High-performance implementation of Chebyshev filter diagonalization for interior eigenvalue computations. (English) Zbl 1376.65055 J. Comput. Phys. 325, 226-243 (2016).

Summary: We study Chebyshev filter diagonalization as a tool for the computation of many interior eigenvalues of very large sparse symmetric matrices. In this technique, the subspace projection onto the target space of wanted eigenvectors is approximated with filter polynomials obtained from Chebyshev expansions of window functions. After the discussion of the conceptual foundations of Chebyshev filter diagonalization, we analyze the impact of the choice of the damping kernel, search space size, and filter polynomial degree on the computational accuracy and effort, before we describe the necessary steps towards a parallel high-performance implementation. Because Chebyshev filter diagonalization avoids the need for matrix inversion, it can deal with matrices and problem sizes that are presently not accessible with rational function methods based on direct or iterative linear solvers. To demonstrate the potential of Chebyshev filter diagonalization for large-scale problems of this kind we include as an example the computation of the $10^2$ innermost eigenpairs of a topological insulator matrix with dimension $10^9$ derived from quantum physics applications.

MSC:

65F15 Numerical computation of eigenvalues and eigenvectors of matrices
65F50 Computational methods for sparse matrices
68M20 Performance evaluation, queueing, and scheduling in the context of computer systems
81V65 Quantum dots as quasi particles

Keywords:
interior eigenvalues; Chebyshev filter polynomials; performance engineering; quantum physics; topological materials

Software:
FEAST; CIRR; ILUPACK; PARDISO; likwid; ARPACK

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