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A methodology for coupling an atomic model with a continuum model using an extended Lagrange function

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Abstract

We propose a hybrid method combining an atomic model and a continuum model, in which the displacement field of the continuum is introduced as a new degree of freedom by extending Andersen's Lagrange function for constant-pressure molecular dynamics. We applied our method to a one-dimensional hybrid model which is composed of an atomic chain and springs. Large-scale fluctuation of the atomic system is found in the hybrid model. The density of states of the phonon is derived, and the large-scale fluctuation induces the generation of a variety of states of phonons. It is shown that the hybrid model proposed by our methodology enables us to perform large-scale simulations without intensive computations.

Recently there has been an increased interest in multiscale modelling as a promising methodology of computational material sciences. Multiscale modelling enables us to analyse non-equilibrium systems, such as dislocations, grain boundaries, and crack propagation, in which microscopic and macroscopic scales closely interact [1, 2]. In these studies, the systems are decomposed into domains characterized by different scales, typical models at these scales are employed, and these models are connected by a hybrid method [3–6].

The key technique in the hybrid method is how to connect the scales across the interfaces between the domains. Many studies have been devoted to connecting the scales. Broughton *et al* [7–9] proposed an interface between an atomic model and a continuum model described by the finite elements (FEs), in which the FE meshes were reduced to the atomic level and the mean-force coupling was introduced. The quasicontinuum technique, which was developed by Tadmor *et al* [10] to simulate defects in solids, provided a mixed continuum and atomic lattice approach at zero temperature. Rudd *et al* [11, 12] proposed a coarse-grained molecular dynamics technique, in which the thermal effect was taken into account through statistical coarse-graining procedures.

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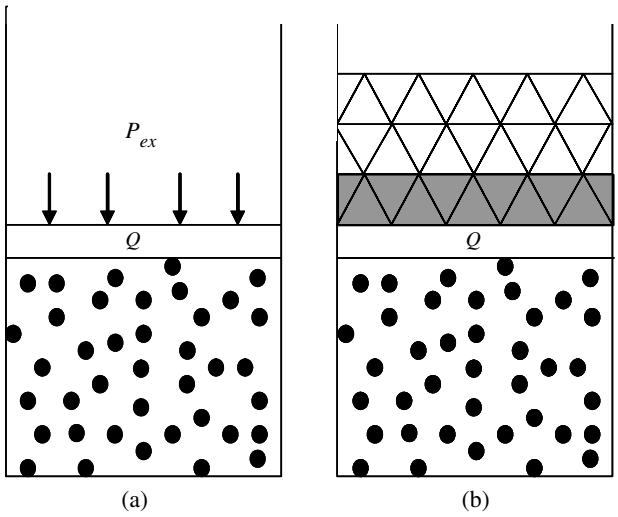

Figure 1. Schematic views of (a) Andersen's model and (b) the hybrid model. (a) In Andersen's model, the atoms (solid circles) in a container are under fixed external pressure $P_{\rm ex}$ through a piston of mass Q. (b) In the hybrid model, the finite elements of the continuum on the piston are drawn as triangles (see the text for details).

In this paper, a new methodology coupling an atomic model and a continuum model will be proposed by extending the well-known Andersen's method [13] for the constant-pressure molecular dynamics (MD) algorithm. In Andersen's method, the volume of the atomic system is introduced as a new degree of freedom, and the dynamics of the 'extended system' generates isobaric trajectories of atoms. Several types of the extended system have been developed by introducing a new degree of freedom [14–16], and these methods have been widely used in the studies of MD simulations, including *ab initio* MD simulation [17]. Our coupling system is a kind of extended system, in which the displacement field of the continuum is introduced as a new degree of freedom. The purposes of this paper are (1) to propose a new methodology for coupling an atomic model and a continuum model using the extended Lagrange function, and (2) to apply the methodology to a simple system: a one-dimensional hybrid model.

In Andersen's method, the constant-pressure MD is realized by introducing the volume V as a new degree of freedom. The Lagrange function of the system of N atoms constrained in isotropically fluctuating volume V under constant hydrostatic pressure $P_{\rm ex}$ is defined as

$$L(\{\mathbf{s}_i, \dot{\mathbf{s}}_i\}, V, \dot{V}) = \sum_i^N \frac{m_i V^{2/3} \dot{\mathbf{s}}_i \cdot \dot{\mathbf{s}}_i}{2} - \Phi(\{V^{1/3}\mathbf{s}_i\}) + \frac{Q\dot{V}^2}{2} - P_{\rm ex}V, \qquad (1)$$

where $\mathbf{s}_i$ and m_i are the normalized position vector and mass of the ith atom, respectively. $\mathbf{s}_i$ is related to the atomic position vector $\mathbf{r}_i$ as $\mathbf{r}_i = V^{1/3}\mathbf{s}_i$. $\dot{\mathbf{s}}_i$ is the time rate of $\mathbf{s}_i$. Φ is the potential energy of interatomic interactions. The parameter Q plays the role of mass. The Lagrange function has a physical meaning, as schematically shown in figure 1(a), where the atomic system in a container is compressed by a piston of mass Q. The first two terms on the right in equation (1) are atomistic kinetic and potential energies. The last two terms can be interpreted as kinetic and potential energies of the piston. The atomic system is under the periodic boundary condition. The equations of motion of the degrees of freedom of $\{\mathbf{s}_i\}$ and V

are derived from equation (1). The equation of motion of V is written as

$$Q\frac{\mathrm{d}\dot{V}}{\mathrm{d}t} = \frac{1}{3V}\left(2K + \sum_{i}^{N} \boldsymbol{r}_i \cdot \boldsymbol{F}_i\right) - P_{\mathrm{ex}}, \tag{2}$$

where K is the kinetic energy of the atomic system and F_i is the total force acting on the ith atom. The first two terms on the right in equation (2) correspond to the internal pressure of the atomic system. It is understood from equation (2) that the driving force of fluctuation of V comes from the imbalance between the internal pressure and the constant external pressure P_{ex}, and the internal pressure fluctuates around at P_{ex}. The timescale for this fluctuation is determined by Q. Time integration of the equations of motion of atoms provides isobaric trajectories in phase space.

We propose a new methodology for coupling an atomic model and a continuum model by extending the above Andersen's method as follows. Let us suppose that the hybrid model is composed of an atomic system and an elastic continuum and that they closely interact. This hybrid model is shown schematically in figure 1(b); the atomic system is connected to the elastic continuum through the piston. The atomic system is under the periodic boundary condition. The continuum is described by triangular elements. On the basis of general elastic theory and the FE algorithm, the energy of the continuum is given as, without body force,

$$E = \tfrac{1}{2}\sum_{\mu}^{N_{\mathrm{e}}}\sum_{l,m}^{l_{\max}}\left[\dot{u}_{\mu,l}\mathbf{M}_{\mu,l,m}\dot{u}_{\mu,m} + u_{\mu,l}\mathbf{K}_{\mu,l,m}u_{\mu,m}\right], \tag{3}$$

where $u_{\mu,l}$ is the displacement of the lth node of the μth finite element, and the subscripts l, m indicate Cartesian directions; therefore, the l, m sum runs over $l_{\max}$: 3×2 for triangular elements in two-dimensional FEs. N_{e} is the number of elements. The first term is the kinetic energy of the elements, where $\mathbf{M}_{\mu,l,m}$ is the mass matrix of the μth element. The second term is the elastic potential energy of the elements, which involves the stiffness matrix $\mathbf{K}_{\mu,l,m}$. It is seen in figures 1(a) and (b) that the elastic stress of the continuum gives the pressure acting on the piston and that the external pressure P_{ex} in Andersen's model is replaced by the elastic stress of the continuum. This means that the potential $P_{\mathrm{ex}}V$ in equation (1) can be replaced by the elastic potential energy,

$$\tfrac{1}{2}\sum_{\mu'}\sum_{l,m}^{l_{\max}} u_{\mu',l}(V)\mathbf{K}_{\mu',l,m}u_{\mu',m}(V). \tag{4}$$

$u_{\mu',l}(V)$ is the displacement of the nodes contacting with the atomic system through the piston and its value depends on the variable volume V and on how the nodes contact with the atomic system spatially. The μ'th element having such nodes is indicated by the grey triangles in figure 1(b). The new degrees of freedom of the displacements of the nodes can be introduced using this elastic potential energy, and the Lagrange function of Andersen's model is extended as

$$\begin{aligned} L(\{\mathbf{s}_i, \dot{\mathbf{s}}_i\}, V, \dot{V}, \{u_{\mu,l}, \dot{u}_{\mu,l}\}) = {} & \sum_{i}^{N}\frac{m_i V^{2/3}\dot{\mathbf{s}}_i \cdot \dot{\mathbf{s}}_i}{2} - \Phi(\{V^{1/3}\mathbf{s}_i\}) + \frac{1}{2}Q\dot{V}^2 \\ & - \tfrac{1}{2}\sum_{\mu'}\sum_{l,m}^{l_{\max}} u_{\mu',l}(V)\mathbf{K}_{\mu',l,m}u_{\mu',m}(V) \\ & + \tfrac{1}{2}\sum_{\mu}^{N_{\mathrm{e}}}\sum_{l,m}^{l_{\max}}\left[\dot{u}_{\mu,l}\mathbf{M}_{\mu,l,m}\dot{u}_{\mu,m} - u_{\mu,l}\mathbf{K}_{\mu,l,m}u_{\mu,m}\right]. \end{aligned} \tag{5}$$

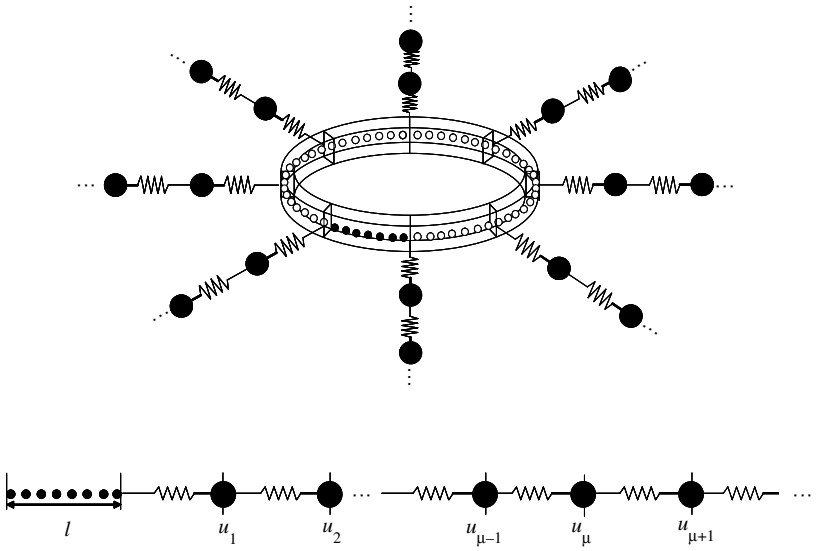

Figure 2. Schematic views of the one-dimensional hybrid model. In the upper panel, the model is illustrated under the periodic boundary condition. Atoms in the basic cell are drawn by solid circles, and atoms in the image cells as open circles. Springs are connected to the atomic chain. In the bottom panel, the detail of the hybrid model is illustrated; an atomic chain of length l is connected to springs. Displacements of the springs are indicated as u_μ.

The first two terms on the right are the atomic energy and the third term is the kinetic energy of the piston. These three terms are also presented in the Lagrange function of equation (1). The fourth term is the above elastic potential energy of equation (4). The last two terms are the kinetic and elastic potential energies of the elements which do not directly contact with the atomic system, and these elements are indicated by the open triangles in figure 1(b). In the new Lagrange function of equation (5), the elastic potential energy $\frac{1}{2}\sum_{\mu'}\sum_{l,m}^{l_{\max}} u_{\mu',l}(V)\mathbf{K}_{\mu',l,m}u_{\mu',m}(V)$ plays the role of bridging between the atomic system and the continuum through V. The equations of motion for the degrees of freedom $\{\mathbf{s}_i\}$, V, and $\{u_{\mu,l}\}$ are derived from the new Lagrange function. The dynamics of the atomic system and the continuum of the hybrid model can be obtained by the time integration of the equations of motion. The element size is of the order of magnitude of the volume of the atomic system; therefore, it is not necessary to reduce the element size to the atomic lattice size.

We applied the above method to a one-dimensional hybrid model as shown in figure 2. The hybrid model is composed of an atomic chain and springs, in which the periodic boundary condition is imposed on the atomic chain. According to the above procedure, the Lagrange function of this model has the form

$$L(\{s_i,\dot{s}_i\},l,\dot{l},\{u_\mu,\dot{u}_\mu\}) = \sum_{i=1}^{N}\frac{m_i(l\dot{s}_i)^2}{2} - \sum_{i,j=1(j<i)}^{N}\phi\left(l|s_i-s_j|\right) + \frac{Q\dot{l}^2}{2}$$
$$- \frac{k_1}{2}(l-l_0-u_1)^2 + \sum_{\mu=1}^{N_s}\frac{m_\mu\dot{u}_\mu^2}{2} - \sum_{\mu=2}^{N_s}\frac{k_\mu}{2}(u_{\mu-1}-u_\mu)^2, \qquad (6)$$

where l is the atomic chain length and l_0 is the equilibrium length. $\phi(l|s_i-s_j|)$ is the pair potential energy between the ith and jth atoms of the atomic chain. N_s is the number of springs. u_μ, m_μ and k_μ are the displacement, mass and spring constant of the μth spring,

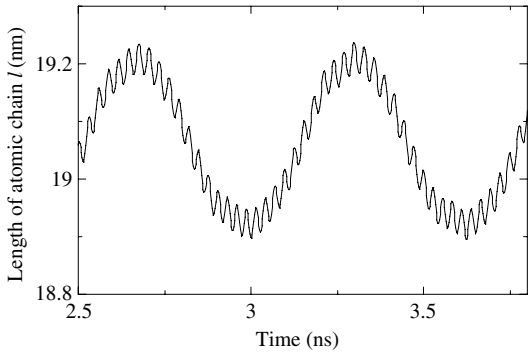

Figure 3. Time evolution of the atomic chain length l of the one-dimensional hybrid model.

respectively. The fourth term, $k_1(l - l_0 - u_1)^2/2$, in equation (6) is the elastic potential energy of the spring that is adjacent to the atomic chain ($\mu = 1$). The last two terms are the kinetic and elastic potential energies of the springs except the adjacent spring ($\mu = 2, 3, \ldots, N_s - 1, N_s$). From function (6), we obtain the equations of motion for $\{s_i\}$, l, and $\{u_\mu\}$:

$$m_i \frac{\mathrm{d}\dot{s}_i}{\mathrm{d}t} = -\frac{1}{l^2}\frac{\partial}{\partial s_i}\sum_{j\neq i}^{N}\phi\left(l|s_i - s_j|\right) - \frac{2m_i\dot{s}_i\dot{l}}{l}, \tag{7}$$

$$Q\frac{\mathrm{d}\dot{l}}{\mathrm{d}t} = \sum_{i=1}^{N} m_i l\dot{s}_i^2 - \frac{\partial}{\partial l}\sum_{i,j=1(j<i)}^{N}\phi\left(l|s_i - s_j|\right) - k_1(l - l_0 - u_1), \tag{8}$$

$$m_\mu\frac{\mathrm{d}\dot{u}_\mu}{\mathrm{d}t} = \begin{cases} k_\mu(l - l_0 - u_\mu) - k_{\mu+1}(u_\mu - u_{\mu+1}), & (\mu = 1) \\ k_\mu(u_{\mu-1} - u_\mu) - k_{\mu+1}(u_\mu - u_{\mu+1}), & (\mu = 2, 3, \ldots, N_s - 1, N_s). \end{cases} \tag{9}$$

The first two terms in equation (8) are the internal pressure (force in the present one-dimensional system) of the atomic chain. The last term in equation (8) is the elastic force caused by the spring ($\mu = 1$), and this term plays the role of connecting the atomic chain to the springs.

In the simulation of the hybrid model, we used the Lennard-Jones pair potential of argon, and the atomic chain was composed of 50 atoms. We connected the atomic chain to nine springs. Each spring had the same mass as that of the atomic chain and the spring constant was derived from the conventional MD simulations of the atomic chain. Gear's algorithm was used to integrate the equations of motion of equations (7)–(9), and the time step was set as 2.15 fs. The temperature was adjusted to 5 K. Initial values of length of atomic chain l and displacements of the springs u_μ and their time rates were set to generate the long-wavelength normal mode in the hybrid model.

The atomic chain length l as a function of time is shown in figure 3. A characteristic feature is found in the curve $l(t)$. The curve $l(t)$ consists of two types of mode: high frequency (period $\approx$0.03 ns) and low frequency (period $\approx$0.6 ns). The high-frequency mode has a small amplitude, and the low-frequency a large amplitude. The high-frequency mode in the curve $l(t)$ comes from the imbalance between the internal force of the atomic chain and the elastic force of the spring ($\mu = 1$). It is shown in the equation of motion for l of equation (8) that the first two terms on the right correspond to the internal force of the atomic chain and the last term to the elastic force of the spring. This imbalance in force gives rise to the high-frequency mode of the $l(t)$. Its frequency depends on the choice of Q. This small fluctuation in the atomic system shows in constant-pressure MD simulations of Andersen's method, in which the volume

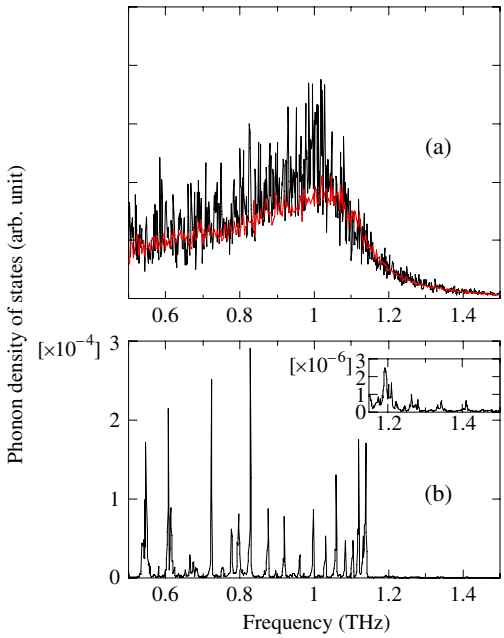

Figure 4. Density of states (DOS) of the phonon calculated by (a) the hybrid model and (b) the conventional MD simulation using 50 atoms. The red line in (a) indicates the DOS calculated by the conventional MD simulation using 500 atoms. In the upper right-hand part of (b), the DOS at the range from 1.2 to 1.5 THz is shown again in a different scale.

fluctuates around an equilibrium volume. The variable elastic force of the spring results in the low-frequency mode of the $l(t)$. The timescale of this mode is determined by the dynamics of the springs. The springs have a long-wavelength normal mode; therefore, the low-frequency mode of $l(t)$ has a large timescale. The large amplitude of the low-frequency mode also comes from the considerably large amplitude of the normal mode of the springs in the hybrid model. This large-scale fluctuation of the atomic system in the hybrid model is a different result from that in Andersen's model.

It is expected that the large-scale fluctuation of the atomic system influences the dynamical properties of atoms. The density of states (DOS) of the atomic vibration mode (phonon) is derived from the Fourier transformation of the velocity auto-correlation function $\psi(t)$ as

$$\psi(t) = \frac{\langle v_i(0) \cdot v_i(t) \rangle}{\langle v_i(0) \cdot v_i(0) \rangle}, \tag{10}$$

where v_i is the velocity of the ith atom, and the bracket $\langle \cdots \rangle$ means time average. The DOS in the above hybrid model is shown in figure 4(a). The DOS is compared with that obtained in the conventional MD simulation using 500 atoms, which is ten times 50 atoms in the atomic system of the hybrid model. Figure 4(b) shows the DOS calculated in the conventional MD simulation using 50 atoms; narrow Gaussians are found in the curve. The DOS in the hybrid model in figure 4(a) can reproduce that obtained in the large system of 500 atoms, while the DOS in the small system of 50 atoms in figure 4(b) is quite different.

The difference in the DOS can be explained as being associated with the large-scale fluctuation of the atomic system in the hybrid model. In the small system of 50 atoms in the conventional MD simulation, a limited number of states of the atomic vibration mode are generated. The limited number of the states results in the narrow Gaussian, as shown in

figure 4(b). In the hybrid model many states of the atomic vibration mode are generated in the atomic system of even 50 atoms. It can be expected that the large-scale fluctuation in the hybrid model causes the generation of a variety of atomic vibration modes, which leads to broadening of the Gaussian in figure 4(b) and to the curve as shown in figure 4(a).

The usefulness of the proposed hybrid method can be pointed out. The derived DOS in the hybrid model reproduces that calculated in the large system of 500 atoms. The hybrid model is composed of the atomic system of 50 atoms and the nine springs, and the size of this model is the same as the large system of 500 atoms. This means that the hybrid model can replace a large-scale atomic model.

In this paper, we have proposed a new methodology coupling an atomic system and a continuum by extending Andersen's molecular dynamics method. The elastic stress of the continuum acts on the atomic system and it replaces the external constant pressure in Andersen's method. The displacement field of the continuum is introduced as a new degree of freedom in the Lagrange function. We applied the method to a one-dimensional hybrid model which was composed of an atomic chain of argon atoms and springs. It is shown from the density of states of the phonon in the hybrid model that our method is effective for implementing large-scale simulations with reasonable computational costs.

References

[1] Vashishta P and Nakano A 1999 *Comput. Sci. Eng.* **1** 20
[2] Nieminen R M 2002 *J. Phys.: Condens. Matter* **14** 2859
[3] Kohlhoff S, Gumbsch P and Fischmeister H F 1991 *Phil. Mag.* A **64** 851
[4] Ogata S, Lidorikis E, Shimojo F, Nakano A, Vashishta P and Kalia R K 2001 *Comput. Phys. Commun.* **138** 143
[5] Rafii-Tabar H, Hua L and Cross M 1998 *J. Phys.: Condens. Matter* **10** 2375
[6] Nakano A, Bachlechner M E, Kalia R K, Lidorikis E, Vashishta P, Voyiadjis G Z, Campbell T J, Ogata S and Shimojo F 2001 *Comput. Sci. Eng.* **3** 56
[7] Broughton J Q, Abraham F F, Bernstein N and Kaxiras E 1999 *Phys. Rev.* B **60** 2391
[8] Abraham F F, Broughton J Q, Bernstein N and Kaxiras E 1998 *Comput. Phys.* **12** 538
[9] Abraham F F, Bernstein N, Broughton J Q and Hess D 2000 *MRS Bull.* **25** 27
[10] Tadmor E B, Ortiz M and Phillips R 1996 *Phil. Mag.* A **73** 1529
[11] Rudd R E and Broughton J Q 1998 *Phys. Rev.* B **58** R5893
[12] Rudd R E and Broughton J Q 2000 *Phys. Status Solidi* b **217** 251
[13] Andersen H C 1980 *J. Chem. Phys.* **72** 2384
[14] Parrinello M and Rahman A 1981 *J. Appl. Phys.* **52** 7182
[15] Nosé S 1984 *Mol. Phys.* **52** 255
[16] Car R and Parrinello M 1985 *Phys. Rev. Lett.* **55** 2471
[17] Senda Y, Shimojo F and Hoshino K 2002 *J. Phys.: Condens. Matter* **14** 3715