

Periodic Boundary Conditions for MR Linear Contact Detection Algorithm in YNANO

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ABSTRACT

The Molecular Dynamics simulation (MD) is an atomistic discontinua simulation tool which has been widely used in computational physics, biology, nano mechanic, nano technology and etc. [1][2][3][4][5] The most time consuming part of a MD simulation is the contact detection process, therefore a good contact detection algorithm is essential to the efficiency of a simulation. MR linear contact detection (linear sort and linear search) algorithm is a widely-used contact detection algorithm because of its linear processing time proportional to the number of atoms. [6] YNANO one such open-source MD code implemented with MR linear contact detection algorithm. However, the MR is developed without a periodic boundary condition (PBC), which greatly limited its application in fluid and gas dynamics simulations.

This paper implements the MR contact detection algorithm with a three dimensional PBC scheme, using a linear contact detection algorithm, MR_PB sort and MR_PB search (PB for periodic boundary).

Validations of the algorithm have been carried out, the CPU time for 10 complete contact detection routines are compared between the MR_PB linear contact detection algorithm and binary contact detection algorithm. Results show that the processing time for the MR_PB sort and MR_IB search both increase linearly to the number of particles. It shows that MR_PB linear contact detection algorithm is suitable for simulations with large number of atoms to improve efficiency and reduce unnecessary computational cost.

This work greatly extends the scope of the MR contact algorithm in the MD simulation realm of nano mechanics. Possible future application may include various topics in nano fluid dynamics simulation and etc.

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