

WAVE-TRANSMITTING BOUNDARY CONDITIONS FOR MOLECULAR DYNAMICS SIMULATIONS: A GREEN'S FUNCTION APPROACH

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Microscale and nanoscale systems and processes are becoming more viable for use in engineering applications. However, our knowledge of their behavior and our ability to model their performance remains limited. In particular, existing continuum-based computational capabilities are not applicable over the full range of operational conditions. The use of molecular dynamics (MD) simulations provides the designer with useful capabilities for investigating the small-scale processes in materials with a regular crystalline structure. However, due to computer power limitations, an MD simulation typically concentrates on a small segment of a full system under analysis, whereas the effect of surrounding media is taken into account in some manner. Physical behavior and properties of simulated segments cannot be unambiguously attributed to a corresponding macroscale system, unless MD boundary conditions most rigorously describe this effect. A similar concern also arises in hybrid multiscale techniques, where the spurious reflection of elastic waves is observed at a boundary of two computational domains with different dispersive characteristics. Though this issue has been studied well in the context of quasi-static systems, the problem of modelling proper dynamic boundary conditions has not yet been addressed satisfactorily. The latter are a larger challenge, since such conditions must accurately represent the dynamic response of the outer region to any possible excitation from the primary MD region; this response can be particularly complicated for realistic crystal lattices. Earlier approaches were typically developed within one-dimensional lattice settings [1] that are difficult to extend to more general cases, or were based on phenomenological schemes. Cai et al. [2] introduced a numerical approach in arbitrary boundary shape is computed. However, their approach requires that response functions, which take the form of large matrices of the size of the number of interface degrees of freedom, be computed using an MD simulation on a domain somewhat larger than the one of interest; this computation must be redone if the problem's geometry changes.

In this paper we show that the MD boundary conditions can be effectively constructed by employing the concept of lattice dynamics Green's function, along with a mixed Laplace-Fourier transform technique. The outer region response is represented in terms of a memory response function, which is related to the lattice Green's function in a particular way. It features two important features: 1) a compact matrix form, whose size is equal to the number of degrees of freedom in one typical lattice cell; 2) uniqueness for a given crystalline lattice, i.e., once obtained, a same function can be used for various problems with this type of crystals. The memory response function describes renormalization of the interatomic interaction at the boundaries of a simulated domain. The performance, dependent on a series of method parameters, is illustrated on benchmark problems.

References

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