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：

NLEP in KS-DFT: Acceleration techniques

邀请人：　　周爱辉研究员

报告时间：**2011** 年 **8** 月 **5** 日（周五）

上午 **10：00-11：00**

报告地点：　　科技综合楼三层 **301**

计算数学所小报告厅

Abstract:

In the 1st part, we present a simple modification of the orbital minimization method (which is among the most promising linear scaling algorithms for electronic structure calculation), by adding a localization step into the algorithm. We show that the addition of the localization step substantially reduces the chances that the iterations get trapped at local minima. In the 2nd part, I will talk about our recent implementation of the density functional theory (DFT) plane wave pseudopotential (PWP) calculation on GPU clusters. This GPU version is developed based on a CPU DFT-PWP code: PEtot. Our test indicates that the GPU version can have a ~10 times speed-up over the CPU version and is about 5 times faster than the legendary VASP code.

欢迎大家参加！