Minimizing Boundary Reflections in Coupled-Domain Simulations

Wei Cai,[1] Maurice de Koning,[1,2] Vasily V. Bulatov,[2] and Sidney Yip[1]
[1]*Department of Nuclear Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*
[2]*Lawrence Livermore National Laboratory, University of California, Livermore, California 94550*
(Received 20 June 2000)

We propose a time-dependent boundary condition coupling an atomistic simulation system to linear surroundings such that reflection of elastic waves across the boundary is minimized. Interdomain interactions expressed in terms of memory kernel functions within linear-response theory are treated in a natural dynamical manner, albeit numerically. The approach is shown to give significantly reduced phonon reflections at the domain boundaries relative to existing coupling methods. In addition, we demonstrate that the framework is also effective in the context of static relaxation of displacement fields associated with embedded inhomogeneities.

PACS numbers: 63.20.Mt, 02.70.Ns, 46.15.–x

A general problem in the domain decomposition approach to modeling discrete systems with localized inhomogeneities (defects) is the spurious reflection of elastic waves due to a change in system description across the domain boundary. Such effects are seen in, for example, the atomistic modeling of dislocation motion [1], crack propagation [2–5], and energetic particle-solid collisions [6,7], while they are also of concern in the recent development of hybrid techniques involving multiple length and/or time scales [8–11]. In order to minimize such reflections, a number of coupling schemes or boundary conditions have been proposed, such as *ad hoc* viscous damping [3–5] and the more physically motivated use of an approximate description of coupling across a domain boundary [7]. Until now, however, none can claim to be free from empiricism and the attendant limitation on general applicability.

In this Letter we describe a method for coupling two crystalline domains, a primary region P and an outer domain Q, for which the P-Q and Q-Q interactions are linear. In the governing equation of motion for the atoms in P, the influence of domain Q is represented in terms of a set of response functions which describe the response of medium Q to disturbances in domain P. These functions are evaluated systematically and without uncontrollable approximations by performing a series of test simulations in domain Q. In this fashion, a numerical boundary condition is derived for the simulation in P, eliminating the infinite number of degrees of freedom of the surrounding region Q from the description, while preserving the correct dynamics in region P. We demonstrate the effectiveness of this method by determining the phonon reflectivity in two model systems, a linear chain and a square lattice, for which previous results are available for comparison. In addition, we demonstrate that the framework is also useful in the context of static relaxation by applying the technique to determine the static displacement field associated with a dislocation configuration embedded in domain P.

Consider a crystalline system P-Q in which the region of interest P may contain inhomogeneities, while medium Q consists of defect-free material. For sufficiently large P and moderate temperatures, it is appropriate to describe the P-Q and Q-Q interactions as harmonic, and one can obtain an equation for P from which the explicit degrees of freedom associated with medium Q have been replaced by an implicit formulation [12,13]:

$$m\ddot{x}_i(t) = -\frac{\partial V}{\partial x_i} + \int_0^t d\tau \sum_{j=1}^{N} \beta_{ij}(\tau)\dot{x}_j(t-\tau) + \sum_{j=1}^{N} \beta_{ij}(t)x_j(0) + R_i(t)\,. \quad (1)$$

Here, x_i represent the N degrees of freedom in P, $V = V(\{x_j\})$ is the potential energy of the entire system with the atoms in Q fixed at their equilibrium positions, $\beta_{ij}(t)$ denote the N^2 elements of the time-dependent memory kernel matrix $\beta(t)$, and $R_i(t)$ is a linear function of the initial displacements and velocities in domain Q. Equation (1) is generally referred to as the generalized Langevin equation [12–14], in which the functions $\beta_{ij}(t)$ describe the response of medium Q to disturbances in region P in the form of P-to-P correlation. The $R_i(t)$ represent the effects on P due to any initial disturbance in Q and are usually treated as random forces to describe the effects of statistical fluctuations in region Q at a nonzero temperature [7,12,13].

Suppose the system is at equilibrium with the atoms in P and Q all at rest. At $t = 0$, one of the atoms in P is given a displacement ϵ, after which all atoms in P are frozen in their initial positions:

$$x_j(t) = x_j(0) = \epsilon\delta_{jk}\,. \quad (2)$$

Allowing the atoms in Q to relax after $t = 0$, the time-dependent forces acting on the atoms in P are given by the right-hand side of Eq. (1),

$$F_i(t) = -\frac{\partial V}{\partial x_i} + \epsilon\beta_{ik}(t)\,, \quad (3)$$

where the convolution terms and the $R_i(t)$ have vanished due to Eq. (2) and the fact that region Q is initially in equilibrium, respectively.

The first term in Eq. (3) represents the static force exerted on x_i if all atoms in Q were to be held fixed in their initial positions (i.e., fixed boundary conditions), while the second term is the time-dependent component arising from the motion of the Q atoms after $t = 0$. It is clear that the response functions $\beta_{ik}(t)$ completely define the P-Q coupling as a space-time dependent P-to-P correlation through medium Q.

Equations (2) and (3) constitute the basis for an algorithm to compute $\beta_{ik}(t)$ from a series of test simulations. Each simulation starts with the perturbation of an x_k according to Eq. (2), followed by a molecular dynamics (MD) run that produces the subsequent response of the atoms in Q under the constraint of fixed positions in P. During each run, the forces $F_i(t)$ are recorded as a function of time, giving directly the N response functions $\beta_{ik}(t)$, $i = 1 \ldots N$, after subtraction of the static force components $-\partial V/\partial x_i$.

In practice, the test simulations are performed over a finite time interval, so that the $\beta_{ij}(t)$ are determined only within a time interval $[0, t_c]$, with t_c being a cutoff time. Given the typical behavior of the matrix elements as a function of time, shown in Fig. 1, it is reasonable to disregard any further variations in the response functions for $t > t_c$, and assume that they remain constant at their cutoff values $\beta_{ij}(t_c)$, provided that t_c is sufficiently large. To be internally consistent, temporal truncation should be accompanied by a spatial cutoff. This means one should neglect all matrix elements that involve atoms separated by a distance larger than a cutoff radius $r_c \sim ct_c$, where c is the sound velocity in Q. In many cases, the number of relevant response functions can be further reduced if the interatomic potential model is finite ranged and the number of degrees of freedom in P that interact directly with those in Q is considerably smaller than N.

As a first demonstration of the effectiveness of the response function boundary condition we are proposing, we apply Eq. (1) to simulate the dynamics in a small section of a linear chain of identical harmonic oscillators with nearest-neighbor interactions. The masses, spring constants, and equilibrium distances are set equal to unity. Fifty oscillators are assigned to a region P which is bracketed by two semi-infinite chains Q_1 and Q_2. Because of the configurational symmetry, there is only one relevant memory kernel in this problem, describing the response of a semi-infinite chain to a displacement in the corresponding boundary oscillator. The test simulation, carried out using a time step $\Delta t = 0.1$, is truncated after a cutoff time $t_c = 50$, when the force fluctuations in the response function have decayed to within approximately 0.15% of the asymptotic value. The numerically computed response function is essentially indistinguishable from the analytical solution [15].

Using the numerically computed response function in (1), an MD simulation is performed to study the time evolution in P after introducing initial displacements $x_i(0)$ according to the wave packet

$$x_i(0) = \cos[k(X_i^0 - b)]\exp[-(X_i^0 - b)^2/2\sigma^2].$$

Here, X_i^0 denotes the equilibrium position of oscillator i and $X = b$ is the position in the center of domain P. As a reference, the motion is also monitored using a full MD simulation in which the oscillators in Q_1 and Q_2 are treated explicitly and no boundary is present. As a measure of the effectiveness of our response function approach, we evaluate the wave reflection at the boundaries between domain P and the chains Q_1 and Q_2. The reflectivity R is defined as the maximum difference between the instantaneous energies stored in region P during the response function simulation and the full MD run, divided by the initial energy in region P.

In Fig. 2, R is plotted as a function of wave vector k with $\sigma = 5$. The results show that the response function approach provides an excellent description of the dynamics

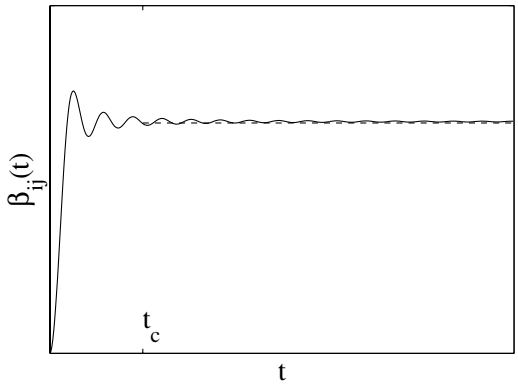

FIG. 1. Typical behavior of the memory kernel matrix elements as a function of time (full line). In practice, the response functions are determined within a time interval $[0, t_c]$, with t_c being a cutoff time. For $t > t_c$ they are assumed to remain constant at their cutoff values $\beta_{ij}(t_c)$ (dashed line).

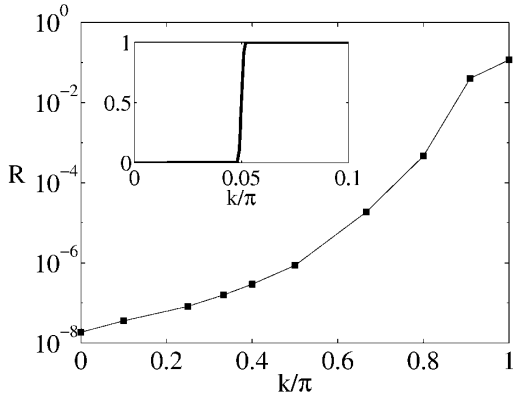

FIG. 2. Phonon reflectivity as a function of wave vector k for a one-dimensional chain of harmonic oscillators. Inset shows reflectivities associated with the CGMD method [10] for the same problem.

in P, featuring a reflectivity below 10^{-3} for approximately 80% of the Brillouin zone, and of the order of only 10^{-1} for k values at the zone boundary. For comparison, the reflectivity results obtained in a coarse-grained molecular dynamics (CGMD) simulation for the same system [10] are shown in the inset. It can be seen that the coupling method in the latter work is much less effective, as only the lower 5% of the Brillouin zone is treated correctly while the components with higher values of k are totally reflected due to the fact that such modes cannot exist in the coarse-grained region.

As a second demonstration, we study wave reflectivity in a two-dimensional version of the previous system, a square lattice of harmonic oscillators with the same specifications. The oscillators are allowed to move only in the direction perpendicular to the plane of the lattice. The primary domain P is defined as a square region containing 3600 lattice sites. Given the symmetry of the configuration and the short range of the interactions, the total number of test simulations required to fully specify the memory kernel matrix is 30. Each simulation is carried out using a time step $\Delta t = 0.1$ and is truncated after a cutoff time $t_c = 50$. Furthermore, an additional spatial truncation is introduced; all matrix elements that involve oscillators separated by a distance larger than a cutoff radius $r_c = 30$ are disregarded.

In order to compare to existing reflectivity results [7], we study the boundary reflectivity as a function of the width of the wave packets. The initial displacements in P are set according to a symmetric two-dimensional Gaussian function of width σ, centered in the middle of domain P. Following the procedure described previously, the reflectivity R is evaluated by comparing the energies stored in domain P during the full MD run and the response function simulation. Figure 3 shows the resulting values of R as a function of the width σ. Our method provides an accurate description of the response of medium Q, showing reflectivity between 10^{-3} and 10^{-5} across a wide range of values for σ. The inset shows reported reflectivity results for similar initial Gaussian displacements in a three-dimensional study using another reflection reduction method [7]; the different curves correspond to different values of the empirical damping coefficient in this scheme. Even though these results and ours do not refer to identical simulations, nonetheless, we believe it is significant that the reflectivity given by our treatment is some 2 orders of magnitude lower. Moreover, the reflectivity of our method can be systematically reduced even further by increasing the cutoff values for t_c and r_c.

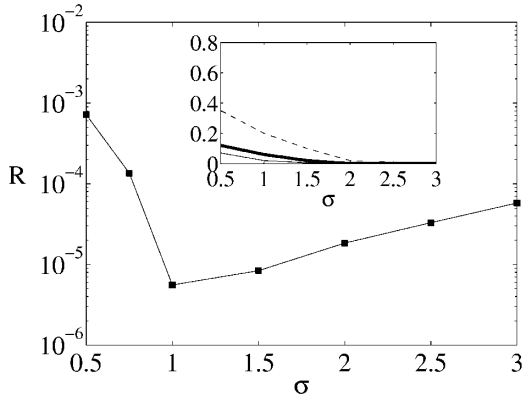

FIG. 3. Reflectivity on a two-dimensional square harmonic lattice as a function of the width σ of initial Gaussian displacements. Inset shows reflectivity results reported in Ref. [7] using another reflection reduction technique for similar Gaussian displacements in a three-dimensional fcc lattice.

In addition to minimizing boundary reflection, the response function framework is also useful in the context of static relaxation of displacement fields associated with a defect embedded in domain P. As a demonstration, we introduce a screw dislocation dipole at the center of the previously described two-dimensional square harmonic lattice. The dipole is created by fixing the displacements of a row of atoms in P at $+0.5$, and those in the adjacent row at

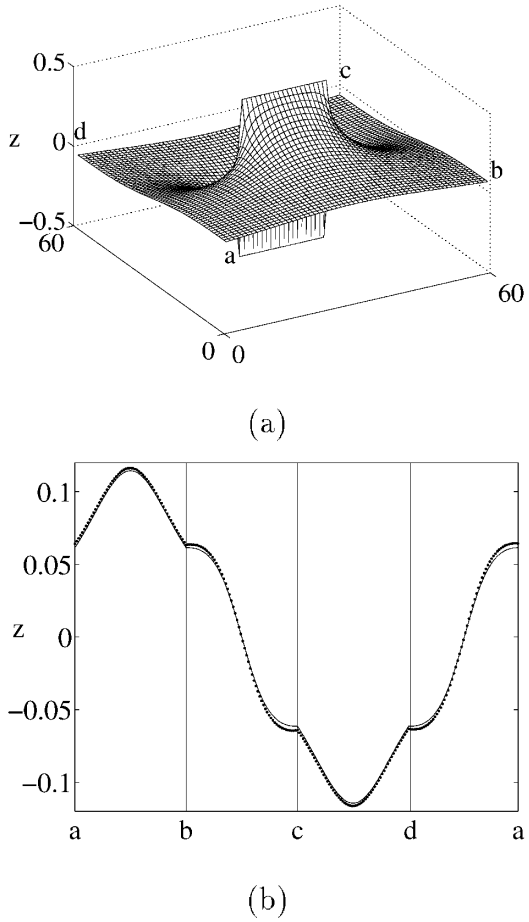

FIG. 4. (a) Displacements in two-dimensional square harmonic lattice containing a screw dislocation dipole in primary region P. (b) Displacement fields of oscillators along the four edges of the boundary a-b-c-d-a; results obtained using conjugate-gradient minimization (full line) and response function relaxation (dotted line).

-0.5, as shown in Fig. 4(a). To obtain the reference static displacement fields for this configuration, we first perform a conjugate-gradient (CG) energy minimization procedure on the entire system employing a sufficiently large Q region to achieve satisfactory convergence.

In order to obtain the relaxed displacement field using the response function method, one may directly integrate the equations of motion (1) until all kinetic energy has dissipated. Using the response functions and cutoff parameters determined in the second application, the static displacement field is thus obtained after about 10^5 MD steps. However, since we are interested only in the static response of medium Q in this application, the same result may be obtained more effectively by neglecting the specific time dependence of the response functions and using only their long-time asymptotic values. In addition, one may also disregard the force components that arise from a particular initial condition. In this manner, the same relaxed displacement fields can be obtained by relaxing the static forces

$$F_i(\{x_j\}) = -\frac{\partial V}{\partial x_i} + \sum_{j=1}^{N} \beta_{ij}(t_c) x_j \,, \tag{4}$$

using the cutoff values $\beta_{ij}(t_c)$ for the asymptotic values of the response functions.

Figure 4(b) shows a comparison between the results obtained with the reference CG procedure (full line) and our response function approach (dotted line). The curves describe the relaxed displacement fields as a function of the oscillator position along the four edges a-b-c-d-a of the P-Q boundary, as indicated in Fig. 4(a). The agreement is seen to be satisfactory, with small discrepancies originating from the errors introduced by the temporal and spatial truncations of the response functions. These errors can be systematically reduced by increasing the values of the cutoff parameters t_c and r_c.

In summary, we have shown how the response of a linear medium surrounding an atomistic simulation system can be treated in a systematic and numerically tractable manner requiring no assumptions beyond linear response theory. The method is found to be optimal in reducing artificial boundary reflections in dynamical simulations, as well as effective in the context of the static relaxation of displacement fields associated with embedded inhomogeneities.

W. C. and S. Y. acknowledge support from the Lawrence Livermore National Laboratory under an ASCI-Level 2 grant. Work of S. Y. is also supported by AFOSR (F49620-00-10082) and NSF (DMR-9980015). M. K. acknowledges support from the Brazilian agency Fundação de Amparo à Pesquisa do Estado de São Paulo under Contract No. 97/14290-6. V. V. B. acknowledges support from the Office of Basic Energy Sciences, the U.S. Department of Energy.

[1] K. Ohsawa and E. Kuramoto, J. Appl. Phys. **86**, 179 (1999).
[2] F. F. Abraham and H. Gao, Phys. Rev. Lett. **84**, 3113 (2000).
[3] S. J. Zhou, P. S. Lomdahl, R. Thomson, and B. L. Holian, Phys. Rev. Lett. **76**, 2318 (1996).
[4] B. L. Holian and R. Ravelo, Phys. Rev. B **51**, 11 275 (1995).
[5] P. Gumbsch, S. J. Zhou, and B. L. Holian, Phys. Rev. B **55**, 3445 (1997).
[6] S. J. Carroll, P. D. Nellist, R. E. Palmer, S. Hobday, and R. Smith, Phys. Rev. Lett. **84**, 2654 (2000).
[7] M. Moseler, J. Nordiek, and H. Haberland, Phys. Rev. B **56**, 15 439 (1997).
[8] F. F. Abraham, J. Q. Broughton, N. Bernstein, and E. Kaxiras, Comput. Phys. **12**, 538 (1998).
[9] J. Q. Broughton, F. F. Abraham, N. Bernstein, and E. Kaxiras, Phys. Rev. B **60**, 2391 (1999).
[10] R. E. Rudd and J. Q. Broughton, Phys. Rev. B **58**, R5893 (1998); Phys. Status Solidi (b) **217**, 251 (2000).
[11] J. A. Smirnova, L. V. Zhigilei, and B. J. Garrison, Comput. Phys. Commun. **118**, 11 (1999).
[12] S. A. Adelman and J. D. Doll, J. Chem. Phys. **61**, 4242 (1974); **62**, 2518 (1975); **64**, 2375 (1976).
[13] J. D. Doll, L. E. Myers, and S. A. Adelman, J. Chem. Phys. **63**, 4908 (1975).
[14] D. Chandler, *Introduction to Modern Statistical Mechanics* (Oxford University Press, New York, 1987).
[15] F. O. Goodman, J. Phys. Chem. Solids **23**, 1269 (1962).