.495 81.230 24.536 |
|        | 3.844 -9.429 -3.615 | -8.959 18.757 9.232 | -5.232 -13.891 -3.995 | 17.495 81.230 24.536 |
| $\sigma_{\text{FEM}}$ | 3.660 -9.992 -3.660 | -9.304 17.387 9.304 | -4.698 -14.060 -4.698 | 21.629 82.435 21.629 |
|        | 3.660 -9.992 -3.660 | -9.304 17.387 9.304 | -4.698 -14.060 -4.698 | 21.629 82.435 21.629 |
| $\sigma_{\text{IH}}$ | 3.660 -9.993 -3.660 | -9.304 17.387 9.304 | -4.698 -14.061 -4.698 | 21.629 82.433 21.629 |
|        | 3.660 -9.993 -3.660 | -9.304 17.387 9.304 | -4.698 -14.061 -4.698 | 21.629 82.433 21.629 |
|        | 0.458 -3.660 -0.975 | 0.618 9.304 14.154 | -4.698 -14.061 -4.698 | 21.629 21.629 82.433 |
|        | 0.458 -3.660 -0.975 | 0.618 9.304 14.154 | -4.698 -14.061 -4.698 | 21.629 21.629 82.433 |

Fig. 6. The tensile stress versus the tensile ratio of uniaxially stretched polymeric material (a). Figures (b) to (f) represent the appearances of the material during deformation at characteristic points shown in Fig. (a). The color represents the magnitude of the stress at the local finite element; blue is low and red is high. The unit of the stress here is $[\epsilon/\sigma]^3$, $\epsilon$ and $\sigma$ are the unit of energy and the unit of size of LJ particle in a coarse-grained polymer, respectively.
Fig. 7. Parallel scaling of multiscale simulation on K computer. The simulation system was composed of one thousand finite elements and each finite element had 10 thousand LJ particles (100 bead-spring chains with 100 beads).

The behavior observed in Fig. 6 is qualitatively consistent with the experimental observation of uniaxially melt-extruded high-density polyethylene films. The yield point has been observed when the tensile ratio is about three, namely the engineering strain is 200%, both in our simulation and in the experiment. The initial condition of polymer in the simulation was amorphous state while that in the experiment was crystalline lamellae. The yield point may depend on the sample size and the direction of stretch. Further investigation, adjusting the conditions between the simulation and the experiment, is still ongoing.

Moreover, we have checked parallel scalability of our multiscale code on K computer. The total number of elements in the FEM model is increased to one thousand, and the total number of particles in a system was increased to 10 millions. Elapsed CPU time [unit s] per a multiscale FEM time step was measured and averaged over 10 FEM steps, which includes the iteration time for running the fine scale CG-PR method in each r-cell. As found in Fig. 7, our multiscale code shows a nearly ideal scaling efficiency when the number of particles per a processor is larger than 100. Generally speaking, parallel scalability of direct MD simulation with 10 million fine scale particles saturates when the number of processors is around one thousand. The reason for the high scaling efficiency of the hybrid method implemented with FEM and LAMMPS may attribute to the facts that (1) the multiscale method, especially the naturally segregated distribution of r-cells, makes efficient use of the massively parallel architecture of the supercomputer used such as K computer, and (2) the CG-PR molecular statics minimization algorithm may have less or no computing overhead.

4 Conclusions

In this work, we have developed a hierarchical multiscale method to bridge finite element method with molecular dynamics by using the large scale atomic/molecular massively parallel simulator (LAMMPS). In this algorithm, QR decomposition has been implemented to couple deformations and stresses at both FEM level as well as MD level, and in between. The coupling algorithm was validated by applying typical deformation patterns on copper crystal model, and good agreement with the result obtained from the CG-PR method was confirmed.

We have applied the multiscale code simulating uniaxial deformation of a polymeric material in a CG-PR multiscale FEM model that is composed of one million fine scale r-cell Lennard-Jones particles and succeeded in observing a typical nonlinear behavior, which is necking of the polymeric material. Indeed, an yield point has appeared when the tensile ratio is about three, which is consistent with the experimental observation.

It is worthy noting that the four-node tetrahedral element (C3D4) has a relative lower interpolation order, and it is often too stiff to be used in inelastic finite deformation computations. The inelastic deformation simulation results reported in this work by using C3D4 element is remarkable, which could not be achieved by using the same type of element in the phenomenological computational plasticity.

In addition, we also examined parallel scalability of the multiscale code using a large FEM model, in which ten million fine scale particles are embedded. The result revealed that the code has a strong, nearly ideal, scaling ability up to ten thousand processors thanks to the highly efficient built-in scalability of LAMMPS. The large scale simulations reported in this paper demonstrated applicability of the multiscale coupling method and algorithm to model and simulate mechanical properties amorphous materials.

Authors contributions

TM designed the con-current coupling algorithm and developed a code to establish interface with LAMMPS. SU developed the multiscale simulation code coupling FEM and LAMMPS, and performed validation tests. TM conducted large scale simulation for the polymeric material. TM and SU wrote simulation parts of the manuscript, and SL supervised the project, wrote and summarized the manuscript. All the authors have read and approved the final manuscript.

Acknowledgements

TM would like to thank Professor M. Isobe who brought TM and SU together. Our collaboration would not have started without his help. TM also thanks to Professor T. Kawakatsu...
and Professor T. Taniguchi for their supports and fruitful discussions. TM was supported by MEXT as “Exploratory Challenge on Post-K computer” (Challenge of Basic Science - Exploring Extremes through Multi-Physics and Multi-Scale Simulations). This research used the computational resources of the K computer provided by the RIKEN Advanced Institute for Computational Science through the HPCI System Research project (Project ID: hp160267, hp170236, hp180176) and the facilities of the Supercomputer Center in the Institute for Solid State Physics at the University of Tokyo.

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