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Stability of Atomic Simulations with Matching Boundary Conditions

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Abstract. We explore the stability of matching boundary conditions in one space dimension, which were proposed recently for atomic simulations (Wang and Tang, Int. J. Numer. Mech. Eng., 93 (2013), pp. 1255–1285). For a finite segment of the linear harmonic chain, we construct explicit energy functionals that decay along with time. For a nonlinear atomic chain with its nonlinearity vanished around the boundaries, an energy functional is constructed for the first order matching boundary condition. Numerical verifications are also presented.

AMS subject classifications: 70-08, 65L99, 34B60

Key words: Stability, matching boundary condition, atomic simulation.

1 Introduction

Atomic and multiscale computations are widely used in materials science and engineering, where the atomic dynamics are resolved only over a subdomain much smaller than the complete underlying systems [8]. As artificial boundaries are introduced numerically, spurious wave reflections may appear, propagate backward and corrupt the local physics. Effective boundary or interfacial conditions are thus crucial for fidel simulations. A class of time history treatments provide exact conditions in linear lattices, yet convolutions cause heavy computing load and considerably reduce the efficiency [1–3, 13, 14, 17]. In addition, they are not exact and sometimes even not applicable for nonlinear lattices, and the kernel functions in a finite computing domain are difficult to obtain in multiple dimensions [9]. In view of these complexities, local approximate boundary treatments

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have been proposed, such as the perfect matched layer method [10, 16], the velocity interfacial conditions [11], and the matching boundary conditions [18]. While the effectiveness for these treatments has been demonstrated numerically, rigorous mathematical proof for the stability are widely open, except for a lowest order velocity interfacial condition [4, 11]. We notice that a semi-discrete finite difference scheme of a wave equation shares the same form with the dynamical equations for atomic chains. For such a scheme, there are studies on stability for boundary treatments, such as the Gustafsson-Kreiss-Sundström theory. However, this theory is based on a wave view for semi-infinite domain, hence only one-sided boundary conditions have been treated [15]. It does not apply to a finite segment of an atomic chain in general. In fact, stability of a finite segment can be a delicate issue, and stability for semi-infinite chain may not imply that for a finite segment [12].

In this work, we establish the stability for several matching boundary conditions on a finite segment of an atomic chain. This class of boundary conditions were proposed by matching the dispersion relation of a linear lattice. They are local in both space and time, hence allow extension to nonlinear lattices by local linearization. Furthermore, for multiple dimensions, the square, triangular, face-centered-cubic and body-centered-cubic lattices have been successfully treated through operator multiplication of such conditions at several selected incident angles [5, 6, 18]. Numerical tests and applications have verified the effectiveness, with reflections well suppressed. For MBC1, MBC2 and MBC3 shown in the next section, we construct energy functionals that decay along with time. These energies, as we shall see afterwards, induce semi-norms. Up to a linear dilation, the atomic chain with these boundary conditions equilibrates. Stability of MBC1 is also established for a nonlinear chain.

The rest of this paper is organized as follows. In Section 2, we describe these matching boundary conditions. Energy functionals for the linear lattice are constructed and verified in Section 3. An energy functional is constructed in Section 4 for nonlinear chains. Some concluding remarks are made in Section 5.

2 Matching boundary conditions

We consider a one-dimensional chain with nearest neighbor interaction. For the k-th atom, its displacement away from equilibrium is denoted by $u_k(t)$. The total potential of the chain consists of pair-wise potentials $J_{l+1/2}(u_{l+1}-u_l)$. With a uniform mass m, the dynamics is governed by the Newton equations.

$$m\ddot{u}_k = -\nabla_{u_k}\Big[\sum_l J_{l+1/2}(u_{l+1}-u_l)\Big] = J'_{k+1/2}(u_{k+1}-u_k) - J'_{k-1/2}(u_k-u_{k-1}), \quad k\in\mathbb{Z}. \tag{2.1}$$

For a harmonic chain, we have $J_{l+1/2}(u_{l+1}-u_l)=\kappa(u_{l+1}-u_l)^2/2$, where κ is the elastic constant. Hence the Newton equations read

$$m\ddot{u}_k = \kappa(u_{k+1}-2u_k+u_{k-1}), \quad k\in\mathbb{Z}. \tag{2.2}$$