

For Favour of Posting



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Joint Colloquium

Random Batch Methods for classical and quantum molecular dynamics

Professor Shi JIN

Institute of Natural Sciences and School of Mathematical Sciences
Shanghai Jiao Tong University, &
The Institute of Mathematical Sciences
The Chinese University of Hong Kong



April 8, 2025 (Tuesday)

3:00pm – 4:00pm

Room 501a, Academic Building No. 1, CUHK

Abstract: Random batch methods were introduced for general interacting particle systems with large number ($N \gg 1$) of particles, with a linear complexity of $O(N)$. We extend this method to molecular dynamics with Coulomb interactions, in the framework of Ewald summation. We will show its superior performance compared to the current state-of-the-art methods (for example PPPM) for the corresponding problems, in both computational efficiency and parallelizability. We use it not only to reduce the cost of long range interactions but also the short-range ones, and as a result we are able to simulate 10 million molecules with just one GPU. We also extend it to quantum Monte-Carlo simulation.

Bio: Shi Jin is the Director of Institute of Natural Sciences, and Chair Professor of Mathematics, at Shanghai Jiao Tong University. He also serves as a co-director of the Shanghai National Center for Applied Mathematics, director of Ministry of Education Key Lab on Scientific and Engineering Computing, and director of Shanghai Jiao Tong University Chongqing Artificial Intelligence Institute.

He received a Feng Kang Prize of Scientific Computing in 2001, a Morningside Silver Medal in 2007. He is an inaugural Fellow of the American Mathematical Society (AMS) (2012), a Fellow of Society of Industrial and Applied Mathematics (SIAM) (2013), an inaugural Fellow of the Chinese Society of Industrial and Applied Mathematics (CSIAM) (2020), and an Invited Speaker at the International Congress of Mathematicians in 2018. In 2021 he was elected a Foreign Member of Academia Europaea and a Fellow of European Academy of Sciences. In 2024 he was awarded a Shanghai Natural Science Prize (first class).

All are Welcome