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RBMD: A Molecular Dynamics Package Enabling to Simulate 10 Million All-Atom Particles in a Single Graphics Processing Unit

Weihang Gao[1,3], Teng Zhao[2,3], Yongfa Guo[3], Jiuyang Liang[1], Huan Liu[3], Maoying Luo[3], Zedong Luo[3], Wei Qin[3], Yichao Wang[4], Qi Zhou[1], Shi Jin[1,2,3] and Zhenli Xu[1,2,5,*]

[1] *School of Mathematical Sciences, Shanghai Jiao Tong University, Shanghai 200240, China.*
[2] *Institute of Natural Sciences, MOE-LSC, and Shanghai National Center for Applied Mathematics, Shanghai Jiao Tong University, Shanghai 200240, China.*
[3] *Shanghai Jiao Tong University-Chongqing Institute of Artificial Intelligence, Chongqing 401329, China.*
[4] *Network & Information Center, Shanghai Jiao Tong University, Shanghai 200240, China.*
[5] *CMA-Shanghai, Shanghai Jiao Tong University, Shanghai 200240, China.*

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Abstract. This paper introduces a random-batch molecular dynamics (RBMD) package for simulations of particle systems at the nano/micro scale. Different from existing packages, the RBMD uses random batch methods for nonbonded interactions of particle systems. The long-range part of Coulomb interactions is calculated in Fourier space by the random batch Ewald algorithm, which achieves linear complexity and superscalability, surpassing classical lattice-based Ewald methods. For the short-range part, the random batch list algorithm is used to construct neighbor lists, significantly reducing computational and memory costs. The RBMD is implemented on GPU-CPU heterogeneous architectures, with classical force fields for all-atom systems. Benchmark systems are used to validate the accuracy and performance of the package. Comparison with the particle-particle particle-mesh and the Verlet list methods in the LAMMPS package is performed on three different NVIDIA GPUs, demonstrating high efficiency of the RBMD on heterogeneous architectures. Our results also show that the RBMD enables simulations on a single GPU with a CPU core up to 10 million particles. Typically, for systems of one million particles, the RBMD allows simulating all-atom systems with a high efficiency of 8.20 ms per step, demonstrating the attractive feature for running large-scale simulations of practical applications on a desktop machine.

AMS subject classifications: 82M37, 65Y05, 65Y20, 68-04

*Corresponding author. *Email addresses:* `xuzl@sjtu.edu.cn` (Z. Xu), `gaowh2019@sjtu.edu.cn` (W. Gao)

Key words: Molecular dynamics, random batch methods, heterogeneous architectures, Coulomb interactions, large-scale simulations.

Program summary

Program Title: RBMD

Developer's repository link: https://github.com/randbatch-md

Licensing provisions: GPL 3.0

Programming language: C++

Nature of problem: Nonbonded interactions, particularly, long-range electrostatic interactions, are the computational bottleneck of molecular dynamics simulations, for which most packages are based on algorithms with the lattice-based Ewald summation and the fast Fourier transform. These algorithms are communication intensive, limiting the parallel efficiency of the algorithm for the GPU calculation. Moreover, for short-range calculations, the building of neighbor lists for each particle is memory intensive, leading to the von Neumann bottleneck for large scale simulations. Therefore, the use of innovative long-range and short-range algorithms is essential for a novel molecular dynamics package that is able to simulate systems beyond the current limitations.

Solution method: In the paper, the random batch methods are introduced under the VTK-m framework to accelerate the nonbonded interactions in molecular dynamics, leading to a novel package, named the random batch molecular dynamics (RBMD). The stochastic nature of the methods significantly improves the efficiency and parallel scalability of the calculations on the GPU-CPU heterogeneous architecture.

1 Introduction

Over the past few decades, molecular dynamics (MD) simulations have achieved tremendous success in a broad range of areas, including biophysics, soft matter, materials modeling, electrochemical energy devices and drug design [1–4]. These advances partly owe to tremendous improvements in hardware [5] that have enabled studies of spatial and temporal scales previously not feasible, such that a more detailed understanding of physical phenomena at micro/macro-scales can be achieved. At present, most traditional MD packages have released multi-CPU and/or GPU versions, such as AMBER [6], GROMACS [7], LAMMPS [8], NAMD [9], and OpenMM [10]. Moreover, the development of accelerators [11] has also promoted the development of machine learning-integrated MD packages [12–14]. Nevertheless, since Moore's law [5] is no longer applicable as the speed improvement of individual processors has been increasing slowly, fast and accurate calculations of pairwise nonbonded interactions on heterogeneous architectures