

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:

**Harmonic surface mapping  
algorithm for fast electrostatic sums**

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报告时间: 2019 年 1 月 4 日 (周五)

下午 15:00-16:00

报告地点: 科技综合楼三层

311 报告厅

## **Abstract:**

The fast and accurate evaluation of electrostatic interactions for particle systems at microscale has been one of the core topics for molecular simulations. We present a harmonic surface mapping algorithm (HSMA) for fast electrostatic sums of finite sources and infinite image sources. Compared to the popular PME method, this algorithm is be useful for more general boundary conditions rather than periodic boundary, and it is much easier for parallelization. The HSMA uses the property that the induced potential due to infinite images is harmonic and can be expanded into a harmonic series. The analytical harmonic series is mapped into a boundary integral over a surface containing the simulation box, which is approximated by a particle system composed of the point sources and a finite number of point image charges, and thus can be efficiently calculated by FMM or the GPU calculations. The performance of the algorithm is shown by numerical examples. The algorithm as a fast Poisson solver is also discussed.

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