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A Two-Way Interfacial Condition for Lattice Simulations

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Abstract. In this paper, we formulate a two-way interfacial condition for simulating lattice dynamics in one space dimension. With a time history treatment, the incoming waves are incorporated into the motion of the boundary atoms accurately. This condition reduces to the absorbing boundary condition when there is no incoming wave. Numerical tests validate the effectiveness of the proposed condition in treating simultaneously incoming waves and outgoing waves.

AMS subject classifications: 70-08, 65L99, 34B60
Key words: Interfacial condition, incoming wave, multiscale computation, time history treatment.

1 Introduction

Multiscale computations have become an indispensable tool in exploring fundamental issues in materials science and their applications in micro, nano and multiscale physics for emerging technologies [7]. In concurrent multiscale computations for a crystalline solid, one selects an atomistic region, where full atomistic computations are performed. The atomistic region is typically a tiny portion of the full solid, where detailed dynamics are demanded to understand nonlinearities, defects, and other important physics. In the complementary region, a coarse grid (continuum) description is used, where short waves are neglected. This greatly reduces the computing load and memory requirement.

Due to the domain decomposition, an artificial interface is introduced between the atomistic and the continuum region. On this interface, suitable conditions are needed to avoid spurious wave reflections. Such spurious waves, if not well suppressed, enter the atomistic region and disturb the local physics in a nonlinear manner. Extensive

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efforts have been made in designing interfacial conditions to reduce the spurious reflections. In the literature, many authors adopted a handshaking region between the atomistic and the continuum regions. In this region, a certain dissipative mechanism is introduced [2]. These interfacial conditions are mostly local in time, namely, requires only information from adjacent grid points at the current time step. A suitable amount of dissipation needs to be tuned in such a way to balance the efficiency and accuracy. They are therefore not accurate treatments of the interface. On the other hand, exact-solution-based interfacial conditions have also been developed more recently. For instance, when time information of an interfacial atom is available, one may reconstruct the displacement at a nearby atom for a linear lattice. This time history treatment was proposed by Adelman and Doll [1] for a harmonic lattice, and further developed for multiscale computations in [3, 8–10]. In contrast to absorbing treatments with a handshaking region, the time history treatment resolves exactly the interface for a linear infinite lattice. In numerical implementations, the accuracy may be reached with sufficiently long time history. For careful analysis, please refer to [5].

In all aforementioned numerical interfacial treatments, fine fluctuations in the continuum region are not taken into account. No wave enters the atomistic region unless it is resolved by the coarse grid. We notice that based on the extended space-time finite element, efforts have been made in incorporating fine scale oscillations into coarse scale solutions [4]. In applications, however, fine scale oscillations do exist in the continuum region and may propagate into the atomistic region. Thermal fluctuation is one such case with great importance. To our knowledge, there is yet quite limited knowledge about how to treat accurately thermal fluctuations in a multiscale computation [6, 12]. Unlike for a continuous wave propagation, a two-way interfacial condition for discrete lattices has not been studied so far in the literature.

In this paper, we develop a two-way interfacial condition for treating both incoming and outgoing waves in one space dimension. With this condition, outgoing waves propagate freely across the interfaces without reflection. With numerical tests, we demonstrate that incoming waves enter the atomistic domain effectively.

The rest of this paper is organized as followings. In Section 2, we derive the two-way interfacial condition. Numerical tests are performed for the linear lattice in Section 3. Some concluding remarks are made in Section 4.

2 Interfacial condition

We consider a harmonic lattice in one space dimension. The displacement u_n of the n-th atom away from its equilibrium is governed by the following rescaled Newton's law.

$$\ddot{u}_n = u_{n+1} - 2u_n + u_{n-1}, \quad n \in \mathbb{N}. \tag{2.1}$$

Consider an atomistic region Ω_D containing the atoms $n = 1, \cdots, N$, and the rest as the continuum region Ω_C. For the sake of clarity, we focus on the discussion of the left interface. The approach applies readily to the right interface. Across the interface, we

refer to the first atom in Ω_D ($n = 1$) as the interfacial atom, and the first atom in Ω_C ($n = 0$) as the ghost point atom. We record time history of the interfacial atom, namely $u_1(\tau)$ for $\tau \in [0, t]$, and reconstruct $u_0(t)$ by a convolution described as follows.

First we decompose the displacement into a left-going component $v_n(t)$, and a right-going component $w_n(t)$. This means $u_n = v_n + w_n$. Due to the linearity, both components satisfy the same Newton's law. In particular, the left-going component evolves according to

$$\ddot{v}_n = v_{n-1} - 2v_n + v_{n+1}. \tag{2.2}$$

Consider the atoms with $n \leq 0$. The motion $v_1(t)$ serves as a boundary condition for the semi-infinite chain. Considering the propagation direction, we assume that $v_n(0) = \dot{v}_n(0) = 0$ for $n \leq 0$.

Taking the vector $V = [v_0\ v_{-1}\ \cdots]^T$, we rewrite the equations in a vector form.

$$\ddot{V} = DV + \begin{bmatrix} v_1 \\ 0 \\ \vdots \end{bmatrix}, \qquad D = \begin{bmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \ddots \end{bmatrix}. \tag{2.3}$$

To solve this system, we start with a finite truncation $V_N = [v_0\ \cdots\ v_{-N+1}]^T$. The dynamics is governed by

$$\ddot{V}_N = D_N V_N + [v_1,\ 0,\ \cdots, 0,\ v_{-N}]^T. \tag{2.4}$$

Here D_N is an $N \times N$ tri-diagonal matrix with entries $1, -2, 1$.

Using the Laplace transform, the linear system is readily solved by ($\hat{}$ denotes the Laplace transform)

$$\hat{V}_N = (s^2 I - D_N)^{-1}[\hat{v}_1,\ 0,\ \cdots,\ 0, \hat{v}_{-N}]^T. \tag{2.5}$$

It is straightforward to compute that the $(1,1)$-th and $(1,N)$-th entries of $(s^2 I - D_N)^{-1}$ are

$$L_{11} = \frac{S^N - S^{-N}}{S^{N+1} - S^{-(N+1)}}, \qquad L_{1N} = \frac{1}{S^{N+1} - S^{-(N+1)}}, \tag{2.6}$$

with $S = (\sqrt{s^2+4} - s)^2/2$. It is easy to show that for $\mathrm{Re}\, s > 0$, we have $|S| < 1$.

Let the inverse transforms of L_{11} and L_{1N} be $\eta_1(t)$ and $\eta_N(t)$, respectively. The exact solution reads

$$v_0(t) = \eta_1(t) * v_1(t) + \eta_N(t) * v_{-N}(t). \tag{2.7}$$

Taking $N \to +\infty$, we have $L_{11} \to S$ and $L_{1N} \to 0$. Therefore, we may approximate

$$\eta_1(t) \to \theta_1(t) \equiv \mathcal{L}^{-1}(S) = \frac{2J_2(2t)}{t}, \quad \eta_N(t) \to 0. \tag{2.8}$$

Therefore, if we have a semi-infinite chain to the left of the atomistic region, the interfacial condition reads

$$v_0(t) = v_1(t) * \theta_1(t). \tag{2.9}$$

This is an exact interfacial condition, i.e., a transparent interfacial condition. It allows all left-going waves leave the atomistic region without reflection. The convolution requires all information from initial state to the current time t. This may not be realized exactly in a numerical simulation. Nevertheless, the numerical algorithm based on this condition absorbs very well the reflected waves. We further remark that for a finite lattice, the previous second limit indicates that we may neglect the numerical boundary at the $-N$-th atom for left-going waves if the lattice is long enough. In the literature, many authors have assumed, sometimes implicitly, to use the interfacial condition corresponds to a semi-infinite long lattice [1, 10].

In the same way, under the assumption of a semi-infinite lattice to the right of the atomistic region, we have

$$w_1 = \theta_1 * w_0. \tag{2.10}$$

From the definition of the left-going and right-going components, we may derive the two-way interfacial condition

$$u_0 = \theta_1 * u_1 + w_0 - \theta_2 * w_0, \tag{2.11}$$

with

$$\theta_2 = \theta_1 * \theta_1 = \mathcal{L}^{-1}(S^2) = \frac{4J_4(2t)}{t}.$$

This is an exact interfacial condition. It transparently absorbs outgoing waves and propagates incoming waves. However, numerical errors exist in real implementations. There is further a trade-off between accuracy and realization cost.

Due to the asymptotic property of the Bessel function, the kernel functions $\theta_1(t)$ and $\theta_2(t)$ decay in the rate of $t^{-3/2}$. See Fig. 1. This decay allows us to perform convolution with a truncated time history of length T. That is, we record $u_1(\tau), w_0(\tau)$ only for $\tau \in [t - T, t]$, and approximate the convolution by neglecting time history before $t - T$. A typical choice of T is about five to ten humps, namely around 15 to 30.

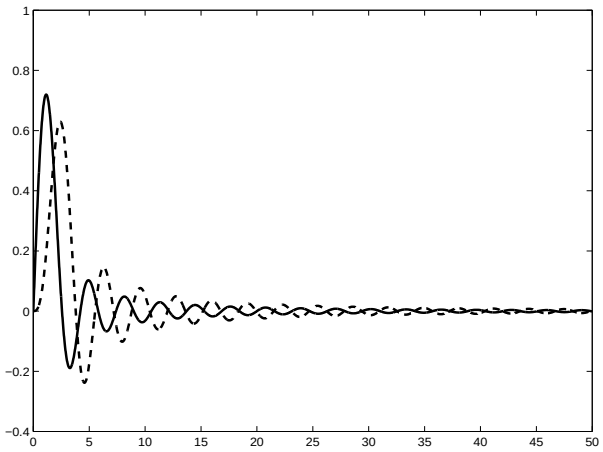

Figure 1: The time history kernel functions: $\theta_1(t)$ (solid) and $\theta_2(t)$ (dashed).

3 Numerical tests

To validate the proposed two-way interfacial condition, we perform several numerical tests. First, we demonstrate that the proposed condition effectively damped out reflections when there are only outgoing waves. Then we show that a monochromatic wave is reproduced with the incoming wave suitably incorporated by the proposed interfacial condition. Finally, more complicated wave packets are considered.

3.1 Absorption for outgoing waves

We take a 201-atom chain in the atomistic region. Following [10], we let the atomistic spacing at equilibrium be $h_a = 0.005$, and the atom position be $x_n = nh_a$. Under this setting, the interfacial conditions are

$$u_0 = \theta_1 * u_1 + w_0 - \theta_2 * w_0, \quad u_{200} = \theta_1 * u_{199} + w_{200} - \theta_2 * w_{200}. \tag{3.1}$$

We take initially a short wave modulated and carried by a Gaussian hump as follows.

$$u_n(0) = \begin{cases} h_a \dfrac{e^{-100(x_n-0.5)^2} - e^{-6.25}}{1-e^{-6.25}} \left(1 + 0.1\cos(80\pi x_n)\right), & \text{for } |x_n - 0.5| \le 0.25; \\ 0, & \text{elsewhere.} \end{cases} \tag{3.2}$$

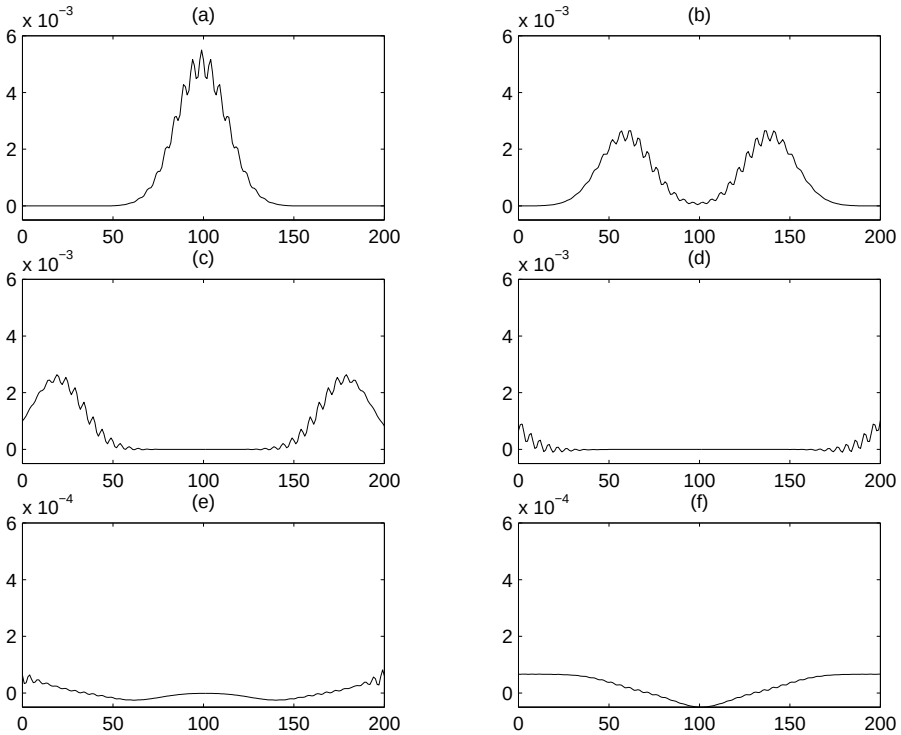

Figure 2: Absorption for outgoing waves: (a) $u_n(0)$; (b) $u_n(40)$; (c) $u_n(80)$; (d) $u_n(120)$; (e) $u_n(160)$; (f) $u_n(200)$.

The initial data contains abundant wave numbers. Because there is no incoming wave, we take

$$w_0 = w_{200} = 0,$$

and initialize the history of u_1 and u_{199} as purely 0. The computation is then performed with a time step size $\triangle t$=0.01, and a time history of length $T = 50$.

The numerical solution at various time is depicted in Fig. 2. Notice that the scale for the last two snapshots is one-tenth of the previous ones. The wave propagates freely towards two boundaries, and the reflection is almost negligible. The amplitude of reflected wave is less than 3% of the initial data. We remark that this is purely an atomistic computation, without any multiscale treatment. Using the PMM method, we may further reduce the reflection [9].

With this test, we demonstrate that the proposed boundary condition is effective in reflection suppression for outgoing waves. As a matter of fact, the condition reduces to that proposed by Adelman and Doll [1].

3.2 Monochromatic wave

Now we include an incoming wave from the left boundary x_0=0. In particular, we examine the simulation of a monochromatic wave

$$u_n(t) = 0.0005\cos(\omega x_n - \lambda t), \quad \text{with} \quad \omega = 10\pi.$$

The frequency is

$$\lambda = 2\sin(\omega\frac{h_a}{2}) = 0.1569,$$

according to the dispersion relation.

More precisely, we take initial data for the 201-atom lattice as follows.

$$u_n(0) = 0.0005\cos(\omega x_n), \quad \dot{u}_n(0) = 0.0005\lambda\sin(\omega x_n). \tag{3.3}$$

The histories for u_1 and u_{199} are initialized as (for $t \leq 0$)

$$u_1(t) = 0.0005\cos(\lambda t - \omega h_a), \quad u_{199}(t) = 0.0005\cos(\lambda t - 199\omega h_a). \tag{3.4}$$

There is an incoming wave from the left. The history as well as the input are given by

$$w_0(t) = 0.0005\cos(\lambda t). \tag{3.5}$$

No wave enters the atomistic domain from the right end, hence w_{200}=0. The numerical solution is depicted in Fig. 3 for time t=0, 10, 20, 30, 40. There is no reflection in the propagation. At t=40, almost one period is completed, as

$$40\lambda = 6.2767 \approx 2\pi.$$

As a comparison, when there is no incoming wave, the wave decays at the left end during the propagation. See Fig. 4.

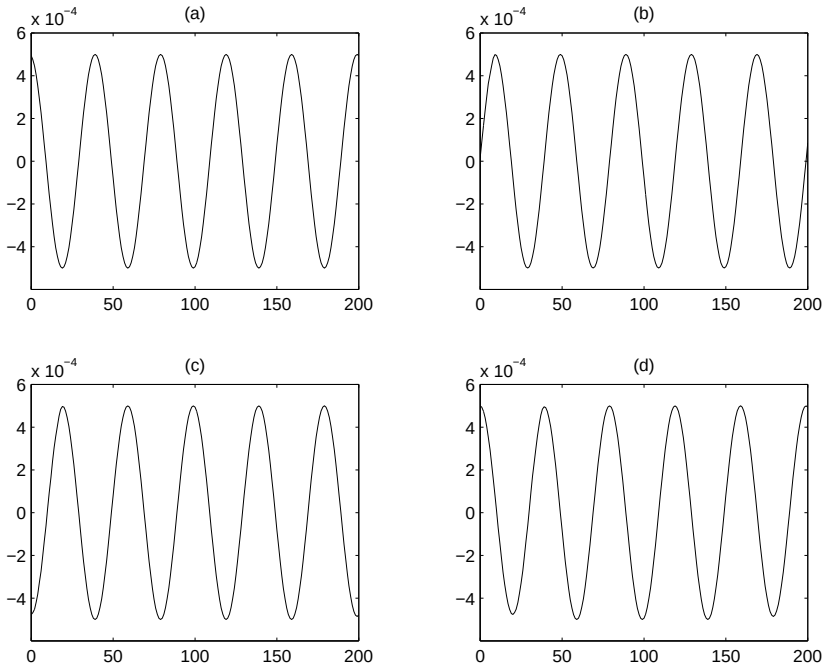

Figure 3: Propagation of monochromatic wave: (a) $u_n(0)$; (b) $u_n(10)$; (c) $u_n(20)$; (d) $u_n(40)$.

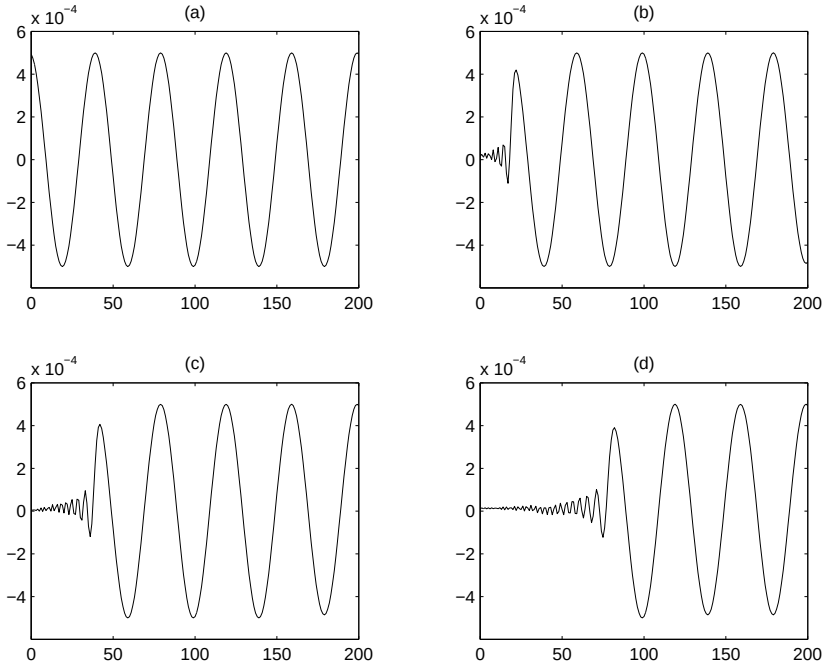

Figure 4: Attenuation of monochromatic wave: (a) $u_n(0)$; (b) $u_n(20)$; (c) $u_n(40)$; (d) $u_n(80)$.

3.3 More examples

To better illustrate the effectiveness of the proposed two-way interfacial condition, we present some more complex examples.

First, we compute for a combination of the previous two examples. We take initial condition as the sum of the Gaussian hump (3.2) and the monochromatic wave (3.3).

$$u_n(0) = \begin{cases} h_a \dfrac{e^{-100(x_n-0.5)^2} - e^{-6.25}}{1-e^{-6.25}} (1 + 0.1\cos(80\pi x_n)) \\ \qquad\qquad +0.1h_a \cos(\omega x_n), & \text{for } |x_n - 0.5| \le 0.25; \\ 0.0005\cos(\omega x_n), & \text{elsewhere.} \end{cases} \tag{3.6}$$

The initial velocity is taken as

$$\dot{u}_n(0) = 0.0005\lambda \sin(\omega x_n). \tag{3.7}$$

The time histories are taken as those for the monochromatic example, because the Gaussian hump has no incoming wave. As shown in Fig. 5, these waves simply superpose and pass across each other, without making any reflection at the boundaries. The Gaussian hump is split into a left-going part and a right-going part. Both parts propagate outward of the atomistic region. Their influence disappears at t between

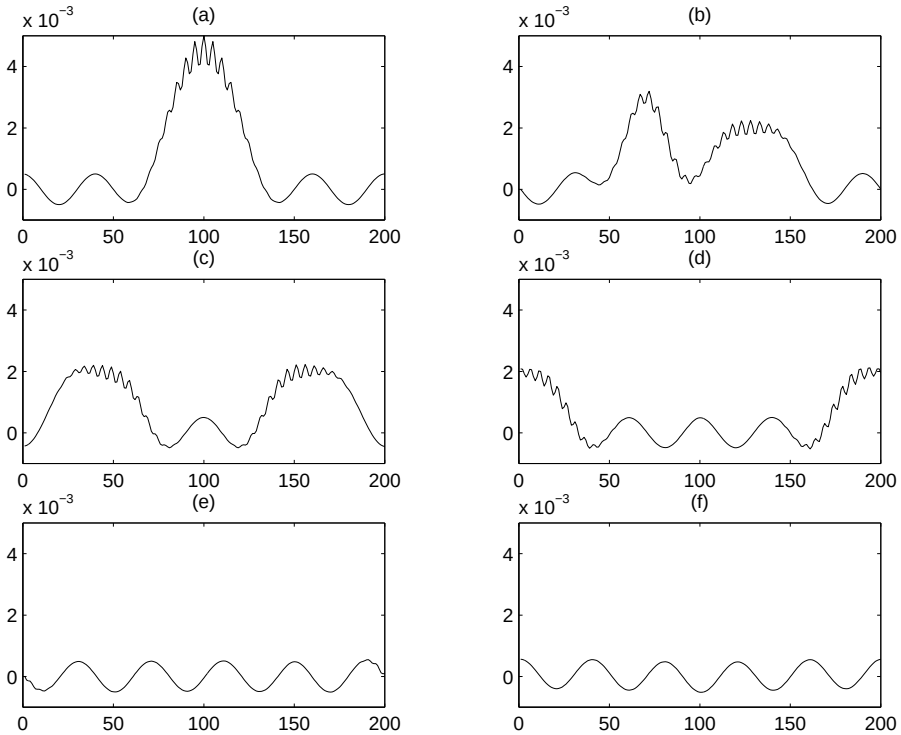

Figure 5: A monochromatic left-going incoming wave overtakes Gaussian hump: (a) $u_n(0)$; (b) $u_n(30)$; (c) $u_n(60)$; (d) $u_n(100)$; (e) $u_n(150)$; (f) $u_n(200)$.

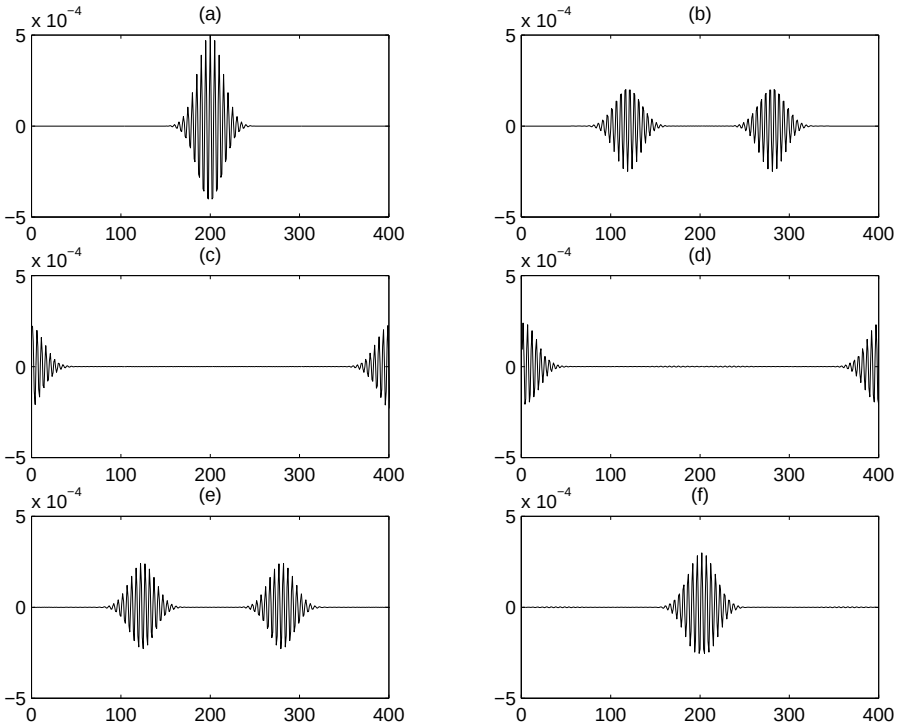

Figure 6: Crossing of polychromatic waves: (a) $u_n(0)$; (b) $u_n(100)$; (c) $u_n(250)$; (d) $u_n(450)$; (e) $u_n(600)$; (f) $u_n(700)$.

150 and 200. Because the monochromatic wave has a definite propagation direction, the wave profiles are not symmetric. The monochromatic wave completely overtakes the Gaussian hump eventually.

Next, we compute the crossing of polychromatic waves. We start with initial data similar to (3.2) in a 401-atom lattice.

$$u_n(0) = \begin{cases} h_a \dfrac{e^{-100(x_n-1)^2} - e^{-6.25}}{1 - e^{-6.25}} \Big(1 + 0.1\cos(80\pi x_n)\Big), & \text{for } |x_n - 1| \le 0.5; \\ 0, & \text{elsewhere.} \end{cases} \tag{3.8}$$

The initial velocity is taken as 0. Similar to the Gaussian hump evolution, the wave packet splits into a left-going wave and a right-going wave. When reaching at the boundary, these two waves produce time histories at the boundary $x_0 = 0$ and $x_{400} = 2$. We record the time histories, and further input these two histories for incoming waves in a later time $t \ge 350$. The history at the 0-th atom is taken as the incoming wave to the 400-th atom; and the history at the 400-th atom is taken as the incoming wave to the 0-th atom. Moreover, the histories are input in a reversed time direction.

The evolution is depicted in Fig. 6. Before $t = 350$, the wave packet propagates toward the boundary atoms and is well absorbed. See the first three subplots. The incoming waves then propagate back to the atomistic region. We notice that the wave

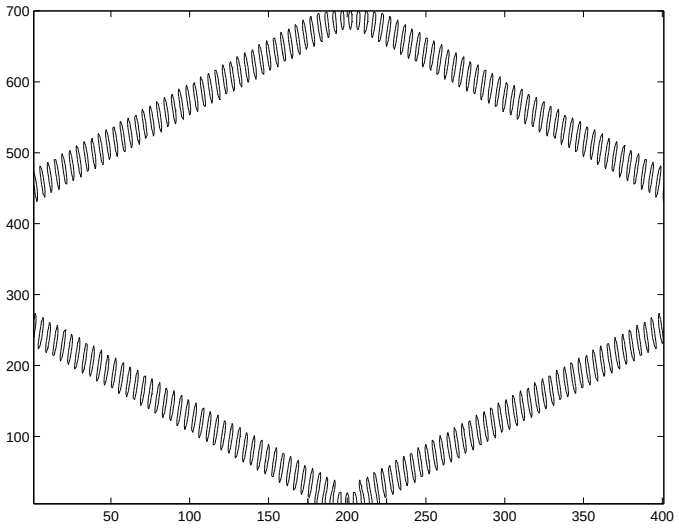

Figure 7: Wave front evolution in the crossing of polychromatic waves. The horizontal axis stands for atomistic numbering n, and the vertical for time t.

profile at $t = 450$ agrees well with that at $t = 250$. In fact, the velocities have a different sign, as they correspond to an incoming state and an outgoing state, respectively. This symmetry holds also for the time pair $t = 600$ and $t = 100$. More careful study shows that there are some phase errors occurred. In particular, the final snapshot for $t = 700$ obviously differs from the initial profile. As a matter of fact, the initial velocity is identically zero, which does not hold for $t = 700$. Nevertheless, the incoming waves are treated efficiently with the proposed two-way interfacial condition. The wave front propagation is further illustrated in a contour plot in Fig. 7.

4 Conclusions

In this study, we propose a two-way interfacial condition for linear atomistic chain. Besides effectively absorbing the outgoing waves, the condition also smoothly incorporates the incoming waves. To our knowledge, this is the first interfacial condition that simultaneously treats both waves for discrete lattices. The efficiency of the proposed condition is examined through several numerical tests.

This condition allows us to enhance the capability of existing concurrent multiscale algorithms. In particular, finite temperature calculations for crystalline solids are of great practical importance, yet remain not well-resolved. As most existing multiscale methods introduce a certain level of unclarified dissipation to absorb the spurious reflection for the outgoing waves, the thermal input can not be accurately accounted across the interfaces/boundaries. The proposed two-way interfacial condition facilitates treating the thermal input in an accurate manner [11].

We remark that the proposed condition is based on the assumption of a linear

lattice, at least linear away from the atomistic region. There is a trade-off for the time history convolution between the cut-off time and the accuracy.

Acknowledgements

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