

Cluster particle dynamics (CPD) for multiscale computation

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Abstract

A cluster particle dynamics (CPD) with the internal degrees of freedom is proposed to reduce the degree of freedom and enlarge the critical time step in molecular simulations. In the CPD, a cluster particle (CP) containing some atoms is first constructed as a structurally less detailed mass point assigned a mass, velocity, momentum, and positions, which is a specific linear combination of corresponding quantities in the subsets of atoms. The motion of CP is very similar to the atomistic motion in MD, and interaction potential between cluster particles are obtained using the least square technique to fit the atomic potential. A newly developed predictor-corrector algorithm is further presented for multiple-scale computations. The integral process consists of CP mean motion and a motion of internal DOF in each period. These two motions are independent, and run alternately in each loop. To balance accuracy and efficiency, a parameter is introduced into the algorithm to determine adaptive the integral time of atoms and CP by the deformation gradient. Intensive numerical studies verify the effectiveness of the proposed method, and show that: (1) Few degrees of freedom are used and the atomistic details can be restored effectively; (2) The high-frequency oscillation components are eliminated, and the larger time steps are allowed; (3) No region decomposition and thus no special treatments for the interface of MD and CP regions.

Keywords: Molecular dynamics; coarse-grained; internal DOF; critical time step; cluster particles