Communication avoiding for sparse matrices and graphs

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Plan

Introduction

Sparse Matrix Matrix multiplication
- Lower bounds for matrices with random sparsity
- Communication optimal algorithms

Sparse Cholesky factorization for SPD matrices
- Combinatorial tools: undirected graphs, elimination trees
- Parallel Cholesky factorization
- Lower bounds for model problems

Graphs: All pairs shortest path

Plan

Lower bounds on communication for sparse LA

- More difficult than the dense case
  - For example computing the product of two (block) diagonal matrices involves no communication in parallel
- Lower bound on communication from dense linear algebra is loose
- Very few existing results:
  - Lower bounds for parallel multiplication of sparse random matrices [Ballard et al., 2013]
  - Lower bounds for Cholesky factorization of model problems [Grigori et al., 2010]

Plan

Introduction

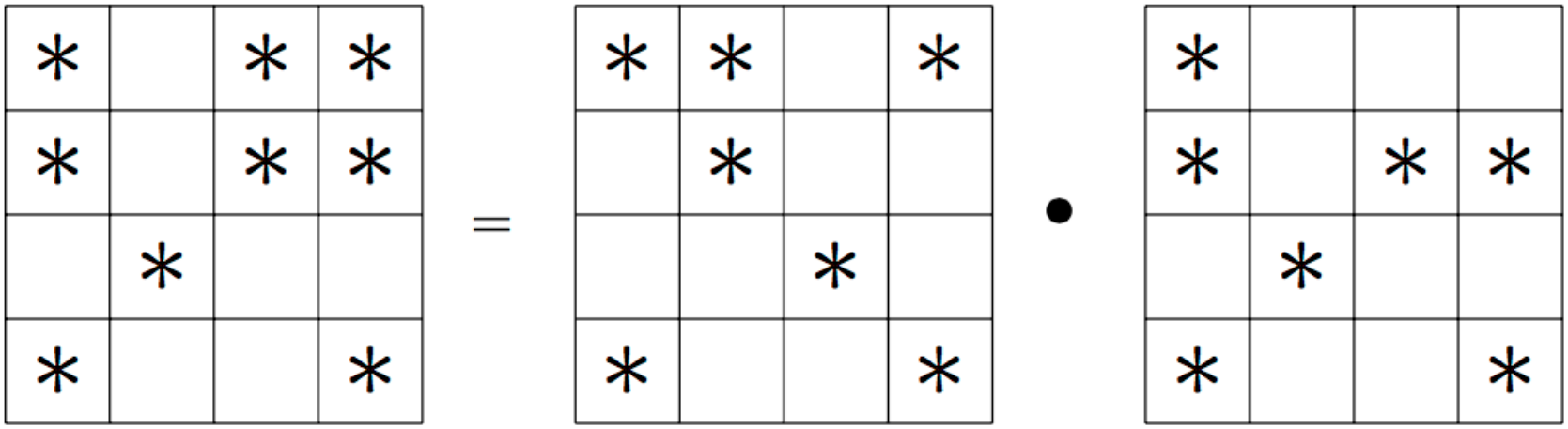
Sparse Matrix Matrix multiplication

- Lower bounds for matrices with random sparsity
- Communication optimal algorithms

Sparse Cholesky factorization for SPD matrices

Graphs: All pairs shortest path

Sparse matrix multiplication (SpGEMM)



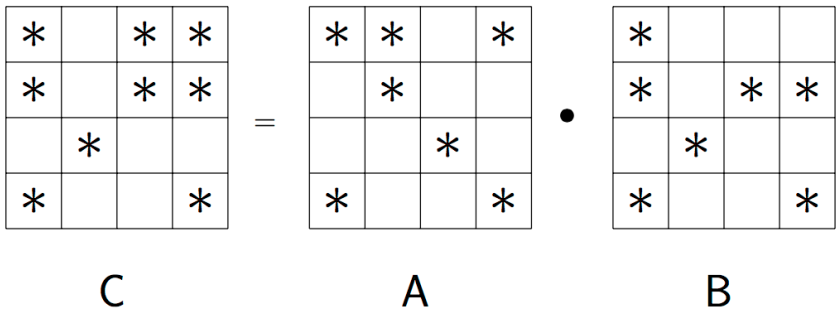
$$C_{ij} = \sum_k A_{ik} B_{kj}$$

Slides with help from G. Ballard, A. Buluc, O. Schwartz. Results from B. Lipshitz thesis

Sequential sparse matrix multiplication

- Column-wise formulation by Gustavson, implemented in Matlab.
- Input matrices of size $n \times n$, stored in compressed sparse column.
- Complexity: $O(flops(A \cdot B) + nnz + n)$, optimal when $flops(A \cdot B) > nnz + n$.

Input: A, B, C
for $j = 1$ to n **do**
  for k where $b_{k,j} \neq 0$ **do**
    $C(:, j) := C(:, j) + A(:, k) \cdot b_{kj}$
  end for
end for



Sparse Matrix Multiplication

- Consider matrices with random sparsity: the adjacency matrices of Erdős - Rényi(n,d) graphs - ER(n,d).
- Let A and B be $n \times n$ ER(n,d) matrices. We assume $d \ll n$. Then:
  - Each entry in A and B is nonzero with probability d/n.
  - The expected number of nonzeros in A and B is dn.
  - The expected number of scalar multiplications in AB is $(d^2/n^2) \cdot n^3 = d^2 n$.
  - The expected number of nonzeros in C is $d^2 n(1 - o(1))$.

Results:

- Lower bounds on communication, improved (higher) with respect to ones derived from dense linear algebra
- Optimal algorithms

Communication bounds for matrix multiplication

Given: A,B of size $n \times n$, local memory of size M, P processors, the lower bound on volume of communication for computing $A \cdot B$ on P processors is:

Dense Classic (cubic flops)

Memory dependent

$$\Omega\left(\frac{n^3}{M^{3/2}} \cdot \frac{M}{P}\right)$$

Memory independent

$$\Omega\left(\frac{n^2}{P^{2/3}}\right)$$

Erdős - Rényi(n,d)

Extension of lower bound for dense matrices to sparse matrices

$$\Omega\left(\frac{\#flops}{M^{3/2}} \cdot \frac{M}{P}\right) = \Omega\left(\frac{d^2 n}{P\sqrt{M}}\right) \leq \Omega\left(\sqrt{\frac{d^2 n}{P}}\right)$$

No algorithm attains this bound.

Communication bounds for Erdős - Rényi(n,d)

Extension of lower bound for dense matrices to sparse matrices

$$\Omega\left(\frac{\#flops}{M^{3/2}} \cdot \frac{M}{P}\right) = \Omega\left(\frac{d^2 n}{P\sqrt{M}}\right) \leq \Omega\left(\sqrt{\frac{d^2 n}{P}}\right)$$

No algorithm attains this bound.

New bound from [Ballard et al., 2013]

$$\Omega\left(\min\left(\frac{dn}{\sqrt{P}}, \frac{d^2 n}{P}\right)\right) = \Omega\left(\frac{dn}{\sqrt{P}} \min\left(1, \frac{d}{\sqrt{P}}\right)\right)$$

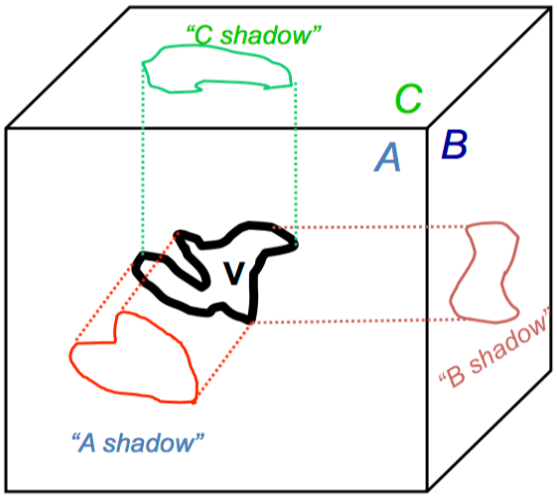
- With some assumptions. Which bound applies depends on ratio $d/\sqrt{P}$.
- Improvement factor of $\sqrt{M} \cdot \max\{1, \sqrt{P}/d\}$ with respect to previous bound
- Two algorithms attain this bound: recursive and 3D iterative.

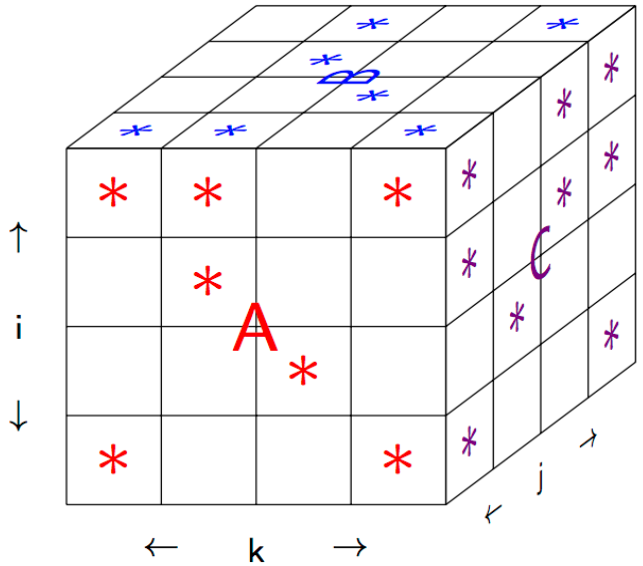
Geometric view of the computation

Computation cube for matrix multiply, with a specified subset of voxels:

- A face for each input/output matrix.
- Voxel (i, j, k) corresponds to the multiplication $a_{ik} \cdot b_{kj}$.
- Loomis & Whitney (1949): Volume of 3D set V satisfies:

$$V \leq (\text{area (A shadow)} \cdot \text{area(B shadow)} \cdot \text{area(C shadow)})^{1/2}$$





Source figure: G. Ballard

Communication bounds for Erdős-Rényi(n,d)

Assumptions:

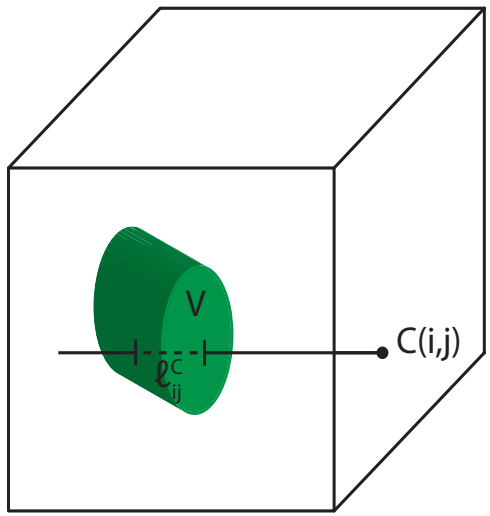
- Sparsity independent algorithms
- Input and output are sparse: $d \leq \sqrt{n}$
- The algorithm is load balanced

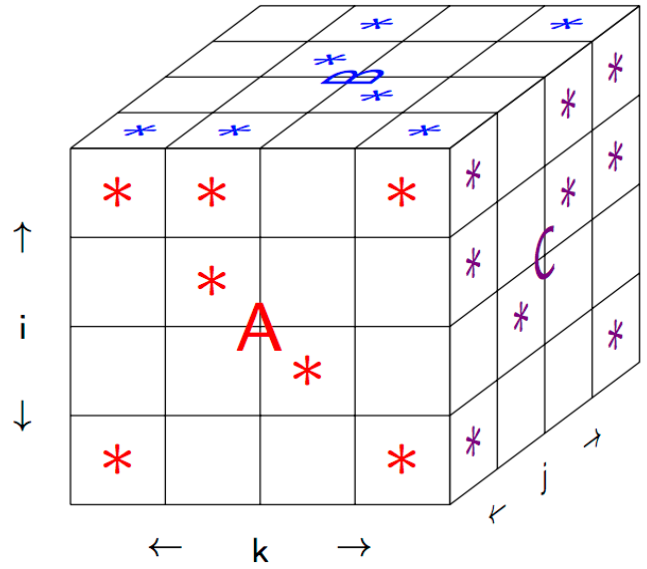
Sparsity independent algorithms:

- Assignement of entries of A, B, C to processors is independent of sparsity pattern of input/output matrices.
- Assignement of computation voxels to processors is independent of sparsity pattern of input/output matrices.
- All known algorithms are sparsity-independent

Lower bound - intuition of the proof

Idea: how many useful flops can be performed by using S inputs/outputs (similar to the dense case).





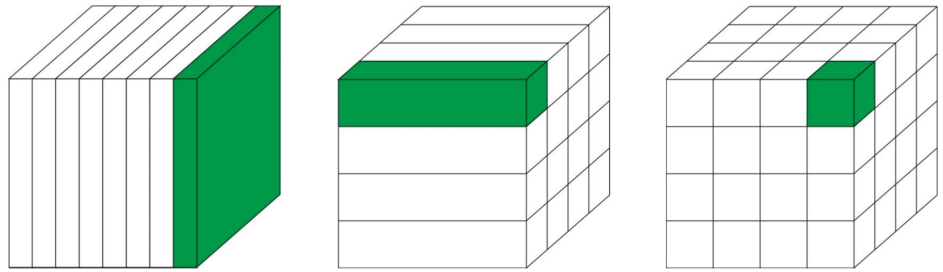
- Distinguish between input shadows and output shadow
- Given a shadow, is it stored on only one processor
- Given an internal grid point, does it correspond to a non-zero: use sparsity independence and randomness

Partitioning the work cube to processes

- Our bounds apply to all sparsity independent algorithms.
- We analyze algorithms that assign contiguous brick-shaped sets of voxels to each processor.

With correctly chosen data distributions:

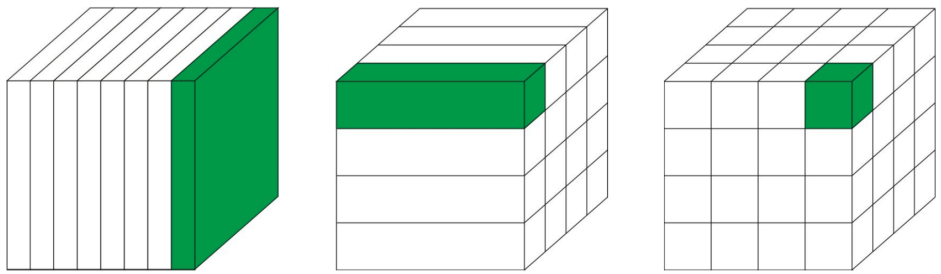
- 1D algorithms communicate entries of only one of the three matrices
- 2D algorithms communicate entries of two of the three matrices
- 3D algorithms communicate entries of all three matrices



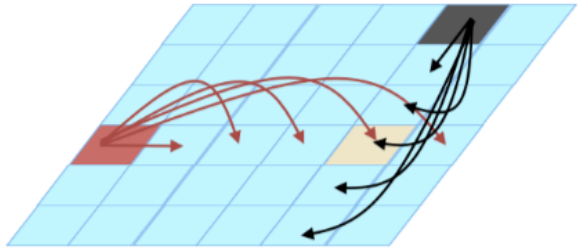
Partitioning the work cube to processes

Details:

- 1D algorithms communicate entries of only one of the three matrices:
  - Block Row: partition A, B, C on procs in a block row fashion. Shift block rows of B around a ring of processors. $W = dn, \quad S = P$
  - Improved Block Row: each proc gathers all required rows of B at once. Point to point communication: $W = d^2n/P, \min\{P, dn/P\}$
  - Outer product: Partition A in block cols, B in block rows, compute outer product, all-to-all to gather C. $W = d^2n/P, \quad S = \log P$
- 2D algorithms communicate entries of two of the three matrices: 2D Sparse SUMMA.
- 3D algorithms communicate entries of all three matrices: 3D Sparse SUMMA, 3D Recursive.



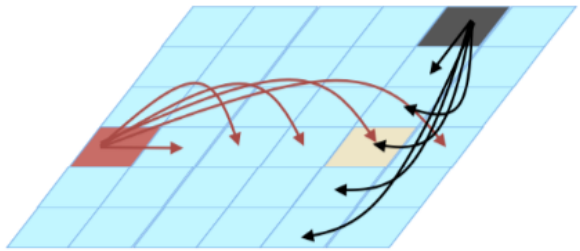
2D Summa



- Process grid $\sqrt{P} \times \sqrt{P}$ (in general does not have to be square)
- $C(i,j)$ is $n/\sqrt{P} \times n/\sqrt{P}$ submatrix of C on processor P_{ij}
- $A(i,k)$ is $n/\sqrt{P} \times b$ submatrix of A on processor P_{ik}
- $B(k,j)$ is $b \times n/\sqrt{P}$ submatrix of B on processor P_{kj}
- $C(i,j) = C(i,j) + \sum_k A(i,k) \cdot B(k,j)$
- To minimize communication, choose b close to $n/\sqrt{P}$ (as in the figure)

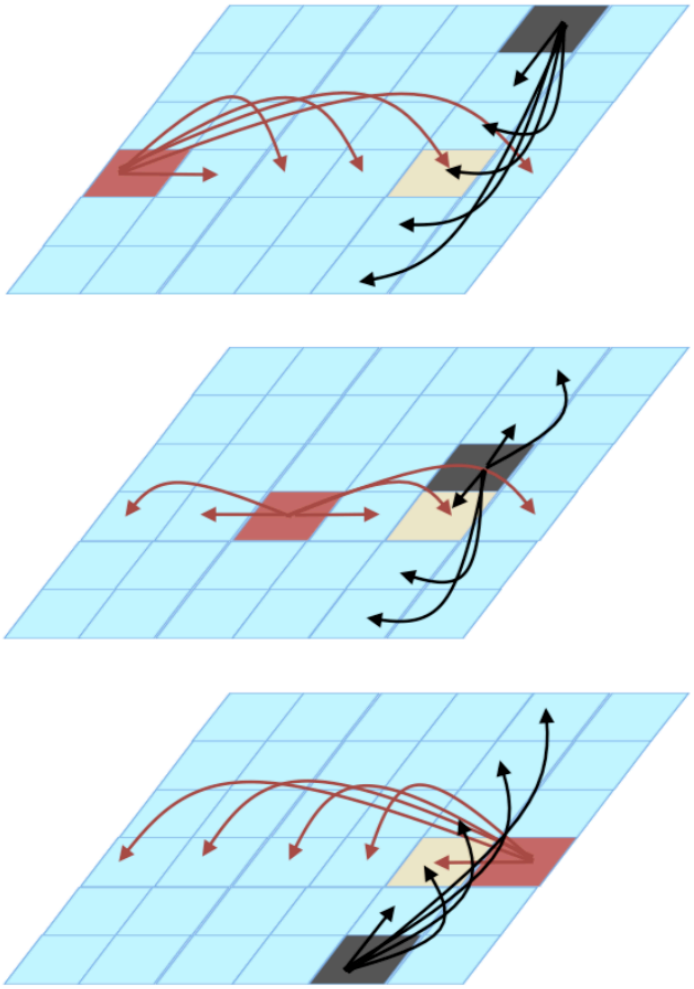
2D Summa (with $b = n/\sqrt{P}$)

- $C(i,j) = C(i,j) + \sum_k A(i,k) \cdot B(k,j)$



1: **for** k=1 to $\sqrt{P}$ **do**
2: **for** all $i,j = 1 \ldots \sqrt{P}$ **do**
3: P_{ik} broadcasts $A(i,k)$ along its row of processors $P_{i,:}$
4: P_{kj} broadcasts $B(k,j)$ along its column of processors $P_{:,j}$
5: $C(i,j) = C(i,j) + A(i,k) \cdot B(k,j)$
6: **end for**
7: **end for**

Dense 3D Summa

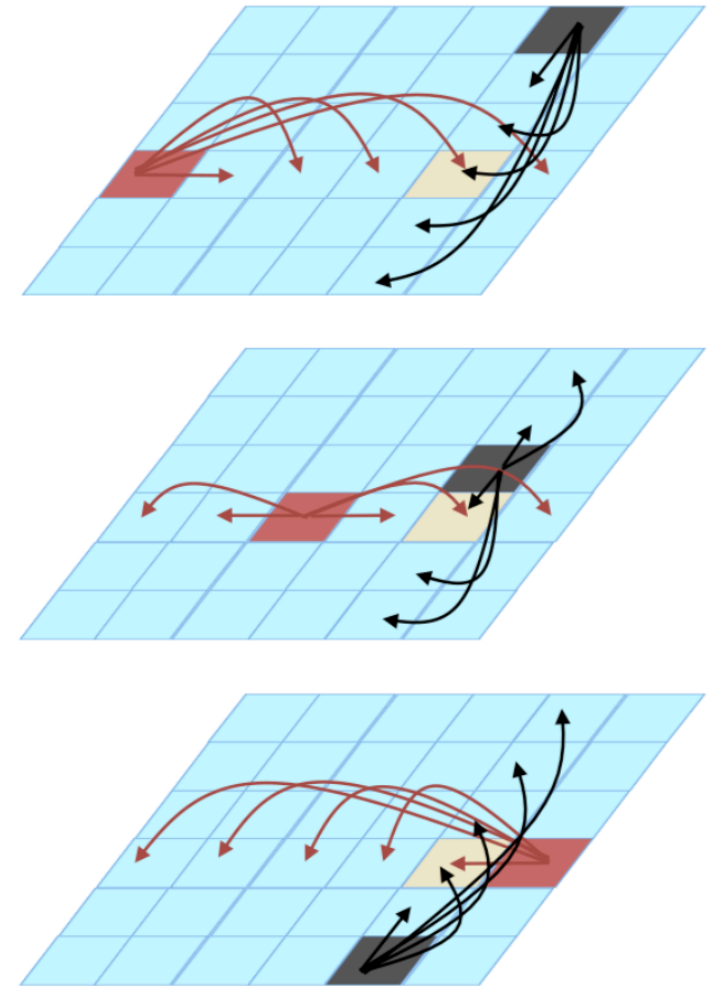


- Assume each processor can store cn^2/P data, $c > 1$
- Process grid: $\sqrt{P/c} \times \sqrt{P}/c \times c$

For $c = 3$

1. Layer 1 stores only $A(:, 1:2)$ and $B(1:2, :)$
2. Layer 2 stores only $A(:, 3:4)$ and $B(3:4, :)$
3. Layer 3 stores only $A(:, 5:6)$ and $B(5:6, :)$

Dense 3D Summa



Process grid: $\sqrt{P/c} \times \sqrt{P}/c \times c$

1. P_{ij0} broadcasts $A(i,j)$ and $B(i,j)$ to P_{ijt}
2. Processors at layer t perform $1/c$-th of SUMMA, i.e. 1/c-th of $\sum_k A(i,k) * B(k,j)$
3. Number of steps is $\sqrt{P/c^3}$
4. At each step, broadcast a block of A and a block of B along rows / columns of the face $\sqrt{P/c} \times \sqrt{P}/c$ process grid
5. Sum-reduce partial sums $\sum_k A(i,k) \cdot B(k,j)$ along t-axis so P_{ij0} owns $C(i,j)$

$$W = O(n^2/\sqrt{Pc}), \quad S = O(\sqrt{P/c^3} + \log c)$$

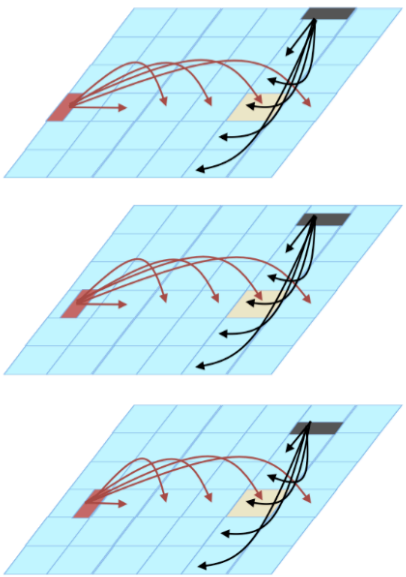
Sparse 3D Summa

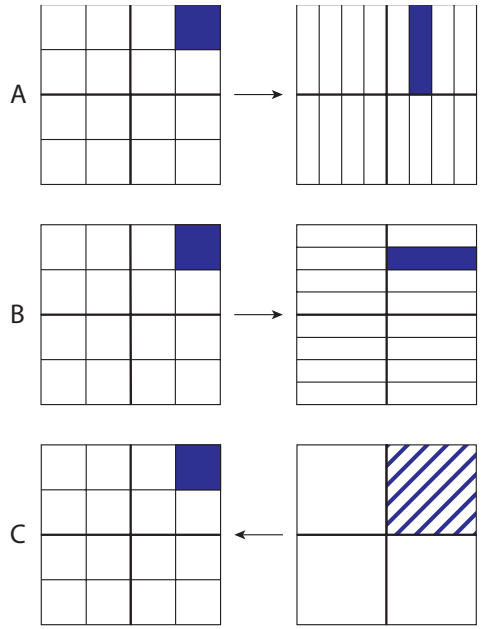
Process grid: $\sqrt{P/c} \times \sqrt{P/c} \times c$, A, B distributed over $\sqrt{P} \times \sqrt{P}$ procs.

- Distribute A and B on c layers: only $1/c$-th of columns of A and rows of B need to be distributed.
  E.g. for A, each proc owns a block of size $n/\sqrt{P/c} \times n/\sqrt{P/c^3}$.
  All-to-all operations performed by blocks of $\sqrt{c} \times \sqrt{c}$ procs.

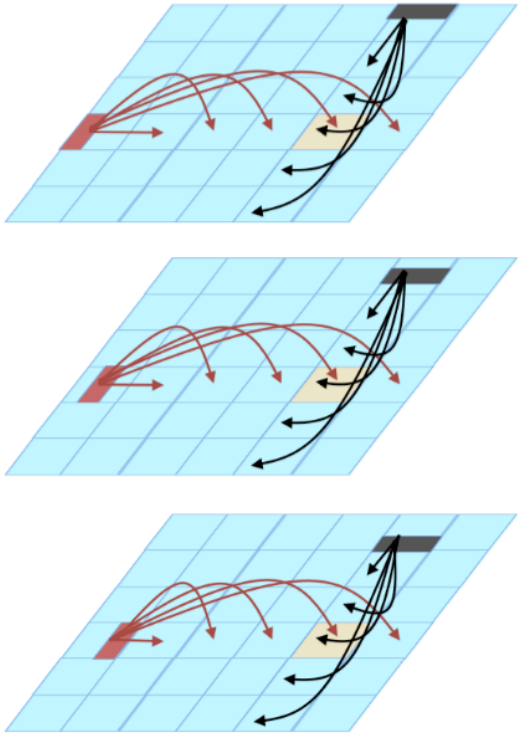
$$W = O(\frac{dn}{P} \cdot \log c), \quad S = O(\log c)$$

Example for $2 \times 2 \times 4$ grid, $c = 4$.





Sparse 3D Summa (contd)



- Processors collect all entries of A and B they need allgather operation among $\sqrt{P/c}$ procs.

$$W = O(\sqrt{P/c} \cdot \frac{dn}{P}) = O(dn/\sqrt{Pc}),$$
$$S = O(\log \sqrt{P/c})$$

- Reduce C on the first layer, and scatter it on all procs
  Sparse case: since each nonzero is contributed by a few flops, use instead gather + merge or all-to-all

$$W = O(\frac{d^2 n}{P} \cdot \log c), \quad S = O(\log c)$$

Optimizing c

Lower bound on communication:

$$\Omega\left(\min\left(\frac{dn}{\sqrt{P}}, \frac{d^2 n}{P}\right)\right)$$

If $d > \sqrt{P}$, then $d^2 n/P > dn/\sqrt{P}$.

Cost of sparse 3D Summa:

$$O\left(\frac{dn}{\sqrt{Pc}} + \frac{d^2 n}{P}\log c\right)$$

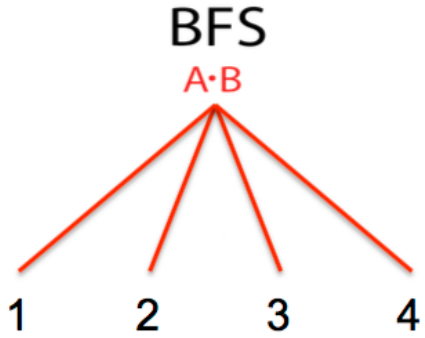
If $d > \sqrt{P}$, choose $c = 1$

If $d < \sqrt{P}$, choose $c = \Theta(P/d^2)$ to balance the two terms in the bandwidth cost.

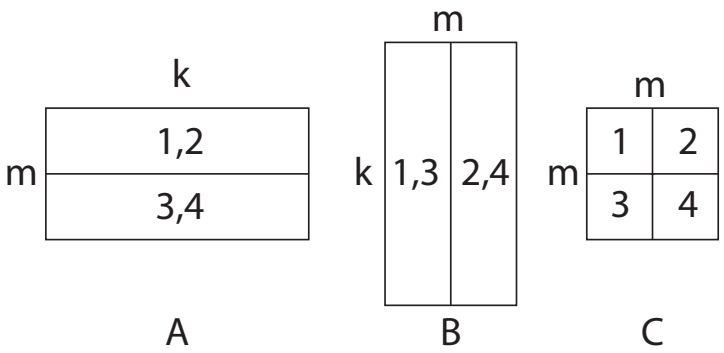
$\rightarrow$ Sparse Summa communication optimal by choosing $c = \min(1, P/d^2)$.
Remark: no increase in memory requirement, which remains $d^2 n/P$.

Recursive algorithm [Ballard et al., 2013]

Divides $A \cdot B$ into 4 sub-problems, each executed on $P/4$ processors.
While $P > 1$, pick the cheapest split

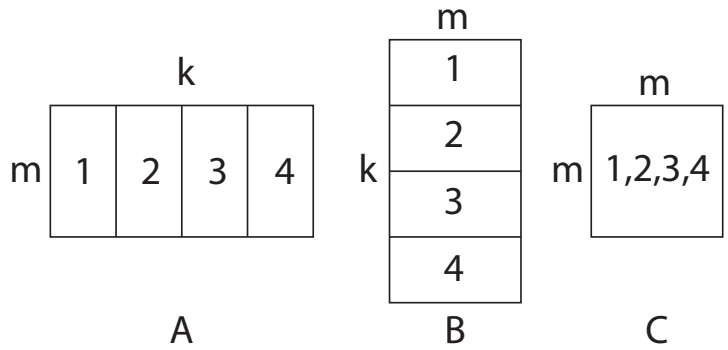


Split 1: Problem $m/2 \times k \times m/2$



Replicates A and B

Split 2: Problem $m \times k/4 \times m$

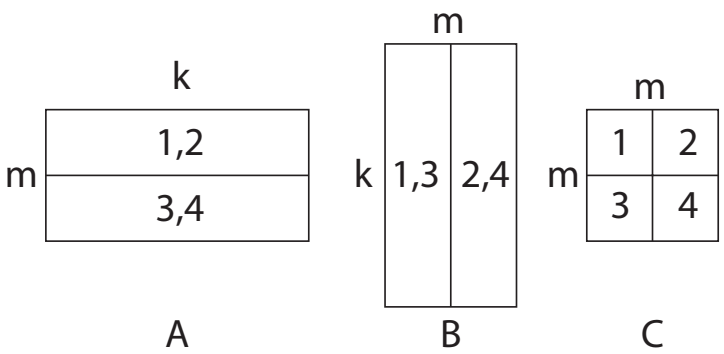


Redistributes and reduces C

Based on [Ballard, Demmel, Holtz, Lipshitz, Schwartz, SPAA'12

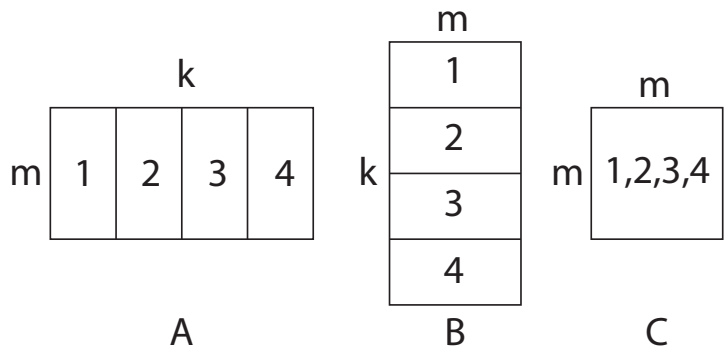
Recursive algorithm [Ballard et al., 2013]

Split 1: Problem $(m/2) \times k \times (m/2)$



Replicates A and B:
Allgather between disjoint pairs of procs
$W = O\left(\frac{dmk}{nP}\right), \quad S = O(1)$

Split 2: Problem $m \times k/4 \times m$



Redistributes and reduces C:
All-to-all between disjoint sets of 4 procs
$W = O\left(\frac{d^2m^2k}{n^2P}\right), \quad S = O(1)$

Recursive algorithm

- Algorithm: while $P > 1$, pick the cheapest split.
- Initially $m = k = n$, split 1 $O(dn/P)$ words is cheaper than split 2 $O(d^2 n/P)$.
- Split 1 cheaper for the first $\log_2 d$ steps.

Case 1: If $P \leq d^2$, Split 1 always cheapest:

$$W = \sum_{i=0}^{\log_4 P - 1} O\left(\frac{d(n/2^i)n}{nP/4^i}\right) = O\left(\frac{dn}{\sqrt{P}}\right), \quad S = O(\log P)$$

Recursive algorithm

Algorithm: while $P > 1$, pick the cheapest split
Case 2: If $P > d^2$, first $log_2 d$ steps use split 1, then use split 2.
After $log_2 d$ steps, subproblem has shape $n/d \times n \times n/d$ and P/d^2 procs.

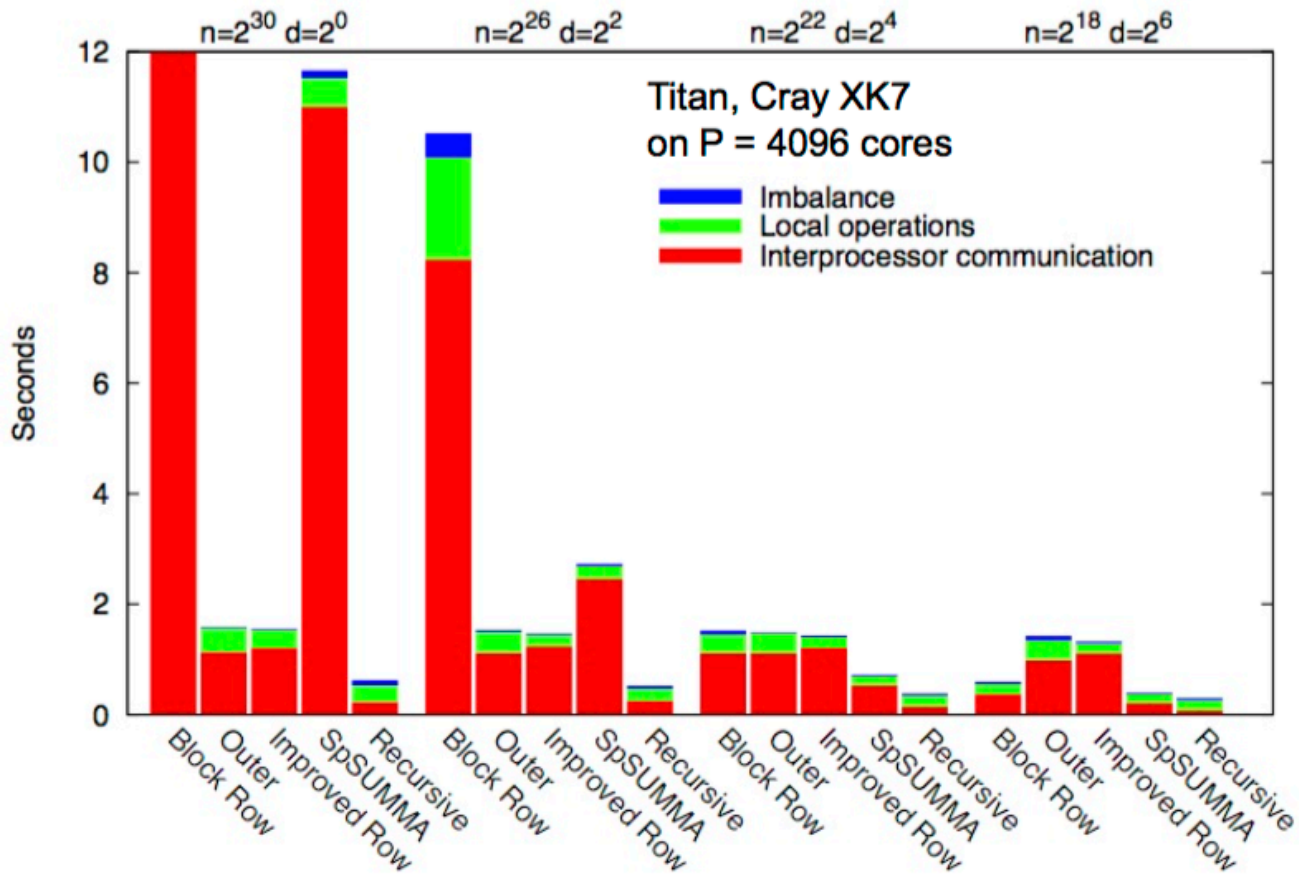
$$
\begin{aligned}
W &= \sum_{i=0}^{\log_2 d - 1} O\left(\frac{d(n/2^i)n}{nP/4^i}\right) + \sum_{i=\log_2 d}^{\log_4 P} O\left(\frac{d^2 n}{P}\right) = O\left(\frac{d^2 n}{P} \log \frac{P}{d^2}\right), \\
S &= O(\log P)
\end{aligned}
$$

- Matches the lower bound of $\Omega\left(\min\left(\frac{dn}{\sqrt{P}}, \frac{d^2 n}{P}\right)\right)$ up to log factor.
- Possible layout: A in block column layout, B in block-row layout, C has blocks of size $n/d \times n/d$, each distributed on a different $\lceil P/d^2 \rceil$ of the processors.
- No need to use DFS, since BFS uses only a constant factor extra memory.

Results for Erdős - Rényi Graph ER(n,d)

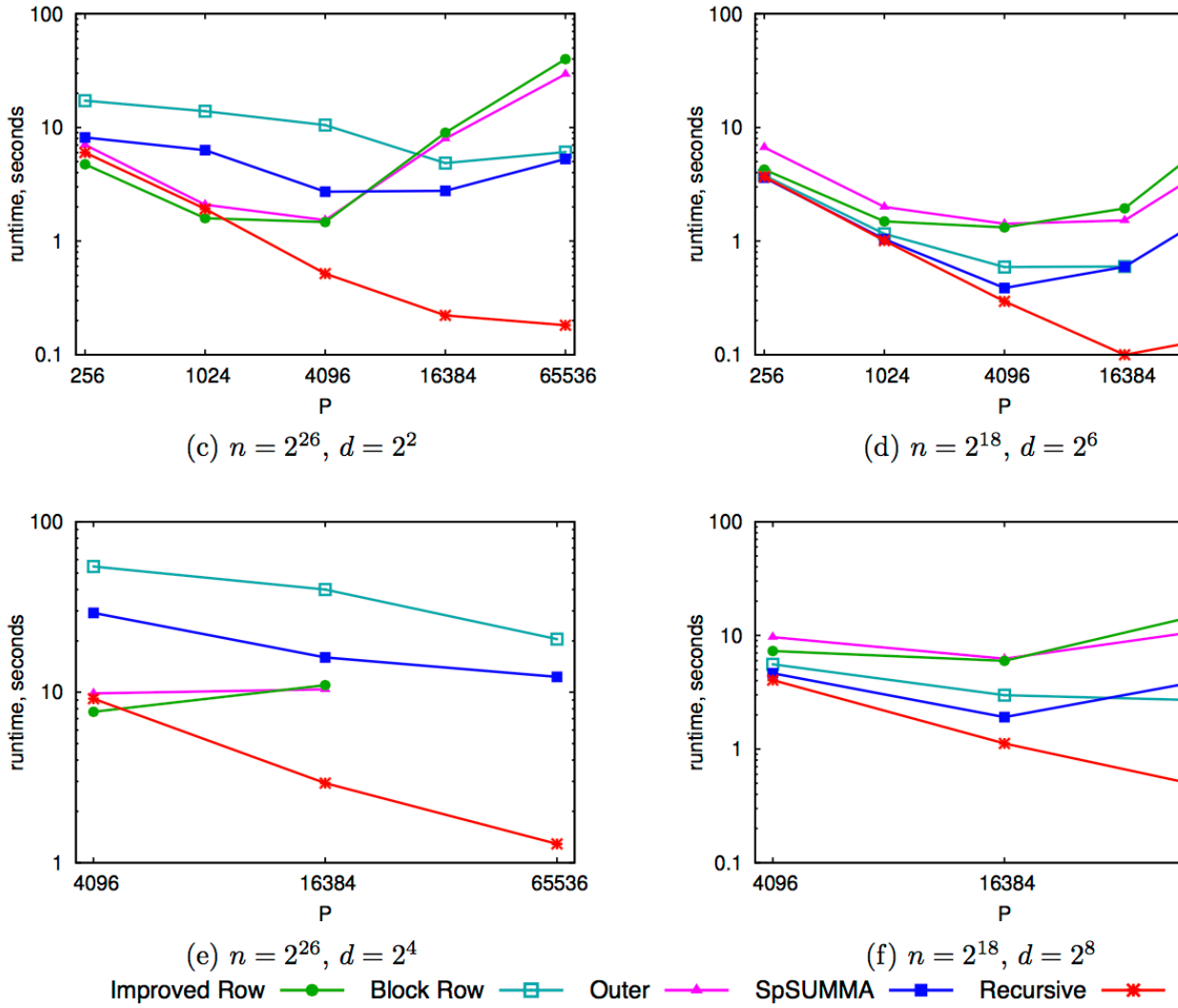
- Machine used: Titan, Cray XK7 from ORNL: 18,688 nodes, each node has 32GB of RAM, a 16 core AMD Opteron 6274 processor, and an Nvidia K20 GPU (not used).
- Experiments: use one core per process (16 MPI processes per node).

Results for Erdős - Rényi Graph



- For each case, expected number of nonzeros in the output is $d^2 n = 2^{30}$.
- For $n = 2^{30}, d = 1$, comm time = 39.3 secs, local operations = 11.9 secs and imbalance = 0.98 secs.

Results for Erdős - Rényi Graph - strong scaling



(c) $n = 2^{26}$, $d = 2^2$

(d) $n = 2^{18}$, $d = 2^6$

(e) $n = 2^{26}$, $d = 2^4$

(f) $n = 2^{18}$, $d = 2^8$

- In general, recursive algorithm outperforms all others
- Among the others: when $d < \sqrt{P}$, Outer product and Improved block row perform best when $d > \sqrt{P}$, sparse SUMMA performs best

Plan

Introduction

Sparse Matrix Matrix multiplication

Sparse Cholesky factorization for SPD matrices

- Combinatorial tools: undirected graphs, elimination trees
- Parallel Cholesky factorization
- Lower bounds for model problems

Graphs: All pairs shortest path

SPD matrices and Cholesky factorization

A is symmetric and positive definite (SPD) if

- $A = A^T$,
- all its eigenvalues are positive,
- or equivalently, A has a Cholesky factorization, $A = LL^T$.

Some properties of an SPD matrix A

- There is no need to pivot for accuracy (just performance) during the Cholesky factorization.
- For any permutation matrix P, PAP^T is also SPD.

Sparse Cholesky factorization

Algebra:

$$
\begin{aligned}
A &= \begin{pmatrix} a_{11} & A_{21}^T \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} \sqrt{a_{11}} & \\ A_{21}./\sqrt{a_{11}} & I \end{pmatrix} \cdot \begin{pmatrix} \sqrt{a_{11}} & A_{21}^T./\sqrt{a_{11}} \\ & A_{22}^s \end{pmatrix} \\
&= \begin{pmatrix} \sqrt{a_{11}} & \\ A_{21}./\sqrt{a_{11}} & L_{22} \end{pmatrix} \cdot \begin{pmatrix} \sqrt{a_{11}} & A_{21}^T./\sqrt{a_{11}} \\ & L_{22}^T \end{pmatrix}, \quad \text{where} \\
& A_{22}^s = A_{22} - (A_{21}./\sqrt{a_{11}}) \cdot (A_{21}^T./\sqrt{a_{11}})
\end{aligned}
$$

Algorithm:

for $k = 1 : n-1$ **do**
  $a_{kk} = \sqrt{a_{kk}}$
  /* $factor(k)$ */
  for $i = k+1 : n$ st $a_{ik} \neq 0$ **do**
    $a_{ik} = a_{ik}/a_{kk}$
  end for
  for $i = k+1 : n$ st $a_{ik} \neq 0$ **do**
    $update(k, i)$
    for $j = i : n$ st $a_{kj} \neq 0$ **do**
      $a_{ij} = a_{ij} - a_{ik}a_{jk}$
    end for
  end for
end for

$L + L^T =$

	1	2	3	4	5	6	7	8	9
1	x	x		x					
2	x	x	x	x	x				
3		x	x	x	x	x			
4	x	x	x	x	x		x		
5		x	x	x	x	x	x	x	
6			x		x	x	x	x	x
7				x	x	x	x	x	
8					x	x	x	x	x
9						x		x	x

Filled graph $G^+(A)$

- Given $G(A) = (V, E)$, $G^+(A) = (V, E^+)$ is defined as:
  there is an edge $(i, j) \in G^+(A)$ iff there is a path from i to j in $G(A)$ going through lower numbered vertices.
- Definition holds also for directed graphs (LU factorization).

- $G(L + L^T) = G^+(A)$, ignoring cancellations.
- $G^+(A)$ is chordal (every cycle of length at least four has a chord, an edge connecting two non-neighboring nodes).
- Conversely, if $G(A)$ is chordal, then there is a perfect elimination order, that is a permutation P such that $G(PAP^T) = G^+(PAP^T)$.

- References: [Parter, 1961, Rose, 1970, Rose and Tarjan, 1978]

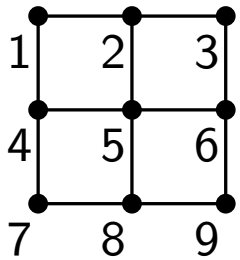
Filled graph $G^+(A)$

$A =$

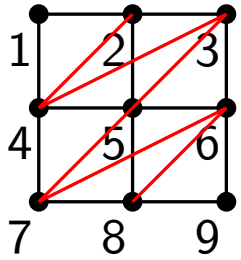
	1	2	3	4	5	6	7	8	9
1	x	x		x					
2	x	x	x		x				
3		x	x			x			
4	x			x	x		x		
5		x		x	x	x		x	
6			x		x	x			x
7				x			x	x	
8					x		x	x	x
9						x		x	x

$L + L^T =$

	1	2	3	4	5	6	7	8	9
1	x	x		x					
2	x	x	x	x	x				
3		x	x	x	x	x			
4	x	x	x	x	x		x		
5		x	x	x	x	x	x	x	
6			x		x	x	x	x	x
7				x	x	x	x	x	
8					x	x	x	x	x
9						x		x	x



$G(A)$



$G^+(A)$

Steps of sparse Cholesky factorization

1. Order rows and columns of A to reduce fill-in

2. Symbolic factorization: based on eliminaton trees
   - Compute the elimination tree (in nearly linear time in $nnz(A)$)
   - Allocate data structure for L
   - Compute the nonzero structure of the factor L, in $O(nnz(L)$

3. Numeric factorization
   - Exploit memory hierarchy
   - Exploit parallelism due to sparsity

4. Triangular solve

Order columns/rows of A

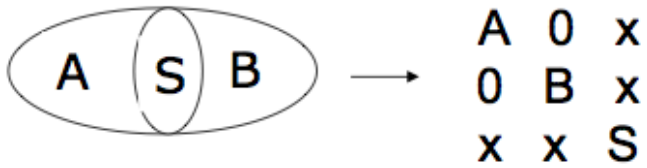
Strategies applied to the graph of A for Cholesky,
to the graph of $A^T A$ for LU with partial pivoting.

Local strategy: minimum degree [Tinney/Walker '67]

- Minimize locally the fill-in.
- Choose at each step (for 1 to n) the node of minimum degree.

Global strategy: graph partitioning approach

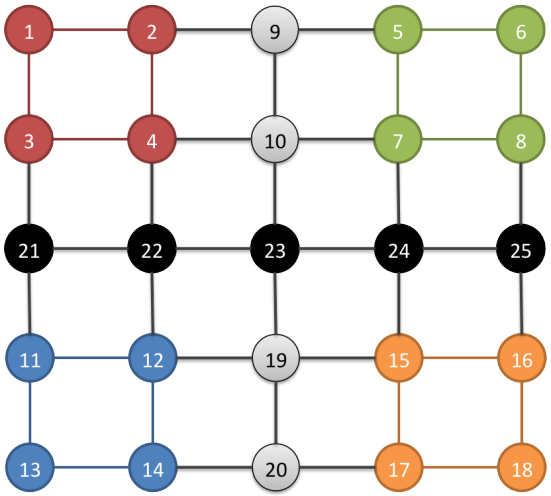
- Nested dissection [George, 1973]
  - First level: find the smallest possible separator S, order last
  - Recurse on A and B
- Multilevel schemes [Barnard/Simon '93, Hendrickson/Leland '95, Karypis/Kumar '95].

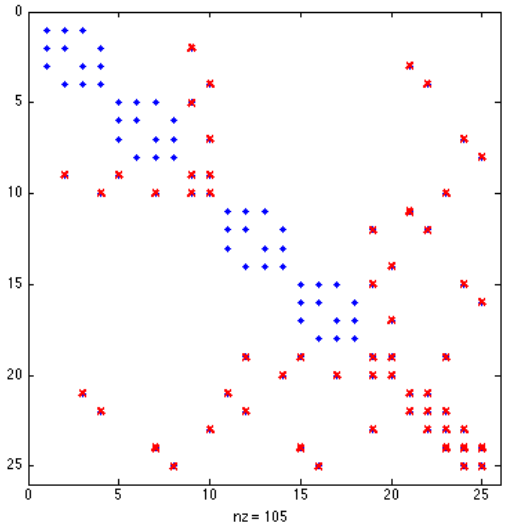


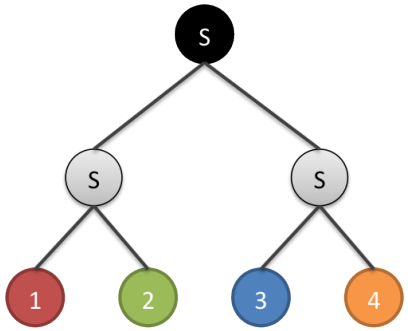
Nested dissection and separator tree

Separator tree:

- Combines together nodes belonging to a same separator, or to a same disjoint graph







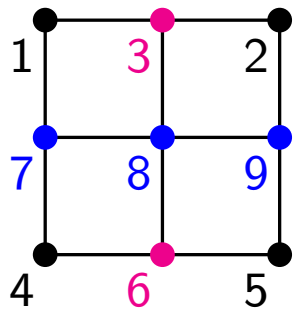
Some available packages:

- Metis, Parmetis (`http://glaros.dtc.umn.edu/gkhome/metis/metis/overview`)
- Scotch, Ptscotch (`www.labri.fr/perso/pelegrin/scotch/`)

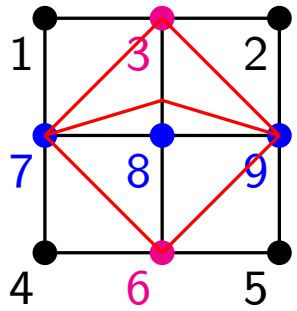
Nested dissection on our 9×9 structured matrix

$$A = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \end{array} \begin{array}{c} \begin{array}{ccccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \end{array} \\ \left(\begin{array}{ccc|ccc|ccc} x & & x & & & & x & & \\ & x & x & & & & & & x \\ \hline x & x & x & & & & & x & \\ \hline & & & x & & x & x & & \\ & & & & x & x & & & x \\ \hline & & & x & x & x & & x & \\ \hline x & & & x & & & x & x & \\ & & x & & & x & x & x & x \\ & x & & & x & & & x & x \end{array} \right) \end{array},$$

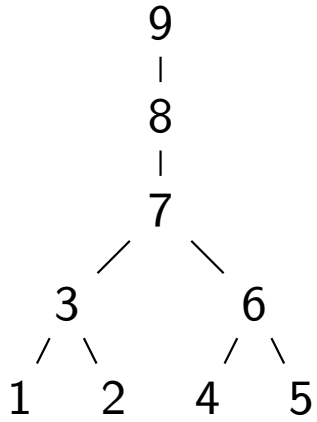
$$L + L^T = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \end{array} \begin{array}{c} \begin{array}{ccccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \end{array} \\ \left(\begin{array}{ccc|ccc|ccc} x & & x & & & & x & & \\ & x & x & & & & & & x \\ \hline x & x & x & & & & x & x & x \\ \hline & & & x & & x & x & & \\ & & & & x & x & & & x \\ \hline & & & x & x & x & x & x & x \\ \hline x & & x & x & & x & x & x & x \\ & & x & & & x & x & x & x \\ & x & x & & x & x & x & x & x \end{array} \right) \end{array}$$



$G(A)$



$G^+(A)$



$T(A)$

Elimination tree (etree)

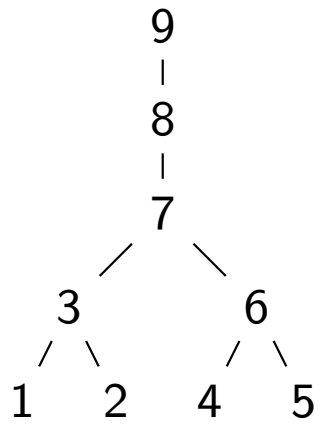
Definition ([Schreiber, 1982] and also [Duff, 1982])

Given $A = LL^T$, the etree $T(A)$ has the same node set as $G(A)$, and k is the parent of j iff

$$k = \min\{i > j : l_{ij} \neq 0\}$$

$L + L^T =$

	1	2	3	4	5	6	7	8	9
1	x		x				x		
2		x	x						x
3	x	x	x				x	x	x
4				x		x	x		
5					x	x			x
6				x	x	x	x	x	x
7	x		x	x		x	x	x	x
8			x			x	x	x	x
9		x	x		x	x	x	x	x



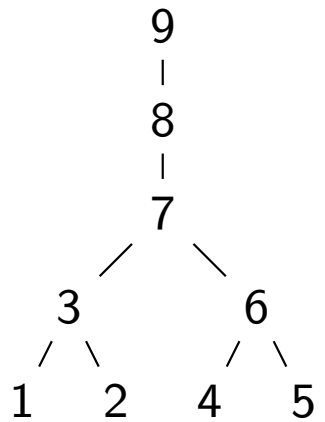
$T(A)$

Column dependencies and the elimination tree

- If $l_{jk} \neq 0$, then
  - $Factor(k)$ needs to be computed before $Factor(j)$.
  - k is an ancestor of j in $T(A)$.
- Columns belonging to disjoint subtrees can be factored independently.
- Topological orderings of $T(A)$ (that number children before their parent)
  - preserve the amount of fill, the flops of the factorization, the structure of $T(A)$

$L + L^T =$

	1	2	3	4	5	6	7	8	9
1	x		x				x		
2		x	x						x
3	x	x	x				x	x	x
4				x		x	x		
5					x	x			x
6				x	x	x	x	x	x
7	x		x	x		x	x	x	x
8			x			x	x	x	x
9		x	x		x	x	x	x	x



$T(A)$

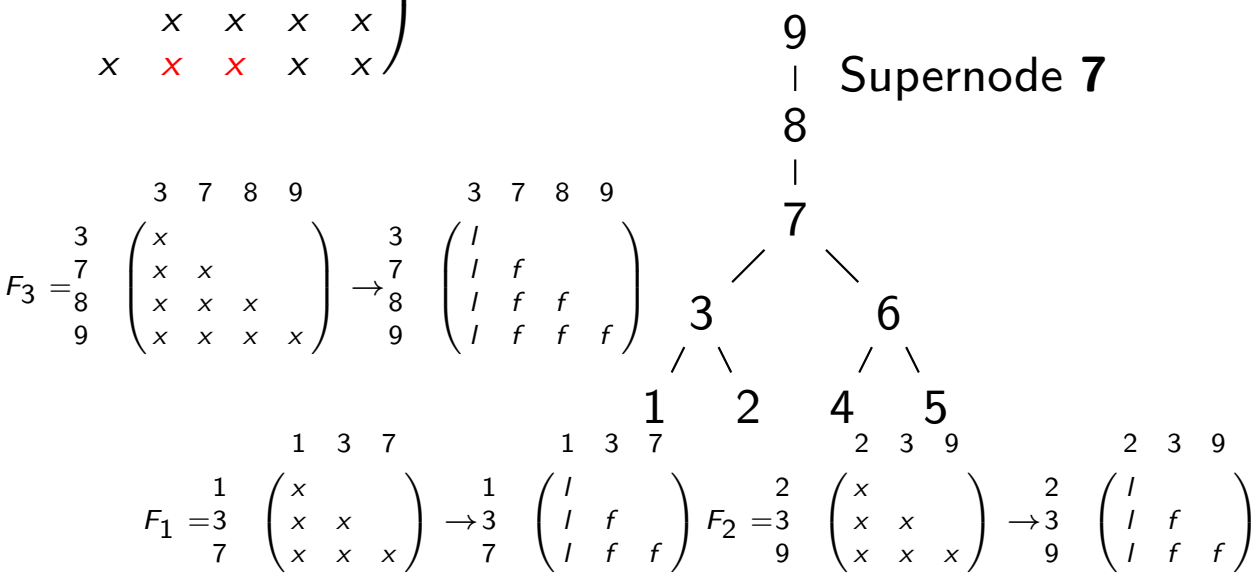
Numeric factorization - multifrontal approach

- Driven by the separator tree of A, a supernodal elimination tree.
- The Cholesky factorization is performed during a postorder traversal of the separator tree.
- At each node k of the separator tree:
  - A frontal matrix F_k is formed by rows and columns involved at step k of factorization:
    - rows that have their first nonzero in column k of A,
    - contribution blocks (part of frontal matrices) from children in $T(A)$.
  - The new frontal matrix is obtained by an extend-add operation.
  - The first rows/columns of F_k corresponding to supernode k are factored.

Numeric factorization - an example

$$L + L^T = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \end{array} \begin{array}{c} \begin{array}{ccccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \end{array} \\ \begin{pmatrix} x & & x & & & & x & & \\ & x & x & & & & & & x \\ x & x & x & & & & x & x & x \\ & & & x & & x & x & & \\ & & & & x & x & & & x \\ & & & x & x & x & x & x & x \\ x & & x & x & & x & x & x & x \\ & & x & & & x & x & x & x \\ & x & x & & x & x & x & x & x \end{pmatrix} \end{array}$$

$$F_{\{7,8,9\}} = \begin{array}{c} \\ 7 \\ 8 \\ 9 \end{array} \begin{array}{c} \begin{array}{ccc} 7 & 8 & 9 \end{array} \\ \begin{pmatrix} x & & \\ x & x & \\ x & x & x \end{pmatrix} \end{array} \rightarrow \begin{array}{c} \\ 7 \\ 8 \\ 9 \end{array} \begin{array}{c} \begin{array}{ccc} 7 & 8 & 9 \end{array} \\ \begin{pmatrix} l & & \\ l & l & \\ l & l & l \end{pmatrix} \end{array}$$



$$F_3 = \begin{array}{c} \\ 3 \\ 7 \\ 8 \\ 9 \end{array} \begin{array}{c} \begin{array}{cccc} 3 & 7 & 8 & 9 \end{array} \\ \begin{pmatrix} x & & & \\ x & x & & \\ x & x & x & \\ x & x & x & x \end{pmatrix} \end{array} \rightarrow \begin{array}{c} \\ 3 \\ 7 \\ 8 \\ 9 \end{array} \begin{array}{c} \begin{array}{cccc} 3 & 7 & 8 & 9 \end{array} \\ \begin{pmatrix} l & & & \\ l & f & & \\ l & f & f & \\ l & f & f & f \end{pmatrix} \end{array}$$

$$F_1 = \begin{array}{c} \\ 1 \\ 3 \\ 7 \end{array} \begin{array}{c} \begin{array}{ccc} 1 & 3 & 7 \end{array} \\ \begin{pmatrix} x & & \\ x & x & \\ x & x & x \end{pmatrix} \end{array} \rightarrow \begin{array}{c} \\ 1 \\ 3 \\ 7 \end{array} \begin{array}{c} \begin{array}{ccc} 1 & 3 & 7 \end{array} \\ \begin{pmatrix} l & & \\ l & f & \\ l & f & f \end{pmatrix} \end{array} \qquad F_2 = \begin{array}{c} \\ 2 \\ 3 \\ 9 \end{array} \begin{array}{c} \begin{array}{ccc} 2 & 3 & 9 \end{array} \\ \begin{pmatrix} x & & \\ x & x & \\ x & x & x \end{pmatrix} \end{array} \rightarrow \begin{array}{c} \\ 2 \\ 3 \\ 9 \end{array} \begin{array}{c} \begin{array}{ccc} 2 & 3 & 9 \end{array} \\ \begin{pmatrix} l & & \\ l & f & \\ l & f & f \end{pmatrix} \end{array}$$

Notation used for frontal matrices F_k:

- x - elements obtained by the extend-add operation,
- l - elements of L computed at node k, f - elements of frontal matrix that will be passed to parent of node k.

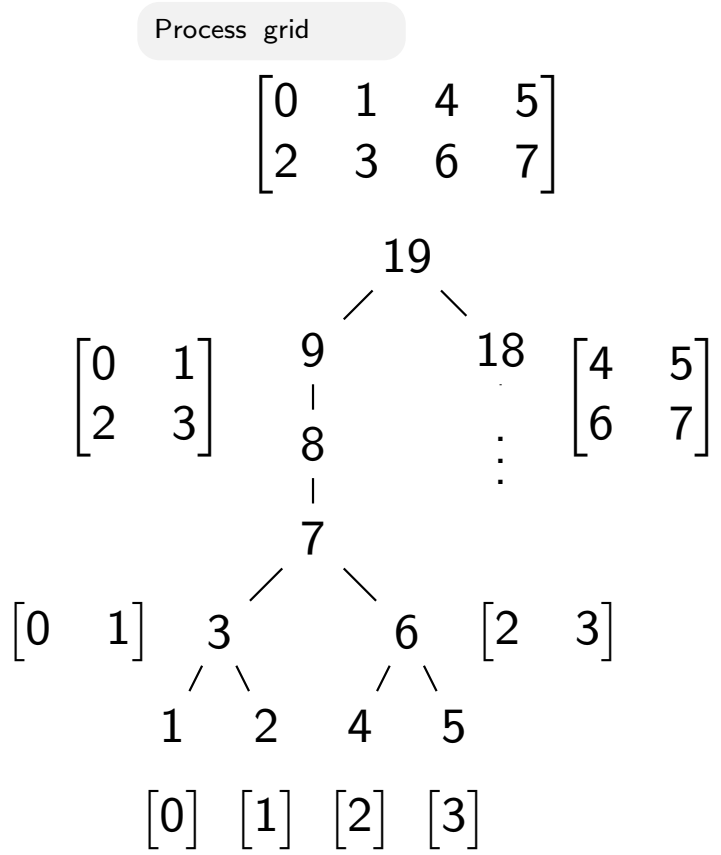
Numeric factorization - PSPASES [Gupta et al., 1995]

- Based on subtree to subcube mapping [George et al., 1989] applied on the separator tree

Subtree to subcube mapping

1. Assign all the processors to the root.
2. Assign to each subtree half of the processors.
3. Go to Step 1 for each subtree which is assigned more than one processor.

The figure displays the process grid used by PSPASES.



Numeric factorization - PSPASES [Gupta et al., 1995]

- Subtree to subcube mapping and bitmask based cyclic distribution:

  Starting at the last level of the separator tree (bottom up traversal), let $i = 1$

  for each two consecutive levels $k, k-1$, based on value of i-th LSB of column/row indices

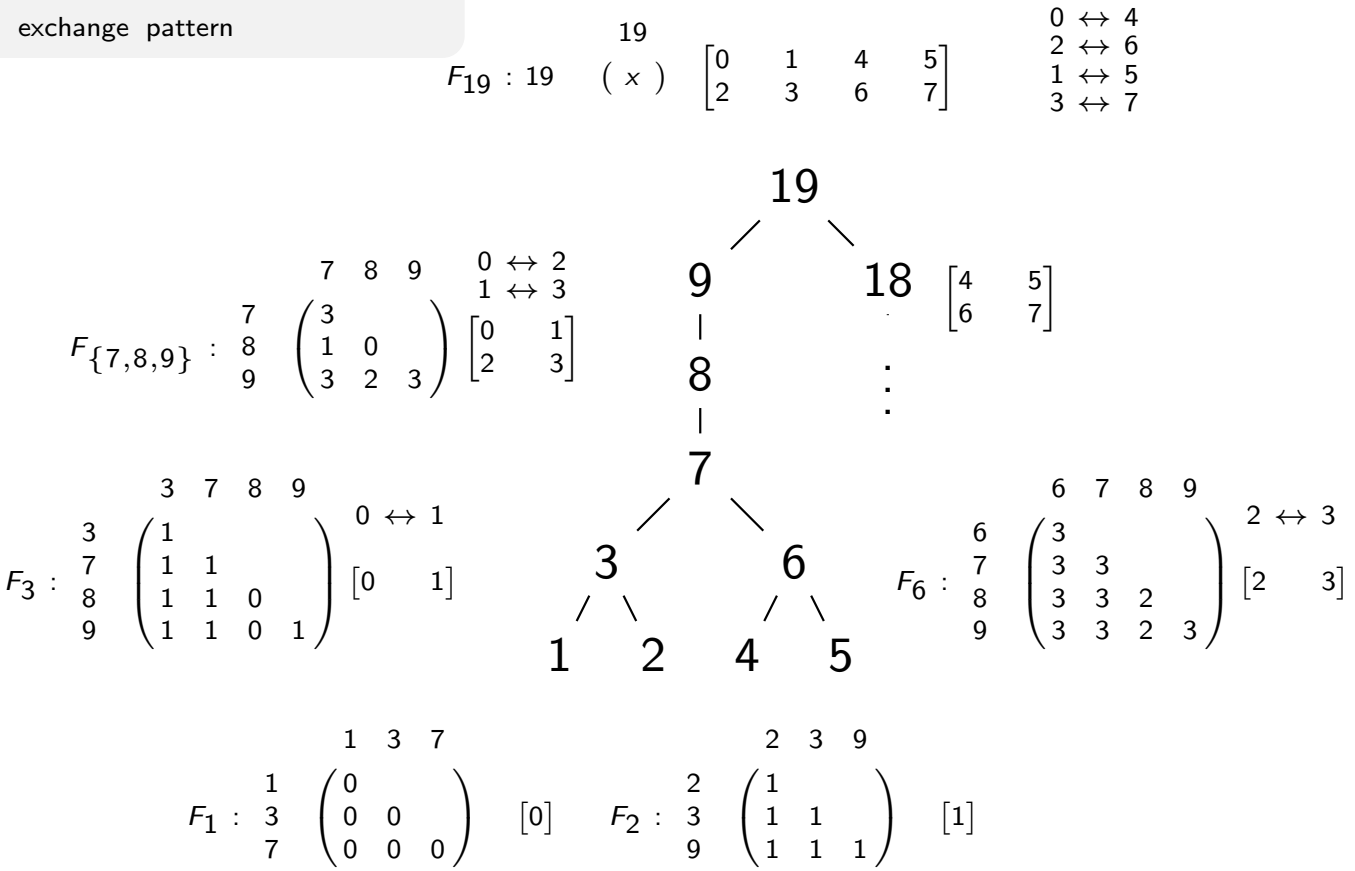
  - For level k:
    Map all even columns to subcube with lower processor numbers
    Map all odd columns to subcube with higher processor numbers
  - For level $k-1$:
    Map all even rows to subcube with lower processor numbers
    Map all odd rows to subcube with higher processor numbers
  - Let $i = i + 1$

PSPASES uses a bitmask based block-cyclic distribution.

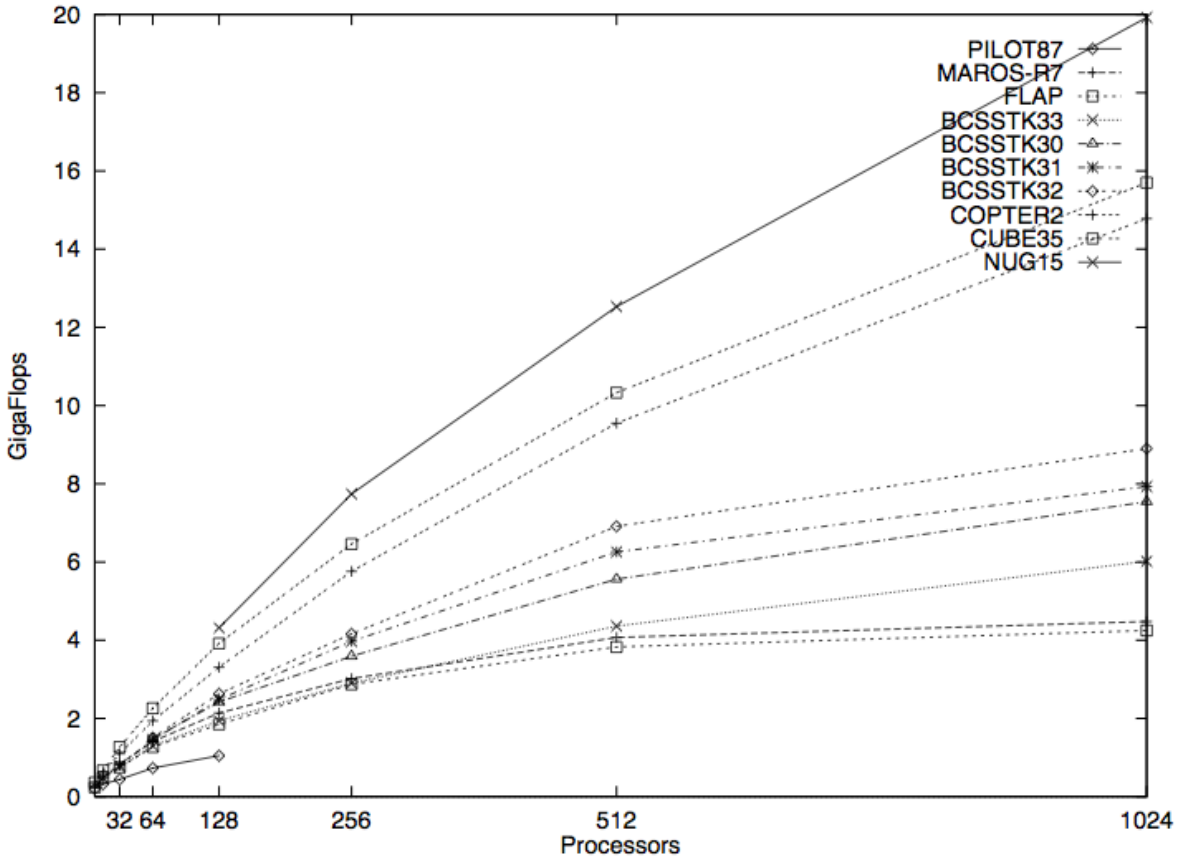
Numeric factorization - PSPASES [Gupta et al., 1995]

- Based on subtree to subcube mapping [George et al., 1989].
- Extend-add operation requires each processor to exchange half of its data with a corresponding processor from the other half of the grid.

Data distribution, process grid and data exchange pattern



Performance results on Cray T3D

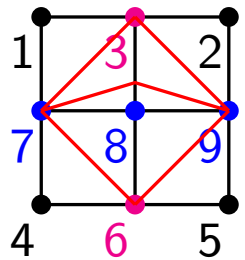


Results from [Gupta et al., 1995]

Lower bounds on communication for Cholesky

- Consider A of size $k^s \times k^s$ results from a finite difference operator on a regular grid of dimension $s \geq 2$ with k^s nodes.
- Its Cholesky L factor contains a dense lower triangular matrix of size $k^{s-1} \times k^{s-1}$.

$$L + L^T = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \end{array} \begin{array}{c} \begin{array}{ccccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \end{array} \\ \begin{pmatrix} x & & x & & & & x & & \\ & x & x & & & & & & x \\ x & x & x & & & & x & x & x \\ & & & x & & x & x & & \\ & & & & x & x & & & x \\ & & & x & x & x & x & x & x \\ x & & x & x & & x & x & x & x \\ & & x & & & x & x & x & x \\ & x & x & & x & x & x & x & x \end{pmatrix} \end{array}$$



$G^+(A)$

- Computing the Cholesky factorization of the $k^{s-1} \times k^{s-1}$ matrix dominates the computation.

Lower bounds on communication

- This result applies more generally to matrix A whose graph $G = (V, E)$, $|V| = n$ has the following property for some l:
  - if every set of vertices $W \subset V$ with $n/3 \leq |W| \leq 2n/3$ is adjacent to at least l vertices in $V - W$,
  - then the Cholesky factor of A contains a dense $l \times l$ submatrix.

Lower bounds on communication

For the Cholesky factorization of a $k^s \times k^s$ matrix resulting from a finite difference operator on a regular grid of dimension $s \geq 2$ with k^s nodes:

$$\#words \geq \Omega\left(\frac{W}{\sqrt{M}}\right), \qquad \#messages \geq \Omega\left(\frac{W}{M^{3/2}}\right)$$

- Sequential algorithm
  - $W = k^{3(s-1)}/3$ and M is the fast memory size
- Work balanced parallel algorithm executed on P processors
  - $W = \frac{k^{3(s-1)}}{3P}$ and $M \approx nnz(L)/P$

Why / how PSPASES attains optimality

- For each node in the separator tree, the communication in the Cholesky factorization dominates the communication in the extend-add step.
- Optimal dense Cholesky factorization needs to be used for each multifrontal matrix ($n \times n$, P procs).
  - optimal block size - minimize communication while increasing flops by a lower order term

$$b = \frac{n}{\sqrt{P}} \log_2^{-2} \sqrt{P}$$

Optimal sparse Cholesky factorization

- Results for $n \times n$ matrix resulting from 2D and 3D regular grids.
- Analysis assumes local memory per processor is $M = O(n \log n/P)$- 2D case and $M = O(n^{4/3}/P)$- 3D case.

	PSPASES	PSPASES with optimal layout	Lower bound
2D grids			
# flops	$O\left(\frac{n^{3/2}}{P}\right)$	$O\left(\frac{n^{3/2}}{P}\right)$	$\Omega\left(\frac{n^{3/2}}{P}\right)$
# words	$O(\frac{n}{\sqrt{P}})$	$O\left(\frac{n}{\sqrt{P}} \log P\right)$	$\Omega\left(\frac{n}{\sqrt{P \log n}}\right)$
# messages	$O(\sqrt{n})$	$O\left(\sqrt{P} \log^3 P\right)$	$\Omega\left(\frac{\sqrt{P}}{(\log n)^{3/2}}\right)$
3D grids			
# flops	$O\left(\frac{n^2}{P}\right)$	$O\left(\frac{n^2}{P}\right)$	$\Omega\left(\frac{n^2}{P}\right)$
# words	$O(\frac{n^{4/3}}{\sqrt{P}})$	$O\left(\frac{n^{4/3}}{\sqrt{P}} \log P\right)$	$\Omega\left(\frac{n^{4/3}}{\sqrt{P}}\right)$
# messages	$O(n^{2/3})$	$O\left(\sqrt{P} \log^3 P\right)$	$\Omega\left(\sqrt{P}\right)$

Optimal sparse Cholesky factorization: summary

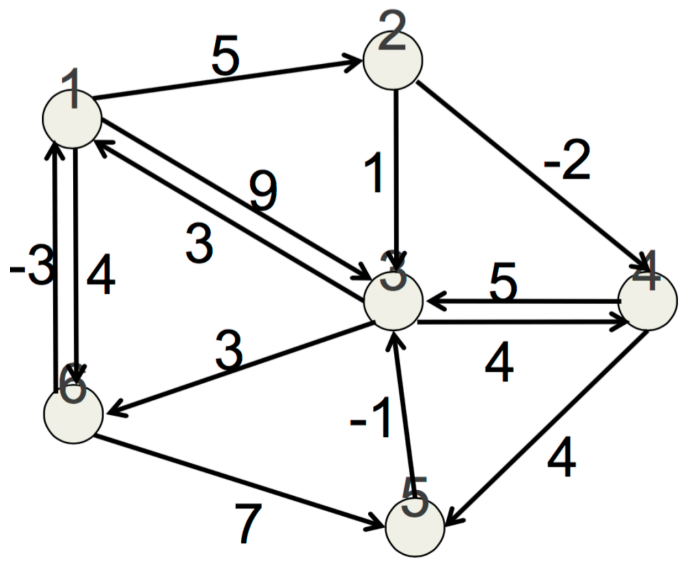
- PSPASES with an optimal layout attains the lower bound in parallel for 2D/3D regular grids:
  - Uses nested dissection to reorder the matrix
  - Distributes the matrix using the subtree to subcube algorithm
  - The factorization of every dense multifrontal matrix is performed using an optimal dense Cholesky factorization
- Sequential multifrontal algorithm attains the lower bound
  - The factorization of every dense multifrontal matrix is performed using an optimal dense Cholesky factorization

Plan

Preliminaries

Graph $G = (V, E)$ is formed by:

- a set of vertices V,
- a set of edges E.



- Edges can be directed or not, can have weights or not.
- A path from v_1 to v_n is formed by a sequence of edges $(v_1, v_2), \ldots (v_{n-1}, v_n)$. Its length is the sum of its weights.

Parallel graph algorithms

- Graph traversals: breadth-first search
- Single Source Shortest Path: Delta-stepping (Meyer and Sanders), randomized approach (Ullman and Yannakakis)
- All Pairs Shortest Path (APSP): Floyd-Warshall, Johnson (based on Dijkstra).
- Graph partitioning

Applications

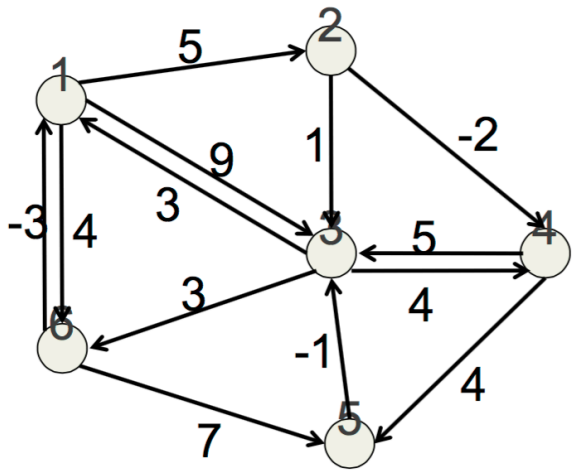
- Routing in transportation networks: compute point to point shortest paths
- Internet and WWW: web search, page rank, document classification and clustering
- Scientific computing: reorderings, graph partitioning, maximum matchings
- APSP: urban planning and simulation, datacenter network design, traffic routing, subroutine in Ullman and Yannakaki's BFS algorithm

All-pairs shortest paths

- Input: directed graphs with weights on edges
- APSP: find shortest paths between all reachable vertex pairs

Floyd-Warshall

for $i,j = 1 : n$, $d(i \to i) := 0$, $d(i \to j) := \infty$
for each edge (i,j)
  $d(i \to j) := w(i \to j)$, $\Pi(i,j) := i$
for k=1 to n **do**
  for $i = 1$ to n **do**
    for $j = 1$ to n **do**
      If $d(i \to k) + d(k \to j) < d(i \to j)$
        $d(i \to j) := d(i \to k) + d(k \to j)$
        $\Pi(i,j) := \Pi(k,j)$
    end for
  end for
end for



$$\begin{bmatrix} 0 & 5 & 9 & \infty & \infty & 4 \\ \infty & 0 & 1 & -2 & \infty & \infty \\ 3 & \infty & 0 & 4 & \infty & 3 \\ \infty & \infty & 5 & 0 & 4 & \infty \\ \infty & \infty & -1 & \infty & 0 & \infty \\ -3 & \infty & \infty & \infty & 7 & 0 \end{bmatrix}$$

- First step: computes the lengths of the paths between all pairs of vertices
- Second step: if required, path reconstruction
- Assume there is no negative cycle

All-pairs shortest paths

APSP problem corresponds to finding the matrix closure on the tropical $(min, +)$ semiring. In the semiring matrix multiplication (distance product)

- replace each multiply with an addition: compute length of a larger path from smaller paths or edges
- replace each add with a minimum operation: get the minimum path if there are multiple paths

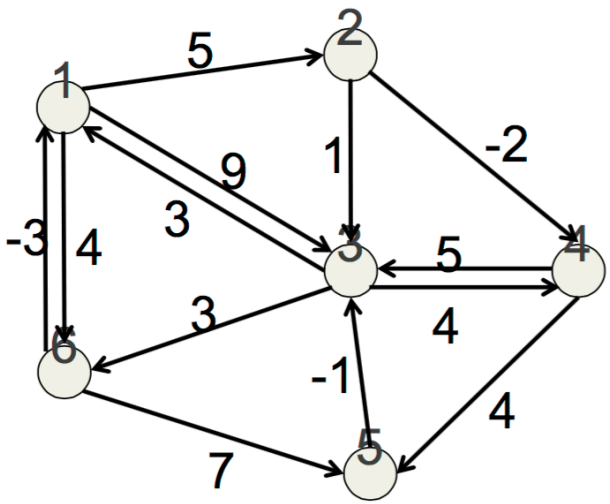
Assume for simplicity adjacency matrices of power of two dimension.

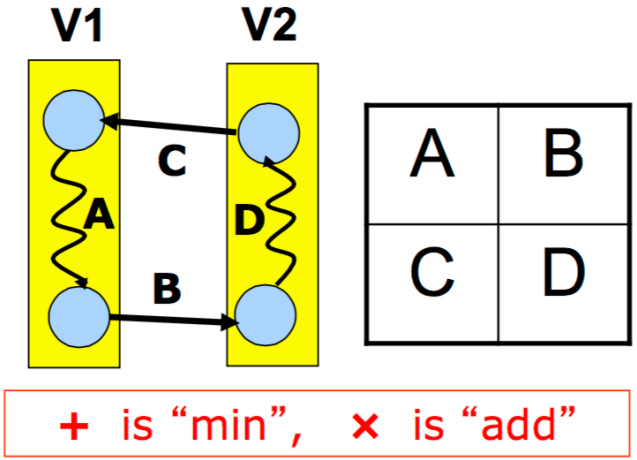
Cost first step: $O(n^3)$ additions and $O(n^2)$ min operations.
Cost path reconstruction: the Shortest-path tree can be calculated for each node in $O(|E|)$ time using $O(n)$ memory to store each tree.

All-pairs shortest paths

- **Floyd-Warshall** more suitable for denser graphs
- In parallel, Floyd-Warshall can be competitive even for sparser graphs, as for example on GPUs [Buluc et al., 2010].
- **Johnson's algorithm**, using for each vertex Dijkstra's single-source shortest path algorithm, requires less flops than Floyd-Warshall for sparse graphs: $O(|E| + |V| \log |V|)$ for each vertex.
- **Divide and Conquer APSP (DC-APSP)**
  - Idea presented in a proof by Aho et al showing equivalence between semiring matrix multiplication and APSP, later presented in papers by Tiskin, Park et al.
  - Faster than the 3 nested loops on GPUs [Buluc et al., 2010].

Divide and conquer APSP



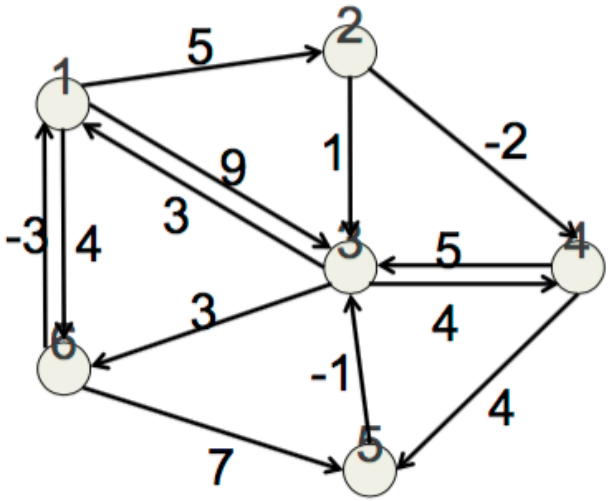


$$\begin{bmatrix} 0 & 5 & 9 & \infty & \infty & 4 \\ \infty & 0 & 1 & -2 & \infty & \infty \\ 3 & \infty & 0 & 4 & \infty & 3 \\ \infty & \infty & 5 & 0 & 4 & \infty \\ \infty & \infty & -1 & \infty & 0 & \infty \\ -3 & \infty & \infty & \infty & 7 & 0 \end{bmatrix}$$

DC-APSP(A,n)
A = DC-APSP(A,n/2);
B = AB; C = CA;
D = D + CB;
D = DC-APSP(D,n/2)
B = BD; C = DC;
A = A + BC;

Source slide: A. Buluç

Divide and conquer APSP



$$\left[\begin{array}{c|cc|ccc} 0 & 5 & 9 & \infty & \infty & 4 \\ \hline \infty & 0 & 1 & -2 & \infty & \infty \\ 3 & \infty & 0 & 4 & \infty & 3 \\ \hline \infty & \infty & 5 & 0 & 4 & \infty \\ \infty & \infty & -1 & \infty & 0 & \infty \\ -3 & \infty & \infty & \infty & 7 & 0 \end{array}\right]$$

DC-APSP(A,n)

find APSP in V_1

A = DC-APSP(A,n/2);

propagate paths from V_1 to V_2

B = AB;

propagate paths from V_2 to V_1

C = CA;

update paths in V_2

D = D + CB;

find APSP in V_2

D = DC-APSP(D,n/2)

find SP from V_1 to V_2, V_2 to V_1

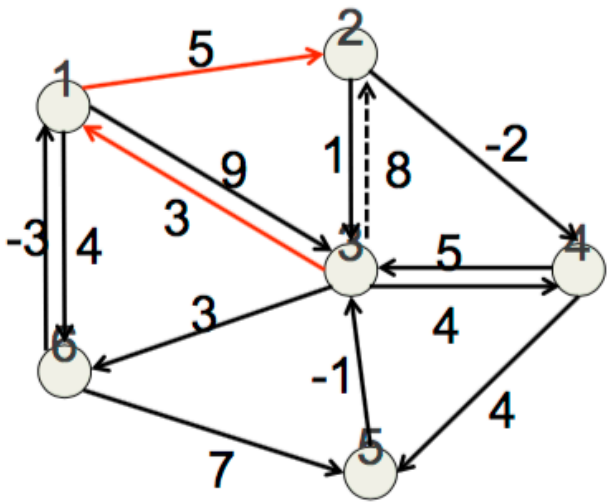
B = BD; C = DC;

find APSP in V_1

A = A + BC;

Source slide: A. Buluç

Divide and conquer APSP



$$\begin{bmatrix} \infty \\ 3 \end{bmatrix} \quad \begin{bmatrix} 5 & 9 \end{bmatrix} = \begin{bmatrix} \infty & \infty \\ 8 & 12 \end{bmatrix}$$

C **B**

The cost of 3-1-2 path

$$d(3,2) = d(3,1) + d(1,2) \xrightarrow{then} \Pi(3,2) = \Pi(1,2)$$

$$\begin{bmatrix} 0 & 5 & 9 & \infty & \infty & 4 \\ \infty & 0 & 1 & -2 & \infty & \infty \\ 3 & \mathbf{8} & 0 & 4 & \infty & 3 \\ \infty & \infty & 5 & 0 & 4 & \infty \\ \infty & \infty & -1 & \infty & 0 & \infty \\ -3 & \infty & \infty & \infty & 7 & 0 \end{bmatrix}$$

Distances

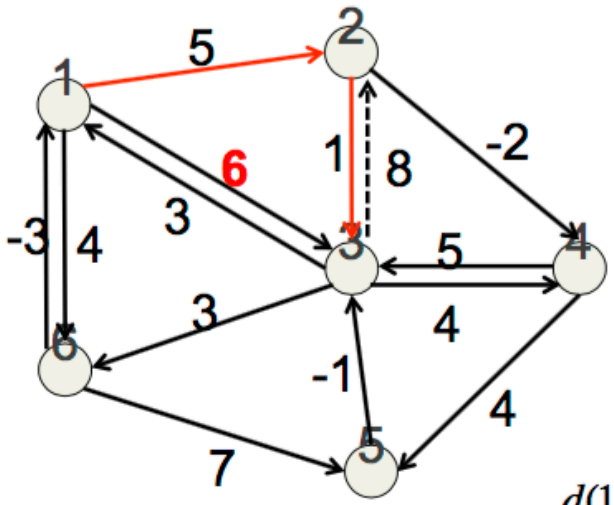
$$\Pi = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 2 & 2 & 2 & 2 & 2 & 2 \\ 3 & \mathbf{1} & 3 & 3 & 3 & 3 \\ 4 & 4 & 4 & 4 & 4 & 4 \\ 5 & 5 & 5 & 5 & 5 & 5 \\ 6 & 6 & 6 & 6 & 6 & 6 \end{bmatrix}$$

Parents

CB: update paths in V_2.

Source slide: A. Buluç.

Divide and conquer APSP



D = DC-APSP(D): no change

$$\begin{bmatrix} 5 & 9 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 8 & 0 \end{bmatrix} = \begin{bmatrix} 5 & 6 \end{bmatrix}$$

B **D**

Path: 1-2-3

$$d(1,3) = d(1,2) + d(2,3) \xrightarrow{then} \Pi(1,3) = \Pi(2,3)$$

$$\begin{bmatrix} 0 & 5 & \mathbf{6} & \infty & \infty & 4 \\ \infty & 0 & 1 & -2 & \infty & \infty \\ 3 & 8 & 0 & 4 & \infty & 3 \\ \infty & \infty & 5 & 0 & 4 & \infty \\ \infty & \infty & -1 & \infty & 0 & \infty \\ -3 & \infty & \infty & \infty & 7 & 0 \end{bmatrix}$$

Distances

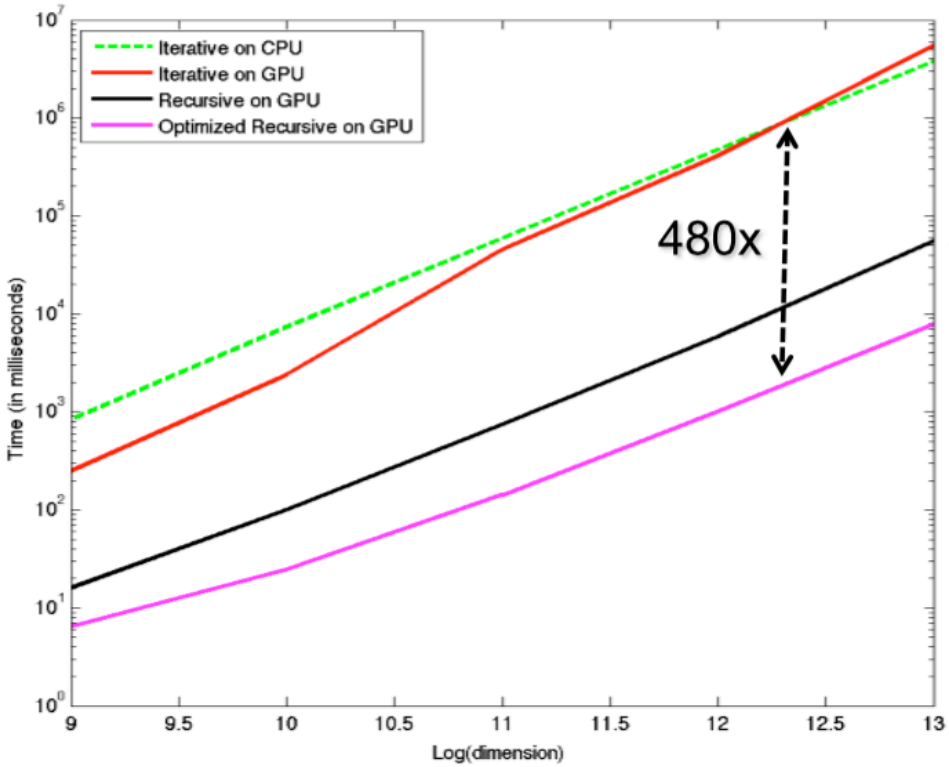
$$\Pi = \begin{bmatrix} 1 & 1 & \mathbf{2} & 1 & 1 & 1 \\ 2 & 2 & 2 & 2 & 2 & 2 \\ 3 & 1 & 3 & 3 & 3 & 3 \\ 4 & 4 & 4 & 4 & 4 & 4 \\ 5 & 5 & 5 & 5 & 5 & 5 \\ 6 & 6 & 6 & 6 & 6 & 6 \end{bmatrix}$$

Parents

BD: find SP from V_1 to V_2.

Source slide: A. Buluç.

Divide and conquer APSP - results



Floyd-Warshall ported to GPU

Naïve recursive implementation

The right primitive (Matrix multiply)

A. Buluç, J. R. Gilbert, and C. Budak. Solving path problems on the GPU. Parallel Computing, 36(5-6):241 - 253, 2010.

- GPU: Nvidia GeForce 8800 Ultra
- Dense graph of at most 8192 vertices
- Matrix multiply optimized by modifying Volkov's code

Lower bounds for APSP

Semiring matrix multiplication has same computational dependency as classic matrix multiplication, and the bounds of [Hong and Kung, 1981], [Irony et al., 2004] apply [Solomonik et al., 2013]:

Memory dependent

$$W = \Omega\left(\frac{n^3}{M^{3/2}} \cdot \frac{M}{P}\right)$$
$$S(M) = \Omega\left(\frac{n^3}{P \cdot M^{3/2}}\right)$$

Memory independent

$$W = \Omega\left(\frac{n^2}{P^{2/3}}\right)$$
$$S = \Omega(\log P)$$

Latency bandwidth trade-off for DC-APSP

Divide and conquer APSP has dependencies similar to 2.5D LU factorization. Hence the same latency-bandwidth trade-off exists [Solomonik et al., 2013]:

If each processor stores $M = cn^2/P$ copies of data, then:

$$S \cdot W = \Omega(\sqrt{cP})$$

and if we want to decrease the bandwidth cost by a factor of $\sqrt{c}$ we obtain:

$$W = \Omega\left(\frac{n^2}{\sqrt{cP}}\right), \quad S = \Omega(\sqrt{cP})$$

Parallelizing APSP

Grid of processors: $\sqrt{P/c} \times \sqrt{P/c} \times c$

Floyd-Warshall: a communication optimal algorithm can be obtained by using the same idea as 2.5D dense matrix multiply $\rightarrow$ 2.5D-SMMM.

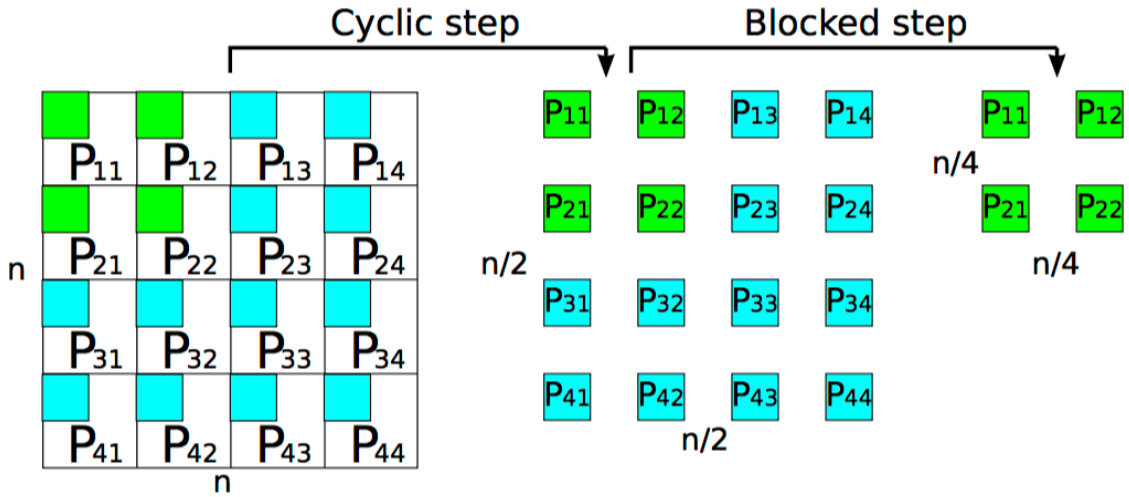
DC-APSP

- To minimize latency, 1/8-th of the processors should be assigned to solving a sub-problem
  $\rightarrow$ but then only 1/8-th of the processors are active

Solution: 2.5D block cyclic DC-APSP [Solomonik et al., 2013]

2.5D block cylic DC-APSP

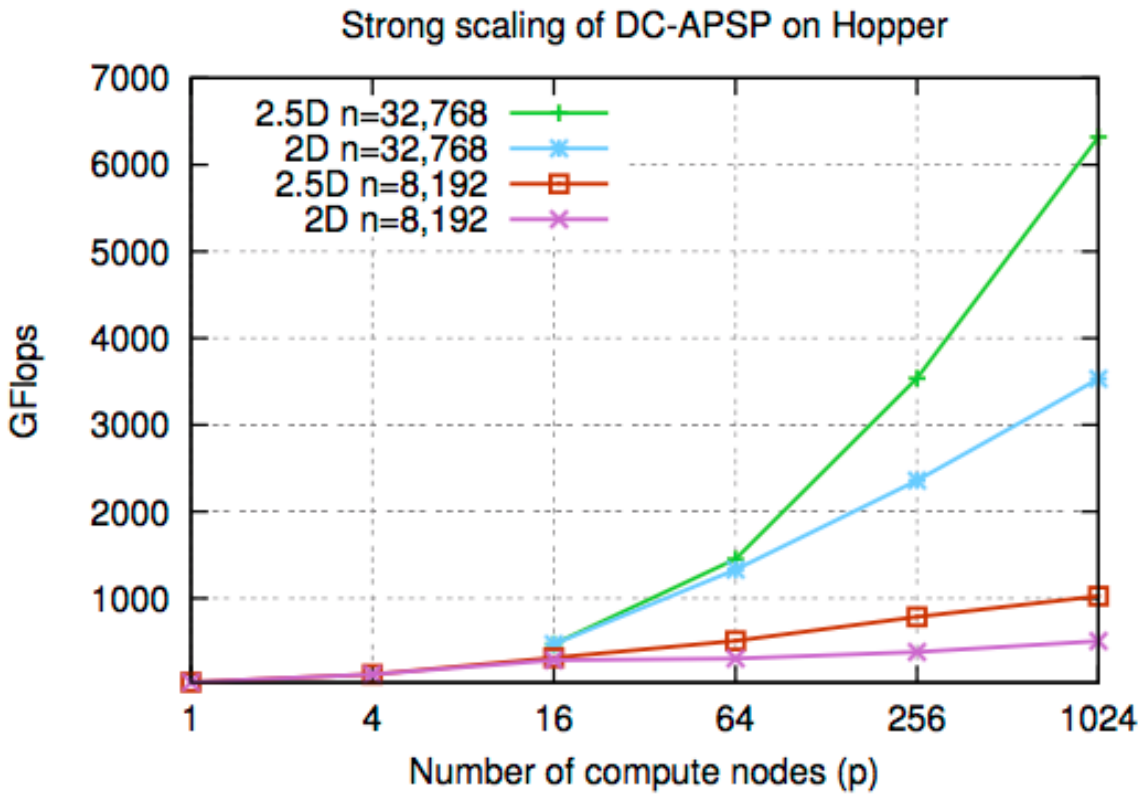
- Use 2.5D block cyclic DC-APSP until $c = 1$
  For block size $b = O(n/c)$, there are $O(\log c)$ recursive steps
- When $c = 1$, $P \geq 1$, switch to 2.5D-SMMM.



Communication optimal:

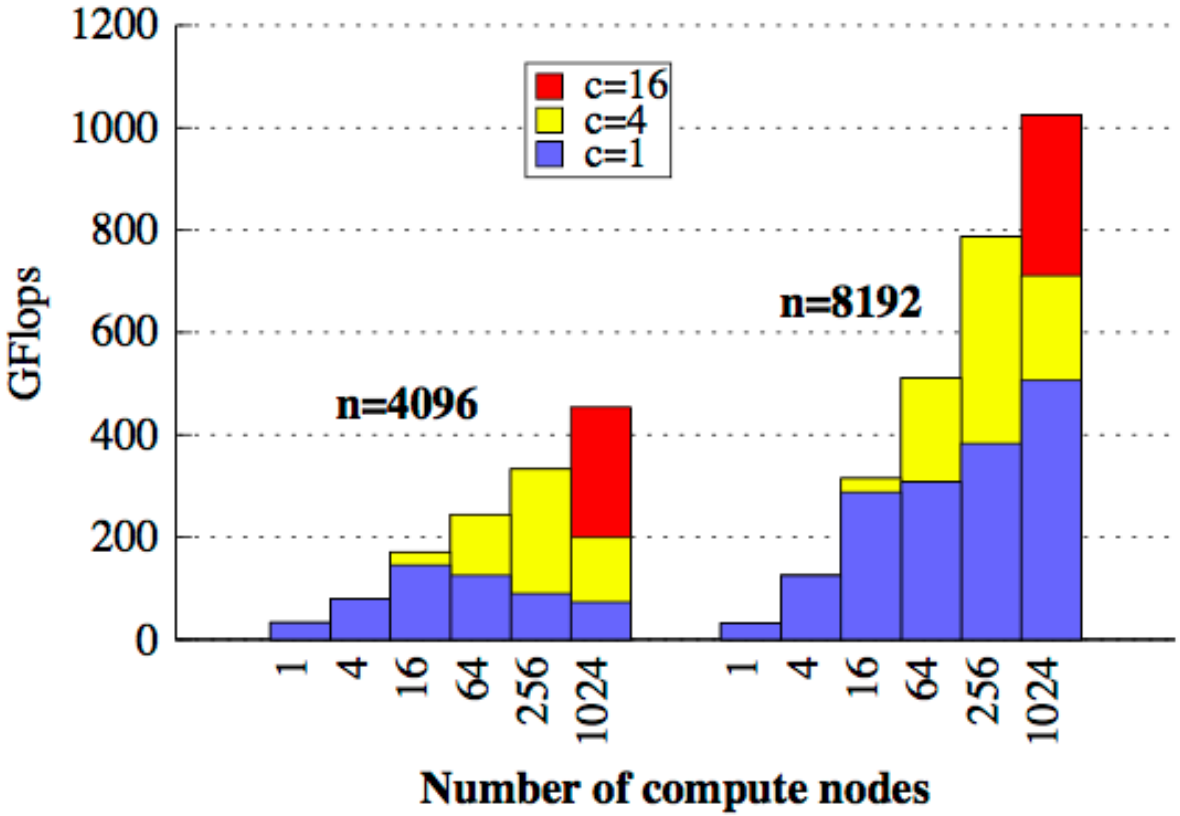
$$W = O(n^2/\sqrt{cP}), \quad S = O(\sqrt{cP}\log^2 P)$$

Experimental results [Solomonik et al., 2013]



- Hopper, Cray XE6, each node is a dual-socket 12-core Magny-Cours Opteron.
- Threaded Semiring-Matrix-Matrix-Multiply achieves 25% of peak performance (13.6 GFlops) on 6 cores (no fused multiply-add operation for the semiring).
- Strong scaling data: best performance for any replication factor c (often $c = 4$).
- On 24,276 cores, 2.5D faster by 1.8x for $n = 8,192$ and 2.0x for $n = 32,768$.

Experimental results [Solomonik et al., 2013]



- In the figure, bars stacked such that $c = 4$ case shows the benefit over $c = 1$ case.
- For $n = 4096$, $c = 16$ leads to a speed-up of 6.2x with respect to $c = 1$.

Conclusions

- Open problems:
  - Identify lower bounds on communication for other operations: LU, QR, etc.
  - Study other graph algorithms

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