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Scalable Matrix Computations on Large Scale-Free Graphs using 2D Graph Partitioning

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Sparse Days, CERFACS, June 17, 2013

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

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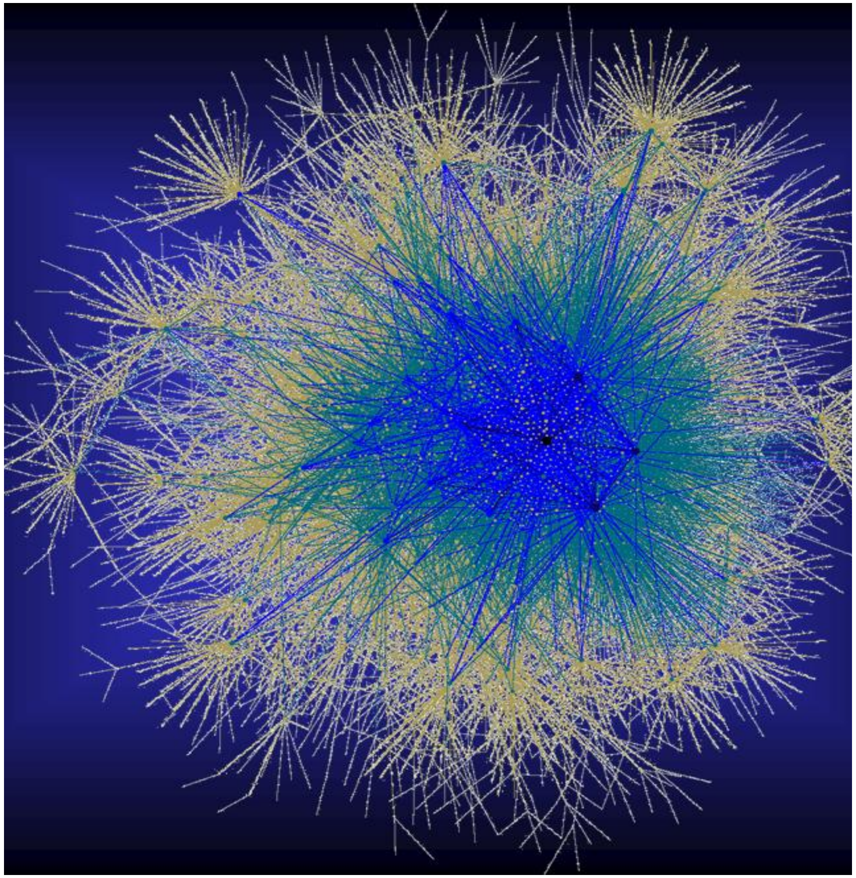
Overview

- We are interested in matrix computations to analyze large graphs on distributed-memory supercomputers
  - In particular, eigensolvers
  - Our focus is on SpMV, a kernel in iterative methods
- We present results of various data distribution strategies for distributed-memory computing on scale-free graphs.
  - 1D vs 2D matrix layout
  - Use of graph and hypergraph partitioners
- We present a new method combining (hyper)graph partitions with 2D distributions, and show its benefit for scale-free graphs.

Background

- Large graphs are pervasive
  - WWW, social networks
- Often scale-free
  - Power-law degree distr.
  - Small diameter
- Very different from PDE discretizations
  - Need to adapt scientific computing methods and tools?



BGP graph (credit: Ross Richardson, Fan Chung)
http://math.ucsd.edu/~fan/graphs/gallery

Matrix Computations: SpMV is key

- Linear algebra is a useful analysis tool for graphs
  - Eigen-analysis using extreme eigenpairs
  - SpMV is core kernel in iterative methods
- Sparse matvec (SpMV) is bottleneck for scale-free graphs on large distributed-memory computers
  - High-degree vertices cause lots of communication
  - Some processors need to communicate with almost all other!

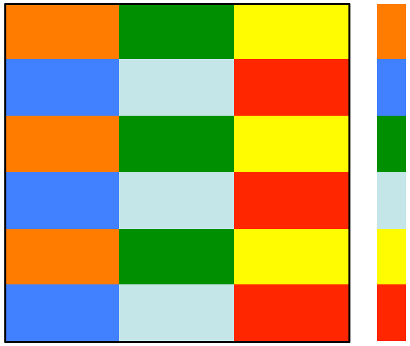
Partitioning

- Graph partitioning generally reduces communication for SpMV
  - Hypergraph model exactly models communication volume (Catalyurek & Aykanat, 2000)
- Graph partitioners are widely regarded as ineffective on scale-free graphs
  - Software tools (e.g., Metis, Scotch, Zoltan) were designed for meshes and PDE discretizations
    - Not optimized for scale-free graphs
  - Focus on communication volume
    - We wish to reduce both #messages and communication volume
- Partitioning strategy depends on type of distribution
  - 1D (row-based) distribution is most common

1D and 2D Matrix Distributions

- 1D matrix distribution:
  - Entire rows (or columns) of matrix assigned to a processor
  - Same mapping used for vectors
  - Default distribution in Trilinos
- 2D matrix distribution:
  - Block-based Cartesian layout
  - Long used in parallel dense solvers (ScaLapack)
  - Also works for sparse matrices (Hendrickson et al. ‘95, Bisseling ‘04)
  - Yoo et al. (SC’11) demonstrated benefit over 1D layouts for eigensolves on scale-free graphs

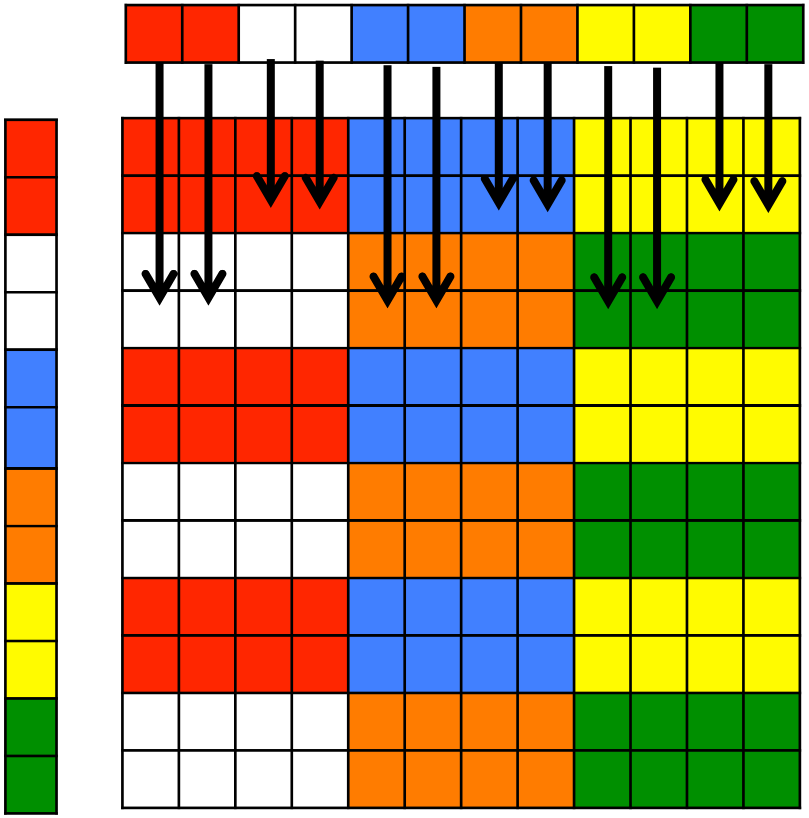
1D row-wise matrix distribution; 6 processes



2D matrix distribution; 6 processes

Benefit of 2D Matrix Distribution

- During matrix-vector multiplication, communication occurs only along rows or columns of processors.
  - Expand (vertical):
    Vector entries x_j sent to column processors to compute local product $y^p = A^p x$
  - Fold (horizontal):
    Local products y^p summed along row processors; $y = \Sigma y^p$
- In 1D, fold is not needed, but expand may be all-to-all.



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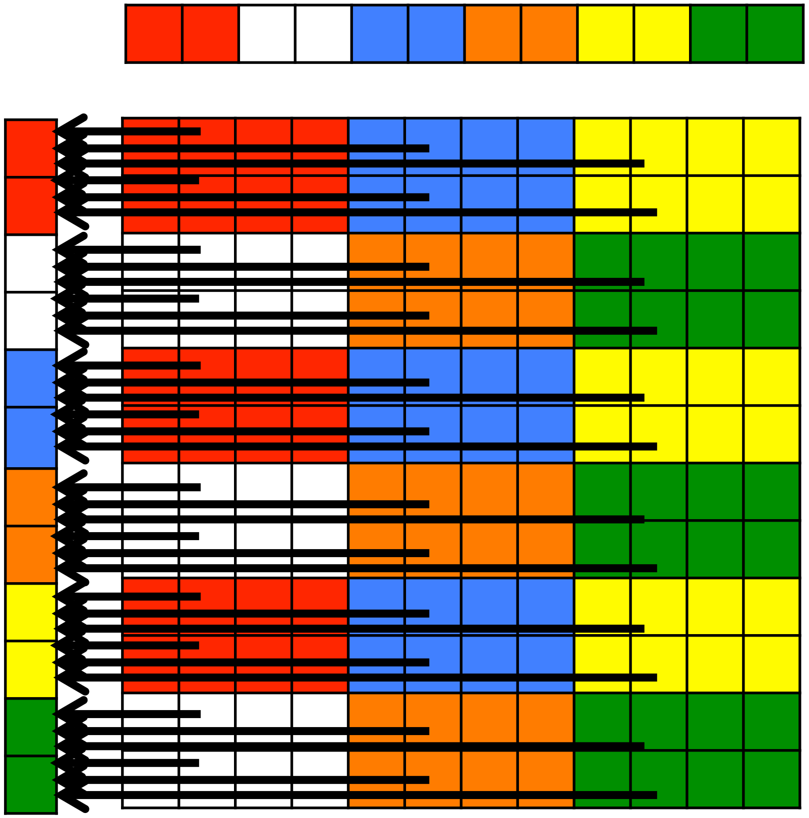


Trilinos Computational Science Toolkit

- Heroux et al., Sandia

- Trilinos Capabilities:
  - Scalable Linear & Eigen Solvers
  - Discretizations, Meshes & Load Balancing
  - Nonlinear, Transient & Optimization Solvers
  - Software Engineering Technologies & Integration

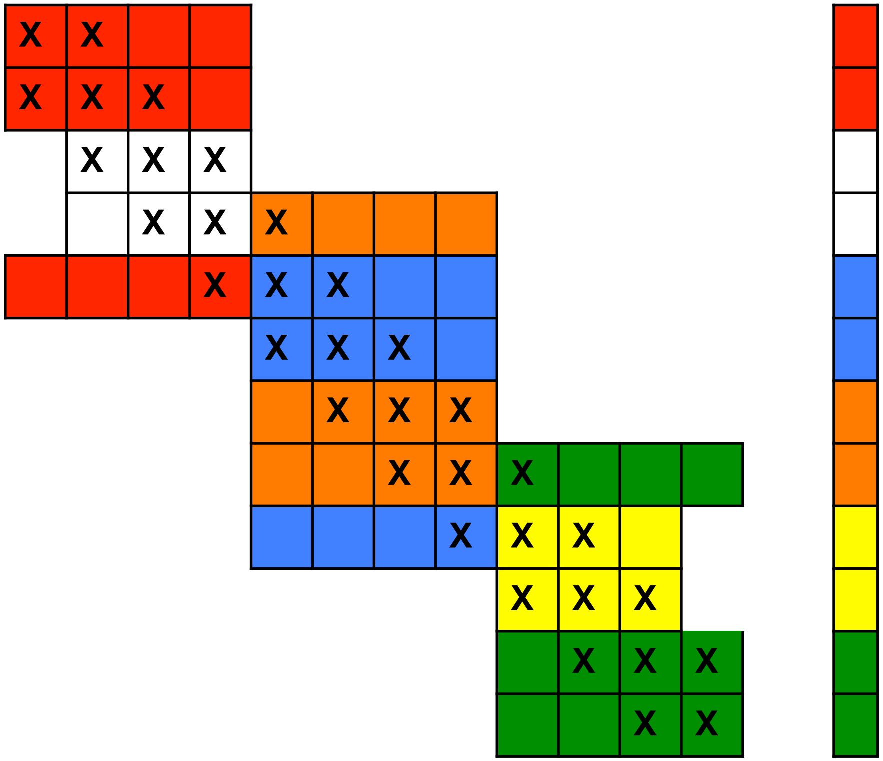
- Trilinos features:
  - Block-based data structures and algorithms
    - Block-based linear and eigen solvers use "multivector" data structures.
  - Toolkit/package-based design
    - Packages can be combined, but not all of Trilinos is needed to get work done.

- In this project, we use Trilinos'…
  - Distributed Matrix/Vector classes *Epetra* and *Epetra64*
  - Eigensolver package *Anasazi*
  - Linear solver package *Belos*
  - Preconditioning package *Ifpack*
  - Utilities package *Teuchos* (e.g., communicators, parameters, ref-counted pointers)

Trilinos Maps

- Maps describe the distribution of global IDs for rows/columns/vector entries to processors.
- Four maps needed in most general case:
  - Row map for matrix
  - Column map for matrix
  - Range map for vector
  - Domain map for vector
- Part of *Epetra* package

Rank 3 (Blue)
Row Map = {4, 5, 8}
Column Map = {4, 5, 6, 7}
Range/Domain Map = {4, 5}



1D vs 2D Strong Scaling Experiments

- Compare times for matrix-vector multiplication with 1D and 2D distributions
- Hera cluster at LLNL (AMD quad-core, quad-socket Opteron processors operating at 2.2/2.3 GHz)
- Matrices from the University of Florida matrix collection
- Symmetrized and largest connected component extracted

Name	Description	Number of Rows	Number of Nonzeros
Hollywood-2009	Hollywood movie actor network (Boldi, Rosa, Santini, Vigna)	1.1M	113M
Wikipedia-20070206	Links between wikipedia pages (Gleich)	3.5M	85M
Ljournal-2008	LiveJournal social network (Boldi, Rosa, Santini, Vigna)	5.6M	99M
Wb-edu	Links between *.edu webpages (Gleich)	8.9M	88M
Cit-Patents	Citation network among US patents (Hall, Jaffe, Trajtenberg)	3.8M	33M

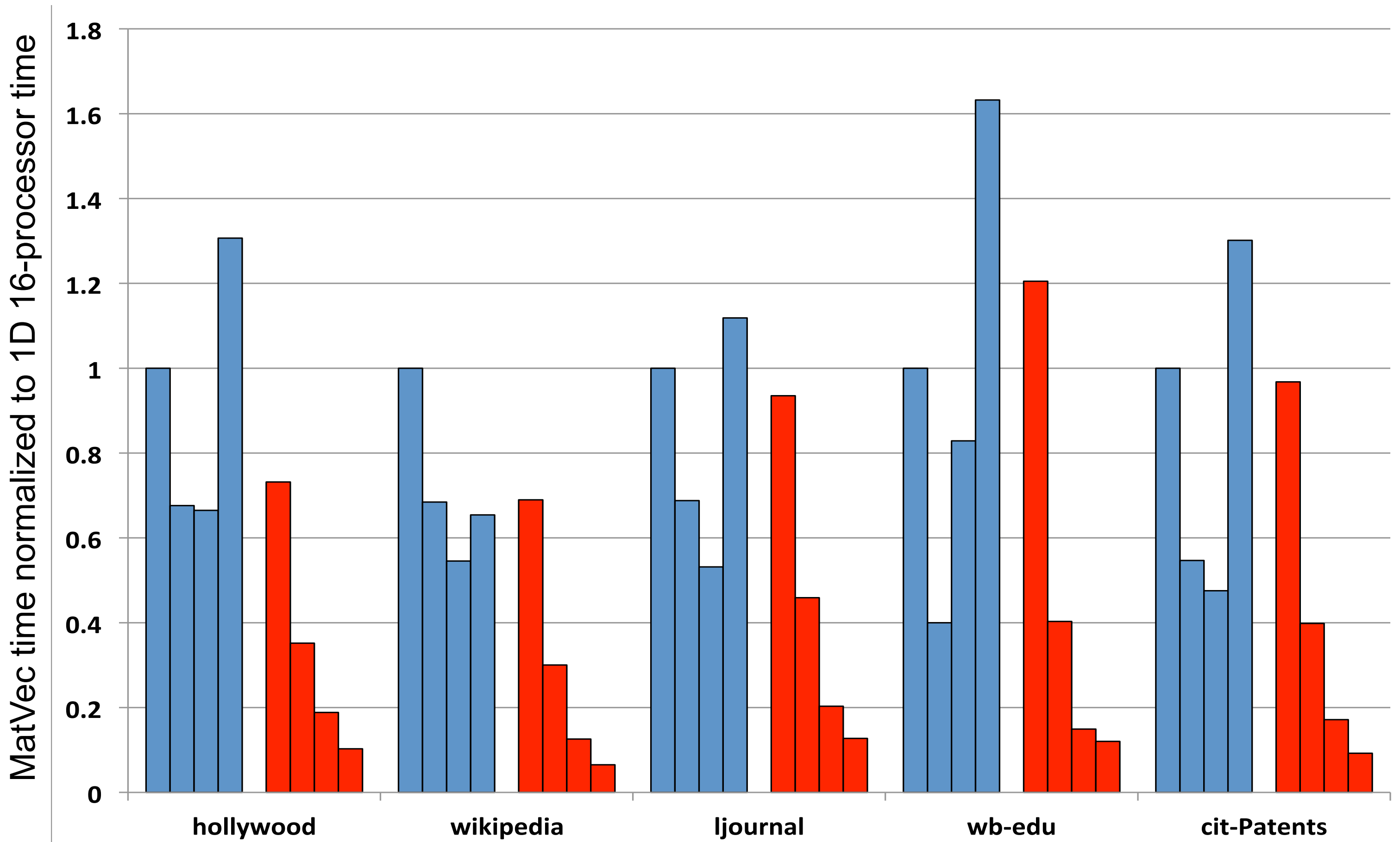
1D vs 2D Strong Scaling experiments

For each matrix:

Blue = Trilinos 1D Matrix Distribution on 16, 64, 256, 1024 processors (left to right)

Red = Trilinos 2D Matrix Distribution on 16, 64, 256, 1024 processors (left to right)

Times are normalized to the 1D 16-processor runtime for each matrix.



Randomization

- On input, randomly permute matrix rows/columns
  - Eliminates any inherent structure in input file (e.g., high degree nodes first)
  - Gives better balance in number of nonzeros per processor for 1D and 2D
  - But can drastically increase communication volume

liveJournal matrix (4M rows; 73M nonzeros) on 1024 processes				
Method	Imbalance in nonzeros (Max/Avg per proc)	Max # Messages per SpMV	Comm. Vol. per SpMV (doubles)	100 SpMV time (secs)
1D-Block	12.8	1023	34.5M	2.14
1D-Random	1.3	1023	55.3M	1.52
2D-Block	11.4	62	43.4M	0.95
2D-Random	1.0	62	64.2M	0.43

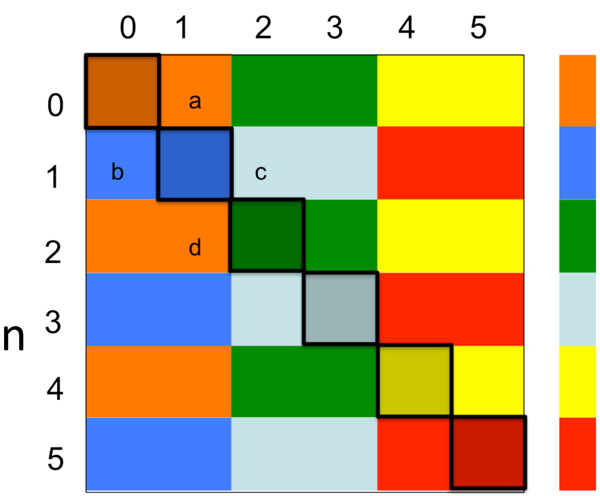
Advanced 2D Partitioning Methods

The Cartesian 2D block distributions are simple to compute but ignore the structure of the graph. Can we do better?

- Coarse-grain hypergraph (Catalyurek & Aykanat '01)
  - Cartesian product, but expensive to compute
  - Requires multiconstraint hypergraph partitioning
- Fine-grain hypergraph (Catalurek & Aykanat '01)
  - Assign each nonzero separately, not Cartesian
  - Much larger hypergraph, impractical for big problems
- Mondriaan (Vastenhouw & Bisseling '05)
  - Recursive hypergraph partitioning
  - Only serial software available

New idea: Graph Partitioning + 2D

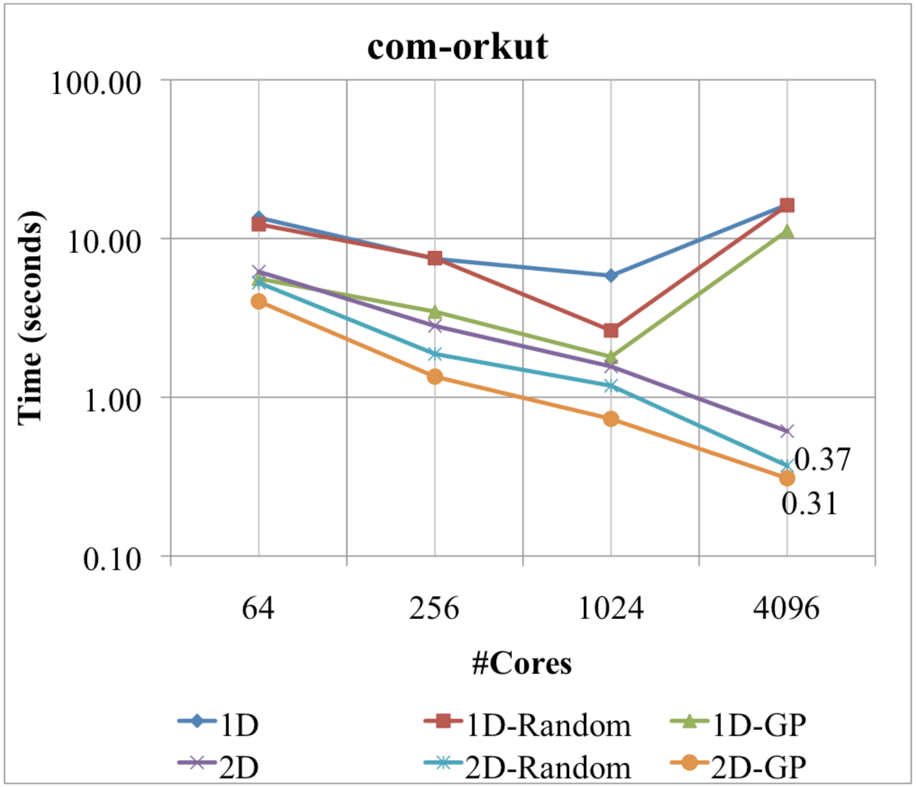
- Cartesian 2D block distributions limit #messages but ignore structure of the graph.
- (Hyper)Graph partitioning (e.g., Zoltan, ParMETIS, Scotch) balances work (nonzeros per process) while attempting to minimize total communication volume.
  - Thought to be ineffective on scale-free graphs
- Our idea: Apply (hyper)graph partitioning and 2D distribution together
  - Compute vertex-based partition of graph using ParMETIS or Zoltan
  - Apply 2D distribution to a logical permutation based on the (hyper)graph partition
- Advantages:
  - Balance the number of nonzeros per process
  - Exploit structure in the graph to reduce communication volume
  - Reduce the number of messages via 2D distribution



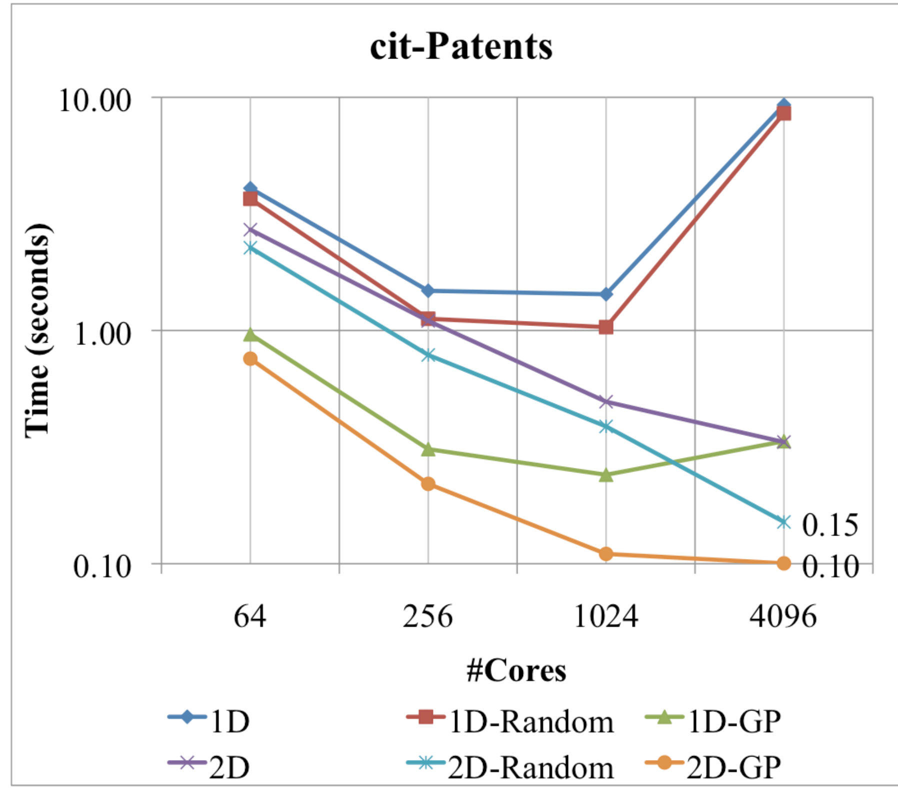
2D-GP: Graph partitioning with 2D Distribution

liveJournal matrix (4M rows; 73M nonzeros) on 1024 processes				
Method	Imbalance in nonzeros (Max/Avg per proc)	Max # Messages per SpMV	Comm. Vol. per SpMV (doubles)	100 SpMV time (secs)
1D-Block	12.8	1023	34.5M	2.14
1D-Random	1.3	1023	55.3M	1.52
1D-GP	1.2	1011	18.9M	0.53
2D-Block	11.4	62	43.4M	0.95
2D-Random	1.0	62	64.2M	0.43
2D-GP	1.4	62	22.4M	0.22

Strong scaling



Orkut social network
3.1M rows; 237M nonzeros
Max nonzeros/row = 33K

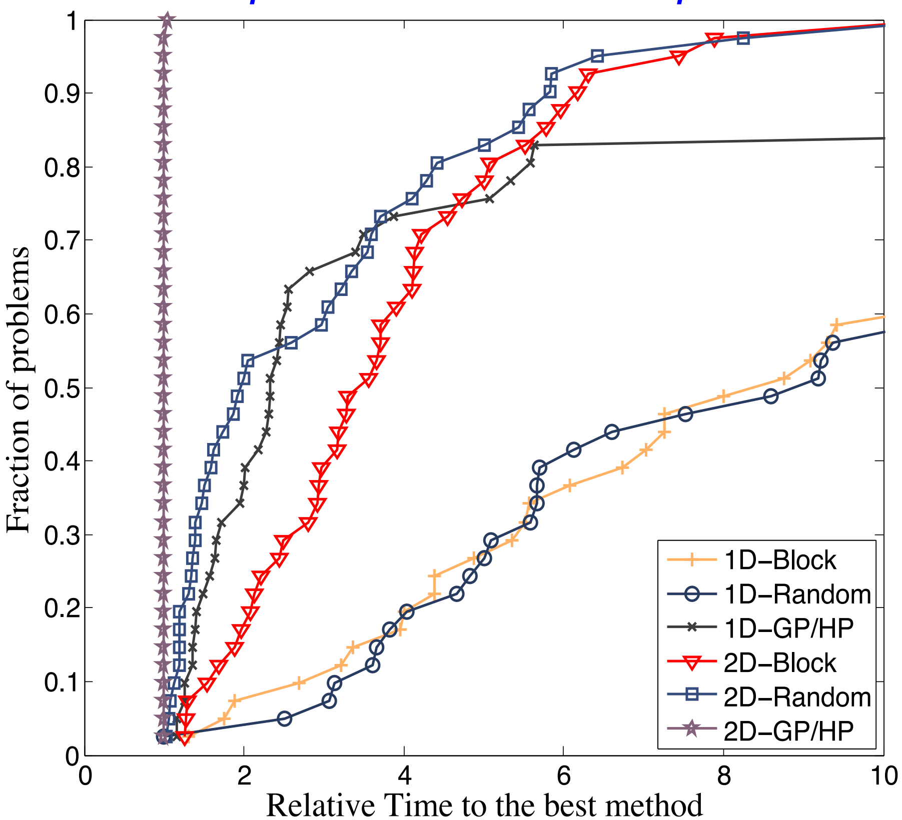


Patent citations network
3.8M rows; 37M nonzeros
Max nonzeros/row = 1K

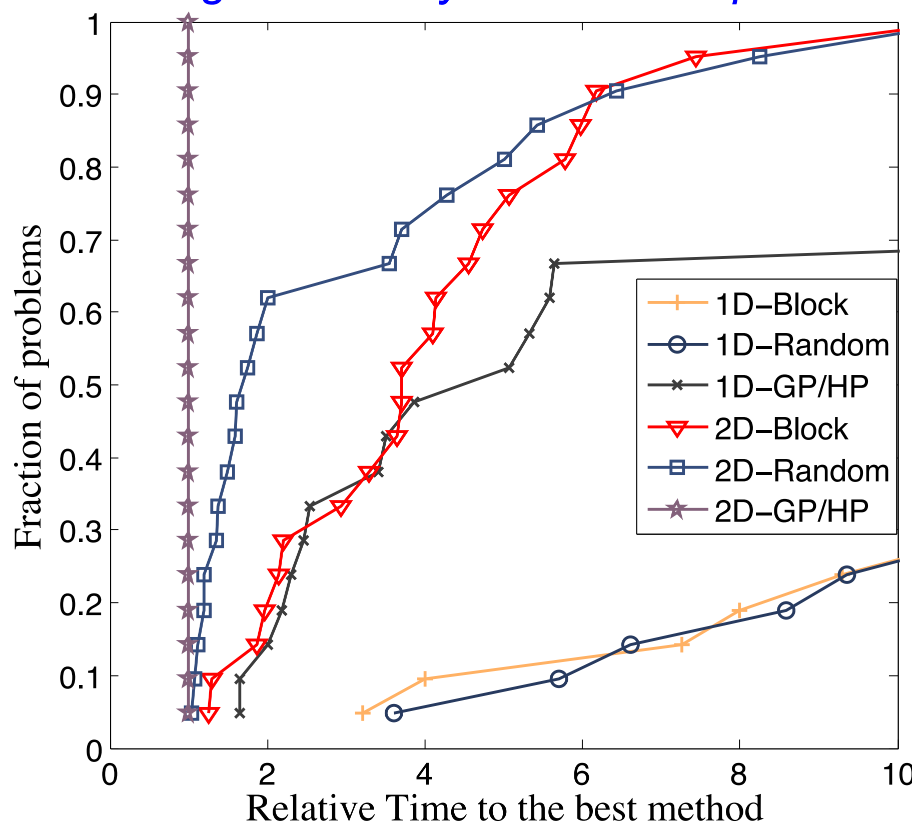
Performance comparisons

- 10 matrices: 1.1M - 67.5M rows; 36M-1.6B nonzeros
- 2D-GP/HP best in all but one experiment
- Benefit even greater for large numbers of processes

All experiments: 64-4096 procs

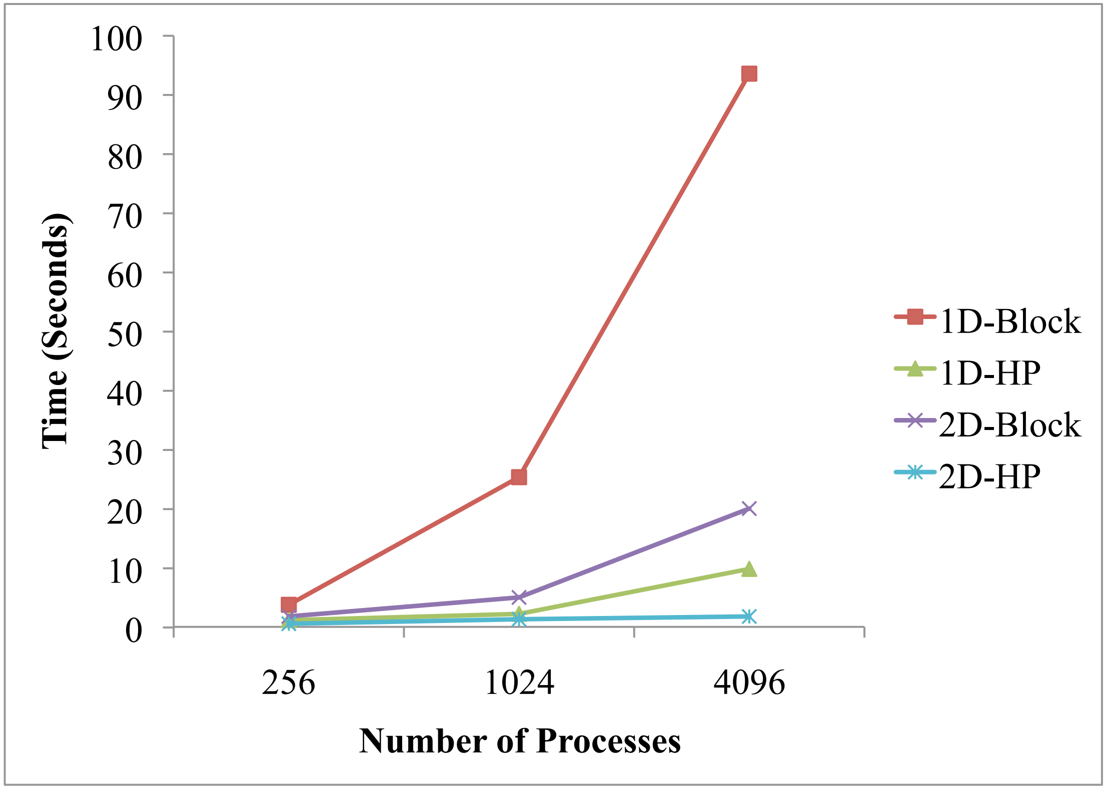


Large runs only: 1024-4096 procs



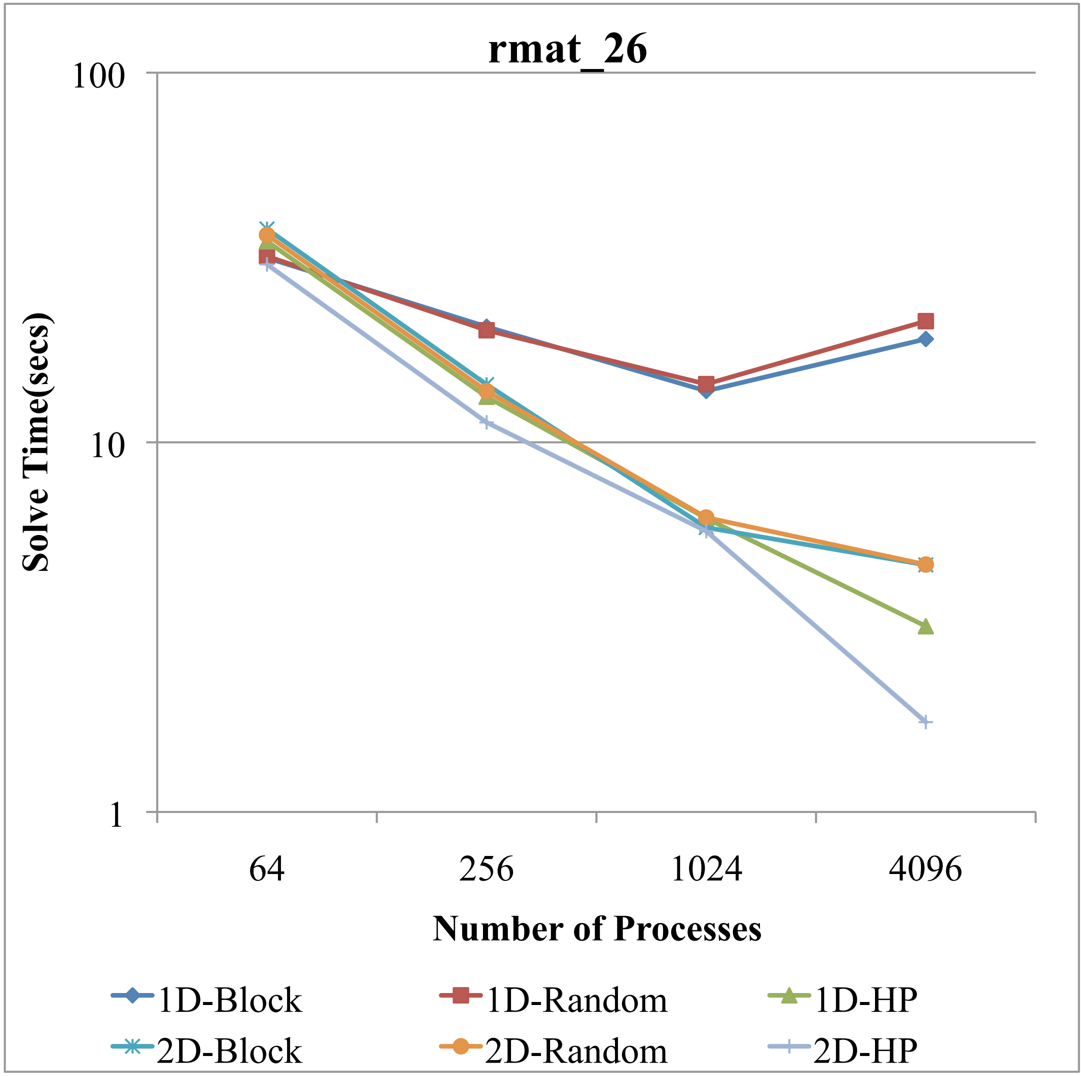
Weak Scaling

- R-MAT matrices (Chakrabarti et al., 2004) with Graph-500 parameters (a=0.57; b=c=0.19; d=0.05)
  - rmat_22 on 256 procs
    - 4.2M vertices
    - 38M edges
  - rmat_24 on 1024 procs
    - 16.8M vertices
    - 151M edges
  - rmat_26 on 4096 procs
    - 67.1M vertices
    - 604M edges
- 2D-HP maintains best weak scaling.



Eigensolver Experiments

- Anasazi Toolkit in Trilinos
  - Baker, Hetmaniuk, Lehoucq, Thornquist; ACM TOMS 2009
  - Block-based eigensolvers: Solve AX = XΛ or AX = BXΛ
- Experiment:
  - Find 10 largest eigenvalues of Laplacian using Block Krylov-Schur (BKS) solver
  - rmat_26 matrix: 67.1M rows; 604M nonzeros
  - HP = Hypergraph partitioning in Zoltan



Conclusions

- 2D distribution has clear benefit for scale-free graphs, especially at high process counts.
  - Reduces max number of messages per process
- Randomization can be effective to restore load balance.
  - But can increase communication volume
- (Hyper)graph partitioning can maintain load balance while keeping communication volume low.
  - More effective for scale-free graphs than thought
- Combining 2D distribution with (hyper)graph partitioning gives best results.
  - Low number of messages, low communication volume, low imbalance
  - Allows reuse of existing partitioning software

Extra Slides

Distributions for Anasazi

- Matrix-vector multiplication an important kernel
  - 55-87% of solve time for hollywood-2009 matrix with block 2D distribution on 64-4096 processes
- Other operations contribute to solve time
  - Remaining time primarily in orthogonalization
  - Balance with respect to vector entries, not matrix entries
- Benefit in balancing BOTH matrix nonzeros and vector entries
  - Randomization can achieve this balance, but increases communication volume drastically.
  - Multiconstraint graph partitioning can be used to achieve balance while keeping communication volume low.
    - Two weights per vertex: [1, number of nonzeros per row]
    - Find one partition that balances both weights.

Example: Eigensolve with multiconstraint graph partitioning

Find 10 largest eigenvalues of hollywood-2009 matrix (1.1M rows; 114M nz) using Anasazi's BKS (0.001 tolerance) on 1024 processes					
Method	Nonzero Imbalance (max/avg)	Vector imbalance (max/avg)	Total Comm Volume for one SpMV (doubles)	SpMV time (secs)	Total Solve time (secs)
2D-Block	26.0	1.0	15.7M	0.93	1.15
2D-Random	1.1	1.0	35.6M	0.44	0.62
2D-GP	1.6	30.3	17.2M	0.33	0.96
2D-GP-MC Multiconstraint	1.6	1.1	17.5M	0.27	0.44

Scaling in Anasazi

- Use Anasazi's Block Krylov Schur method to find ten largest eigenvalues of the normalized Laplacian matrix (tol=0.001)