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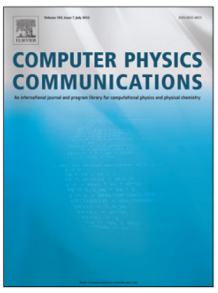

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A Hybrid Parallel Architecture for Electrostatic Interactions in the Simulation of Dissipative Particle Dynamics

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Abstract:

In this work, we upgraded the electrostatic interaction method of CU-ENUF (S.-C. Yang, Y.-L. Wang, *et al.*, J. Comput. Chem. 37, 2016, 378–387) which first applied CUNFFT (nonequispaced Fourier transforms based on CUDA) to the reciprocal-space electrostatic computation and made the computation of electrostatic interaction done thoroughly in GPU. The upgraded edition of CU-ENUF runs concurrently in a hybrid parallel way that enables the computation parallelizing on multiple computer nodes firstly, then further on the installed GPU in each computer. By this parallel strategy, the size of simulation system will be never restricted to the throughput of a single CPU or GPU. The most critical technical problem is how to parallelize a CUNFFT in the parallel strategy, which is conquered effectively by deep-seated research of basic principles and some algorithm skills. Furthermore, the upgraded method is capable of computing electrostatic interactions for both the atomistic molecular dynamics (MD) and the dissipative particle dynamics (DPD). Finally, the benchmarks conducted for validation and performance indicate that the upgraded method is able to not only present a good precision when setting suitable parameters, but also give an efficient way to compute electrostatic interactions for huge simulation systems.

PROGRAM SUMMARY

Program title: HP-ENUF

Program Files doi: http://dx.doi.org/10.17632/zncf24fhpv.1

Licensing provisions: GNU General Public License 3 (GPL)

Programming language: C, C++, and CUDA C

Supplementary material:

The program is designed for effective electrostatic interactions of large-scale simulation systems, which runs on particular computers equipped with NVIDIA GPUs. It has been tested on (a) single computer node with Intel(R) Core(TM) i7-3770 @ 3.40GHz (CPU) and GTX 980 Ti (GPU), and (b) MPI parallel computer nodes with the same configurations.

Nature of problem:

For molecular dynamics simulation, the electrostatic interaction is the most time-consuming computation because of its long-range feature and slow convergence in simulation space, which approximately take up most of the total simulation time. Although the parallel method CU-ENUF [40] based on GPU has achieved a qualitative leap compared with previous methods in electrostatic interactions computation, the computation capability is limited to the throughput capacity of a single GPU for super-scale simulation system. Therefore, we should look for an effective method to handle the calculation of electrostatic interactions efficiently for a simulation system with super-scale size.