THE HONG KONG POLYTECHNIC UNIVERSITY
香港理工大學

DEPARTMENT OF APPLIED MATHEMATICS
應 用 數 學 系

The Hong Kong Polytechnic University
Department of Applied Mathematics

Colloquium

Random-Batch Ewald Method for High-Scalable MD simulations

By

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Abstract

The development of efficient methods for long-range systems plays important role in all-atom simulations of biomolecules and drug design. We present a random-batch Ewald (RBE) method for molecular dynamics simulations of particle systems with long-range Coulomb interactions. The RBE takes advantage of the random minibatch strategy for the force calculation between particles, leading to an order N algorithm. It is based on the Ewald splitting of the Coulomb kernel and the random importance sampling is employed in the Fourier part such that the force variance can be reduced. This new simulation method avoids the use of the FFT and greatly improves the scalability of the molecular simulations. We also discuss the treatment of the short-range interactions by using random batch idea. Numerical results, including protein solution and phase-separated electrolytes, are presented to show the attractive performance of the algorithm.

Date: 25 February 2022 (Friday)
Time: 9:00-10:00 (Hong Kong Standard Time GMT +8)
Venue: Online Talk via Zoom (Meeting ID: 964 0569 7605)
Speaker: Prof. Zhenli Xu, Shanghai Jiao Tong University
Host: Prof. Zhonghua Qiao, The Hong Kong Polytechnic University
Click to join:
https://polyu.zoom.us/j/96405697605?pwd=THlWYlNINE8xUXVWUzBZdDFCdFMxZz09

Click to join

*** * * ALL ARE WELCOME * * ***

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