LBNL Status Update

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with ...

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funded by TOPS and AST

Our Mission

- To develop and deploy large scale linear solvers and eigensolvers in support of SciDAC Applications
  - Research into how to incorporate/work around unique characteristics of Accelerator Applications

Old Business

- Exact Shift-Invert Lanczos for Generalized Eigenvalue Problems
  - Integrated into Omega3P
  - Combines distributed memory SuperLU and ARPACK
  - Special optimizations for clusters of SMPs
  - Largest problem solved n=7.5M nnz=302M on IBM SP at NERSC
  - Good proof-of-concept for direct solvers
    - Used for solving larger problems (L. Lee)

- Standalone version almost ready
  - "Generic" OO style allowing substitution of different linear solvers
  - BABELized version next

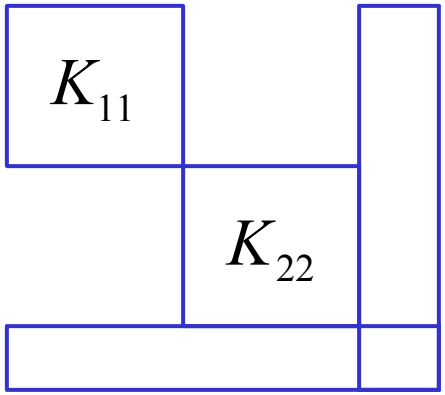
New Business

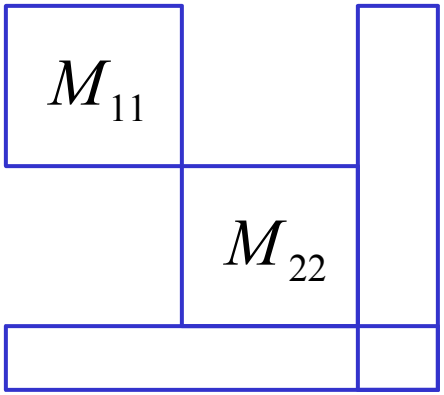
- Straightforward application of direct solvers incurs too much fill
  - Use of SuperLU in preconditioners
  - AMLS
    - Divide and Conquer (sort of) for eigenvalue calculations

Algebraic Sub-structuring

$$Kx = \lambda M x \,,\; K \text{ symmetric} \,,\; M \text{ SPD}$$

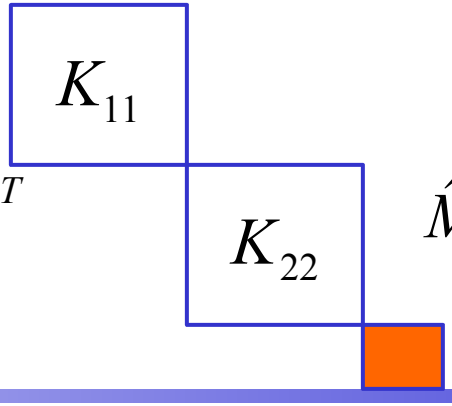
1. Matrix Partition



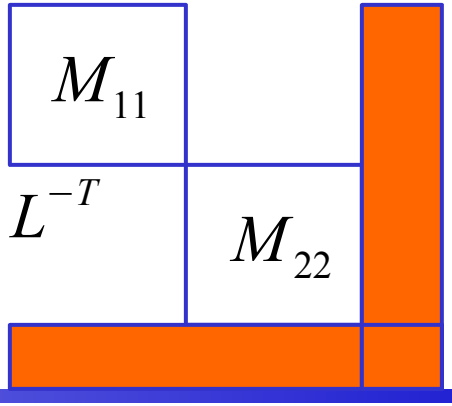


2. Block elimination (congruent trans)

$$\hat{K} = L^{-1} K L^{-T}$$



$$\hat{M} = L^{-1} M L^{-T}$$



Algebraic Sub-structuring (cont)

3. Sub-structure calculation (mode selection)

$$K_{11} v^{(1)} = \mu^{(1)} M_{11} v^{(1)}$$
$$K_{22} v^{(2)} = \mu^{(2)} M_{22} v^{(2)}$$

4. Subspace assembly

$$S_1 = \left(v_1^{(1)} v_2^{(1)} \ldots v_{k_1}^{(1)} \right)$$
$$S_2 = \left(v_1^{(2)} v_2^{(2)} \ldots v_{k_2}^{(2)} \right)$$

$$S = \begin{pmatrix} S_1 & & \\ & S_2 & \\ & & I \end{pmatrix}$$

Algebraic Sub-structuring (cont)

5. Projection (Rayleigh-Ritz)

$$(S^T \hat{K} S) q = \theta (S^T \hat{M} S) q$$

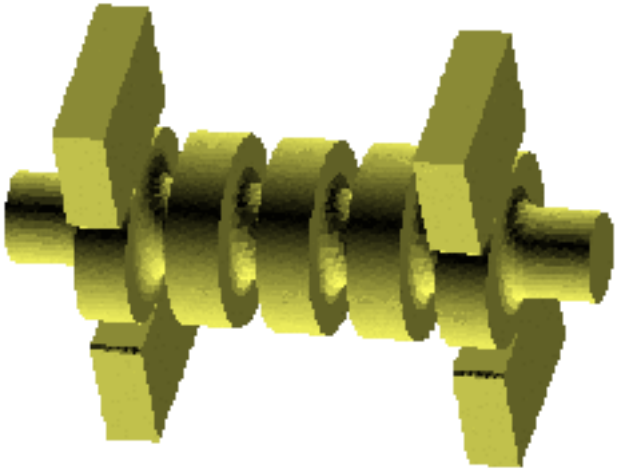
6. Unravel

$$D = diag(\theta_1, \theta_2, \ldots, \theta_m), U = L^{-T} S Q_m$$
$$Q_m = (q_1 q_2 \ldots q_m), \hat{K} = L^{-1} K L^{-T}$$

Status and Plans

- Algebraic Analysis and Error Estimates
  - Mode selection heuristic for single level and extremal eigenpairs
    - Examines components of eigenvectors…
    - Todo: Multi-level analysis
      Interior eigenpairs
- Sequential implementation complete
  - Uses: METIS, SuperLU, ARPACK, …
  - Can handle large null space in K
- Comparison and evaluation on more accelerator problems
- Parallel implementation to follow
  - Coordinate factorizations, updates, eigenvalue computations, …

Some results: Accelerator Model

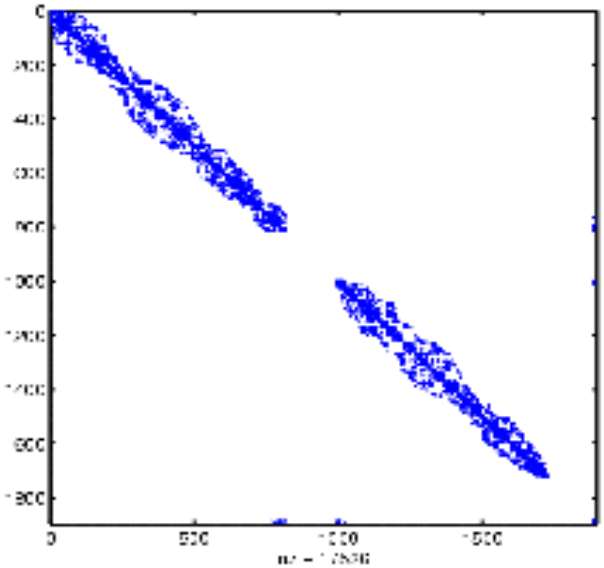


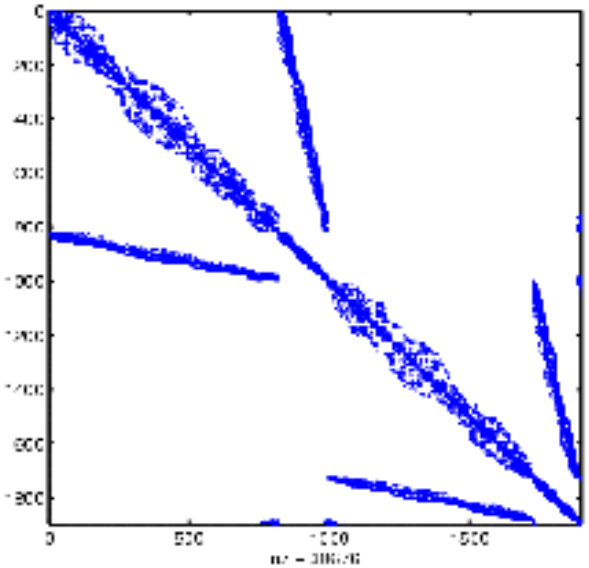
$$n = 1898$$

$$n_1 = 995$$

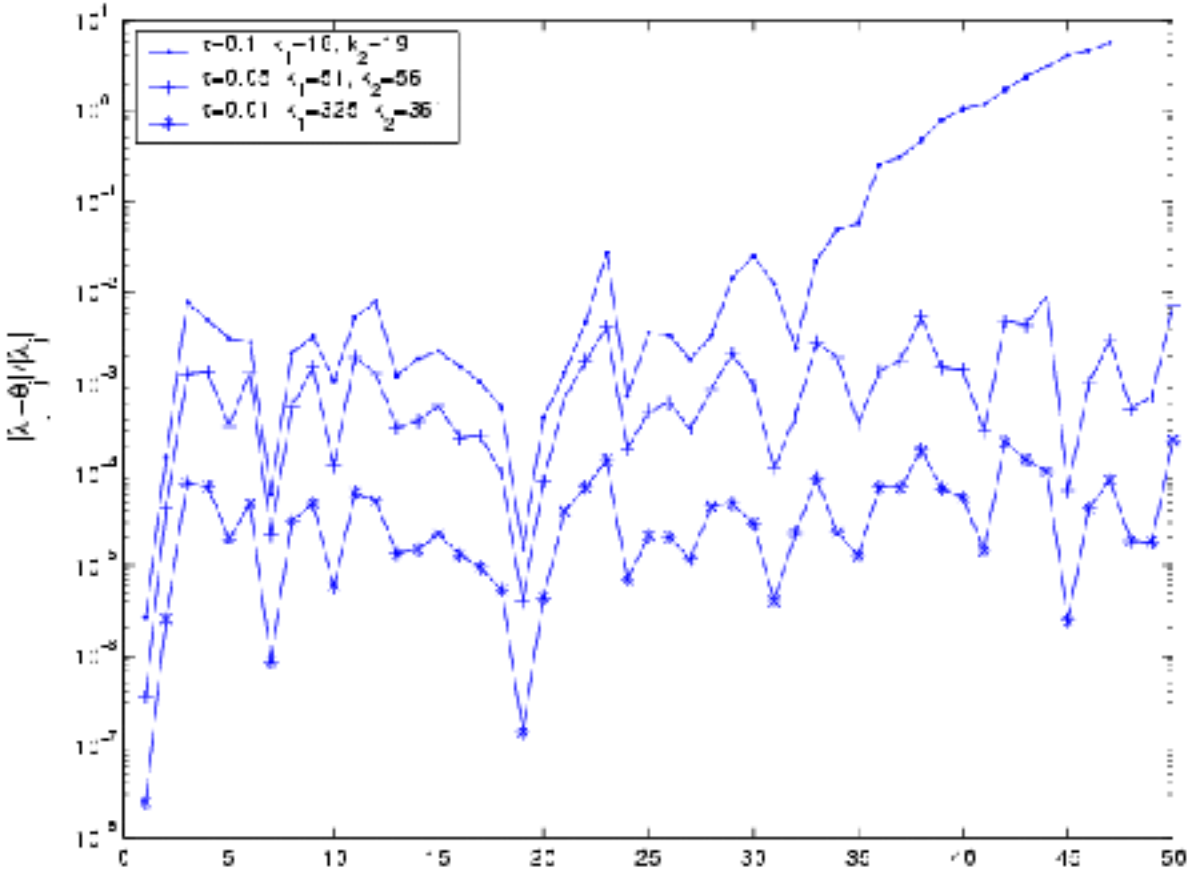
$$n_2 = 887$$

$$n_3 = 6$$





Relative error (Accelerator Model)



Future Plans

- Handle new models and formulations
  - Quadratic Eigenvalue Problems
  - Linear Systems with special properties from optimization

$$\begin{pmatrix} K - \lambda M & Mv \\ (Mv)^T & 0 \end{pmatrix}$$

- More Software Engineering
  - Vectorization & Communication optimizations on X1 & other new architectures
    - Initial experiments with SuperLU underway