Scalable Preconditioned Eigenvalue Solver in Hypre

\[ B^{-1}(A-I)u = 0 \]

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Abstract

We develop a scalable preconditioned eigenvalue solver for partial eigenvalue problems for large symmetric matrices on massively parallel computers, using the multigrid technology and incomplete factorization preconditioning of the HYPRE software for the Scalable Linear Solvers project at the Lawrence Livermore National Laboratory (LLNL), Center for Applied Scientific Computing. The solver implements the locally optimal block preconditioned conjugate gradient (LOBPCG) method described in: A. V. Knyazev, Toward the Optimal Preconditioned Eigensolver: Locally Optimal Block Preconditioned Conjugate Gradient Method, SIAM Journal on Scientific Computing 23 (2001), no. 2, pp. 517-541. The LOBPCG solver computes one or more of the smallest eigenvalues and the corresponding eigenvectors of a symmetric matrix using preconditioning directly, without using the shift-and-invert scheme and inner-outer iterations.

We discuss the implementation approach for a flexible matrix free parallel algorithm and the capabilities of the developed software. The code performance is demonstrated on a set of model large-scale test problems.

The following HYPRE preconditioners have been tested in the eigenvalue solver: AMG-PCG, DS-PCG, ParaSails-PCG, Schwarz-PCG and Euclid-PCG. The code has been mainly developed and tested on a Beowulf cluster at CU Denver. This system includes 36 nodes, 2 processors per node, PIII 933MHz processors, 2GB memory per node running Linux RedHat, and a 7.2SCI Dolphin supercomputer interconnect. The code has also been tested on several LLNL clusters using Compaq and IBM hardware, running Unix and/or Linux.