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Stability of matching boundary conditions for diatomic chain and square lattice

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Abstract. Stability of MBC1, a specific matching boundary condition, is proved for atomic simulations of a diatomic chain. The boundary condition and the Newton equations that govern the atomic dynamics form a coupled system. Energy functions that decay along with time are constructed for both the boundary with the same type atoms and the one with different type atoms. For a nonlinear chain, MBC1 is also shown stable. Numerical verifications are presented. Moreover, MBC1 is proved to be stable for a two dimensional square lattice.

Keywords: stability; matching boundary condition; diatomic chain; two-dimensional square lattice; energy function

1. Introduction

Atomic simulations are widely used in the study of mechanical properties for materials and dynamics for structures, yet usually limited to the scale of microns. To include atomic features beyond this scale, concurrent multiscale algorithms have been developed in the past two decades, e.g., see an introduction in Liu (2005). For such an algorithm, the most challenging part is the numerical boundary (interface) treatment. An exact boundary condition in terms of convolution was invented for atomic simulations by Adelman (1974), and later further developed under the name of time history treatment, e.g., Cai (2000), Wagner (2003), Karpov (2005), Tang (2006a, b), Dreher (2008). To alleviate numerical costs of convolutions and difficulty in computing the kernel functions, local boundary conditions have been developed. Perfectly matched layer method was one among them, first invented for treating electromagnetic fields Berenger (1994), Thirunavukkarasu (2011). Some other accurate boundary treatments based on wave point of view include the variational boundary condition Engquist (1979), Li (2008), velocity interfacial condition Tang (2008), and matching boundary condition Wang (2010a, 2013). A boundary condition and the Newton equations of the atomic dynamics form a coupled dynamical system.

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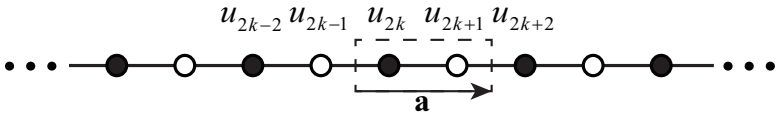


Fig. 1 Diatomic chain

For boundary conditions, one of the fundamental properties is its stability. An unstable condition may lead to divergent result and contaminate the multiscale computation. There are extensive studies for the continuous boundary value problems for partial differential equations, e.g., Baffet (2011) for wave equation with Higdon absorbing boundary condition, Zhang (2014) for first and second order absorbing boundary conditions, Eriksson (2017) for nonreflecting boundary conditions of an incomplete parabolic system, etc. There are relatively limited results for atomic dynamics with numerical boundary conditions. These include Trefethen (1985) for Gustafsson-Kreiss-Sundström theory, Li (2009) for molecular dynamics simulations in semi-infinite domain. For finite computational domain, results were obtained for velocity interfacial conditions Fang (2012), and matching boundary condition Tang (2014).

In this work, the stability for MBCs in a finite domain is discussed. MBCs are local in both space and time, designed by matching the dispersion relations. It applies to simulations not only for simple lattices, but also for complex lattices, with diatomic chain as a representative. The stability of MBC1 for linear diatomic chain using different boundary atoms, is studied systematically. Its stability can be proved by constructing energy function which is positive and monotone decreasing over time. In addition, stability of MBC1 for nonlinear diatomic chain and square lattice is also studied.

The rest of this paper is organized as follows. In Section 2, we prove stability of MBC1 for linear diatomic chain by constructing energy functions. Numerical tests are presented in Section 3. We discuss stability for nonlinear diatomic chain and square lattice in Section 4 and Section 5, respectively.

2. Stability of MBC1 for diatomic chain

Diatomic chain is the simplest complex lattice. Its unit cell (minimal periodic unit) is made of two atoms, shown as a solid circle and a hollow one in Fig. 1. Their masses are m_1 and m_2, respectively. We consider the diatomic chain with nearest neighbour interaction. Displacements of the $2k$-th and $(2k+1)$-th atoms away from equilibrium are denoted by $u_{2k}(t)$ and $u_{2k+1}(t)$. The pair-wise potential energy of the chain is $J_{2k+1/2}(u_{2k+1}-u_{2k})$. The total energy of the chain can be written as Tang (2014)

$$\begin{aligned} E_{diatomic} =& \frac{1}{2}\sum_k (m_1\dot{u}_{2k}^2 + m_2\dot{u}_{2k+1}^2) + \sum_k \big[J_{2k+1/2}(u_{2k+1}-u_{2k}) \\ &+ J_{2k-1/2}(u_{2k}-u_{2k-1})\big]. \end{aligned} \tag{1}$$

The dynamic equations of the diatomic chain are

$$\begin{cases} m_1\ddot{u}_{2k} = J'_{2k+1/2}(u_{2k+1}-u_{2k}) - J'_{2k-1/2}(u_{2k}-u_{2k-1}), \\ m_2\ddot{u}_{2k+1} = J'_{2k+3/2}(u_{2k+2}-u_{2k+1}) - J'_{2k+1/2}(u_{2k+1}-u_{2k}), k\in\mathbb{Z}. \end{cases} \tag{2}$$

For a harmonic chain, in another word, $J_{2k+1/2}(u_{2k+1}-u_{2k})=\kappa(u_{2k+1}-u_{2k})^2/2$, where κ is the elastic constant, the Newton Eq. (2) read

$$\begin{cases} m_1\ddot{u}_{2k}=\kappa(u_{2k+1}-2u_{2k}+u_{2k-1}), \\ m_2\ddot{u}_{2k+1}=\kappa(u_{2k+2}-2u_{2k+1}+u_{2k}), k\in\mathbb{Z}. \end{cases} \tag{3}$$

We rescale time by $\sqrt{\kappa/m_1}$, and denote $\gamma=m_1/m_2>0$ the mass ratio of the two atoms. Eq. (3) can be written as

$$\begin{cases} \ddot{u}_{2k}=u_{2k+1}-2u_{2k}+u_{2k-1}, \\ \ddot{u}_{2k+1}=\gamma(u_{2k+2}-2u_{2k+1}+u_{2k}), k\in\mathbb{Z}. \end{cases} \tag{4}$$

2.1 MBC1 for diatomic chain

We sketch the derivation of MBC1 as follows Wang (2010a). MBC1 involves the velocity and displacement of the boundary atom and its neighbour. For the diatomic chain, consider a solution for Eq. (4) in the wave form

$$\begin{cases} u_{2k}=U_1e^{i(\omega t-2k\xi)}, \\ u_{2k+1}=U_2e^{i(\omega t-(2k+1)\xi)}, k\in\mathbb{Z}, \end{cases} \tag{5}$$

where ω is the frequency, and ξ is the wave number. Then we obtain an eigenvalue problem

$$\begin{bmatrix} \omega^2-2 & 2\cos\xi \\ 2\gamma\cos\xi & \omega^2-2\gamma \end{bmatrix}\begin{bmatrix} U_1 \\ U_2 \end{bmatrix}=0. \tag{6}$$

This gives dispersion relation

$$\omega_\pm^2=(1+\gamma)\pm\sqrt{(1-\gamma)^2+4\gamma\cos^2\xi}, \tag{7}$$

and the relative amplitude of two type atoms

$$\begin{bmatrix} U_1 \\ U_2 \end{bmatrix}_\pm=\begin{bmatrix} \cos\xi \\ \frac{1}{2}\left[1-\gamma\mp\sqrt{(1-\gamma)^2+4\gamma\cos^2\xi}\right] \end{bmatrix}. \tag{8}$$

If the boundary atom is even-numbered, we suppose MBC1 to be

$$\dot{u}_{2N}+c_1\dot{u}_{2N-1}=b_1(u_{2N-1}-u_{2N}), \tag{9}$$

where c_1 and b_1 are undetermined coefficients Wang (2010b, 2013). The residual function is defined as

$$\Delta(\xi)=i\omega(\xi)\left[U_1(\xi)+c_1U_2(\xi)e^{i\xi}\right]-b_1\left[U_2(\xi)e^{i\xi}-U_1(\xi)\right]. \tag{10}$$

By requiring $\Delta(0)=0,\Delta'(0)=0,\Delta''(0)=0$, we calculate the coefficients

$$c_1=\frac{1}{\gamma},b_1=\sqrt{2\left(1+\frac{1}{\gamma}\right)}, \tag{11}$$

Fig. 2 A finite chain with boundary of the same type atoms

and obtain MBC1

$$\dot{u}_{2N} + \frac{1}{\gamma}\dot{u}_{2N-1} = \sqrt{2\left(1+\frac{1}{\gamma}\right)}(u_{2N-1} - u_{2N}). \tag{12}$$

If the boundary atom is odd-numbered, we can obtain similarly

$$\dot{u}_{2N+1} + \gamma\dot{u}_{2N} = \sqrt{2\gamma(1+\gamma)}(u_{2N} - u_{2N+1}). \tag{13}$$

To investigate the stability, we consider a finite chain with boundary condition MBC1. We define an energy function of atomic velocities and displacements, which is positive and monotone decreasing over time.

2.2 Boundary of the same type atoms

For simplicity, we assume that two boundary atoms are both the even-numbered atoms as shown in Fig. 2. Then the equations of the finite chain with boundary conditions are

$$\begin{cases} \ddot{u}_{2k} = u_{2k+1} - 2u_{2k} + u_{2k-1}, k = -N+1, -N+2, ..., N-2, N-1, \\ \ddot{u}_{2k+1} = \gamma(u_{2k+2} - 2u_{2k+1} + u_{2k}), k = -N, -N+1, ..., N-2, N-1, \\ \dot{u}_{-2N} + \frac{1}{\gamma}\dot{u}_{-2N+1} = \sqrt{2\left(1+\frac{1}{\gamma}\right)}(u_{-2N+1} - u_{-2N}), \\ \dot{u}_{2N} + \frac{1}{\gamma}\dot{u}_{2N-1} = \sqrt{2\left(1+\frac{1}{\gamma}\right)}(u_{2N-1} - u_{2N}). \end{cases} \tag{14}$$

Let energy function be

$$\begin{aligned} E_{same}(t) =& \frac{1}{2}\sum_{k=-N+1}^{N-1}\dot{u}_{2k}^2 + \frac{1}{2\gamma}\sum_{k=-N}^{N-1}\dot{u}_{2k+1}^2 + \frac{1}{2}\sum_{k=-N+1}^{N-1}\left[(u_{2k+1}-u_{2k})^2 + (u_{2k-1}-u_{2k})^2\right] \\ &+ \frac{\gamma}{1+\gamma}\left[\frac{1}{2}(u_{-2N+1}-u_{-2N})^2 + \frac{1}{2}(u_{2N-1}-u_{2N})^2\right]. \end{aligned} \tag{15}$$

Fig. 3 A finite chain with boundary of different types atoms

It is positive, and direct calculations show that

$$\begin{aligned}
\frac{dE_{same}}{dt} =& \sum_{k=-N+1}^{N-1} \dot{u}_{2k}(u_{2k+1} - 2u_{2k} + u_{2k-1}) + \sum_{k=-N}^{N-1} \dot{u}_{2k+1}(u_{2k+2} - 2u_{2k+1} + u_{2k}) \\
&+ \sum_{k=-N+1}^{N-1} [(\dot{u}_{2k+1} - \dot{u}_{2k})(u_{2k+1} - u_{2k}) + (\dot{u}_{2k-1} - \dot{u}_{2k})(u_{2k-1} - u_{2k})] \\
&+ \frac{\gamma}{1+\gamma} [(\dot{u}_{-2N+1} - \dot{u}_{-2N})(u_{-2N+1} - u_{-2N}) \\
&+ (\dot{u}_{2N-1} - \dot{u}_{2N})(u_{2N-1} - u_{2N})] \\
=& \dot{u}_{-2N+1}(u_{-2N} - u_{-2N+1}) - \frac{\gamma}{1+\gamma}(\dot{u}_{-2N+1} - \dot{u}_{-2N})(u_{-2N} - u_{-2N+1}) \\
&+ \dot{u}_{2N-1}(u_{2N} - u_{2N-1}) - \frac{\gamma}{1+\gamma}(\dot{u}_{2N-1} - \dot{u}_{2N})(u_{2N} - u_{2N-1}) \\
=& -\frac{\gamma}{1+\gamma}\left[(\dot{u}_{-2N} + \frac{1}{\gamma}\dot{u}_{-2N+1})(u_{-2N+1} - u_{-2N}) \right. \\
&\left. + (\dot{u}_{2N} + \frac{1}{\gamma}\dot{u}_{2N-1})(u_{2N-1} - u_{2N})\right] \\
=& -\sqrt{\frac{2\gamma}{1+\gamma}}\left[(u_{-2N+1} - u_{-2N})^2 + (u_{2N-1} - u_{2N})^2\right] \leqslant 0.
\end{aligned} \tag{16}$$

So the energy function is monotone decreasing over time. The boundary condition (14) is hence stable for diatomic chain with any mass ratio.

2.3 Boundary of different type atoms

Without loss of generality, we assume that the right boundary atom is even-numbered atom and the left one is odd-numbered as shown in Fig. 3. Then the equations of the finite chain with boundary conditions are

$$\begin{cases}
\ddot{u}_{2k} = u_{2k+1} - 2u_{2k} + u_{2k-1}, \\
\ddot{u}_{2k+1} = \gamma(u_{2k+2} - 2u_{2k+1} + u_{2k}), k = -N+1, -N+2, ..., N-2, N-1, \\
\dot{u}_{-2N+1} + \gamma\dot{u}_{-2N+2} = \sqrt{2\gamma(1+\gamma)}(u_{-2N+2} - u_{-2N+1}), \\
\dot{u}_{2N} + \frac{1}{\gamma}\dot{u}_{2N-1} = \sqrt{2\left(1+\frac{1}{\gamma}\right)}(u_{2N-1} - u_{2N}).
\end{cases} \tag{17}$$

We define an energy function

$$\begin{aligned} E_{diff}(t) =& \frac{1}{2}\sum_{k=-N+1}^{N-1}\dot{u}_{2k}^2+\frac{1}{2\gamma}\sum_{k=-N+1}^{N-1}\dot{u}_{2k+1}^2+\frac{1}{2}\sum_{k=-N+1}^{N-1}(u_{2k+1}-u_{2k})^2 \\ &+\frac{1}{2}\sum_{k=-N+2}^{N-1}(u_{2k-1}-u_{2k})^2+\frac{1}{2(1+\gamma)}(u_{-2N+2}-u_{-2N+1})^2 \\ &+\frac{\gamma}{2(1+\gamma)}(u_{2N-1}-u_{2N})^2. \end{aligned} \tag{18}$$

The function is positive and

$$\begin{aligned} \frac{dE_{diff}}{dt} =& \sum_{k=-N+1}^{N-1}\dot{u}_{2k}(u_{2k+1}-2u_{2k}+u_{2k-1}) \\ &+\sum_{k=-N+1}^{N-1}\dot{u}_{2k+1}(u_{2k+2}-2u_{2k+1}+u_{2k}) \\ &+\sum_{k=-N+1}^{N-1}[(\dot{u}_{2k+1}-\dot{u}_{2k})(u_{2k+1}-u_{2k})] \\ &+\sum_{k=-N+2}^{N-1}[(\dot{u}_{2k-1}-\dot{u}_{2k})(u_{2k-1}-u_{2k})] \\ &+\frac{1}{1+\gamma}[(\dot{u}_{-2N+1}-\dot{u}_{-2N+2})(u_{-2N+1}-u_{-2N+2})] \\ &+\frac{\gamma}{1+\gamma}[(\dot{u}_{2N-1}-\dot{u}_{2N})(u_{2N-1}-u_{2N})] \\ =&\dot{u}_{-2N+1}(u_{-2N+2}-u_{-2N+1}) \\ &-\frac{1}{1+\gamma}(\dot{u}_{-2N+1}-\dot{u}_{-2N+2})(u_{-2N+2}-u_{-2N+1}) \\ &+\dot{u}_{2N-1}(u_{2N}-u_{2N-1})-\frac{\gamma}{1+\gamma}(\dot{u}_{2N-1}-\dot{u}_{2N})(u_{2N}-u_{2N-1}) \\ =&-\frac{1}{1+\gamma}(\dot{u}_{-2N+1}+\gamma\dot{u}_{-2N+2})(u_{-2N+2}-u_{-2N+1}) \\ &-\frac{\gamma}{1+\gamma}(\dot{u}_{2N}+\frac{1}{\gamma}\dot{u}_{2N-1})(u_{2N-1}-u_{2N}) \\ =&-\sqrt{\frac{2\gamma}{1+\gamma}}\left[(u_{-2N+2}-u_{-2N+1})^2+(u_{2N-1}-u_{2N})^2\right]\leqslant 0. \end{aligned} \tag{19}$$

So, it is monotone decreasing over time.

The boundary condition (17) is hence stable for diatomic chain with different type boundary atoms.

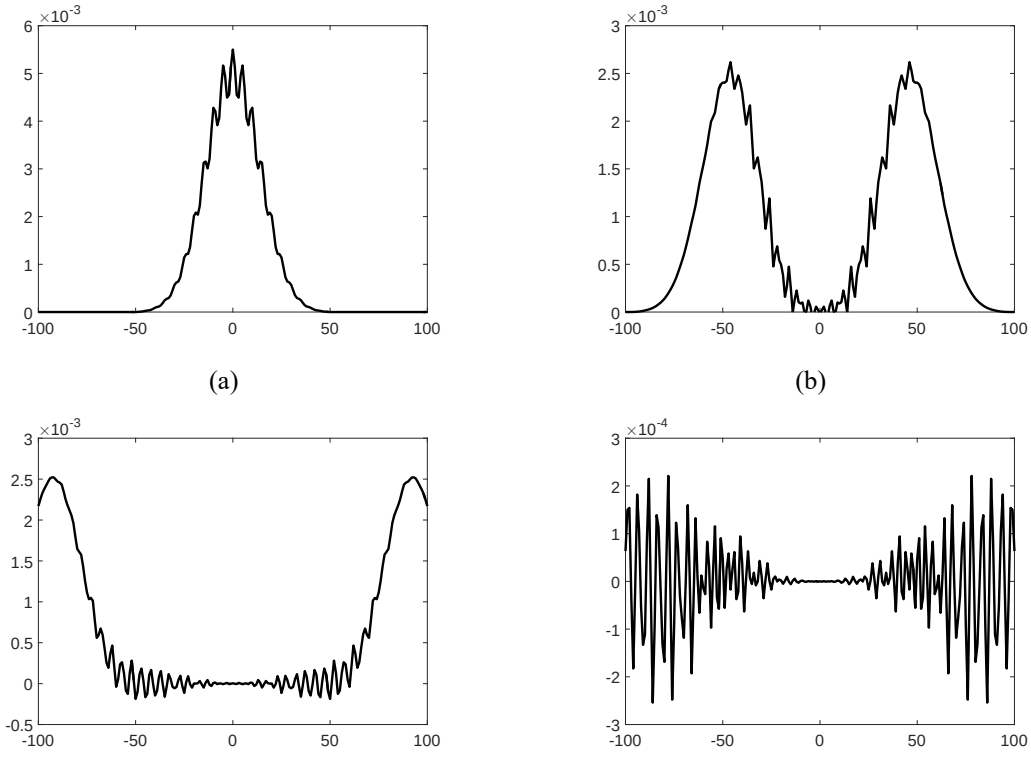


Fig. 4 Displacements with same boundary: (a) $u_n(0)$; (b) $u_n(40)$; (c) $u_n(80)$; (d) $u_n(120)$. The horizontal axis represents the atomic numbering, and the vertical axis represents the displacement

3. Numerical test

In this section, we compute diatomic chains, with 201 atoms ($N = 100$ in the Eq. (14)) for the boundary with same type atoms; and with 200 atoms ($N = 100$ in the Eq. (17)) for the boundary with different type atoms by speed verlet algorithm with time step size $\Delta t = 0.01$. The mass ratio $\gamma = 2$. We take initial data as in Tang (2006a)

$$u_n(0) = \begin{cases} 0.005\,[1 + 0.1\cos(0.4\pi n)]\,\dfrac{e^{-0.0025n^2} - e^{-6.25}}{1 - e^{-6.25}}, & -50 < n < 50, \\ 0, & elsewhere. \end{cases} \tag{20}$$

The velocity is uniformly zero initially. The displacements are shown in Figs. 4 and 5. From Fig. 6, we know that the reflection is about 3%. The choice of boundary atoms makes little difference in terms of the reflection.

The energy decay rate is shown in Fig. 7. The numerically calculated decay rate and the one calculated by the boundary terms are almost the same. As asserted by the theoretical results, both types of boundaries are stable.

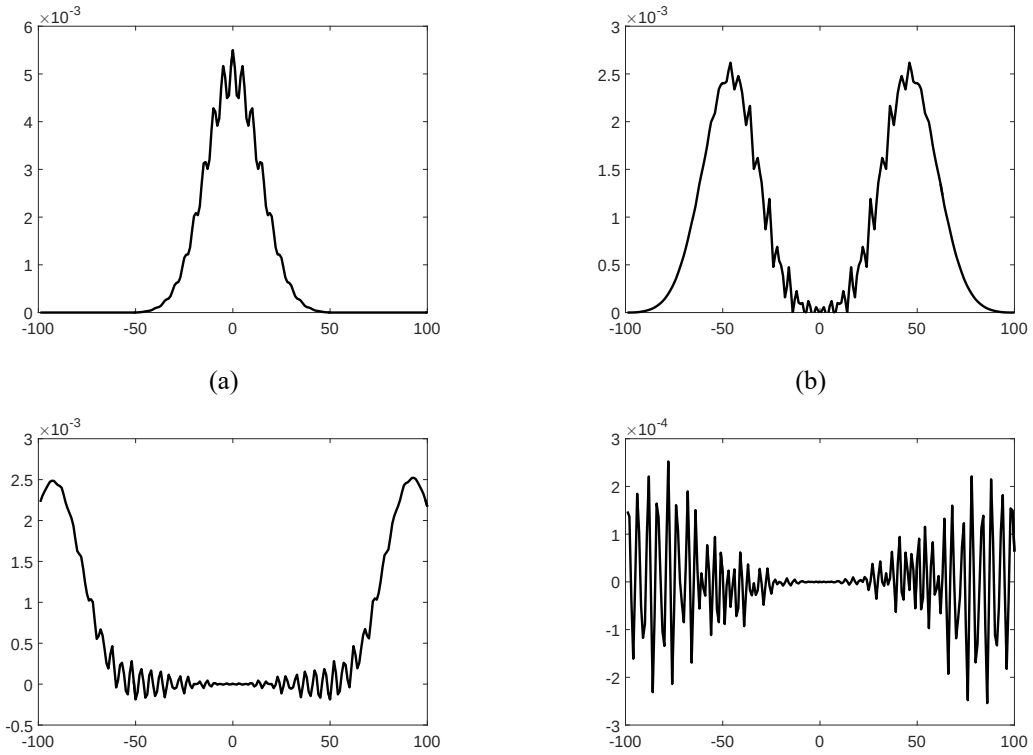


Fig. 5 Displacements with different boundaries: (a) $u_n(0)$; (b) $u_n(40)$; (c) $u_n(80)$; (d) $u_n(120)$. The horizontal axis represents the atomic numbering, and the vertical axis represents the displacement

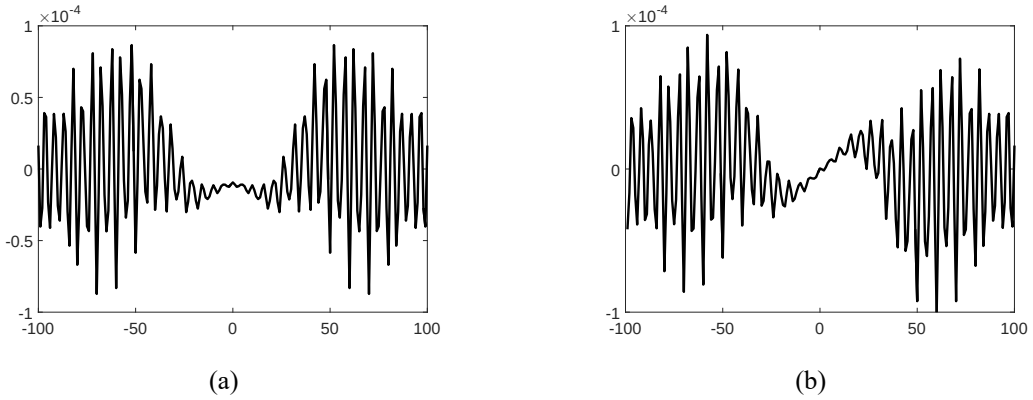
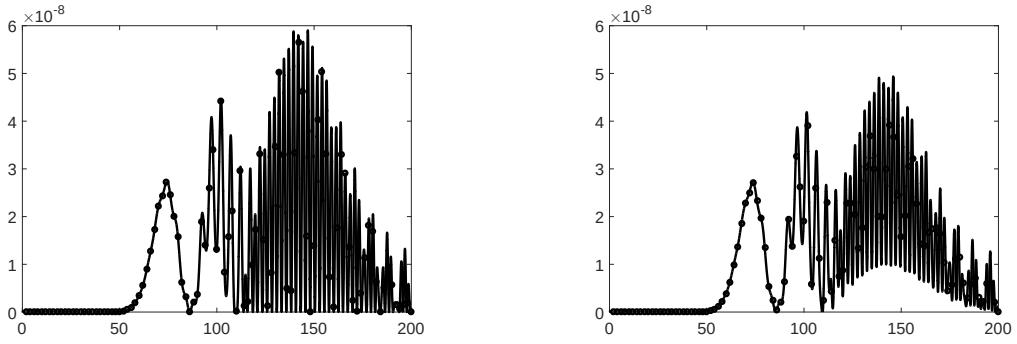


Fig. 6 Comparison of $u_n(200)$ with different boundary atoms: (a) boundary with same type atoms; (b) boundary with different type atoms. The horizontal axis represents the atomic numbering, and the vertical axis represents the displacement



(a) (b)

Fig. 7 Energy decay rate for MBC1: solid curve for numerically calculated $-\dot{E}(t)$ and circle for (a) $\sqrt{2\gamma/(1+\gamma)}[(u_{-2N}-u_{-2N+1})^2+(u_{2N-1}-u_{2N})^2]$ (boundary with the same type atoms); (b) $\sqrt{2\gamma/(1+\gamma)}[(u_{-2N+1}-u_{-2N+2})^2+(u_{2N-1}-u_{2N})^2]$ (boundary with the different type atoms). The horizontal axis represents time, and the vertical axis represents the rate

4. Stability of MBC1 for nonlinear diatomic chain

For nonlinear diatomic chain (2), MBC1 with sound speed is as follows **?**.

$$\begin{cases} \dot{u}_{-2N}+\dfrac{1}{\gamma}\dot{u}_{-2N+1}=C_L(t)\sqrt{2\left(1+\dfrac{1}{\gamma}\right)}(u_{-2N+1}-u_{-2N}), \\ \dot{u}_{2N}+\dfrac{1}{\gamma}\dot{u}_{2N-1}=C_R(t)\sqrt{2\left(1+\dfrac{1}{\gamma}\right)}(u_{2N-1}-u_{2N}), \end{cases} \tag{21}$$

where

$$\begin{aligned} &C_L(t)= \\ &\sqrt{\left[J'_{-2N+3/2}(u_{-2N+2}-u_{-2N+1})-J'_{-2N+1/2}(u_{-2N+1}-u_{-2N})\right]\Big/(u_{-2N+2}-2u_{-2N+1}+u_{-2N})} \\ &>0, \\ &C_R(t)= \\ &\sqrt{\left[J'_{2N-3/2}(u_{2N-1}-u_{2N-2})-J'_{2N-1/2}(u_{2N}-u_{2N-1})\right]\Big/(u_{2N-2}-2u_{2N-1}+u_{2N})} \\ &>0. \end{aligned} \tag{22}$$

Here we take same type atoms for the boundary as an example. Let energy function

$$\begin{aligned} E_{nonlinear}(t) =& \frac{1}{2}\sum_{k=-N+1}^{N-1}\dot{u}_{2k}^2+\frac{1}{2\gamma}\sum_{k=-N}^{N-1}\dot{u}_{2k+1}^2+\sum_{k=-N+1}^{N-1}\big[J_{2k+1/2}(u_{2k+1}-u_{2k}) \\ & -J_{2k-1/2}(u_{2k}-u_{2k-1})\big]+\frac{\gamma}{1+\gamma}J_{-2N+1/2}(u_{-2N+1}-u_{-2N}) \\ & +\frac{\gamma}{1+\gamma}J_{2N-1/2}(u_{2N}-u_{2N-1}). \end{aligned} \tag{23}$$

We calculate

$$\begin{aligned} \frac{dE_{nonlinear}}{dt} =& \sum_{k=-N+1}^{N-1}\dot{u}_{2k}\ddot{u}_{2k}+\frac{1}{\gamma}\sum_{k=-N}^{N-1}\dot{u}_{2k+1}\ddot{u}_{2k+1} \\ & +\sum_{k=-N+1}^{N-1}(\dot{u}_{2k+1}-\dot{u}_{2k})\Big[J'_{2k+1/2}(u_{2k+1}-u_{2k}) \\ & -(\dot{u}_{2k}-\dot{u}_{2k-1})J'_{2k-1/2}(u_{2k}-u_{2k-1})\Big] \\ & +\frac{\gamma}{1+\gamma}(\dot{u}_{-2N+1}-\dot{u}_{-2N})J'_{-2N+1/2}(u_{-2N+1}-u_{-2N}) \\ & +\frac{\gamma}{1+\gamma}(\dot{u}_{2N}-\dot{u}_{2N-1})J'_{2N-1/2}(u_{2N}-u_{2N-1}) \\ =& -\dot{u}_{-2N+1}J'_{-2N+1/2}(u_{-2N+1}-u_{-2N})+\dot{u}_{2N-1}J'_{2N-1/2}(u_{2N}-u_{2N-1}) \\ & +\frac{\gamma}{1+\gamma}(\dot{u}_{-2N+1}-\dot{u}_{-2N})J'_{-2N+1/2}(u_{-2N+1}-u_{-2N}) \\ & +\frac{\gamma}{1+\gamma}(\dot{u}_{2N}-\dot{u}_{2N-1})J'_{2N-1/2}(u_{2N}-u_{2N-1}) \\ =& -\frac{\gamma}{1+\gamma}(\dot{u}_{-2N}+\frac{1}{\gamma}\dot{u}_{-2N+1})J'_{-2N+1/2}(u_{-2N+1}-u_{-2N}) \\ & +\frac{\gamma}{1+\gamma}(\dot{u}_{2N}+\frac{1}{\gamma}\dot{u}_{2N+1})J'_{-2N+1/2}(u_{2N}-u_{2N-1}) \\ =& -C_L(t)\sqrt{\frac{2\gamma}{1+\gamma}}(u_{-2N+1}-u_{-2N})J'_{-2N+1/2}(u_{-2N+1}-u_{-2N}) \\ & -C_R(t)\sqrt{\frac{2\gamma}{1+\gamma}}(u_{2N}-u_{2N-1})J'_{-2N+1/2}(u_{2N}-u_{2N-1}). \end{aligned} \tag{24}$$

Because the diatomic chain itself is stable, the atomic motion is always in a potential well. The inter-atomic forces and displacement difference have inverse signs. This means

$$\begin{cases} -(u_{-2N+1}-u_{-2N})J'_{-2N+1/2}(u_{-2N+1}-u_{-2N})<0, \\ -(u_{2N}-u_{2N-1})J'_{-2N+1/2}(u_{2N}-u_{2N-1})<0. \end{cases} \tag{25}$$

So

$$\frac{dE_{nonlinear}(t)}{dt}<0. \tag{26}$$

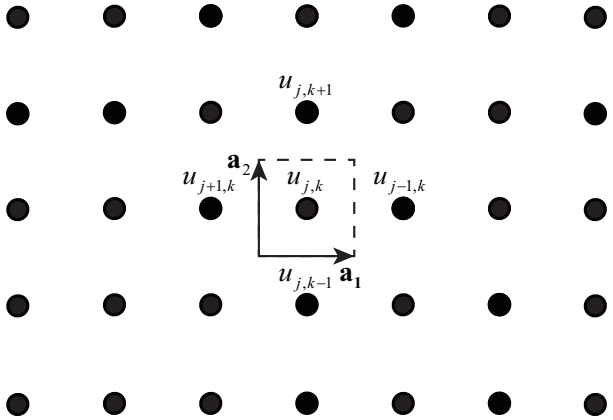


Fig. 8 Square lattice

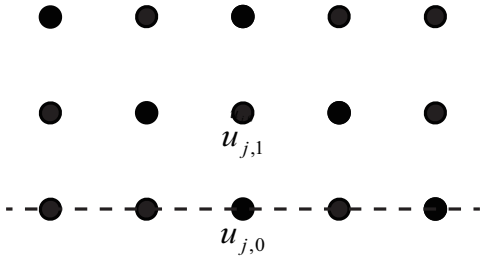


Fig. 9 The bottom boundary of square lattice.

MBC1 (21) is stable for the nonlinear diatomic chain.

We remark that even the sound speeds $C_L(t)$ and $C_R(t)$ are chosen in other forms, stability still holds.

5. Stability of MBC1 for square lattice

Dimensionless linearized equations of square lattice shown in Fig. 8 are

$$\ddot{u}_{j,k} = u_{j+1,k} + u_{j,k+1} + u_{j-1,k} + u_{j,k-1} - 4u_{j,k}, j, k \in \mathbb{Z}. \tag{27}$$

For the bottom boundary (Figure 9), MBC1 was proposed in Wang (2013)

$$\dot{u}_{j,0} + \dot{u}_{j,1} = 2(u_{j,1} - u_{j,0}), j \in \mathbb{Z}. \tag{28}$$

To investigate stability, we consider a finite system with MBC1 as follows

$$\begin{cases} \ddot{u}_{j,k} = u_{j+1,k} + u_{j,k+1} + u_{j-1,k} + u_{j,k-1} - 4u_{j,k},\ j = 1, 2, ...M-1,\ k = 1, 2, ..., N-1, \\ \dot{u}_{j,0} + \dot{u}_{j,1} = 2(u_{j,1} - u_{j,0}), \dot{u}_{j,N} + \dot{u}_{j,N-1} = 2(u_{j,N-1} - u_{j,N}),\ j = 1, 2, ...M-1, \\ \dot{u}_{0,k} + \dot{u}_{1,k} = 2(u_{1,k} - u_{0,k}), \dot{u}_{M,k} + \dot{u}_{M-1,k} = 2(u_{M-1,k} - u_{M,k}),\ k = 1, 2, ..., N-1. \end{cases} \tag{29}$$

Let energy function be

$$E_{square}(t) = \frac{1}{2}\sum_{j=1}^{M-1}\sum_{k=1}^{N-1}\Big[\dot{u}_{j,k}^2 + \frac{1}{2}\left(u_{j+1,k}-u_{j,k}\right)^2 + \frac{1}{2}\left(u_{j-1,k}-u_{j,k}\right)^2 + \frac{1}{2}\left(u_{j,k+1}-u_{j,k}\right)^2 + \frac{1}{2}\left(u_{j,k-1}-u_{j,k}\right)^2\Big]. \tag{30}$$

It is positive, and

$$\begin{aligned}
\frac{dE_{square}}{dt} =& \sum_{j=1}^{M-1}\sum_{k=1}^{N-1}\dot{u}_{j,k}(u_{j+1,k}+u_{j-1,k}+u_{j,k+1}+u_{j,k-1}-4u_{j,k}) \\
&-\frac{1}{2}\sum_{j=1}^{M-1}\sum_{k=1}^{N-1}\dot{u}_{j,k}(u_{j+1,k}+u_{j-1,k}+u_{j,k+1}+u_{j,k-1}-4u_{j,k}) \\
&+\frac{1}{2}\sum_{j=2}^{M}\sum_{k=1}^{N-1}\dot{u}_{j,k}(u_{j,k}-u_{j-1,k})+\frac{1}{2}\sum_{j=0}^{M-2}\sum_{k=1}^{N-1}\dot{u}_{j,k}(u_{j,k}-u_{j+1,k}) \\
&+\frac{1}{2}\sum_{j=1}^{M-1}\sum_{k=2}^{N}\dot{u}_{j,k}(u_{j,k}-u_{j,k-1})+\frac{1}{2}\sum_{j=1}^{M-1}\sum_{k=0}^{N-2}\dot{u}_{j,k}(u_{j,k}-u_{j,k+1}) \\
=&\frac{1}{2}\sum_{k=1}^{N-1}[\dot{u}_{M,k}(u_{M,k}-u_{M-1,k})-\dot{u}_{1,k}(u_{1,k}-u_{0,k}) \\
&-\dot{u}_{M-1,k}(u_{M-1,k}-u_{M,k})+\dot{u}_{0,k}(u_{0,k}-u_{1,k})] \\
&+\frac{1}{2}\sum_{j=1}^{M-1}[\dot{u}_{j,N}(u_{j,N}-u_{j,N-1})-\dot{u}_{j,1}(u_{j,1}-u_{j,0}) \\
&-\dot{u}_{j,N-1}(u_{j,N-1}-u_{j,N})+\dot{u}_{j,0}(u_{j,0}-u_{j,1})] \\
=&-\frac{1}{2}\sum_{k=1}^{N-1}[(\dot{u}_{0,k}+\dot{u}_{1,k})(u_{1,k}-u_{0,k})+(\dot{u}_{M,k}+\dot{u}_{M-1,k})(u_{M-1,k}-u_{M,k})] \\
&-\frac{1}{2}\sum_{j=1}^{M-1}[(\dot{u}_{j,0}+\dot{u}_{j,1})(u_{j,1}-u_{j,0})+(\dot{u}_{j,N}+\dot{u}_{j,N-1})(u_{j,N-1}-u_{j,N})] \\
=&-\sum_{k=1}^{N-1}\left[(u_{1,k}-u_{0,k})^2+(u_{M-1,k}-u_{M,k})^2\right] \\
&-\sum_{j=1}^{M-1}\left[(u_{j,1}-u_{j,0})^2+(u_{j,N-1}-u_{j,N})^2\right]\leqslant 0.
\end{aligned} \tag{31}$$

So the MBC1 is stable for two-dimensional square lattice.

6. Discussions

Stability of a boundary condition for atomic chains is an important issue, but is difficult to establish in general. There are extensive studies for continuous systems, such as the von Neumann analysis for finite difference method of the Cauchy problem for general linear systems. However, they can not be readily extended to discrete systems. For a finite and discrete system, eigenvalue analysis and Lyapunov method may be used to investigate stability. Eigenvalue analysis works for linear systems. Eigenvalues change with the number of equations, and accuracy can be an issue particularly when the order is high unless one has analytical expressions. Lyapunov method may be used to study stability for both linear and nonlinear systems, yet the Lyapunov function is difficult to construct in general. Here we obtain such functions only for several particular cases.

In this paper, the stability for MBCs in finite domain is established. The stability of MBC1 for linear diatomic chain under different choices of boundary atoms is proved by constructing energy function (Lyapunov function). Numerical tests verify our theoretical results. Then we generalize the form of the energy function to prove the stability for a nonlinear diatomic chain. In addition, for two dimensional square lattice, MBC1 is proved stable as well.

In this paper, we only considered nearest neighboring interaction. Challenges are well expected for chains with non-nearest neighboring interaction. Furthermore, there is yet no general way for constructing the energy functions. Studies along this line are desirable.

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