

数学与系统科学研究院  
计算数学所定期学术报告

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报告题目:

**Parallelizable Algorithms for  
Optimization Problems with  
Orthogonality Constraints**

报告时间: 2018 年 12 月 6 日 (周四)

下午 16:00-17:00

报告地点: 思源楼一层

报告厅

## **Abstract:**

To construct a parallel approach for solving optimization problems with orthogonality constraints is usually regarded as an extremely difficult mission, due to the low scalability of the orthogonalization procedure. However, such demand is particularly huge in some application domains such as material computation. In this talk, we propose two infeasible algorithms, based on augmented Lagrangian penalty function, for solving optimization problems with orthogonality constraints. Different with the classic augmented Lagrangian method, our algorithms update both the prime variables and the dual variables by new strategies. The orthogonalization procedure is only invoked once as the last step of the above mentioned two algorithms. Consequently, the main parts of these two algorithms can be parallelized naturally. We establish global subsequence convergence results for our proposed algorithms. Worst-case complexity and local convergence rate are also studied under some mild assumptions. Numerical experiments, including tests under parallel environment, illustrate that our new algorithms attain good performances and a high scalability in solving discretized Kohn-Sham total energy minimization problems.

**欢迎大家参加！**