Parallel Eigensolver for Electronic Structure Calculations

E.L. Briggs, C.T. Kelley, J. Bernholc
North Carolina State University, Raleigh, North Carolina, 27695-7518

We describe a parallel eigensolver designed for electronic structure calculations. For large problems, diagonalization becomes computationally dominant in all standard Kohn-Sham DFT codes. While universal packages such as LAPACK and ScaLapack are widely used in electronic structure, they fail to take advantage of specific characteristics of the problem. Our new diagonalizer, a partitioned folded spectrum method (PFSM), executes up to an order of magnitude faster than the standard solvers while achieving the same level of accuracy and convergence. It is currently implemented in the Real Space Multigrid (RMG) code developed at NCSU, but it is not specific to this code. RMG is open source and runs on Linux, Windows and MacIntosh systems. It has achieved over 6.5 PFLOPS running on 18k nodes of a Cray XK7, and can be downloaded at sourceforge.net/projects/rmgdft/. For more information about PFSM, see the preprint at arxiv.org/abs/1502.07806. A stand-alone implementation of PSFM will also be distributed as open-source software.