Implementation of a Scalable Preconditioned Eigenvalue Solver Using Hypre

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Implementation of LOBPCG Eigensolver Using Hypre

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Implementation of a Scalable Preconditioned Eigenvalue Solver Using Hypre

Background

- LOBPCG - Locally Optimal Block Preconditioned Conjugate Gradient Method
- Authors of code for Hypre – Andrew Knyazev & Merico Argentati both from the University of Colorado at Denver
LOBPCG Algorithm

- LOBPCG solver finds the smallest eigenvalues of a symmetric positive definite matrix.
- The algorithm is matrix free since the multiplication of a vector by the matrix $A$ and an application of the preconditioner $T$ to a vector are needed only as functions.
- For computing only the smallest eigenpair, the algorithm implements a local optimization of a 3-term recurrence

$$x^{n+1} \in \text{span}\{x^n, x^{n-1}, T(Ax^n - \lambda(x^n)x^n)\}$$

- If finding $m$ smallest eigenpairs of $A$, the Rayleigh-Ritz method on a $3m$-dimensional trial subspace, is used during each iteration for the local optimization.
Previously Developed LOBPCG Software

- MATLAB
- C-language based on LAPACK/BLAS libraries
- Initial PETSc version
**Hypre (High Performance Preconditioners)**

- Hypre is a software library for solving large, sparse linear systems on massively parallel computers
- The primary goal is to provide users with advanced parallel preconditioners
- The Hypre libraries are designed to provide robustness, ease of use, flexibility and interoperability
LOBPCG Hypre Implementation

- C-language
- Hypre libraries (hypre-1.6.0) and LAPACK/BLAS libraries
- Implementation is based on Hypre Linear Algebraic (IJ) Interface for applications with sparse linear systems
- User interface to solver is a “Hypre style” API
- User provided functions for MATVEC multiply and preconditioner/solve
- LOBPCG Hypre implementation utilizes Hypre parallel vector manipulation routines and MGS for orthonormalization
LOBPCG Hypre Implementation (cont.)

- Test driver IJ_eigen_solver.c, is modified version of IJ_linear_solvers.c which retains much of its functionality/capability
- Test driver allows for input of Matrix Market files and internally generated matrices (Laplacians of several different types and sizes)
- Shell script IJ_eigen_solver.sh provides basic suite of tests
- LOBPCG Hypre based code will be included in the next Beta Release of the Hypre Project
LOBPCG Software Implemented Using Hypre

- IJ_eigen_solver.c
- lobpcg.c
- lobpcg_matrix.c
- lobpcg_utilities.c
- lobpcg.h
- Hypre Include Files

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LOBPCG User Interface (API)

I. Setup Functions
HYPRE_LobpcgCreate(HYPRE_LobpcgData *lobpcg);
HYPRE_LobpcgSetup(HYPRE_LobpcgData lobpcg);
HYPRE_LobpcgSetVerbose(HYPRE_LobpcgData lobpcg);
HYPRE_LobpcgSetMaxIterations(HYPRE_LobpcgData lobpcg,int max_iter);
HYPRE_LobpcgSetTolerance(HYPRE_LobpcgData lobpcg,double tol);
HYPRE_LobpcgSetBlockSize(HYPRE_LobpcgData lobpcg,int bsize);
HYPRE_LobpcgSetSolverFunction(HYPRE_LobpcgData lobpcg,
    int (*FunctSolver)(HYPRE_ParVector x,HYPRE_ParVector y));
HYPRE_LobpcgDestroy(HYPRE_LobpcgData lobpcg);

II. Lobpcg Solver
HYPRE_LobpcgSolve(HYPRE_LobpcgData lobpcgdata,
    int (*FunctA)(HYPRE_ParVector x,HYPRE_ParVector y),
    HYPRE_ParVector *v,double **eigval);

III. Output Functions
HYPRE_LobpcgGetEigval(HYPRE_LobpcgData lobpcg,double **eigval);
HYPRE_LobpcgGetResvec(HYPRE_LobpcgData lobpcg,double ***resvec);
HYPRE_LobpcgGetEigvalHistory(HYPRE_LobpcgData lobpcg,double ***eigvalhistory);
Compiling and Testing

- Make files for various hardware configurations and compilers are provided
- A test program IJ_eigen_solver.sh, similar to IJ_linear_solvers.sh, has been developed
- LOBPCG code has been compiled and tested on the CU Denver cluster using scali and mpich libraries and using gcc, pgcc and mpicc compilers
Compiling and Testing (cont.)

- The beowulf cluster at CU Denver includes:
  - 36 nodes, 2 processors each
  - each node: 2 PIII 933MHz, 2GB memory
  - linux Redhat 7.2
  - SCI Dolpin interconnect, management interconnect

- Lobpcg has been compiled and tested on a subset of the OCF Production Systems at LLNL, including ASCI blue, M&IC tera, gps and lx
Compiling and Testing (cont.)

- Testing has been done using a variety of internally generated Laplacians and several matrix market files that were used as input.

- Quality and accuracy of code, using multiple processors, seems to be quite good based in this limited testing.

- Preconditioning is implemented through calls to Hypre preconditioned PCG linear solvers. In our tests, only a few (2-10) inner iterations typically provide the best performance and increasing the number of the inner iterations does not improve the final convergence.
Hypre Preconditioners Tested with LOBPCG

- AMG-PCG: algebraic multigrid
- DS-PCG: diagonal scaling
- ParaSails-PCG: approximate inverse of $A$ is generated by attempting to minimize $\|I - AM\|_F$
- Schwarz-PCG: additive Schwarz
- Euclid-PCG: incomplete LU
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LOBPCG Performance vs Preconditioner Iterations

7-Point 3-D Laplacian, 8,000,000 x 8,000,000 matrix, 55,760,000 nz, Preconditioner/Solve: Schwarz-PCG, 10 Processors.
Timing Results – Scalability

<table>
<thead>
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<th>Nproc</th>
<th>Nz</th>
<th>Prec. setup</th>
<th>Apply Prec.</th>
<th>LOBPCG Lin. Alg.</th>
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<td>112,000,000</td>
<td>671.0</td>
<td>163.8</td>
<td>38.9</td>
</tr>
</tbody>
</table>

7-Point 3-D Laplacian, Block size: 1, Lobpcg iterations: 10, Inner (pcg) interations: 3, Preconditioner/Solve: Schwarz-PCG.
Timing Results – Scalability (cont.)

TOTAL EXECUTION TIME as PROBLEM SIZE INCREASES

- Prec. Setup
- Apply Prec.
- Lobpcg Lin. Alg.

Time (Seconds)

Number of Processors

2, 4, 8, 16, 32

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Conclusions

- Implementation illustrates that the LOBPCG matrix free algorithm can be implemented using parallel libraries

- User interface routines
  - provide ease of use for a variety of users
  - have been developed with the goal of using the Hypre standard API
  - provide flexible capability for the user to provide MATVEC multiply and preconditioned solver functions, which leverage the power of Hypre preconditioners

- Initial scalability looks promising, but more testing is needed by other users on larger problems

- Enhancements are possible to improve robustness, efficiency and readability/clarity of code