数学与系统科学研究院

计算数学所学术报告

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报告题目：

On the numerical accuracy of the particle-mesh Ewald method.

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报告时间：**2017** 年 **6** 月 **22** 日（周四）

上午 **10:00-11:00**

报告地点：　　数学院南楼七层

714 教室

Abstract:

Computing the electrostatic interactions is a non-trivial task in molecular dynamics (MD) simulations, and usually becomes the bottleneck in large scale parallelism. The particle-mesh Ewald method is the standard algorithm for calculating the point-charge electrostatic interactions in modern MD packages. In this talk, we establish the theoretical framework for estimating the numerical error of the particle-mesh Ewald method. The error estimate is proved to be precise in uncorrelated charge systems, and is shown to be of satisfactory quality in correlated charge systems. Based on the error estimate, the multiple-staggered mesh and the optimal interpolation basis are proposed to reduce the error. It is demonstrated that the new methods are always more accurate and more efficient than the standard particle-mesh Ewald method, and can be implemented without substantial change in existing MD codes. Finally we demonstrate that the error estimate is of crucial importance in automatically determining the optimal working parameters for the particle mesh Ewald method.

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