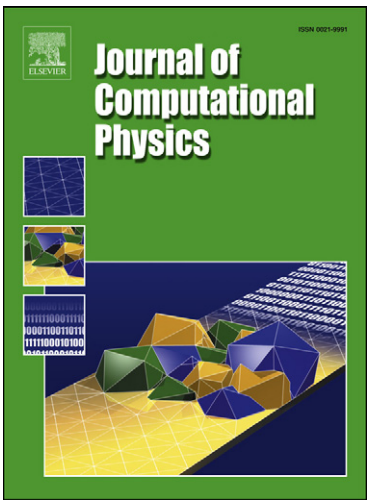

A projected preconditioned conjugate gradient algorithm for computing a large eigenspace of a Hermitian matrix

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PII: S0021-9991(15)00100-X
DOI: http://dx.doi.org/10.1016/j.jcp.2015.02.030
Reference: YJCPH 5734

To appear in: *Journal of Computational Physics*

Received date: 27 July 2014
Revised date: 2 January 2015
Accepted date: 20 February 2015

Please cite this article in press as: E. Vecharynski et al., A projected preconditioned conjugate gradient algorithm for computing a large eigenspace of a Hermitian matrix, *J. Comput. Phys.* (2015), http://dx.doi.org/10.1016/j.jcp.2015.02.030

A Projected Preconditioned Conjugate Gradient Algorithm for Computing a Large Eigenspace of a Hermitian Matrix[☆]

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Abstract

We present an iterative algorithm for computing an invariant subspace associated with the algebraically smallest eigenvalues of a large sparse or structured Hermitian matrix A. We are interested in the case in which the dimension of the invariant subspace is large (e.g., over several hundreds or thousands) even though it may still be small relative to the dimension of A. These problems arise from, for example, density functional theory (DFT) based electronic structure calculations for complex materials. The key feature of our algorithm is that it performs fewer Rayleigh–Ritz calculations compared to existing algorithms such as the locally optimal block preconditioned conjugate gradient or the Davidson algorithm. It is a block algorithm, and hence can take advantage of efficient BLAS3 operations and be implemented with multiple levels of concurrency. We discuss a number of practical issues that must be addressed in order to implement the algorithm efficiently on a high performance computer.

1. Introduction

We are interested in efficient algorithms for computing a small percentage of eigenpairs of a large Hermitian matrix A that is either sparse or structured (i.e., the matrix–vector product Ax can be computed efficiently.) Often these

[☆]This material is based upon work supported by the U.S. Department of Energy, Office of Science, under Scientific Discovery through Advanced Computing (SciDAC) program funded by the Offices of Advanced Scientific Computing Research and Basic Energy Sciences contract number DE-AC02-05CH11231.

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