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Using 2D Matrix Distributions in Trilinos

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U.S. DEPARTMENT OF ENERGY
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Motivation

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- Default row-based distribution in Trilinos is satisfactory for many scientific applications.
  - Nice, regular matrix structure.
  - Roughly equal number of nonzeros per row.
  - Data dependencies localized by finite difference stencil, finite element support, particle field radius, etc.
- Matrix structure for many graph applications is not so “nice.”
  - Scale-free graphs: web graphs, social networks, etc.
  - Power-law degree distribution in graphs leads to large variation in number of nonzeros per row (load imbalance)
  - No locality in data dependencies (high communication costs)
  - Row-based distributions can lead to All-to-All communication patterns.
    - Max. number of messages per process is 80-100% of number of processors.

1D and 2D Matrix distributions

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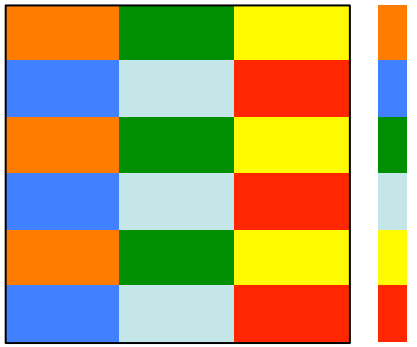
- 1D matrix distribution:
  - Entire rows (or columns) of matrix assigned to a processor
  - Same mapping used for vectors
  - Epetra's default distribution
- 2D Cartesian matrix distribution:
  - Block-based layout of matrix within processors
  - In effect, partitioning the nonzeros of the matrix (i.e., the edges of the graph).
  - Long used in parallel direct solvers
  - 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

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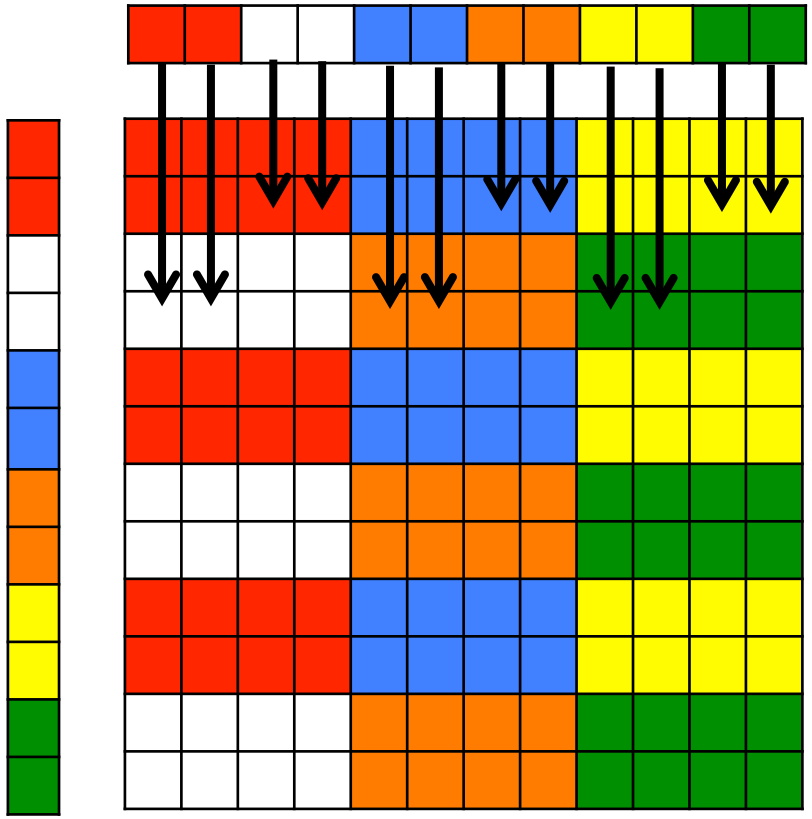
- During matrix-vector multiplication, communication occurs only along rows or columns of processors.
  - Expand (vertical): Vector entries x_j sent to column processors to compute local product $y^p = A^p x$
  - Fold (horizontal): Local products y^p summed along row processors; $y = \sum y^p$
- In 1D,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



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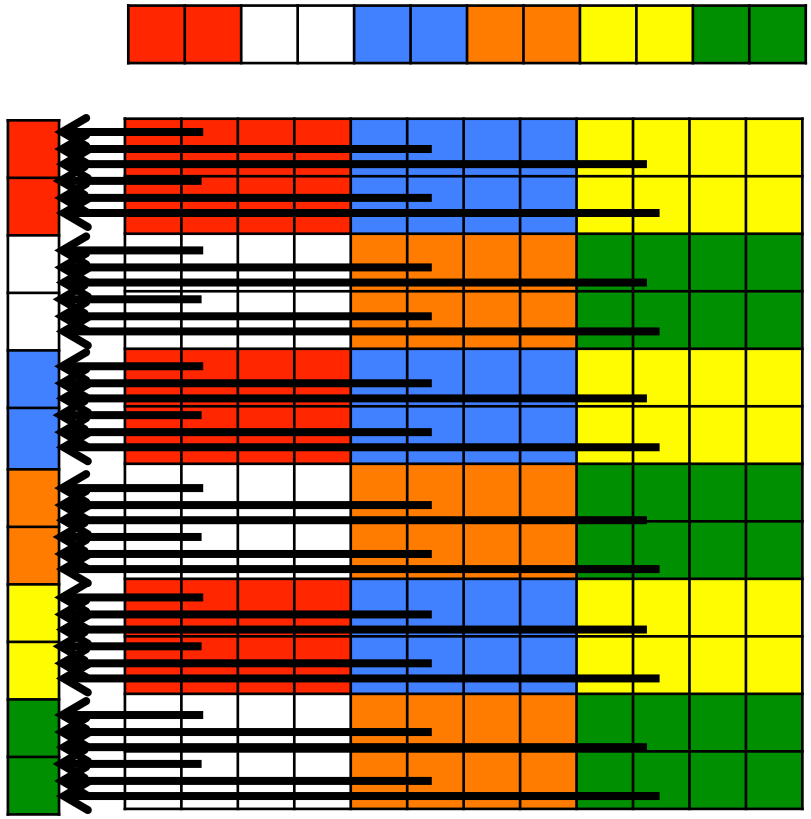

Epetra Maps Support 2D Distributions

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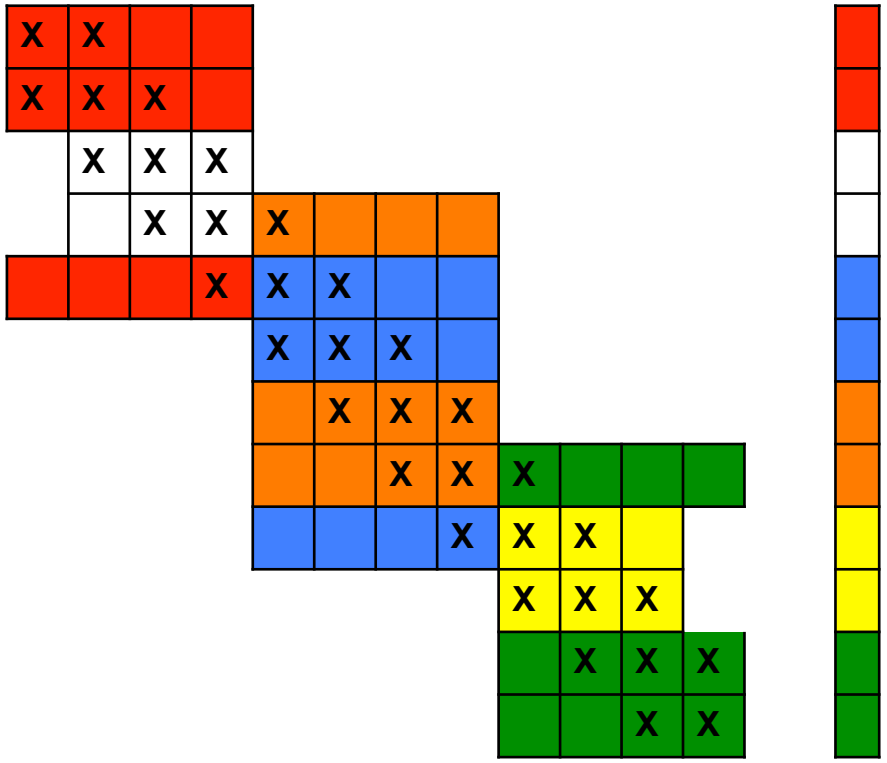
- In Petra Object Model, maps describe the distribution of global IDs to processors.
  - Row & column maps for matrix
  - Range & domain maps for vector
- Expand done by matrix's Importer; Fold done by matrix's Exporter.
- Important to keep the row map sparse during matrix construction
  - Memory for dense row maps doesn't scale; 2D layout has N/sqrt(P) rows per processor.
  - For locally empty rows, dense row maps still communicate zero-valued entries in fold.
- Let Epetra compute the Column map in FillComplete.
  - Similar reasons as above.

Rank 2 (Blue)
Row Map = {4, 5, 8}
Column Map = {4, 5, 6, 7}
Range/Domain Map = {4, 5}



Example: Common Parallel Distributions for Scale-Free Graphs

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- Randomization can restore load balance for 1D and 2D distributions.
- 2D distributions have fewer messages per processor, making them faster than 1D (despite higher 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

New idea: Graph Partitioning + 2D

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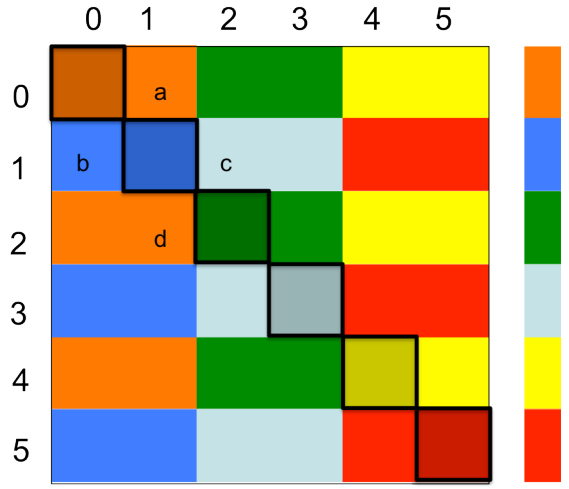
- 2D Cartesian block-based layouts ignore structure of the graph.
- (Hyper)Graph partitioning (e.g., Zoltan, ParMETIS, Scotch) balances work (nonzeros per process) while attempting to minimize total communication volume.
  - Doesn't significantly reduce the number of messages.
- Idea: Apply (hyper)graph partitioning and 2D distribution together
  - Compute row-based partition of matrix 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



"Scalable Matrix Computations on Large Scale-Free Graphs using 2D Graph Partitioning."
E. Boman, K. Devine, S. Rajamanickam. To appear, Proceedings of SC13

2D-GP: Graph partitioning with 2D Distribution

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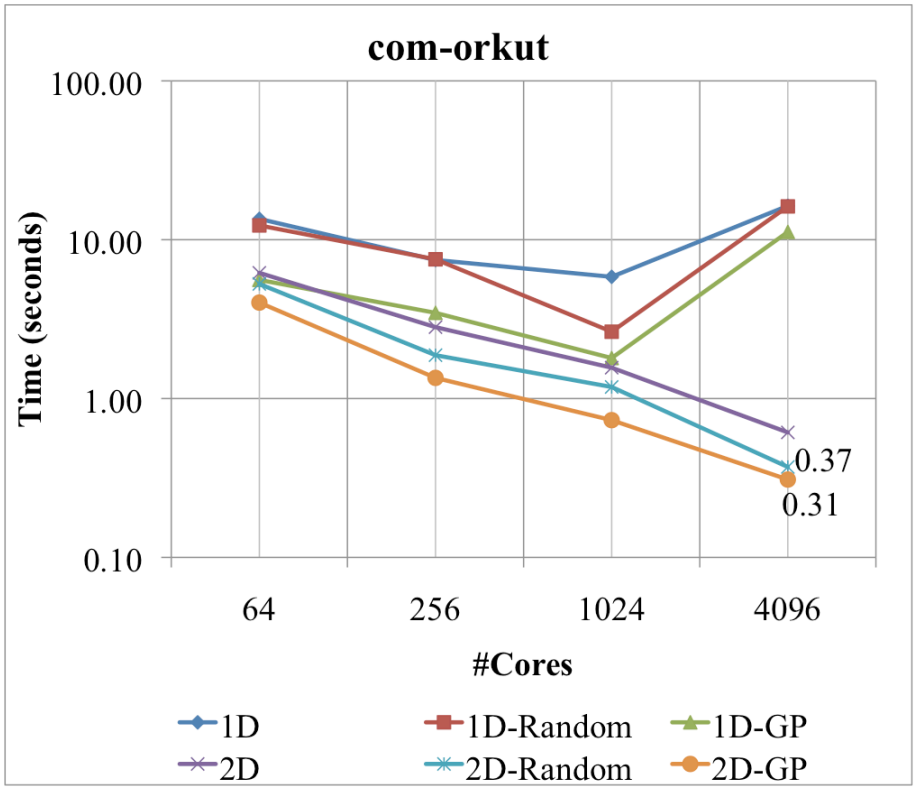
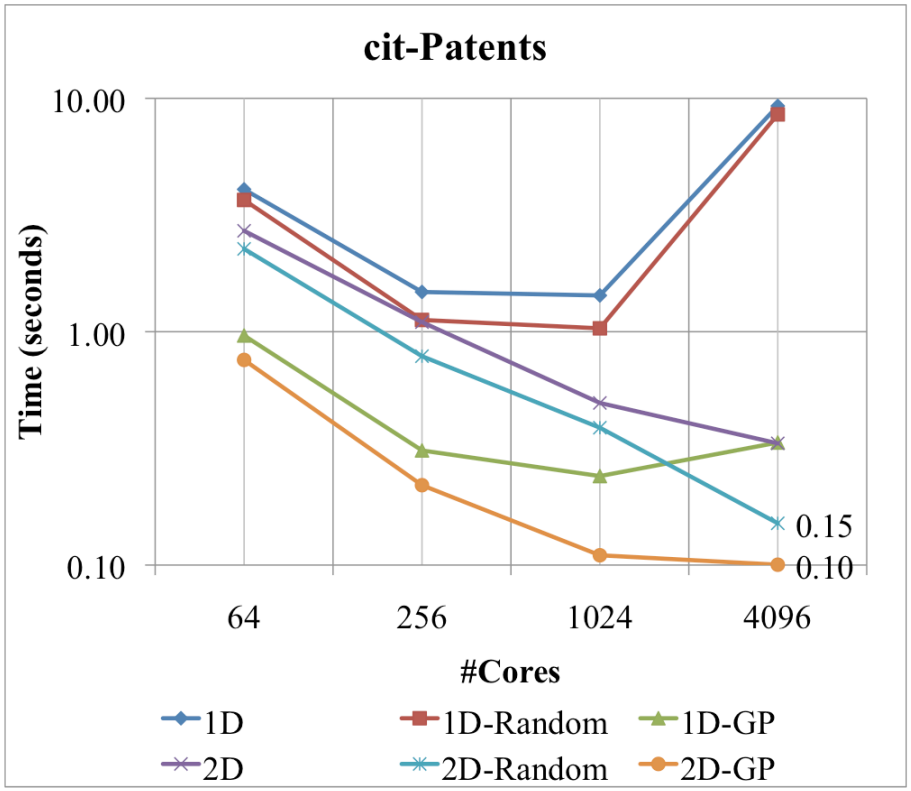
liveJournal matrix (4M rows; 73M nonzeros) on 1024 processes				
Method	Imbalance in nonzeros (Max/Avg per proc)	Max # Messages per SpMV	Comm. Vol. per SpMV (doubles)	100 SpMV time (secs)
1D-Block	12.8	1023	34.5M	2.14
1D-Random	1.3	1023	55.3M	1.52
1D-GP	1.2	1011	18.9M	0.53
2D-Block	11.4	62	43.4M	0.95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

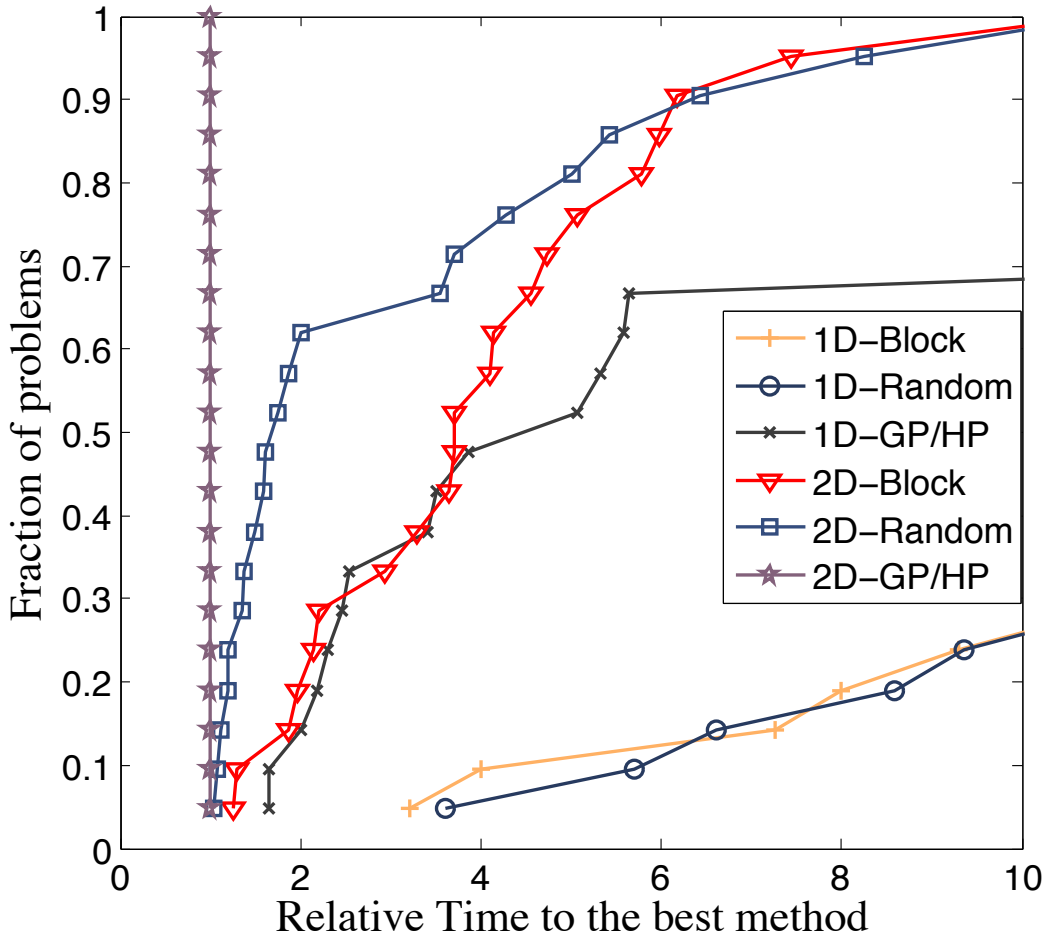


Patent citations network
3.8M rows; 37M nonzeros
Max nonzeros/row = 1K

Performance comparison

- 10 scale-free graphs from SNAP and UF matrix collections:
  1.1M - 67.5M rows;
  36M-1.6B nonzeros
- 1024-4096 processes

- 2D layout has clear benefits.
  - Reduces max number of messages per process
- 2D-GP/HP gives best results.
  - Low number of messages, low communication volume, low imbalance



Conclusions

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- 2D distribution has definite benefit, 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

Questions for the audience

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- Will 2D distributions work as seamlessly in TPetra?
- How does one efficiently redistribute matrices into 2D distributions?
- Which preconditioners work for 2D distributions?
- How does one precondition matrices from scale-free graphs?
  - Boman and Deweese have some ideas.
- Does Trilinos' development path extend beyond scientific applications and into data-centric applications?
  - How do we get it done? Staffing? Funding?