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CORRECTION

Correction to: FastNBL: fast neighbor lists establishment for molecular dynamics simulation based on bitwise operations

Kun Li[1,2] · Shigang Li[1] · Shan Huang[1,2] · Yifeng Chen[3] · Yunquan Zhang[1]

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The first main paragraph of the paper contains errors. The correct wording is given below.

Molecular dynamics simulation is widely used to investigate the physical properties, biological structures, or chemical processes for a large number of particles [25]. Many mature molecular dynamics packages, including GROningen MAchine [1,26] (GROMACS), Large-scale Atomic/Molecular Massively Parallel Simulator [10, 23, 29, 30] (LAMMPS), Nanoscale Molecular Dynamics [19, 28] (NAMD) and HOOMD-blue, have been developed exhaustively in recent years. These packages could provide efficient molecular dynamics simulation not available in experiments by rich calculation models and analysis tools in different applications [36]. However, though the molecular dynamics simulation is extensively enabled by these simulation packages, it is still difficult to ignore the computation cost of interaction forces during the simulation which is extremely time-consuming [20]. This is mainly because the force computation requires to calculate the interactions between each pair of particles in the system, giving rise to $O(N^2)$ evaluations of the interaction in each time step, where N is the total number of particles. It is very costly to carry out such a calculation when a great quantity of particles is simulated. Some typical optimization methods are designed for reducing the cost in this process.

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✉ Shigang Li
shigangli.cs@gmail.com

[1] State Key Laboratory of Computer Architecture, Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China

[2] School of Computer and Control Engineering, University of Chinese Academy of Sciences, Beijing, China

[3] HCST Key Lab at School of EECS, Peking University, Beijing, China

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