MATCHING BOUNDARY CONDITIONS FOR LATTICE DYNAMICS

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Summary We design a class of accurate and efficient absorbing boundary conditions for molecular dynamics simulations of crystalline solids. By matching the dispersion relation, we propose matching boundary conditions (MBC's) for one dimensional chains. For multiple dimensional lattices, we further construct multi-directional MBC's via operator multiplications. Reflection coefficient analysis and numerical studies verify the effectiveness of MBC's for spurious reflection suppression.

MOTIVATION

Artificial boundary treatment of atomic simulations is one of the core techniques for atomic-to-continuum multiscale simulations. This is especially important for dynamic problems. Rough treatments lead to large numerical spurious reflections at the artificial boundaries of the molecular dynamics (MD) domain, leading to severe pollution in the MD solutions (see Fig.1), sometimes even numerical instability.

In this paper, we develop a new class of accurate and efficient absorbing boundary conditions (ABC's), named as matching boundary conditions (MBC's), which are effective to suppress spurious reflection at artificial boundaries for molecular dynamics simulations of crystalline solids.

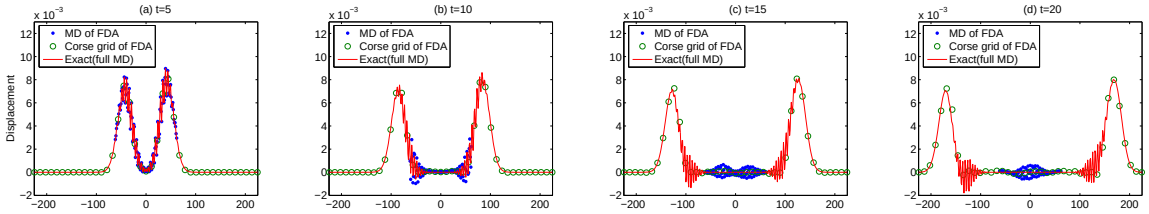

Figure 1. Multiscale numerical solution of a monatomic chain with the Lennard-Jones potential under the framework of the finite difference approach (FDA) with VIC1 (the velocity interfacial conditions involving displacement of one interior atom) [1] at: (a) $t = 5$; (b) $t = 10$; (c) $t = 15$; (d) $t = 20$. The apparent spurious reflection in the MD domain is due to the rough interfacial treatment.

MATCHING BOUNDARY CONDITIONS

We systematically develop MBC's for simple lattices in one space dimension and two space dimensions, as well as for compound lattices. The effectiveness of the proposed MBC's is demonstrated by reflection coefficient analysis and numerical tests.

MBC's for one dimensional monatomic chains

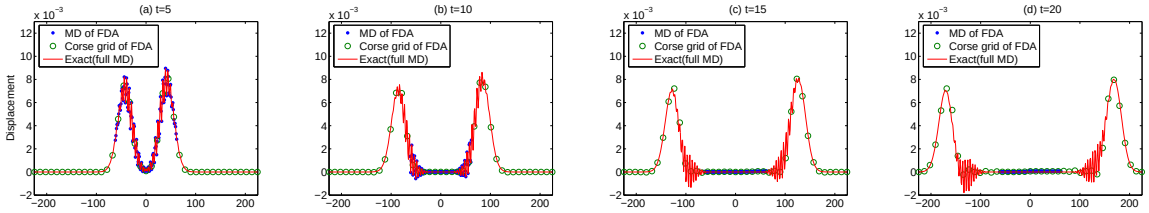

Figure 2. Multiscale numerical solution of a monatomic chain with the Lennard-Jones potential by the FDA with MBC2 involving displacement and velocity of two interior atoms at: (a) $t = 5$; (b) $t = 10$; (c) $t = 15$; (d) $t = 20$.

For one dimensional monatomic chains, MBC's take a form of linear combination of displacement and velocity at atoms near the boundary, with the coefficients determined by matching the dispersion relation of the lattice vibrations. We propose a group velocity rule for matching the dispersion relation, namely, one identifies outgoing waves and treats primarily waves with large group velocity. Perfect absorption may be reached for the outgoing waves at selected wave numbers. Reflection suppression is enhanced progressively by involving more neighboring atoms in the conditions. In particular, high accuracy can be reached in the long wave limit. MBC's with a few atoms can suppress spurious reflection effectively (see Fig.2).

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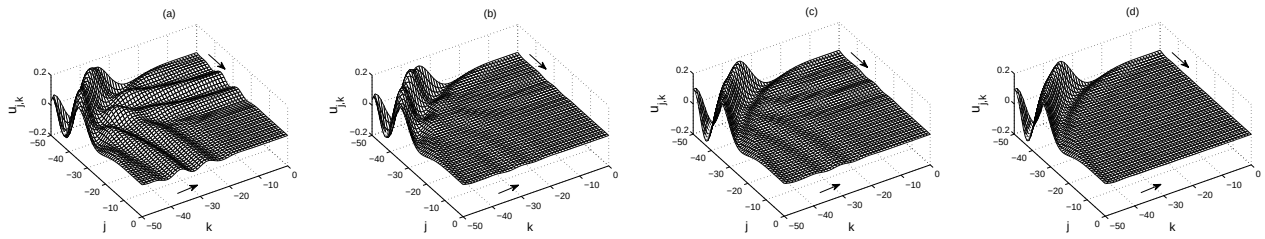

Figure 3. Numerical solutions at $t = 70$ in a test of an out-of-plane wave propagation problem in the square lattice with one of the following ABC's imposed on the four artificial boundaries: (a) VIC1; (b) MBC1; (c) V1V1; (d) M1M1. Due to the symmetry, only a quarter of the computing domain is shown. Arrows illustrate the propagation directions of reflection waves.

MBC's for multiple dimensional lattices

For scalar and vector wave problems in two dimensional lattices, following the Higdon ABC's for continuous waves [2], we construct multi-directional MBC's by using the product of MBC operators that effectively absorb incident waves at certain directions. For instance, M1M1 is constructed by using the product of two MBC1 operators. The operator multiplication MBC's considerably improve the absorption in all directions.

The effectiveness of an operator multiplication ABC depends on the effectiveness of the corresponding operator factor ABC's. For instance, the multi-directional ABC's based on MBC1 are more effective than those based on VIC1. See Fig. 3.

MBC's for compound lattices

For compound lattices, we perform the first systematical exploration on the artificial boundary treatment of one dimensional diatomic chains. Adopting the extended zone scheme of the dispersion relation, we design MBC's that effectively treat both the acoustic and optical phonons simultaneously [3].

We point out that the extended zone scheme of the dispersion relation should be adopted rather than the commonly used reduced zone scheme. This is crucial for the stability of one-way-wave ABC's, as the propagation direction of optical phonons is specified correctly only by the extended zone scheme.

CONCLUSIONS

In this paper, we develop a new class of accurate and efficient absorbing boundary conditions to suppress spurious reflections at MD artificial boundaries for simulations of crystalline solids.

The novelty of our work is as follows. The general form of linear combination of velocity and displacement is proposed for the first time. The method of matching the dispersion relation is first applied to design ABC's for discrete lattices. Based on the efficient MBC's, multi-directional ABC's are further constructed for multi-dimensional lattices by using the product of MBC operators. For compound lattices, we point out that the extended zone scheme of the dispersion relation should be adopted rather than the commonly used reduced zone scheme.

With clear physical interpretations, the proposed MBC's take a compact and general form. The coefficients are precalculated with selected wave numbers and selected incident angles as the only tunable parameters. They reach high efficiency, namely, excellent reflection suppression at the cost of negligible computational costs. Furthermore, the spatial and temporal locality allows a direct and effective application to nonlinear lattices in multiple spatial dimensions. For most applications, MBC's with a few atoms near the boundary suffice for the accuracy requirements. The implementation is easy and straightforward, and extension to other lattices is direct.

In conclusion, MBC's provide effective treatment with wide application prospects for the atomic simulations and multiscale computations of crystalline solids.

References

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[2] Higdon R.L. : Absorbing Boundary Conditions for Difference Approximations to the Multi-dimensional Wave Equation. *Math. Comp.* **47**: 437–459, 1986.

[3] Wang X., Tang S.: Matching Boundary Conditions for Diatomic Chains. *Comput. Mech.* **46**: 813–826, 2010.