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:

Solving large-scale generalized eigenvalue problems

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<u>报告地点</u>:科技综合楼三层 311 计算数学所报告厅

Abstract:

Generalized eigenvalue problems arise naturally in a wide range of science and engineering applications. In this talk we first survey a few representative algorithms for generalized eigenvalue problems, then we discuss the main challenges facing large scale problems. It is well-known that the cost for global orthogonalization is significant for large eigen-problems. In addition, the cost for the Rayleigh-Ritz refinement is no longer insignificant when the number of eigenvalues to be computed becomes large, say 10,000 of a matrix-pencil with dimension over 1 million. Eigen-algorithms that can scale better on modern supercomputers need to require far less cost on global reorthogonalization as well as on the Rayleigh-Ritz refinement than standard algorithms.

We present a framework that combines the Chebyshev filtered subspace iteration and the spectral slicing using shift-invert iteration. This combination leads to an algorithm that has fast convergence for both the exterior and the interior eigenvalues. The algorithm is naturally suitable for parallel execution, it has less global reorthogonalization cost and less Rayleigh-Ritz refinement cost. We will present preliminary numerical results on generalized eigenvalue problems arising from DFT calculations discretized by an adaptive finite element method.

欢迎大家参加!