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A REAL-SPACE ABSORBING BOUNDARY CONDITION FOR MOLECULAR DYNAMICS

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A non-reflection boundary condition is essential for any molecular dynamics (MD) simulation involving elastic wave transmission. The study of non-reflection boundary conditions for a discrete lattice dated back to 1970s and has recently been systematically extended to obtain time history kernel functions for crystal lattices [1]. However, the method is derived in the frequency domain based on the assumption of the periodically repeating crystal lattice thus limits its usage to simple geometric boundaries, e.g., the planar boundary.

In this talk, we will present a generalized real-space absorbing boundary condition for molecular dynamics simulation. The time history kernel functions are derived in the real space instead of in the frequency domain. The assumption of periodically repeating crystal lattice adopted in the frequency domain is thus relaxed. The time history kernel functions for 1D atomic chain, 2D square lattice and 2D triangular lattice are derived to demonstrate the generality of the proposed method. The real-space method proposed herein relies on the choice of neighbouring atoms outside the simulation domain. We show how to choose neighbouring atoms for planar and corner boundaries of 2D lattices. The influence of atoms far from the domain is found to be negligible.

REFERENCES

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