

数学与系统科学研究院

计算数学所学术报告

报告人: **Prof. Weiguo Gao**

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报告题目:

**NLEP in KS-DFT: Numerical
methods**

邀请人: 周爱辉研究员

报告时间: **2011 年 8 月 5 日 (周五)**

上午 9: 00-10: 00

报告地点: **科技综合楼三层 301**

计算数学所小报告厅

Abstract:

In each SCF iteration, we need to solve a large scale linear eigenvalue problem. In particular, a lot of eigenpairs are desired for big systems. We present our new implementation of LOBPCG method which avoids unnecessary orthogonalization without affecting its convergence. This algorithm has been implemented in our FEM code with a real space preconditioner presented. On the other hand, we examine the possibility of using standard Newton's method for solving the nonlinear eigenvalue problems. We show that the Jacobian matrix associated with this nonlinear system has a special structure that can be exploited to reduce the computational complexity.

欢迎大家参加!