SAND2015-2983C

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Distributing Linear Systems for Parallel Computation

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Sandia National Laboratories

AWM Research Symposium, April 2015

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

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Leveraging investments in computing

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- Decades of research in parallel, high-performance computing for scientific applications in the national laboratories
  - Driven by stockpile stewardship mission: ensure reliability and safety of nuclear weapons without nuclear testing
- Large investments in infrastructure and people
  - Hardware design, purchases, operations
  - Operating systems, file systems, runtime systems
  - Libraries of linear/nonlinear/eigensolvers, optimization algorithms, uncertainty quantification methods, partitioners
- Relatively straightforward transfer to other PDE-based applications
  - Climate simulation, reactor design and safety, carbon sequestration, nanotechnology, etc.
- New exciting research areas: e.g., "big data" analysis, cybersecurity
- Can we leverage our scientific computing investment to address broader range of application areas?

Case study:
Partitioning for Parallel Computing

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- First step in parallel computing: distributing work among the processors
- Partitioning: Divide work so that total execution time is minimized
  - Constraint: Processors have equal amounts of work
    - Processors are not waiting for other processors to finish computation
  - Objective: Interprocessor communication (data movement) is minimized
- Note: this definition differs from that often used in graph-analysis
  - Here, think "load balancing," not "clustering"
- Use matrix distribution for matrix-vector multiplication as model problem
  - Key kernel of many scientific applications (e.g., finite element analysis)
  - Important in graph analysis (e.g., spectral analysis using extreme eigenpairs)
  - Distribute matrix and vector to minimize matrix-vector multiplication time

Partitioning software

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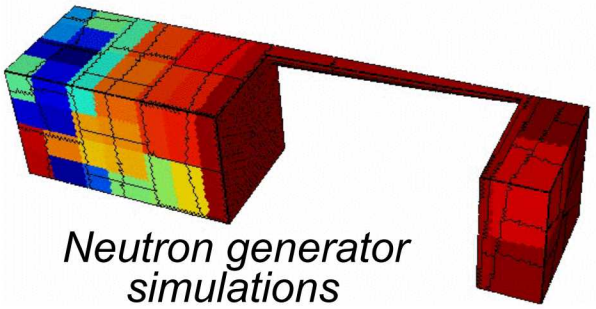
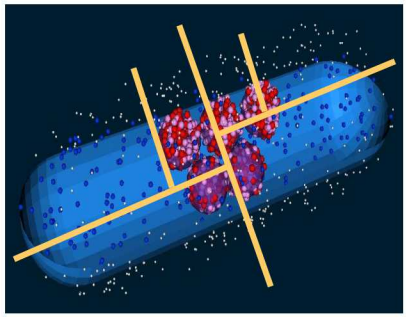
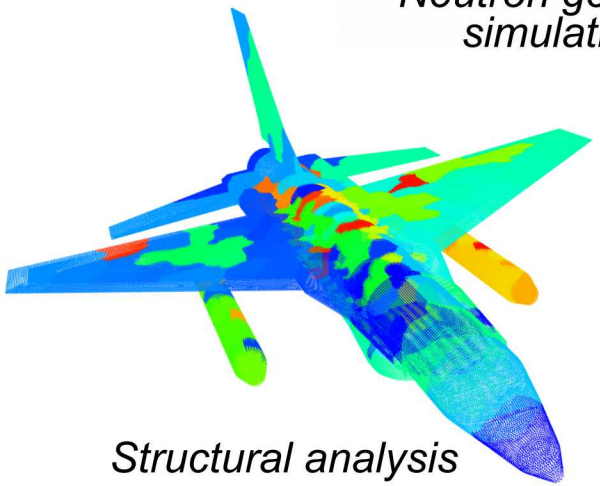
- Many high quality parallel partitioning tools developed for physics-based applications
  - Zoltan toolkit of geometric, graph & hypergraph partitioners (Sandia)
  - ParMETIS (U. Minnesota) & PT-Scotch (U. Bordeaux) graph partitioners



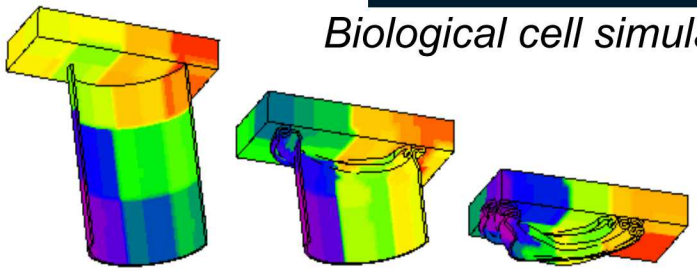
Neutron generator simulations



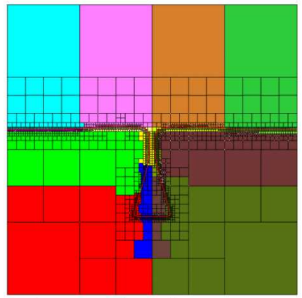
Biological cell simulations



Structural analysis



Contact detection in crash simulations



Chemical vapor deposition

Typical matrix partition

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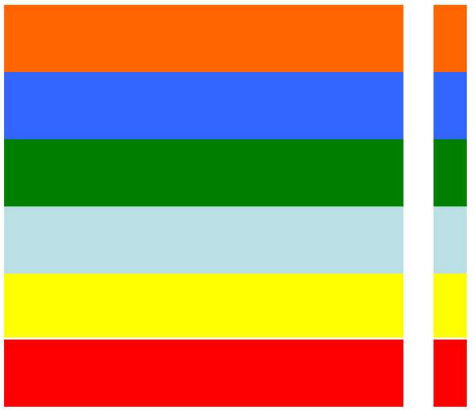
- 1D Distribution:
  - Entire row (or column) of matrix assigned to a single processor
  - Vector uses same distribution
  - During SpMV, processor receives (via communication) vector entries needed to match non-zeros in owned rows.



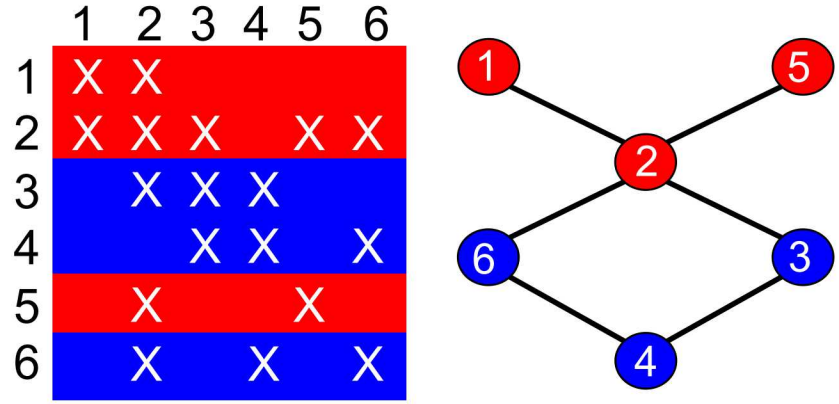
1D row-wise matrix distribution; 6 processes

- 1D-Block distribution of *N* x *N* matrix onto *p* processors:
  - First *N/p* rows given to processor 0
  - Next *N/p* rows given to processor 1
  - And so on…
  - Default in many parallel linear algebra libraries (e.g., Trilinos)

Graph partitioning: 1D-GP

(Kernighan, Lin, Schweikert, Fiduccia, Mattheyes, Simon, Hendrickson, Leland, Kumar, Karypis, et al.)

- Explicitly attempts to minimize communication costs induced by partition
- Represent matrix *A* as a graph:
  - One vertex *j* per row a_j
  - Edge (*i, j*) exists iff $a_{ij} \neq 0$
  - Vertex weights = # nonzeros in row



- Goal: Assign equal vertex weight to parts while minimizing weight of edges between parts (i.e., cut by part boundary)
- Highly effective for mesh-based PDE problems
  - Mostly local connectivity (e.g., local support for basis functions)
  - Regular structure (e.g., dual graph of mesh)

Example: Finite element matrix

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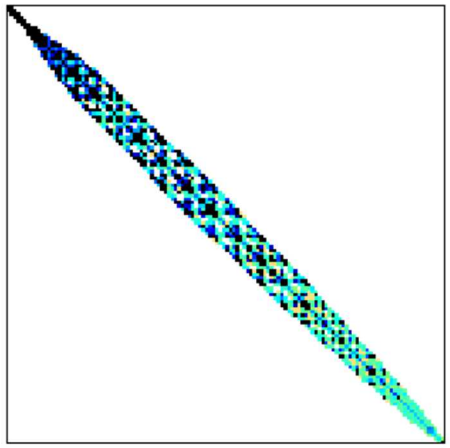
- Structural problem discretizing a gas reservoir with tetrahedral finite elements
- Platform: SNL Redsky cluster
  - 2.93 GHz dual socket/quad core Nehalem X5570 procs
  - 3D torus InfiniBand network
- Graph partition gives 25% reduction in SpMV time relative to 1D-Block
  - Improves load balance
  - Reduces communication volume



Serena matrix
Janna & Ferronato
U.Florida Sparse Matrix Collection

Serena: 1.4M rows; 65M nonzeros; Max 249 nz/row; Avg 46 nz/row 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	1.2	55	4.4M	0.20
1D-Random	1.0	1023	62.1M	13.62
1D-GP	1.1	98	1.1M	0.15

CounterExample: Social network matrix

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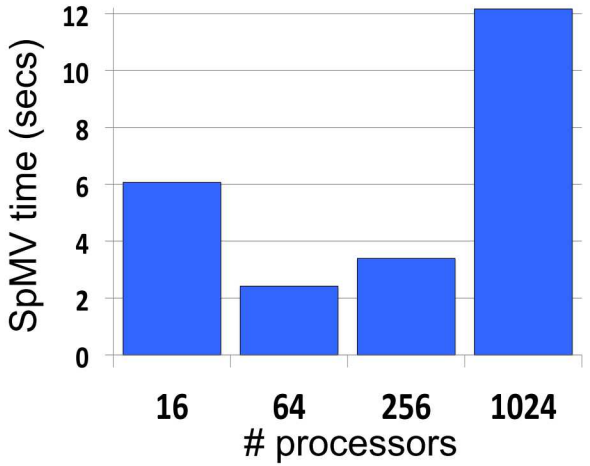
- Social networks, web graphs, etc., have very different structure from PDE discretizations
  - Power-law degree distributions; scale-free properties
- Graph partitioning can reduce SpMV time
  - Reduces imbalance and communication volume
- But large number of messages hurts scaling
  - Nearly all-to-all communication



Strong scaling of 1D-GP for com-liveJournal matrix
Yang & Leskovec
Stanford SNAP collection

com-liveJournal: 4M rows; 73M nonzeros; Max 15K nz/row; Avg 18 nz/row 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	14.72
1D-Random	1.3	1023	66.3M	14.00
1D-GP	1.2	1011	18.9M	12.17

Goal: Reduce number of messages

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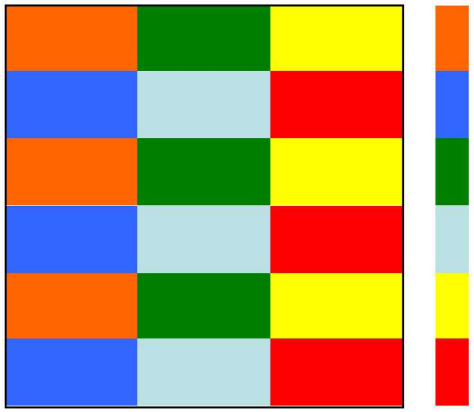
- 1D distribution:
  - Entire rows (or columns) of matrix assigned to a processor
- 2D distribution:
  - Cartesian methods: Each process owns intersection of some rows & columns
  - Processes are *logically* arranged in a 2D grid
  - Limits max #messages per process to *O(sqrt(#processors))*
  - Long used in parallel dense solvers (ScaLapack)
  - Beneficial also for sparse matrices (Fox et al. '88, Lewis & van de Geijn '93, Hendrickson et al. '95)
  - 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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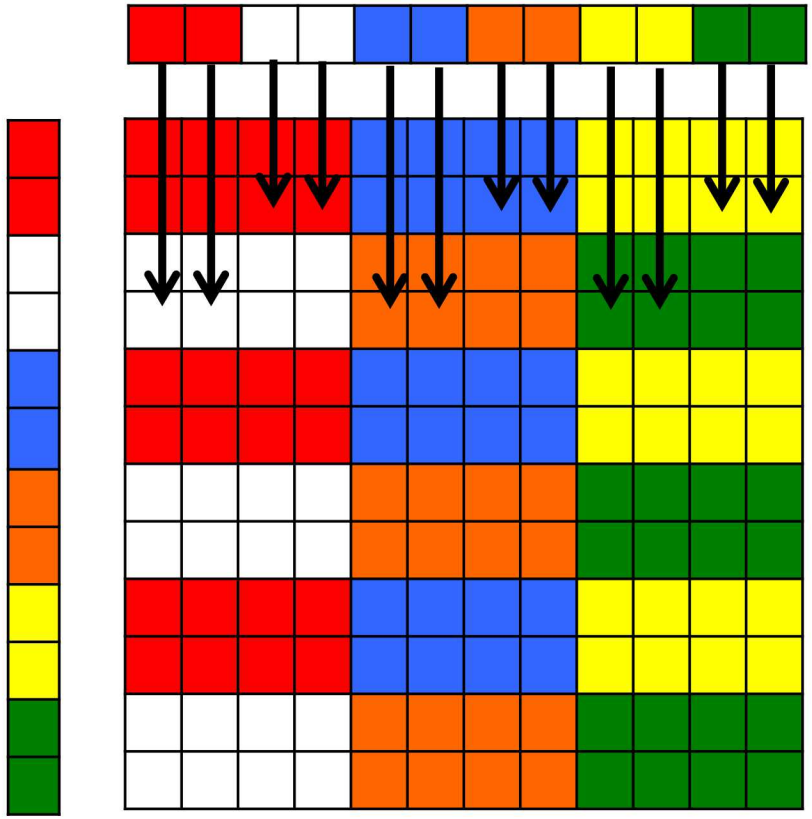
- During matrix-vector multiplication (y=Ax), communication occurs only along rows or columns of processors.
  - Expand (vertical): Vector entries x_j sent to column processors to compute local product $y^p = A^p x$
  - Fold (horizontal): Local products y^p summed along row processors; $y = \sum y^p$
- In 1D, fold is not needed, but expand may be all-to-all.



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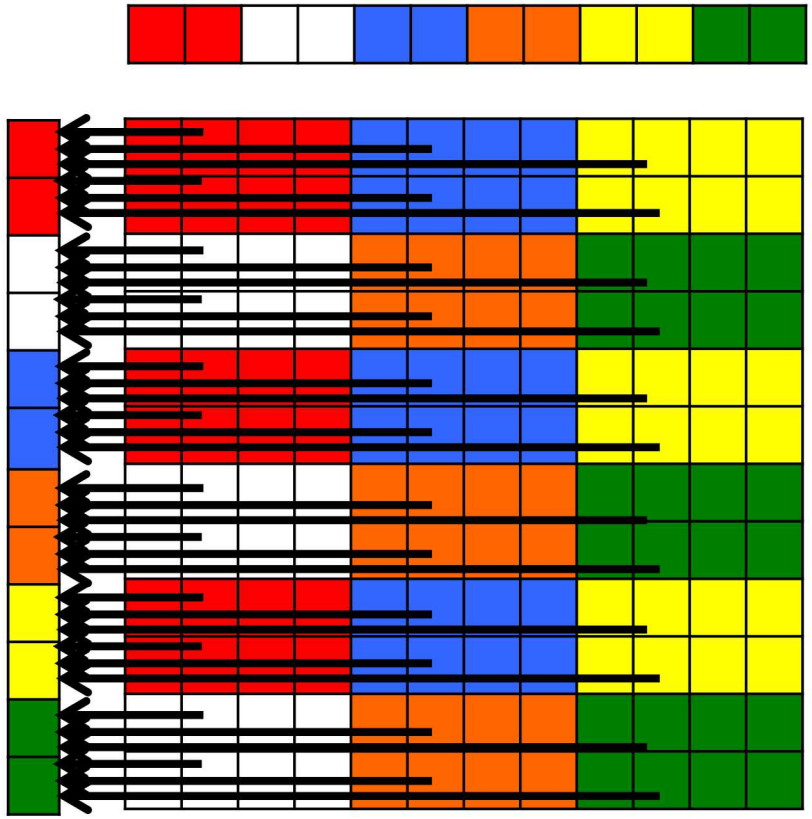

2D Partitioning of Social Network

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- Drastic reduction in max number of messages and SpMV time
  - Even with expand & fold, max number of messages is smaller
- Communication volume high with 2D partitions
  - Ignoring the non-zero structure of the matrix.
  - Can we exploit it as we did with 1D-GP?

liveJournal: 4M rows; 73M nonzeros; Max 15K nz/row; Avg 18 nz/row 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	14.72
1D-Random	1.3	1023	66.3M	14.00
1D-GP	1.2	1011	18.9M	12.17
2D-Block	11.4	62	43.4M	1.31
2D-Random	1.0	62	64.2M	0.97

New Method: 2D + Graph Partitioning

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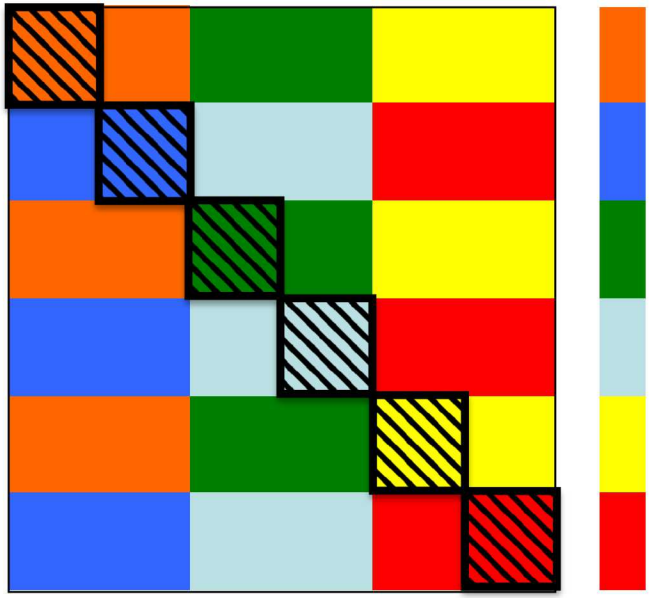
- Existing research into direct 2D partitioning of nonzeros (treat nonzeros as graph/hypergraph vertices)
  - Catalyurek & Aykanat; Vastenhouw & Bisseling
  - Much larger problem → very expensive
  - Only serial software available
- Our idea: Apply parallel graph partitioning and 2D distribution together
  - Compute 1D-GP row (vertex) partition of matrix (graph)
  - Apply 2D distribution to the resulting permuted matrix (graph)
- Advantages:
  - Balance the number of nonzeros per process,
  - Exploit structure in the graph to reduce communication volume, AND
  - Reduce the number of messages via 2D distribution
- Don't optimize a single objective but try do fairly well in all

2D Graph Partitioning (2D-GP)

- Partition rows (vertices) of original matrix (graph) into p parts
  - Using standard graph partitioner
- Implicitly, let $A_{perm} = PAP^T$
  - Where P is permutation from partitioning above
- Assign A_{perm} to processes using Cartesian block 2D layout

Due to partitioning, diagonal blocks of A_{perm} will be denser:



Results 1D vs 2D (Block, Random, GP)

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- With 2D-GP,
  - Low number of messages as with 2D-Block, 2D-Random
  - Reduced communication volume due to using structure of matrix
  - Reduced SpMV execution time

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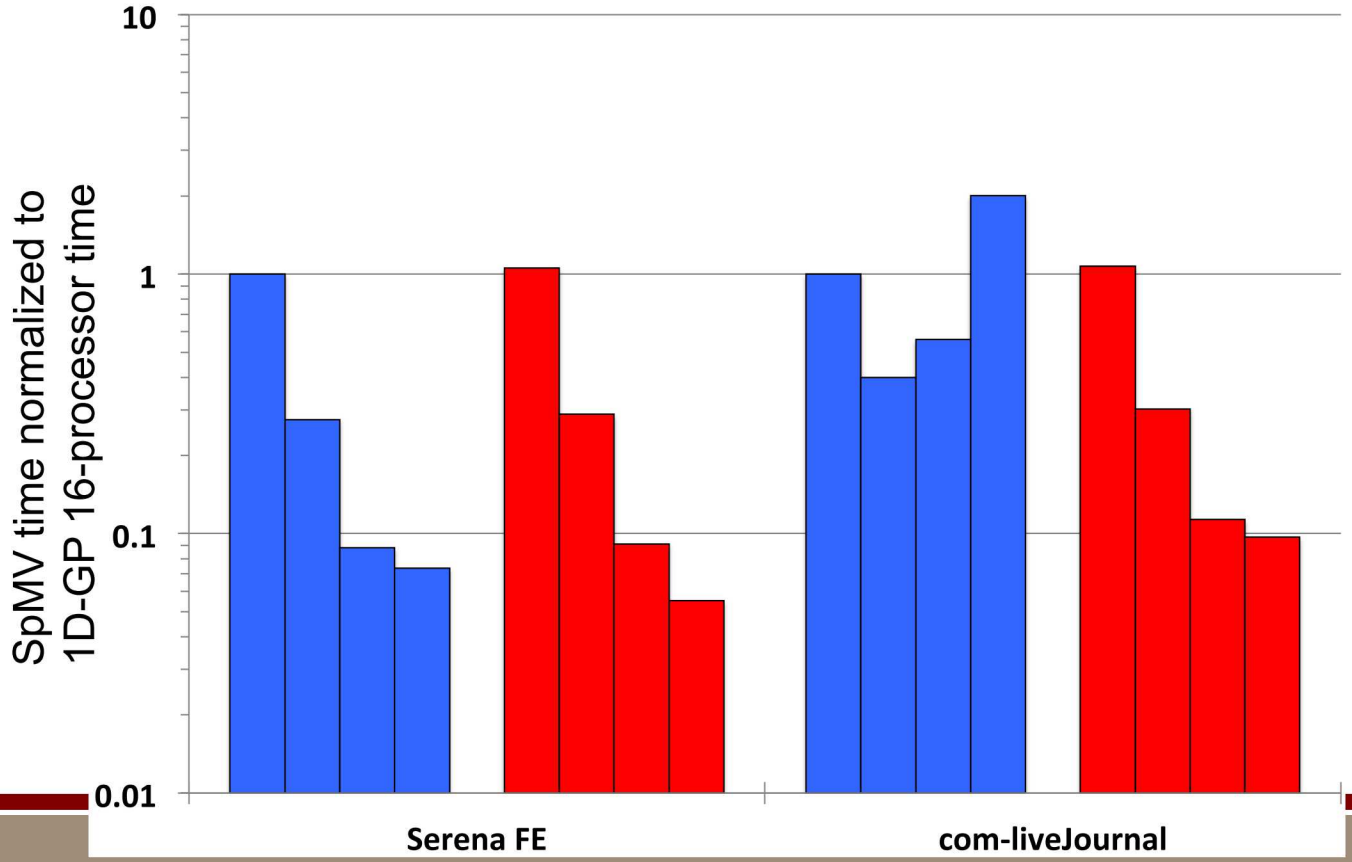
2D-Block	11.4	62	43.4M	1.31
2D-Random	1.0	62	64.2M	0.97
2D-GP	1.4	62	22.4M	0.59

Strong scaling: 1D-GP vs 2D-GP

- Performance for fixed problem as increase number of processors
- For each matrix:
  - **Blue = 1D-GP on 16, 64, 256, 1024 processors (left to right)**
  - **Red = 2D-GP on 16, 64, 256, 1024 processors (left to right)**
  - Times are normalized to the 1D-GP 16-processor runtime

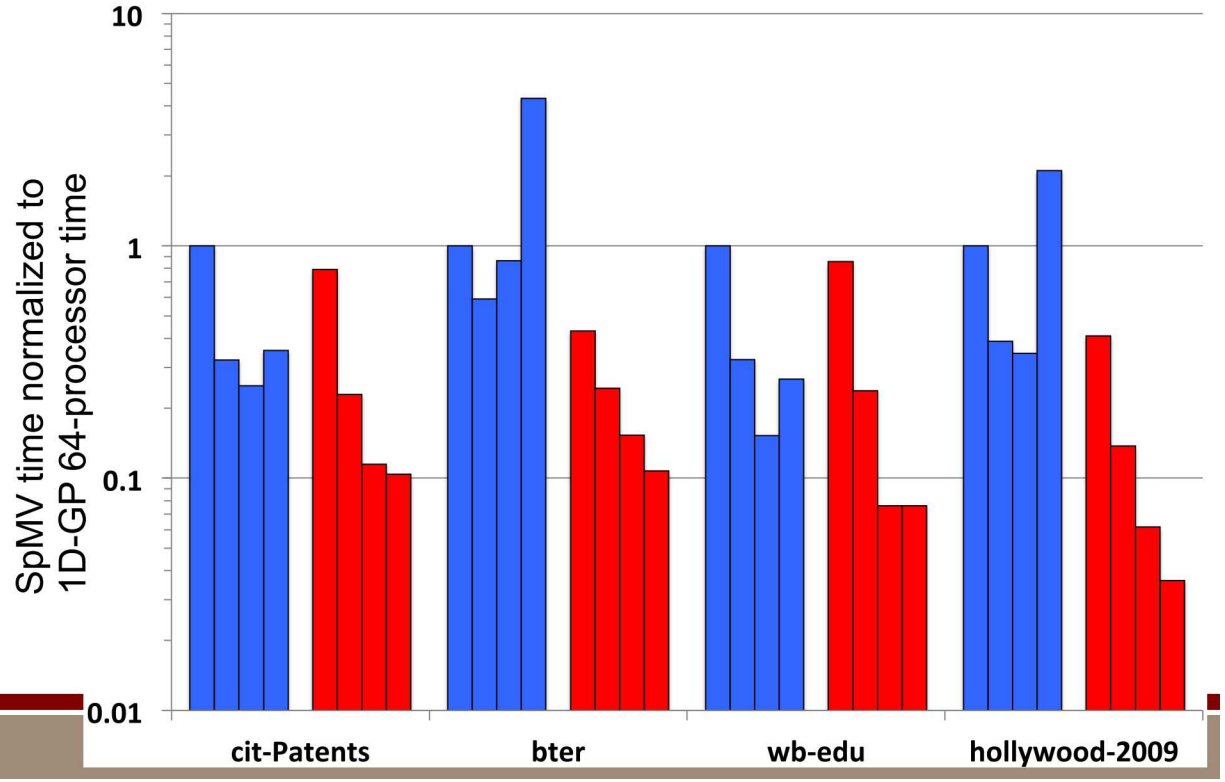


More 1D vs 2D experiments

Platform: cab cluster at LLNL (2.6GHz Intel Xeon E5 16-core nodes, Infiniband)

Name	Description	# Rows	# Nonzeros
cit-patents (UFL)	Citation network of US patents (Hall, Jaffe, Trajtenberg)	3.8M	33M
bter (generated)	Block Two-Level Erdös-Rényi (Seshadhri, Kolda, Pinar)	3.9M	63M
wb-edu (UFL)	Links between *.edu webpages (Gleich)	8.9M	88M
hollywood-2009 (UFL)	Hollywood movie actor network (Boldi, Rosa, Santini, Vigna)	1.1M	113M

- For each matrix:
  - Blue = 1D-GP on 64, 256, 1024, 4096 processors (left to right)
  - Red = 2D-GP on 64, 256, 1024, 4096 processors (left to right)
  - Times are normalized to the 1D-GP 64-processor runtime



Conclusions

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- Parallel distribution strategies depend on structure of data
  - Sparsity, regularity, dimensions of matrix are important
  - Demonstrated with Finite Element vs Social Network matrices
- Tools developed for PDEs can be applied *cleverly* in other application domains
  - Exploited partitioners and linear algebra libraries (developed for scientific computing) in network analysis scenario
  - Partitioners: Zoltan (SNL) and ParMETIS (U. Minnesota)
  - Matrix/Vector classes: Trilinos (SNL) using Map class to describe 1D and 2D distributions
- Challenging and exciting opportunities for cross-utilization of hardware, systems, algorithms and software

For more information…

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- "Scalable Matrix Computations on Large Scale-Free Graphs Using 2D Graph Partitioning."
  Erik Boman, Karen Devine, and Sivasankaran Rajamanickam
  Proc. of the International Conference on High Performance Computing, Networking, Storage and Analysis (SC13)

- Trilinos home page: http://trilinos.org
- Zoltan home page: http://www.cs.sandia.gov/Zoltan

- Email: kddevin@sandia.gov