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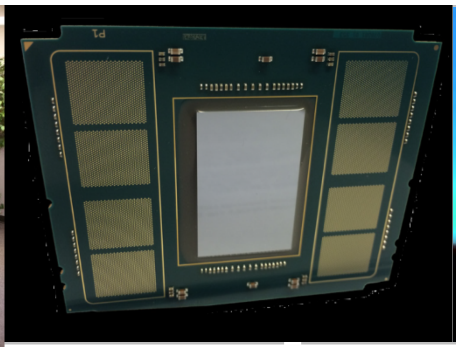
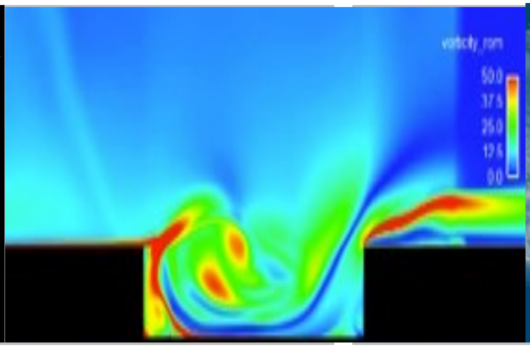
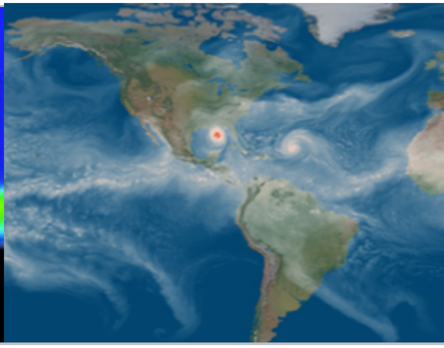

A Parallel Hierarchical Low-Rank Solver for General Sparse Matrices

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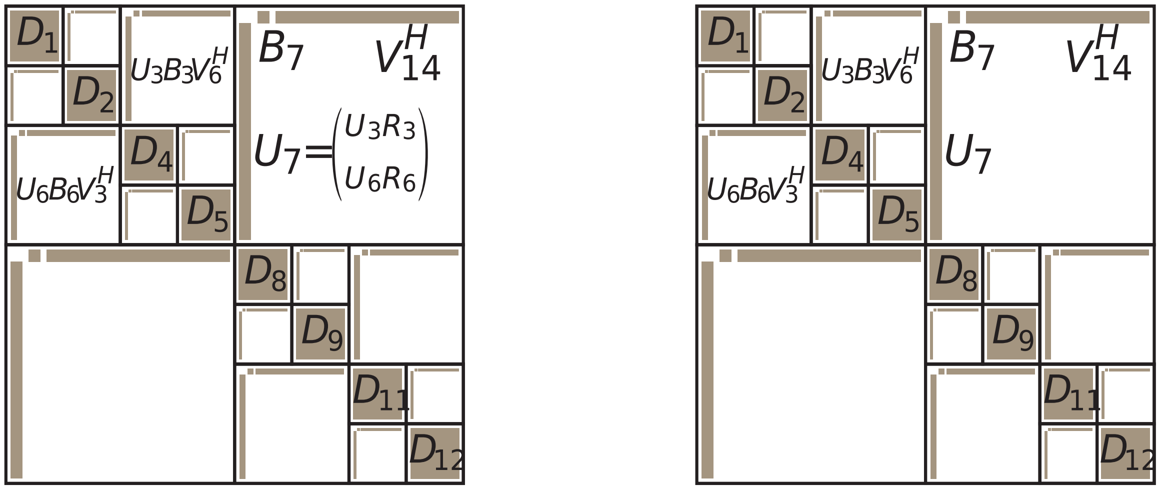
U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

Hierarchical Low-Rank (HLR) Matrices and Solvers

- Low-rank structure is common in applications
- Hierarchical (low-rank) matrices and solvers are *"hot"*
  - Early work by Hackbusch, 1999-2000 (H-matrix)
  - HSS and BLR formats most popular now
- Key insight: Many matrices have useful (rank) structure
  - Blocks far from diagonal can be approximated using low-rank
    - Holds for elliptic PDEs, some other (e.g., advection-diffusion problems)
    - Similar intuition as for Fast Multipole Methods (FMM)
    - May also apply to data science (e.g. covariance matrix)
- Our goals
  - Develop new solver/preconditioner with less memory (and flops)
  - Speed up sparse direct solvers (high accuracy)
  - Use as preconditioner (low accuracy)

Low-Rank Structure

- Low-rank structure often occurs in *off-diagonal blocks in*
  - The matrix A
  - The inverse of A
  - The LU factors of A
- Ex: Hierarchical low-rank structure (Figure from Wang et al.)

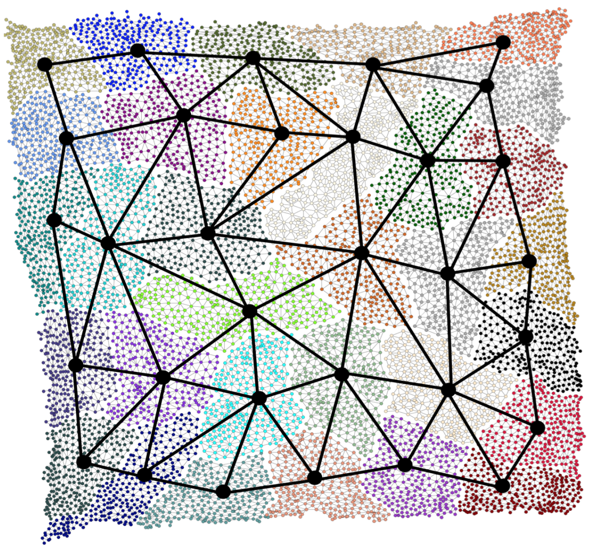


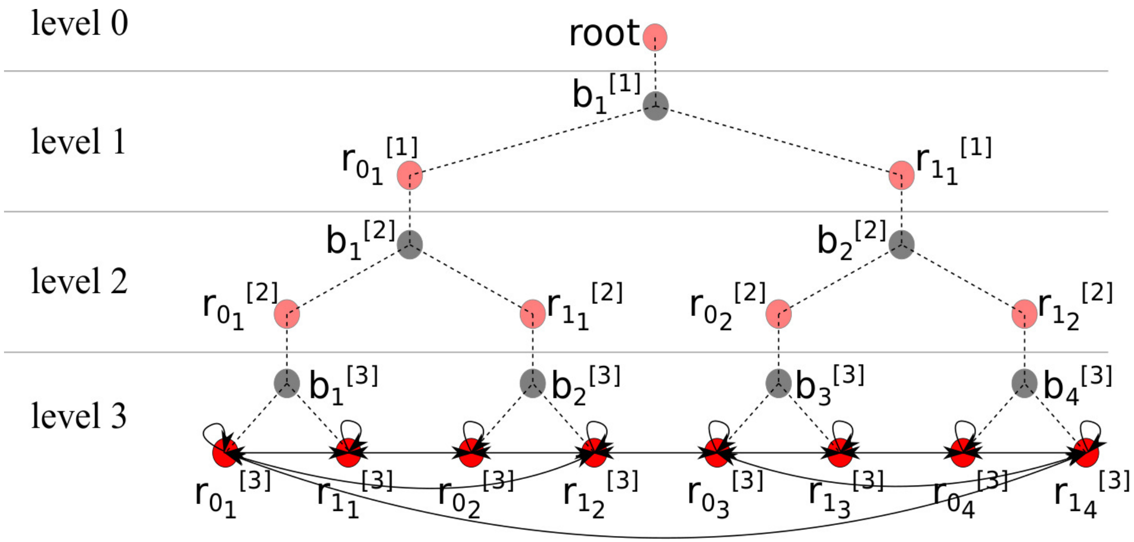
(a) HSS matrix. (b) HODLR matrix.

- Problem: rank growth in off-diagonal blocks
  - We use H2 format (allows further splitting, standard admissibility)

The LoRaSp/H2 Method

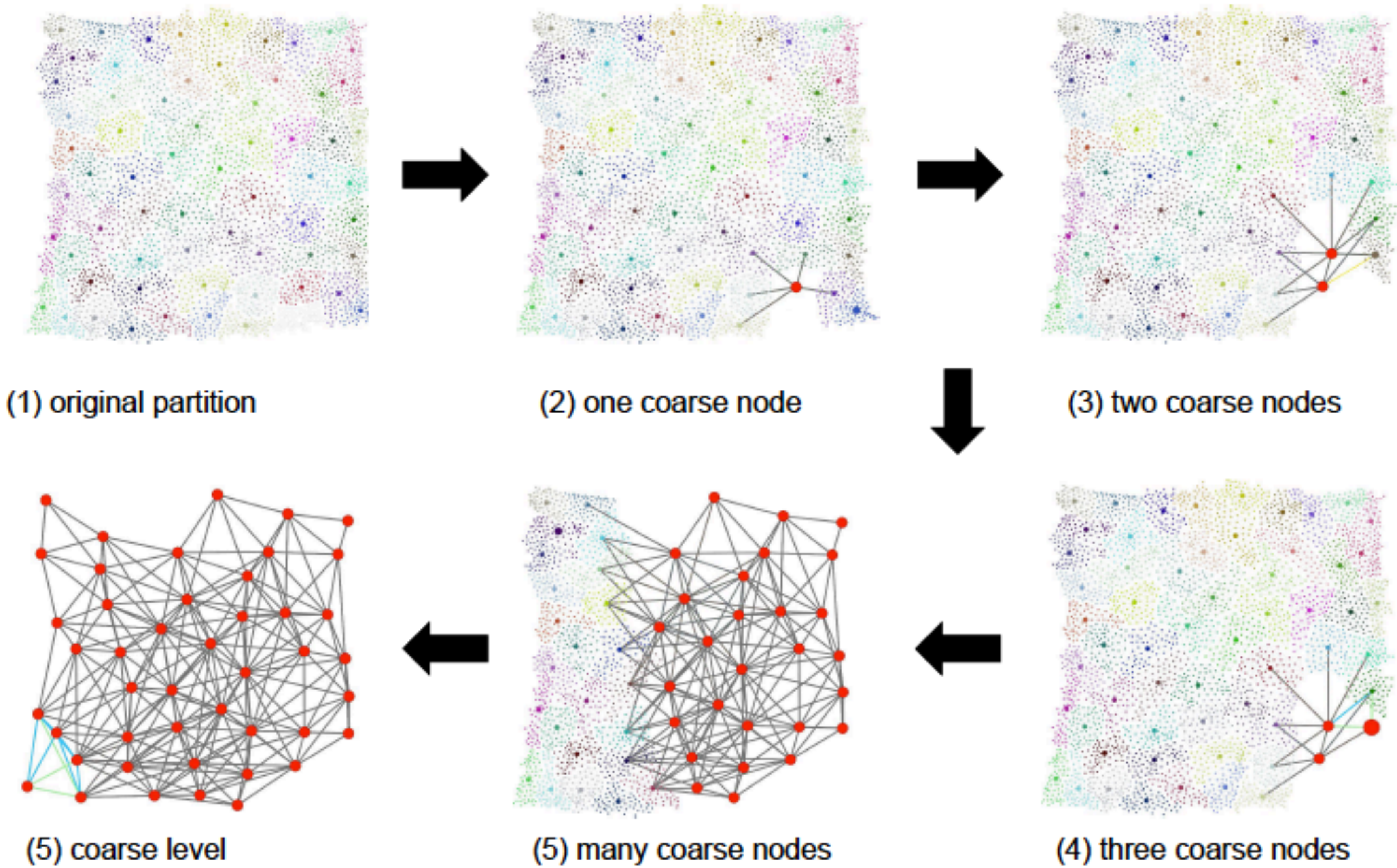
- Pouransari, Coulier, Darve, SISC 2017
- Partition graph via recursive bisection, construct tree
- Eliminate “clusters” (blocks) starting at leaf level
  - Approximate block LU factorization
  - New “coarse” dof via *extended sparsification*
- Merge neighbors, repeat for each level in the hierarchy (bottom up)





Figures courtesy Chen et al., and Pouransari et al.

Algorithm: Fine to Coarse Level



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Multilevel Block Incomplete Factorization

- Strong ILU connection:
  - LoRaSp/H2 solver is really a Block ILU(0) factorization where the “dropped” blocks are approximated using low-rank method
    - A= LU+E, where E has low-rank blocks
  - We compensate for the dropped blocks by adding new rows/columns to the matrix (*extended sparsification*)
  - Typically, “fill” blocks have low-rank structure
- We eliminate the *fine* vertices (clusters)
  - The Schur complement for remaining *coarse* vertices is a much smaller matrix
  - Solve for this recursively
- Similarities to
  - ARMS (Saad, 2002)
  - AMG

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Extended Sparsification

- For simplicity, assume symmetric A (can be extended)
- Suppose the off-diagonal blocks are (approx) low-rank:

$$\begin{pmatrix} A_1 & UV^T \\ VU^T & A_2 \end{pmatrix}$$

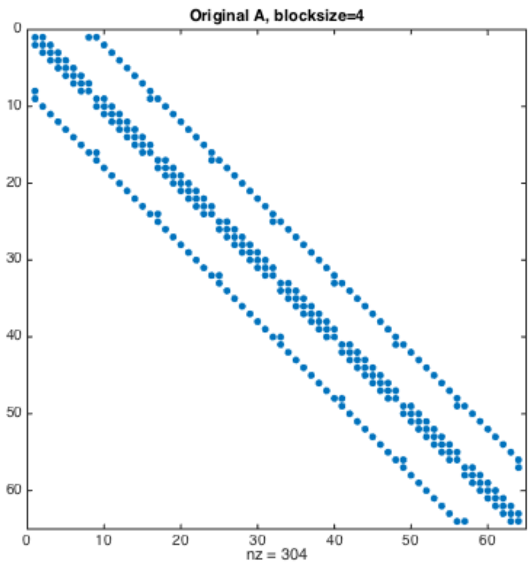
- We solve the equivalent extended system

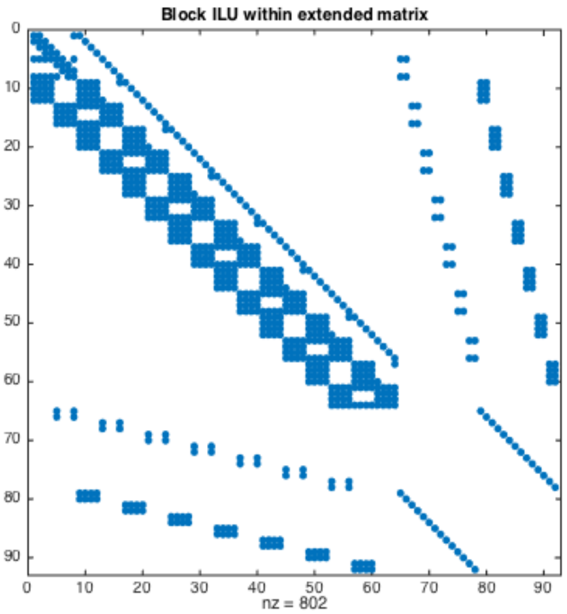
$$\begin{pmatrix} A_1 & 0 & U & 0 \\ 0 & A_2 & 0 & V \\ U^T & 0 & 0 & -I \\ 0 & V^T & -I & 0 \end{pmatrix}$$

- We sparsify the original matrix, but add extra rows/cols that also need to be factored.
- The lower the ranks of U,V, the smaller extended system

ILU and Extended Sparsification

- Note: Fill blocks in the block LU factors often have low rank
  - Schur complements in the Gaussian elimination
- Approach: Compute blocks in ILU(0) exactly, and
  - Approximate blocks in ILU(1) (not in ILU(0)) using low-rank
  - Extend matrix with new rows/cols





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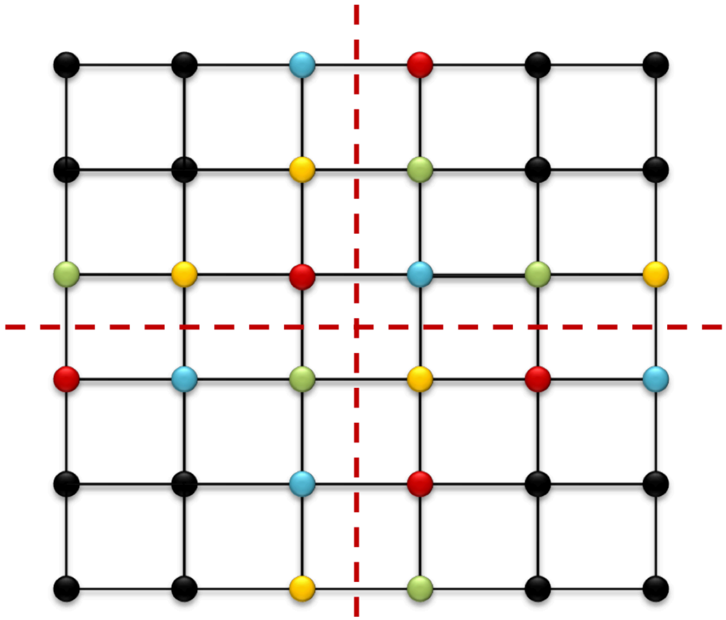
Our Parallel Algorithm

- Data parallel: Each processor works on a subgraph (subdomain).
- Consider the cluster graph:
  - Only boundary vertices need communication.
  - Interior vertices can be eliminated independently in parallel.
- Use graph coloring on the boundary to find concurrent work.
- #synchronization points = #colors
- Can overlap communication and computation.
- Repeat for each level.
- Future: Task-based; dynamic sched.



Example: 4 processors. Each vertex (node) corresponds to a cluster of variables.

Experiments

- Parallel H2 solver (and results) by Chao Chen
  - Parallel extension of LoRaSp serial code
  - MPI everywhere
  - Eigen library for dense linear algebra (on node)

- SVD for low-rank compression
  - a) Fixed eps in matrix approx. (ranks vary)
  - b) Fixed rank in matrix approx. (quality varies)
    - used in most of the experiments

- Platform: Cray XC30 (Edison/NERSC)
  - Used 16 (out of 24) cores per node
  - Used up to 16 nodes (256 cores)

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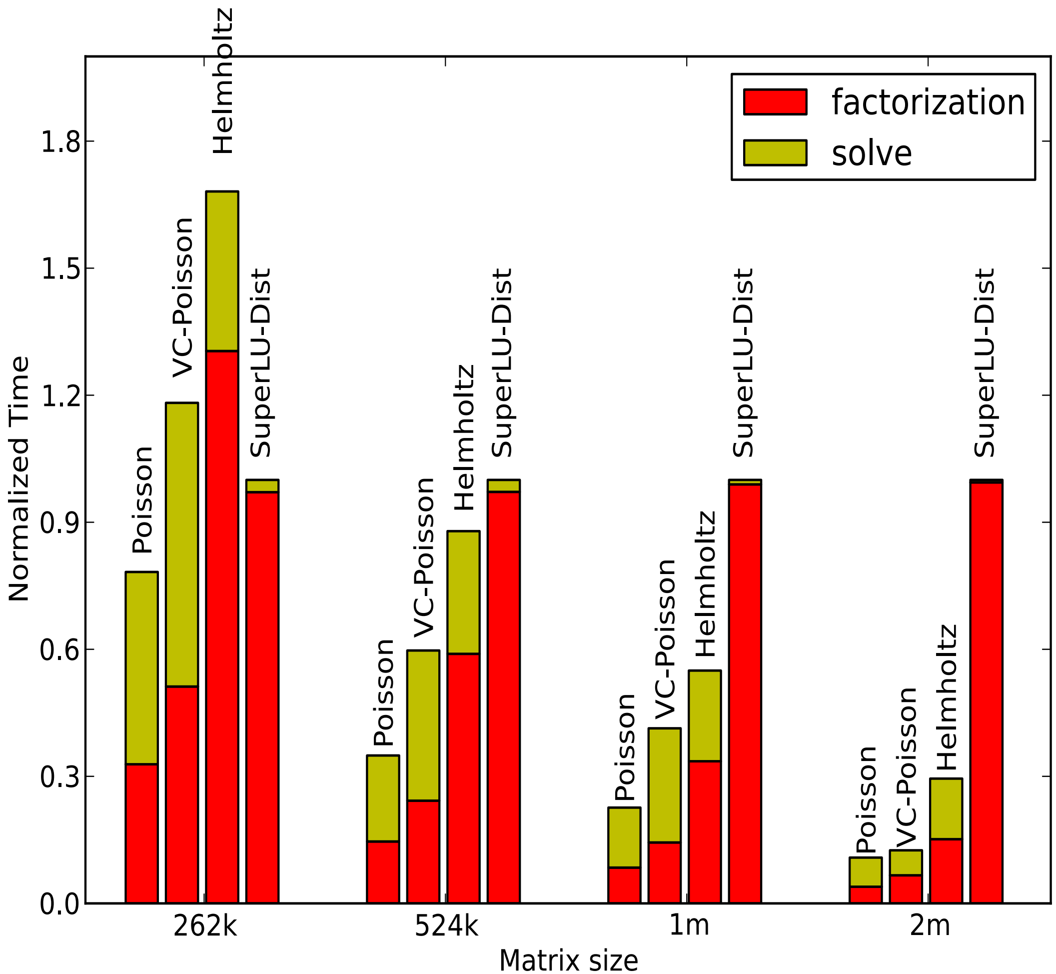
Results: Structured Mesh Case

Compare hierarchical solver as preconditioner vs. SuperLU-Dist direct solver on three 3D PDE model problems. 16 processors (MPI ranks).



(a) Total time

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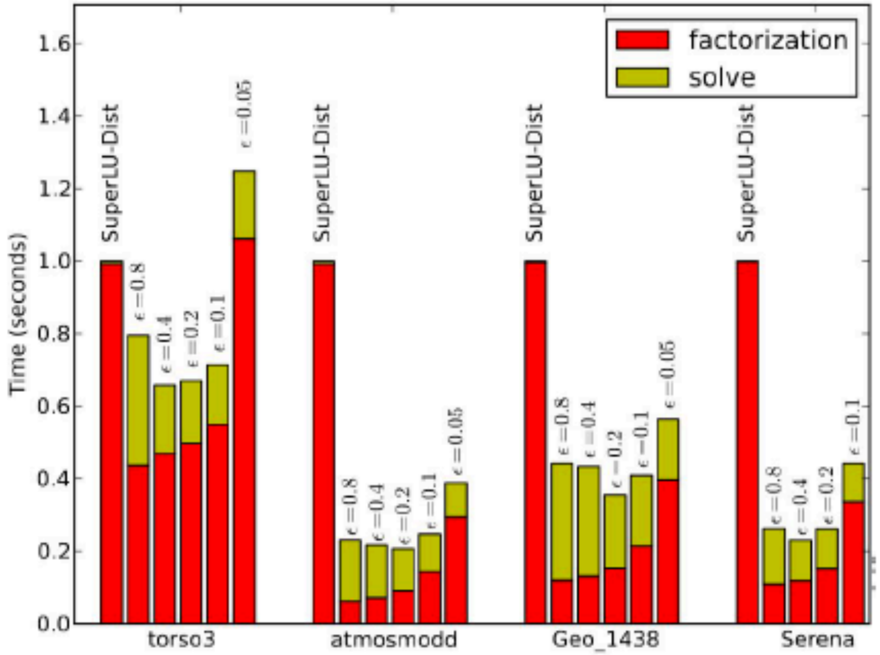
Results: Unstructured Case

Compare hierarchical solver as preconditioner vs. SuperLU-Dist on unstructured matrices, including nonsymmetric cases.

Table 1: General matrices from the University of Florida Sparse Matrix Collection

Matrices	size	# nonzero	symbolic pattern symmetry	numeric value symmetry	positive definite
torso3	0.26M	4.4M	no	no	no
atmosmodd	1.3M	8.8M	yes	no	no
Geo_1438	1.4M	60.2M	yes	yes	yes
Serena	1.4M	64.1M	yes	yes	yes



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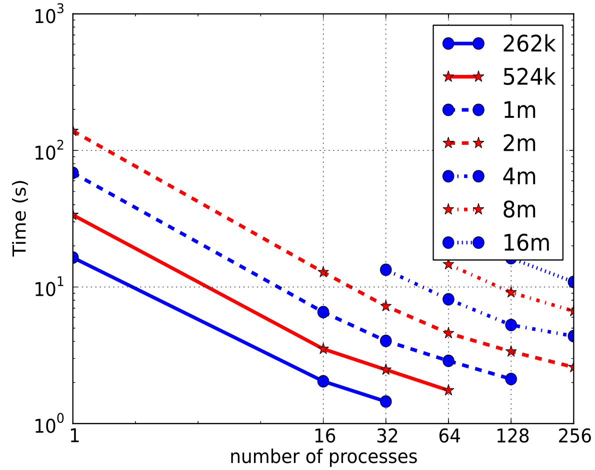
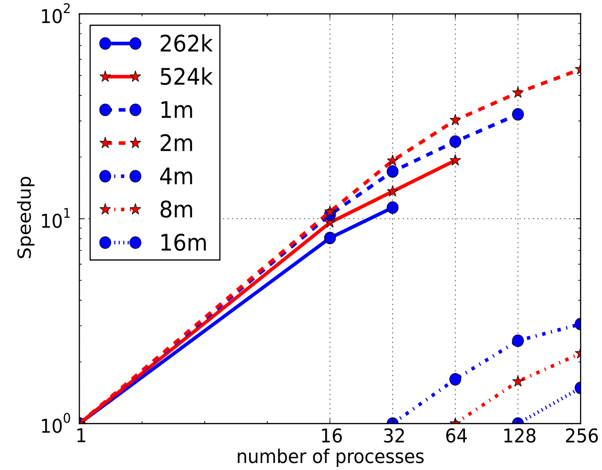
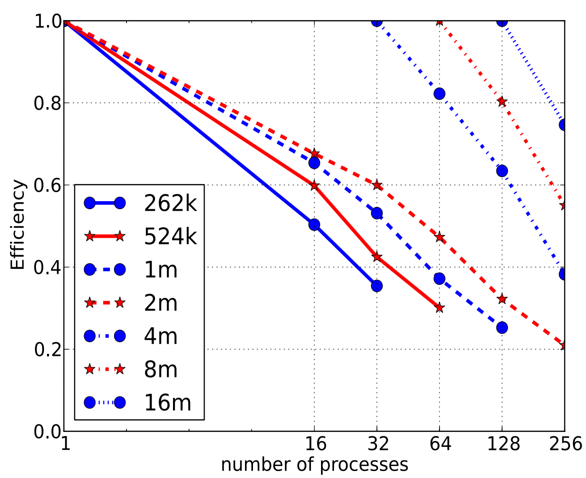
Results: 3D Poisson Eqn.



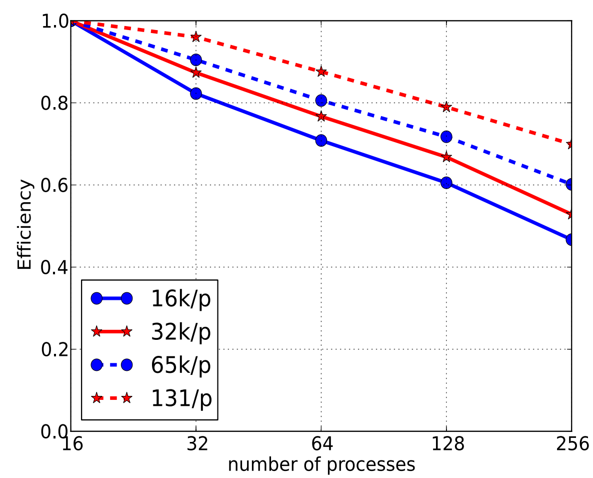
(a) Factorization time



(b) Factorization speedup



(c) Fixed total problem size



(d) Fixed problem size per processor

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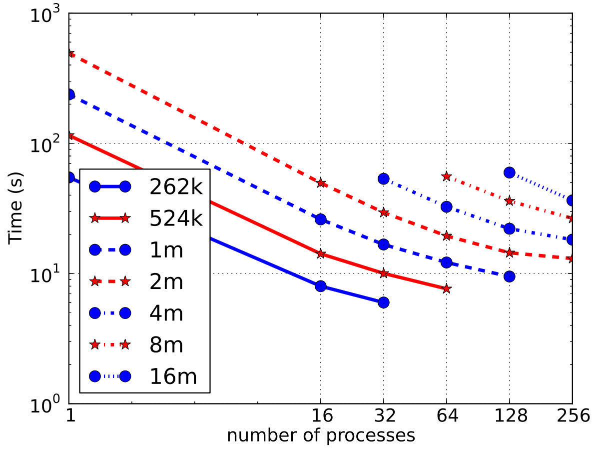
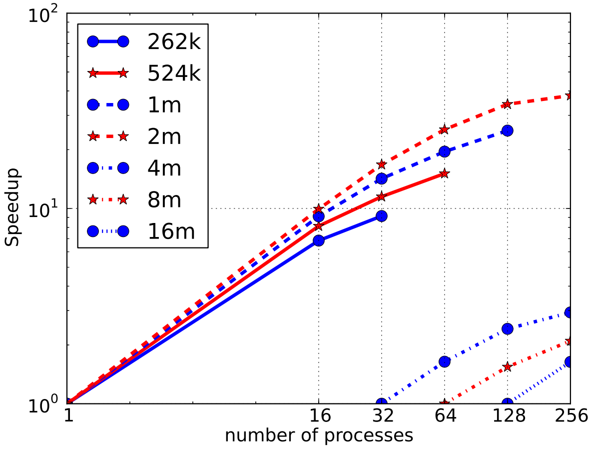
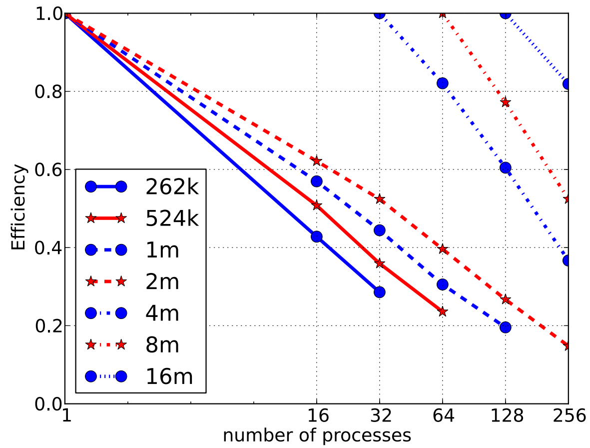
Results: Helmholtz eqn.



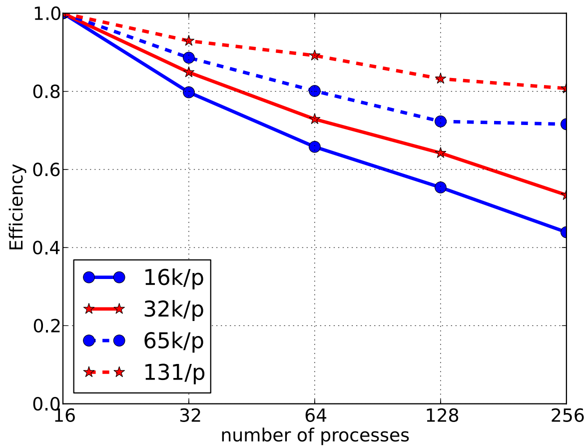
(a) Time



(b) Speedup



(c) Fixed total problem size



(d) Fixed problem size per processor

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In Progress: Preserve Near-Null-Space

Laplace with Neumann bc's except Robin on bottom with $\beta = 100$ on ¼ of surface & $\beta = 0$ on the rest

standard method with vertical clusters

mesh	its	nnz/n
16 x 16 x 8	9	133.4
32 x 32 x 8	11	156.0
64 x 64 x 8	17	167.7
128 x 128 x 8	26	173.6

modified so 1st level compression accounts for constant

mesh	its	nnz/n
16 x 16 x 8	6	146.5
32 x 32 x 8	9	187.4
64 x 64 x 8	11	208.9
128 x 128 x 8	17	219.9
256 x 256 x 8	28	225.5

- Credit: Tuminaro (Matlab)
- Based on idea by Yang
- Only 1st level implemented so far

Conclusions (1)

- Hierarchical low-rank methods (HLR) augment the current solver/preconditioner ecosystem.
- Faster than sparse direct
- Most useful as preconditioner
- User must choose accuracy (input arg.)
- Setup phase can be expensive.
  - Can often amortize this cost over multiple rhs
- Theory promises near-linear complexity for many PDE problems
  - Potentially more robust than multigrid/AMG (at a cost)

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Conclusions (2)

- Well suited for modern architectures
  - Most work is in dense linear algebra (even for sparse problems)
    - High arithmetic intensity
  - Many small dense matrices at same time
    - Could use batched BLAS/LAPACK
- Our hierarchical solver
  - Is motivated by H2 but can also be interpreted as multilevel ILU
  - Many options/variations still to explore
    - Low rank: SVD, RRQR, RRLU, ACA, ID, …
- Early days:
  - Several algorithm options, best choice unclear
  - Codes are still immature but rapidly improving

References

- Pouransari, Coulier, Darve, “Fast Hierarchical Solvers for Sparse Matrices using Extended Sparsification and Low-Rank Approximation”, SIAM J. Sci. Comp. 39(3), 2017.
- Chen, Pouransari, Rajamanickam, Boman, Darve, “A Distributed-Memory Hierarchical Solver for Sparse Linear Systems”, Parallel Computing, in revision.

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