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Fast Coarse-Grained Particle Method and Its Hybridization with Molecular Dynamics

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Understanding fundamental processes of engineering materials such as fracture, friction, corrosion, and erosion, which are inherently multi-physics and multi-scaled phenomena, is important to predict their lifetimes and to advance their performance. Because of the long-range nature of the phenomena, direct atomistic treatment of the whole system is impractical. Therefore a concurrent, hybrid simulation scheme is often adopted, in which a continuum or coarse-graining method is applied to peripheral regions where atomistic simulation is not crucial, to reduce total computational cost [1]. A variety of continuum and/or coarse-graining methods have been proposed for such hybrid simulation of "hard" and "soft" matters [2,3]. The Finite Element (FE) and Quasi-Continuum (QC) [2] are well known methods mainly for hard matters. In both methods, a target system is partitioned into the elements; accurate treatment of the deformation field usually requires experienced arrangement of the elements. Recently a novel coarse-graining approach has been proposed [4] assuming the local statistical equilibrium, in which virtual particles that distribute in the system are introduced and the inter-particle interaction is calculated through the partition function of the atomic Hamiltonian in the harmonic approximation with a constraint. Among the interesting features, we note that the method has higher physical accuracies than the FE or QM method and the coarse-grained Hamiltonian is identical to the atomistic Hamiltonian at the lowest coarse-graining level, thus we consider that the method is suitable for the hybridization with the atomistic simulation.

With application to a large-scale multi-component system in mind, we improve the method to formulate the fast coarse-grained particle (FCGP) method. The principal improvements include: (i) we formulate a recursive coarse-graining scheme (Fig.1), with which we can coarse-grain a target system by many orders without sacrificing the elastic description; (ii) we extend the method to be applicable to a multi-component system, with which both optical and acoustic phonon dispersion relations are reproduced well; (iii) we take into account the local rotation of the system; (iv) we incorporate the anharmonic correction to the stiffness matrix between the particles, which is important in simulation at finite temperatures. The FCGP method plays important roles to bridge the huge spatiotemporal scale-gap between the atomistic and continuum descriptions such as the fluid dynamics. We develop a hybrid atomistic/coarse-grained simulation scheme. To couple the atomistic and the coarse-grained regions, we adopt the buffered-cluster method [5] that is free from the ghost force occurring usually at the atomistic-continuum interfaces in other hybrid schemes [2].

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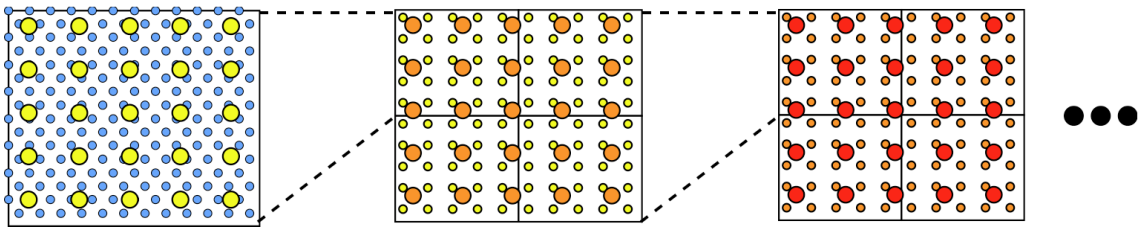

FIG. 1. Schematic illustration of the recursive coarse-graining method. At first we coarse-grain the atomic system (light-blue balls) to obtain the coarse-grained system (yellow balls). The coarse-grained system (yellow balls) is extended assuming the periodic boundary condition and the system is again coarse-grained. Continuing this procedure recursively, we can obtain massively coarse-grained system.

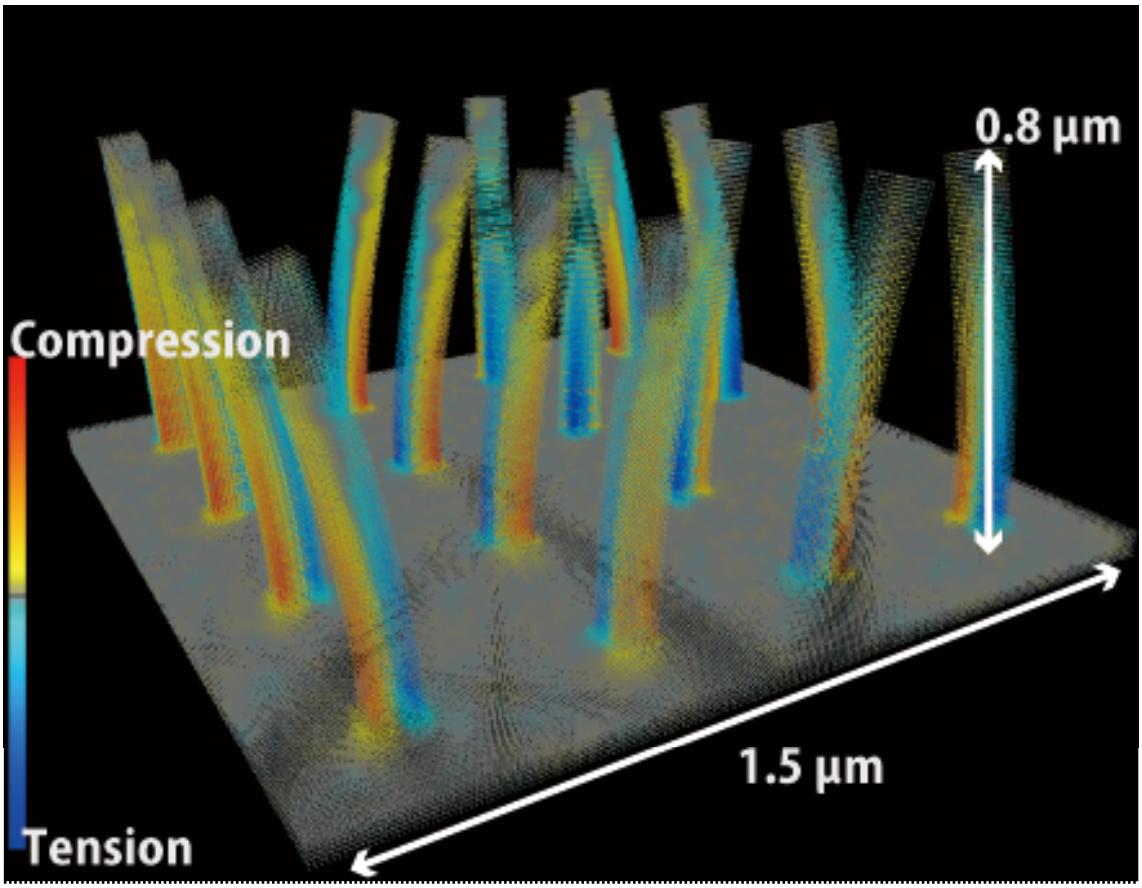

FIG. 2. A snapshot of the FCGP simulation of the oscillating nanorods. About 16,000 atoms are coarse-grained to one particle in this simulation.