高性能 EDA 算法校企联合实验室

学术报告系列

报告人

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上海大学

报告题目

Fast algorithms for modified Poisson-Boltzmann equations with correlation effects

报告时间

2024 年 8 月 9 日　下午 3:00 – 4:00

报告地点

光华楼东主楼 1513 室

报告摘要

The modified Poisson-Boltzmann (MPB) equations are often used to describe the equilibrium particle distribution of ionic systems. In this work, we propose a fast algorithm to solve the MPB equations with the self Green's function as the self-energy in two/three dimensions, where the solution of the self Green's function poses a computational bottleneck due to the requirement of solving a high-dimensional partial differential equation. Our algorithm combines the selected inversion with hierarchical interpolative factorization for the self Green's function. By strategically exploiting the locality and low-rank characteristics of the corresponding operators, algorithms with linear complexity in two dimensions and quasi-linear complexity in three dimensions are achieved. Extensive numerical results are conducted to demonstrate the accuracy and efficiency of the proposed algorithm for problems in two/three dimensions.

报告人简介

涂一辉，上海大学理学院讲师。2017 年在上海交通大学致远学院本科毕业，2023 年博士毕业于上海交通大学，获计算数学博士学位。2021 年至 2022 年，在美国普渡大学进行联合培养。2023 年加入上海大学。当前研究方向为偏微分方程数值解和深度学习算法，主要研究内容包括：离子输运问题中的快速算法，基于神经网络的快速求解器和相场方程的高效计算等。

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