

数学与系统科学研究院
计算数学所网络学术报告

报告人: Associate Prof. Guanghui Hu

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报告题目:

**Towards efficient numerical
simulations in density functional
theory**

邀请人: 谢和虎 研究员

报告时间: 2021 年 12 月 15 日 (周三)

上午 10:00-11:00

报告工具: 腾讯会议 (ID: 279-816-754)

会议链接:

<https://meeting.tencent.com/dm/d7zE1uiGxgYF>

Abstract:

In this talk, the background and recent development of numerical methods for density functional theory will be briefly reviewed first. Then focusing on efficiency of simulations, several numerical issues such as convergence of SCF iteration, adaptive mesh methods, orthonormalization constraint for wavefunctions, parallel computing, will be introduced. The solutions of above issues, within our h-adaptive finite element framework, will be described in detail. Numerical experiments show the effectiveness, as well as some potential issues of our method.

欢迎大家参加！