



高性能 EDA 算法
校企联合实验室

学术报告系列



报告人

干则成

香港科技大学 (广州)

报告题目

Fast algorithm for particle-based simulation of quasi-2D Coulomb systems

报告时间

2024 年 8 月 9 日 下午 2:00 – 3:00

报告地点

光华楼东主楼 1513 室

报告摘要

Quasi-2D Coulomb systems are of fundamental importance and have attracted much attention in many areas nowadays. Their reduced symmetry gives rise to interesting collective behaviors, but also brings great challenges for particle-based simulations. We propose a novel algorithm framework to address the $O(N^2)$ simulation complexity associated with the long-range nature of Coulomb interactions. First, we introduce an efficient Sum-of-Exponentials approximation for the long-range kernel associated with Ewald splitting, achieving uniform convergence in terms of inter-particle distance, which reduces the complexity to $O(N^{7/5})$. We then introduce a random batch sampling method in the periodic dimensions, the stochastic approximation is proven to be both unbiased and with reduced variance via a tailored importance sampling strategy, further reducing the computational cost to $O(N)$. The performance of our algorithm is demonstrated via various numerical examples. Notably, it achieves a speedup of 2-3 orders of magnitude comparing with Ewald2D method, enabling molecular dynamics simulations with up to 10^6 particles on a single core. The present approach is therefore well-suited for large-scale particle-based simulations of Coulomb systems under confinement, making it possible to investigate the role of Coulomb interaction in many practical situations.

报告人简介

Zecheng Gan is an assistant professor in the Thrust of Advanced Materials at HKUST(GZ), and assistant professor of mathematics, at HKUST. He obtained his PhD from SJTU, under the supervision of Prof. Zhenli Xu (2010-2016), and worked as a postdoc assistant professor in mathematics at University of Michigan, Ann Arbor (2016-2019) and then postdoc associate at Courant institute, New York university until August 2021 before joining HKUST. His research interest includes applied and computational mathematics, scientific computing, machine learning and data-driven methods, and their applications in interdisciplinary sciences.

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