SAND2012-4160P

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Eigensolvers on HPC Platforms

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Goals

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- Integrate SNL's Trilinos eigensolver package Anasazi with the Megraphs graph framework for Cray-XMT
- Develop preconditioners and eigenanalysis theory to advance use of eigensolvers for graph problems
- Collaborate closely with LLNL in eigensolver comparisons and theoretical development

Modular Environment for Graph Research and Analysis with Persistent Hierarchical Storage

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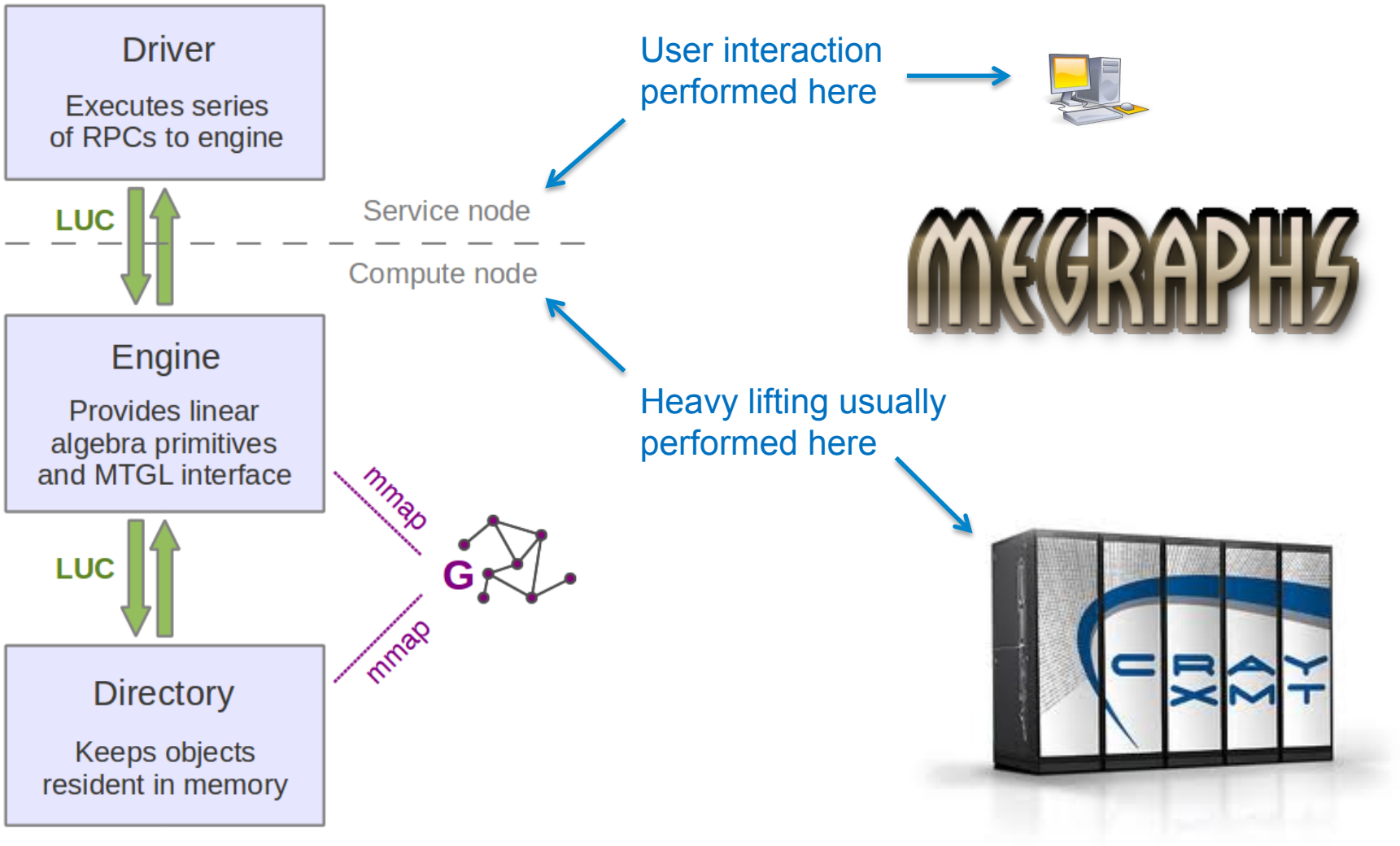

Anasazi Eigensolver in the Trilinos Solver Toolkit

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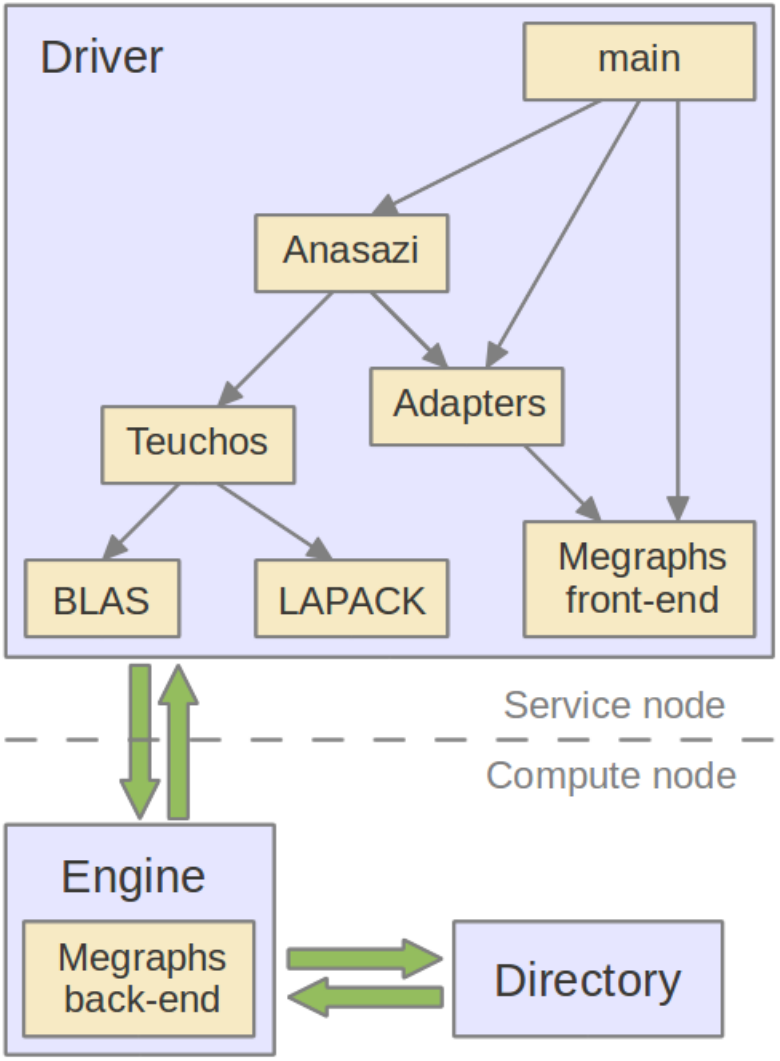
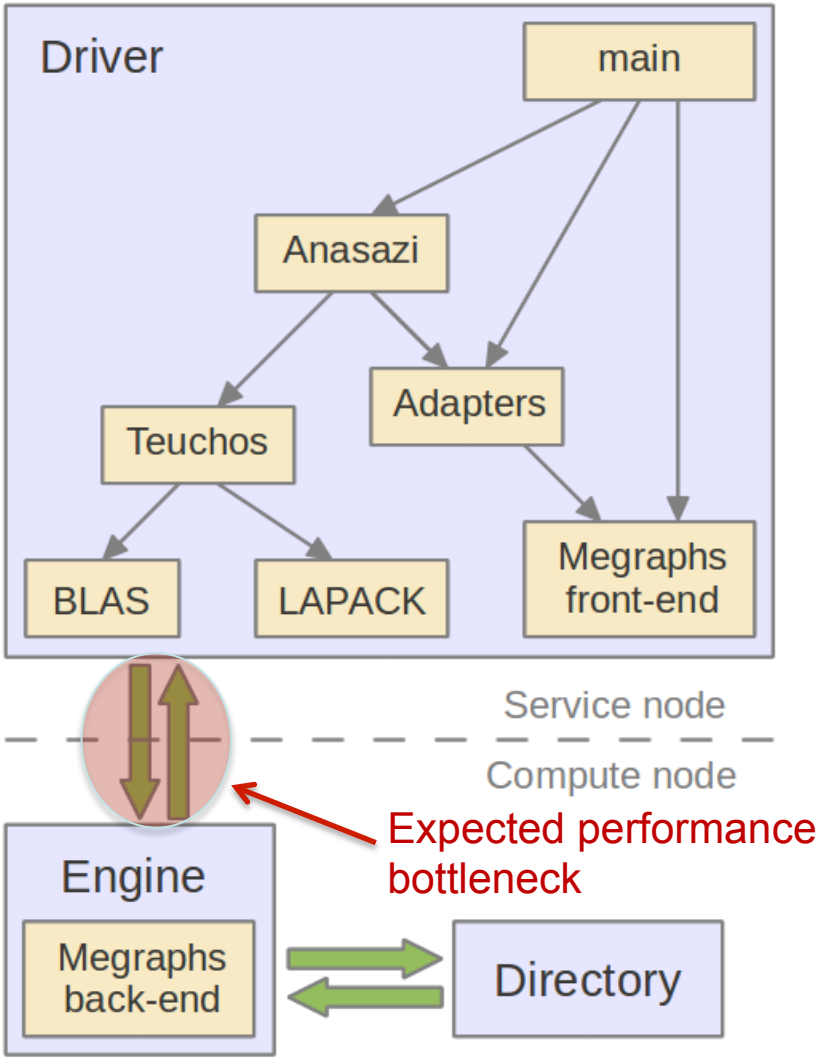
- Generic framework for large-scale iterative eigensolvers
- Block-based eigensolvers: Solves $AX = X\Lambda$ or $AX = BX\Lambda$
  - Reliably determine multiple and/or clustered eigenvalues
  - Achieve better cache locality for operator-vector products
  - Example applications: Modal/stability/bifurcation analysis, commute time
- Four eigensolvers:
  - *LOBPCG Locally Optimal Block Preconditioned Conjugate Gradient (Knyasev, 2002; Hetmaniuk & Lehoucq, 2006)*
  - Block Krylov-Schur (a block extension of Stewart, 2000)
  - Block Davidson (Arbenz, Hetmaniuk, Lehoucq, Tuminaro, 2005)
  - IRTR Implicit Riemannian Trust Region (Absil, Baker, Gallivan, 2006)
- Software written in templated C++
  - Distributed with Trilinos' Epetra and Tpetra matrix/vector class adapters
  - Templated interface allows use of alternate matrix/vector classes (e.g., Megraphs) .

Hybrid Approach to Megraphs/Anasazi Integration



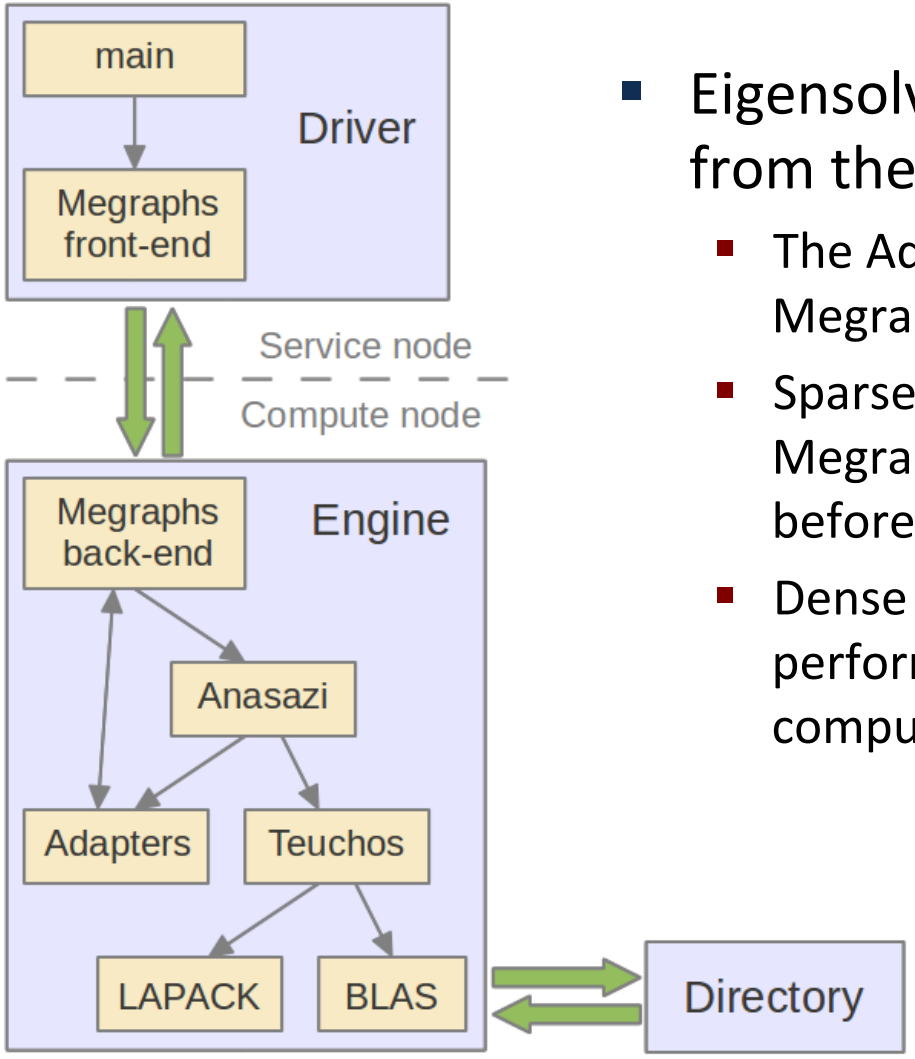
- Eigensolve is orchestrated by Anasazi from the service node:
  - The Adapters allow Anasazi to make use of Megraphs kernels via the Megraphs front-end.
  - Dense matrix operations are performed by BLAS/LAPACK on the XMT service node.
  - Sparse matrix operations are performed by Megraphs on the XMT compute nodes.

Hybrid Approach to Megraphs/Anasazi Integration



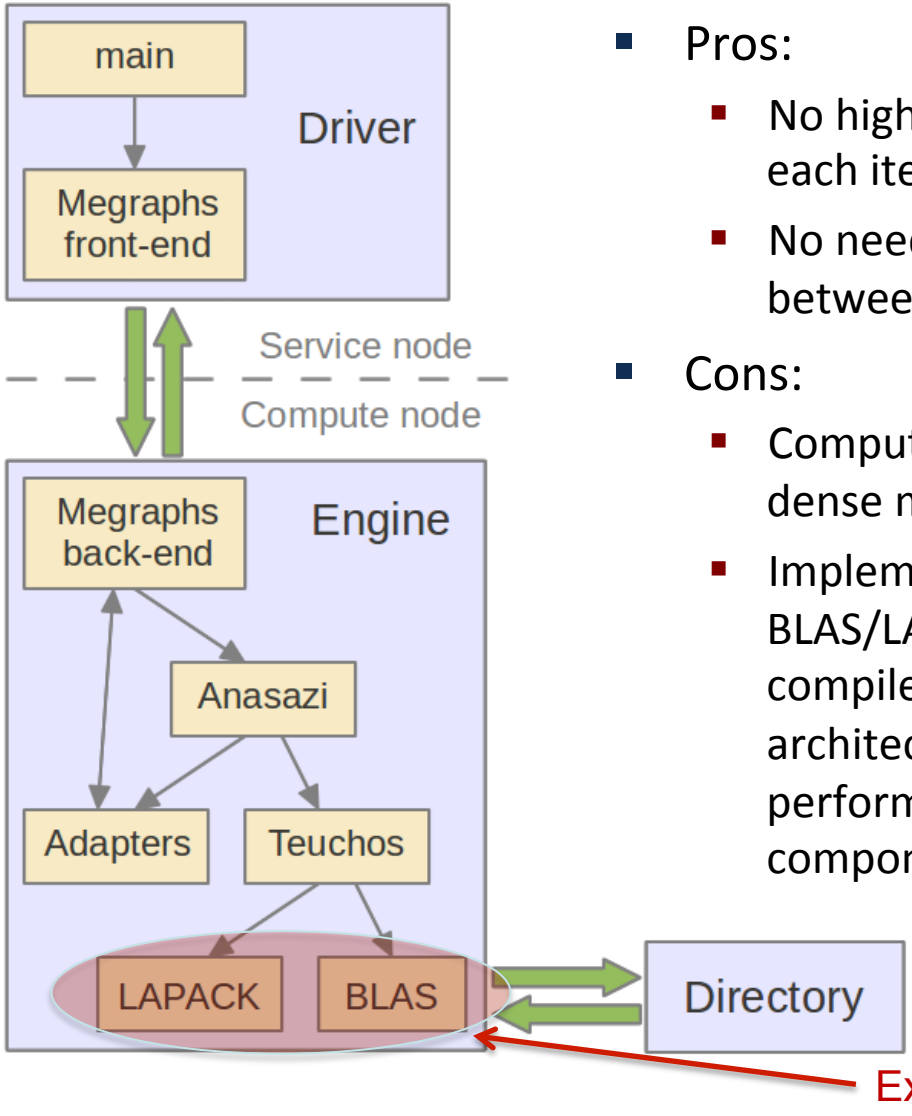
- Pros:
  - Takes advantage of the service node's floating point performance and the compute nodes' ability to hide memory latency.
  - Straight-forward implementation (the service node is just a Linux box).
- Cons
  - High-latency communication is required on each iteration of the eigensolve.
  - Dense matrices must be transferred between the service and compute nodes on each iteration.

Full Compute-Node Approach to Integration



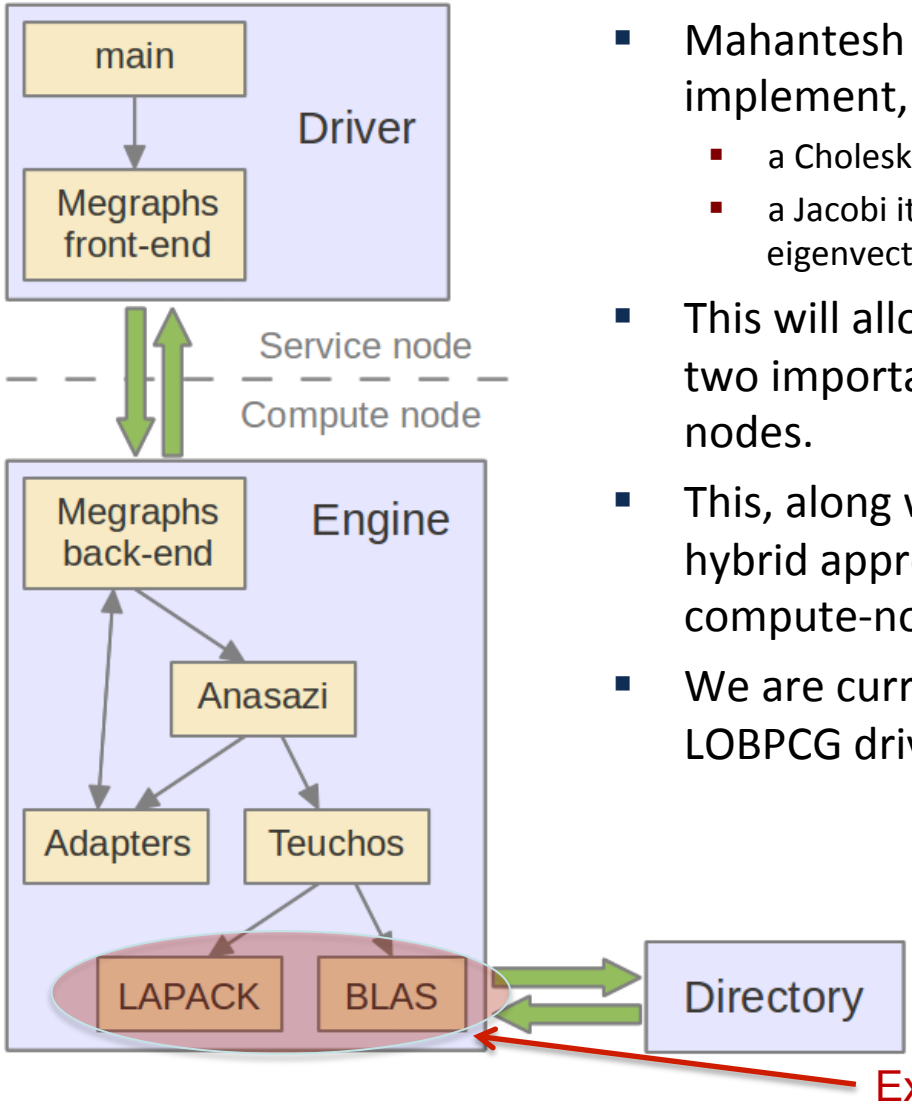
- Eigensolve is orchestrated by Anasazi from the compute nodes:
  - The Adapters allow Anasazi to make use of Megraphs kernels directly.
  - Sparse matrix operations are performed by Megraphs on the XMT compute nodes, as before.
  - Dense matrix operations are now performed by BLAS/LAPACK on the XMT compute nodes.

Full Compute-Node Approach to Integration



- Pros:
  - No high-latency communication required on each iteration of the eigensolve.
  - No need to repeatedly transfer dense matrices between the service and compute nodes.
- Cons:
  - Compute nodes were not designed for efficient dense matrix operations.
  - Implementation is very labor-intensive: no BLAS/LAPACK library provided; no Fortran compiler available; architectural peculiarities; architecture-specific parallelization and performance optimization are required for all components.

Full Compute-Node Approach to Integration



- Mahantesh Halappanavar (PNNL) has agreed to implement, for the XMT compute nodes,
  - a Cholesky factorization and forward/backward solves and
  - a Jacobi iteration for computing the eigenvalues/ eigenvectors of a symmetric matrix.
- This will allow us to ascertain the performance of two important dense matrix kernels on the compute nodes.
- This, along with performance measurements of the hybrid approach, will allow us to decide if the full compute-node approach is worth pursuing.
- We are currently debugging the adapters and an LOBPCG driver needed for the hybrid approach.

Preconditioning Eigensolvers

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- Interested in support-graph preconditioners for solving eigenproblems on graph data.
- Experiments to determine benefit of existing preconditioners:
  - Integrated Trilinos' Ifpack preconditioner package with Anasazi eigensolvers
  - Computed five smallest eigenvalues (tol=10^{-5}) of combinatorial Laplacians of public real-world graphs
  - Ran Anasazi's LOBPCG method on serial Linux workstation

Graph	n	m	No pre.	Jacobi	SGS	IC(0)
pgp_cc	10,680	24,316	33.0 s (2444 it.)	6.9 s (315 it.)	5.7 s (201 it.)	4.4 s (362 it.)
dblp-ubc	93,156	178,145	523 s (3769 it.)	78.6 s (344 it.)	83.9 s (230 it.)	55.3 s (385 it.)
flickr_cc	513,969	3,190,452	19,240 s (22,328 it)	1540 s (673 it.)	Failed	363 s (367 it.)

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Results courtesy of Erik Boman, SNL

SNL/LLNL Collaboration

- Preconditioners:
  - SNL will develop serial support-graph preconditioners.
  - LLNL will adapt AMGe for graph problems.
  - Future work: Use support-graph preconditioner as inexact solve (smoother) within 2-level AMGe to obtain a scalable, parallel algorithm.
- Tutorials:
  - Rich Lehoucq & Karen Devine, Anasazi how-to document.
  - Erik Boman, Support Graph Preconditioning (March 23).
  - Panayot Vassilevski, Element Based Algebraic Multigrid (April 20).
- Comparison of Eigensolvers and Platforms:
  - Agreed on common experiments for comparing eigensolvers and platforms.
  - Sharing data sets from SNL's BTER generator and LLNL's preferential attachment generator.
  - Sharing software installations on LLNL and SNL platforms.
  - Will work together to run and analyze experiments.

Evaluation of Eigensolvers on HPC Platforms: SNL & LLNL

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- Phase 0: Software development
  - Drivers for various solver libraries, input formats, analyses, performance tests
  - Megraphs/Anasazi integration for Cray XMT
- Phase 1: Find smallest eigenvalues & corresponding eigenvectors of graph Laplacians
  - Number of eigenvalues sought: 10, 20, 50 , 100
  - Input graphs: Yoo's preferential attachment, Kolda's BTER, public domain (e.g., twitter, flickr, snap); 1M-100M vertices
  - Platforms: hera 800-node AMD quad-core cluster at LLNL; Cray XMT as Megraphs/ Anasazi matures.
  - Solvers: Anasazi, SLEPc, hypre's LOBPCG; block vs non-block methods
  - Metrics: robustness for various data, ability to find multiplicities, run time, scalability
- Later phases:
  - Experiments on Dark Storm and sponsor platforms with sponsor data
  - Experiments with very large graphs (more than 2B edges/vertices)
  - More detailed comparisons of MPI clusters vs XMT
  - Effects of preconditioning

Continuing work

- Evaluation of Anasazi/Megraphs integration on XMT
- Implementation/evaluation of support-graph preconditioners
  - With summer student Kevin Deweese (UCSB, advisor = John Gilbert)
- Collection/analysis of HPC eigensolver comparison results
- Further investigation of …
  - Relationships between classical, graph and nonlocal Laplacians
  - Variational characterization of relationships for commute time and statistical ranking