Parallel Numerical Algorithms

Chapter 4 – Sparse Linear Systems
Section 4.1 – Direct Methods

Michael T. Heath and Edgar Solomonik

Department of Computer Science
University of Illinois at Urbana-Champaign

CS 554 / CSE 512

Outline

Sparse Matrices

- Matrix is *sparse* if most of its entries are zero
- For efficiency, store and operate on only nonzero entries, e.g., $a_{jk} \cdot x_k$ need not be done if $a_{jk} = 0$
- But more complicated data structures required incur extra overhead in storage and arithmetic operations
- Matrix is “usefully” sparse if it contains enough zero entries to be worth taking advantage of them to reduce storage and work required
- In practice, grid discretizations often yield matrices with $\Theta(n)$ nonzero entries, i.e., (small) constant number of nonzeros per row or column

Graph Model

- *Adjacency Graph* $G(\boldsymbol{A})$ of symmetric $n \times n$ matrix $\boldsymbol{A}$ is undirected graph having n vertices, with edge between vertices i and j if $a_{ij} \neq 0$
- Number of edges in $G(\boldsymbol{A})$ is the number of nonzeros in $\boldsymbol{A}$
- For a grid-based discretization, $G(\boldsymbol{A})$ is the grid
- Adjacency graph provides visual representation of algorithms and highlights connections between numerical and combinatorial algorithms
- For nonsymmetric $\boldsymbol{A}$, $G(\boldsymbol{A})$ would be directed
- Often convenient to think of a_{ij} as the weight of edge (i, j)

Sparse Matrix Representations

- *Coordinate (COO)* (naive) format – store each nonzero along with its row and column index
- *Compressed-sparse-row (CSR)* format
  - Store value and column index for each nonzero
  - Store index of first nonzero for each row
- Storage for CSR is less than COO and CSR ordering is often convenient
- CSC (compressed-sparse column), blocked versions (e.g. CSB), and other storage formats are also used

Sparse Matrix Distributions

- Dense matrix mappings can be adapted to sparse matrices
  - 1-D blocked mapping – store all nonzeros in n/p consecutive rows on each processor
  - 1-D cyclic or randomized mapping – store all nonzeros in some subset of n/p rows on each processor
  - 2-D block mapping – store all nonzeros in a $n/\sqrt{p} \times n/\sqrt{p}$ block of matrix
- 1-D blocked mappings are best for exploiting locality in graph, especially when there are $\Theta(n)$ nonzeros
- Row ordering matters for all mappings, randomization and cyclicity yield load balance, blocking can yield locality

Sparse Matrix Vector Multiplication

- *Sparse matrix vector multiplication (SpMV)* is

  $$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$$

  where $\boldsymbol{A}$ is sparse and $\boldsymbol{x}$ is dense

- CSR-based matrix-vector product, for all i (in parallel) do

  $$y_i = \sum_j a_{i,c(j)} x_{c(j)} = \sum_{j=1}^{n} a_{ij} x_j$$

  where $c(j)$ is the index of the jth nonzero in row i

- For random 1-D or 2-D mapping, cost of vector communication is same as in corresponding dense case

SpMV with 1-D Mapping

- For 1D blocking (each processor owns n/p rows), number of elements of x needed by a processor is the number of columns with a nonzero in the rows it owns
- In general, want to order rows to minimize maximum number of vector elements needed on any processor
- Graphically, we want to partition the graph into p subsets of n/p nodes, to minimize the maximum number of nodes to which any subset is connected, i.e., for $G(\boldsymbol{A}) = (V, E)$,

  $$V = V_1 \cup \cdots \cup V_p, \quad |V_i| = n/p$$

  is selected to minimize the largest number of external vertices adjacent to any partition,

  $$\max_i(|\{v : v \in V \setminus V_i, \exists w \in V_i, (v, w) \in E\}|)$$

Surface Area to Volume Ratio in SpMV

- The number of external vertices the maximum partition is adjacent to depends on the *expansion* of the graph
- Expansion can be interpreted as a measure of the surface-area to volume ratio of the subgraphs
- For example, for a $k \times k \times k$ grid, a subvolume of $k/p^{1/3} \times k/p^{1/3} \times k/p^{1/3}$ has surface area $\Theta(k^2/p^{2/3})$
- Communication for this case becomes a neighbor *halo exchange* on a 3-D processor mesh
- Thus, finding the best 1-D partitioning for SpMV often corresponds to *domain partitioning* and depends on the physical geometry of the problem

Other Sparse Matrix Products

- SpMV is of critical importance to many numerical methods, but suffers from a *low flop-to-byte ratio* and a potentially high communication bandwidth cost
- In graph algorithms *SpMSpV* ($\boldsymbol{x}$ and $\boldsymbol{y}$ are sparse) is prevalent, which is even harder to perform efficiently (e.g., to minimize work need layout other than CSR, like CSC)
- *SpMM* ($\boldsymbol{x}$ becomes dense matrix $\boldsymbol{X}$) provides a higher flop-to-byte ratio and is much easier to do efficiently
- *SpGEMM* (SpMSpM) (matrix multiplication where all matrices are sparse) arises in e.g., algebraic multigrid and graph algorithms, efficiency is highly dependent on sparsity

Solving Triangular Sparse Linear Systems

Given sparse lower-triangular matrix $\boldsymbol{L}$ and vector $\boldsymbol{b}$, solve

$$\boldsymbol{L}\boldsymbol{x} = \boldsymbol{b}$$

- all nonzeros of $\boldsymbol{L}$ must be in its lower-triangular part
- Sequential algorithm: take $x_i = b_i/l_{ii}$, update

$$b_j = b_j - l_{ji}x_i \quad \text{for all} \quad j \in \{i+1, \ldots, n\}$$

- If $\boldsymbol{L}$ has $m > n$ nonzeros, require $Q_1 \approx 2m$ operations

Parallelism in Sparse Triangular Solve

- We can adapt any dense parallel triangular solve algorithm to the sparse case
  - Again have fan-in (left-looking) and fan-out (right-looking) variants
  - Communication cost stays the same, computational cost decreases
- In fact there may be additional sources of parallelism, e.g., if $l_{21} = 0$, we can solve for x_1 and x_2 concurrently
- More generally, can *concurrently prune leaves* of directed acyclic adjacency graph (DAG) $G(\boldsymbol{A}) = (V, E)$, where $(i, j) \in E$ if $l_{ij} \neq 0$
- Depth of algorithm corresponds to diameter of this DAG

Parallel Algorithm for Sparse Triangular Solve

- *Partition*: associate fine-grain tasks with each (i, j) such that $l_{ij} \neq 0$
- *Communicate*: task (i, i) communicates with task (j, i) and (i, j) for all possible j
- *Agglomerate*: form coarse-grain tasks for each column of $\boldsymbol{L}$, i.e., do 1-D agglomeration, combining fine-grain tasks $(\star, i)$ into agglomerated task i
- *Map*: assign coarse-grain tasks (columns of $\boldsymbol{L}$) to processors with blocking (for locality) and/or cyclicity (for load balance and concurrency)

Analysis of 1-D Parallel Sparse Triangular Solve

- Cost of 1-D algorithm will clearly be less than the corresponding algorithm for the dense case
- Load balance depends on distribution of nonzeros, cyclicity can help distribute dense blocks
- Naive algorithm with 1-D column blocking exploits concurrency only in fan-out updates
- Communication bandwidth cost depends on surface-to-volume ratio of each subset of vertices associated with a block of columns
- Higher concurrency and better performance possible with dynamic/adaptive algorithms

Cholesky Factorization

- Symmetric positive definite matrix $\boldsymbol{A}$ has *Cholesky factorization*

  $$\boldsymbol{A} = \boldsymbol{L}\boldsymbol{L}^T$$

  where $\boldsymbol{L}$ is lower triangular matrix with positive diagonal entries

- Linear system

  $$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$$

  can then be solved by forward-substitution in lower triangular system $\boldsymbol{L}\boldsymbol{y} = \boldsymbol{b}$, followed by back-substitution in upper triangular system $\boldsymbol{L}^T\boldsymbol{x} = \boldsymbol{y}$

Computing Cholesky Factorization

- Algorithm for computing Cholesky factorization can be derived by equating corresponding entries of $\boldsymbol{A}$ and $\boldsymbol{L}\boldsymbol{L}^T$ and generating them in correct order
- For example, in 2×2 case

$$\begin{bmatrix} a_{11} & a_{21} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} \ell_{11} & 0 \\ \ell_{21} & \ell_{22} \end{bmatrix} \begin{bmatrix} \ell_{11} & \ell_{21} \\ 0 & \ell_{22} \end{bmatrix}$$

so we have

$$\ell_{11} = \sqrt{a_{11}}, \quad \ell_{21} = a_{21}/\ell_{11}, \quad \ell_{22} = \sqrt{a_{22} - \ell_{21}^2}$$

Cholesky Factorization Algorithm

```
for $k = 1$ to $n$
    $a_{kk} = \sqrt{a_{kk}}$
    for $i = k + 1$ to $n$
        $a_{ik} = a_{ik} / a_{kk}$
    end
    for $j = k + 1$ to $n$
        for $i = j$ to $n$
            $a_{ij} = a_{ij} - a_{ik}\, a_{jk}$
        end
    end
end
```

Cholesky Factorization Algorithm

- All n square roots are of positive numbers, so algorithm well defined
- Only lower triangle of $\boldsymbol{A}$ is accessed, so strict upper triangular portion need not be stored
- Factor $\boldsymbol{L}$ computed in place, overwriting lower triangle of $\boldsymbol{A}$
- Pivoting is not required for numerical stability
- About $n^3/6$ multiplications and similar number of additions are required (about half as many as for LU)

Parallel Algorithm

Partition

- For $i, j = 1, \dots, n$, fine-grain task (i, j) stores a_{ij} and computes and stores

  $$\begin{cases} \ell_{ij}, & \text{if } i \geq j \\ \ell_{ji}, & \text{if } i < j \end{cases}$$

  yielding 2-D array of n^2 fine-grain tasks

- Zero entries in upper triangle of $\boldsymbol{L}$ need not be computed or stored, so for convenience in using 2-D mesh network, ℓ_{ij} can be redundantly computed as both task (i, j) and task (j, i) for $i > j$

Fine-Grain Tasks and Communication

$$\begin{tikzcd}
\substack{a_{11}\\ \ell_{11}} \arrow[r] \arrow[d] & \substack{a_{21}\\ \ell_{21}} \arrow[r] \arrow[d] & \substack{a_{31}\\ \ell_{31}} \arrow[r] \arrow[d] & \substack{a_{41}\\ \ell_{41}} \arrow[r] \arrow[d] & \substack{a_{51}\\ \ell_{51}} \arrow[r] \arrow[d] & \substack{a_{61}\\ \ell_{61}} \arrow[d] \\
\substack{a_{21}\\ \ell_{21}} \arrow[r] \arrow[d] & \substack{a_{22}\\ \ell_{22}} \arrow[r] \arrow[d] & \substack{a_{32}\\ \ell_{32}} \arrow[r] \arrow[d] & \substack{a_{42}\\ \ell_{42}} \arrow[r] \arrow[d] & \substack{a_{52}\\ \ell_{52}} \arrow[r] \arrow[d] & \substack{a_{62}\\ \ell_{62}} \arrow[d] \\
\substack{a_{31}\\ \ell_{31}} \arrow[r] \arrow[d] & \substack{a_{32}\\ \ell_{32}} \arrow[r] \arrow[d] & \substack{a_{33}\\ \ell_{33}} \arrow[r] \arrow[d] & \substack{a_{43}\\ \ell_{43}} \arrow[r] \arrow[d] & \substack{a_{53}\\ \ell_{53}} \arrow[r] \arrow[d] & \substack{a_{63}\\ \ell_{63}} \arrow[d] \\
\substack{a_{41}\\ \ell_{41}} \arrow[r] \arrow[d] & \substack{a_{42}\\ \ell_{42}} \arrow[r] \arrow[d] & \substack{a_{43}\\ \ell_{43}} \arrow[r] \arrow[d] & \substack{a_{44}\\ \ell_{44}} \arrow[r] \arrow[d] & \substack{a_{54}\\ \ell_{54}} \arrow[r] \arrow[d] & \substack{a_{64}\\ \ell_{64}} \arrow[d] \\
\substack{a_{51}\\ \ell_{51}} \arrow[r] \arrow[d] & \substack{a_{52}\\ \ell_{52}} \arrow[r] \arrow[d] & \substack{a_{53}\\ \ell_{53}} \arrow[r] \arrow[d] & \substack{a_{54}\\ \ell_{54}} \arrow[r] \arrow[d] & \substack{a_{55}\\ \ell_{55}} \arrow[r] \arrow[d] & \substack{a_{65}\\ \ell_{65}} \arrow[d] \\
\substack{a_{61}\\ \ell_{61}} \arrow[r] & \substack{a_{62}\\ \ell_{62}} \arrow[r] & \substack{a_{63}\\ \ell_{63}} \arrow[r] & \substack{a_{64}\\ \ell_{64}} \arrow[r] & \substack{a_{65}\\ \ell_{65}} \arrow[r] & \substack{a_{66}\\ \ell_{66}}
\end{tikzcd}$$

Fine-Grain Parallel Algorithm

```
**for** $k = 1$ **to** $\min(i, j) - 1$
    recv broadcast of $a_{kj}$ from task $(k, j)$
    recv broadcast of $a_{ik}$ from task $(i, k)$
    $a_{ij} = a_{ij} - a_{ik}\, a_{kj}$
**end**
**if** $i = j$ **then**
    $a_{ii} = \sqrt{a_{ii}}$
    broadcast $a_{ii}$ to tasks $(k, i)$ and $(i, k)$, $k = i + 1, \dots, n$
**else if** $i < j$ **then**
    recv broadcast of $a_{ii}$ from task $(i, i)$
    $a_{ij} = a_{ij} / a_{ii}$
    broadcast $a_{ij}$ to tasks $(k, j)$, $k = i + 1, \dots, n$
**else**
    recv broadcast of $a_{jj}$ from task $(j, j)$
    $a_{ij} = a_{ij} / a_{jj}$
    broadcast $a_{ij}$ to tasks $(i, k)$, $k = j + 1, \dots, n$
**end**
```

Agglomeration Schemes

Agglomerate

- Agglomeration of fine-grain tasks produces
  - 2-D
  - 1-D column
  - 1-D row

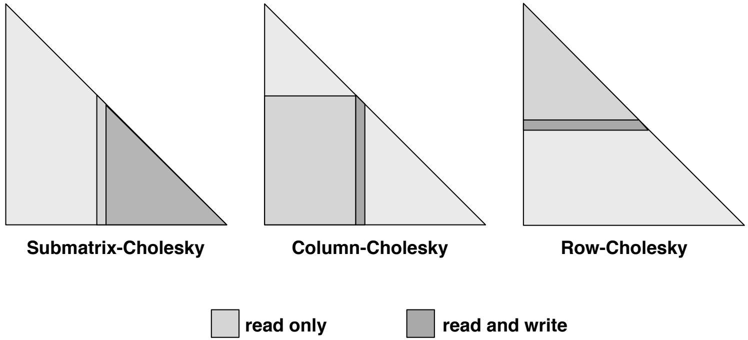
  parallel algorithms analogous to those for LU factorization, with similar performance and scalability

Loop Orderings for Cholesky

Each choice of i, j, or k index in outer loop yields different Cholesky algorithm, named for portion of matrix updated by basic operation in inner loops

- *Submatrix-Cholesky*: (fan-out) with k in outer loop, inner loops perform rank-1 update of remaining unreduced *submatrix* using current column
- *Column-Cholesky*: (fan-in) with j in outer loop, inner loops compute current *column* using matrix-vector product that accumulates effects of previous columns
- *Row-Cholesky*: (fan-in) with i in outer loop, inner loops compute current *row* by solving triangular system involving previous rows

Memory Access Patterns



Column-Oriented Cholesky Algorithms

Submatrix-Cholesky

```
for $k = 1$ to $n$
    $a_{kk} = \sqrt{a_{kk}}$
    for $i = k+1$ to $n$
        $a_{ik} = a_{ik}/a_{kk}$
    end
    for $j = k+1$ to $n$
        for $i = j$ to $n$
            $a_{ij} = a_{ij} - a_{ik}\, a_{jk}$
        end
    end
end
```

Column-Cholesky

```
for $j = 1$ to $n$
    for $k = 1$ to $j-1$
        for $i = j$ to $n$
            $a_{ij} = a_{ij} - a_{ik}\, a_{jk}$
        end
    end
    $a_{jj} = \sqrt{a_{jj}}$
    for $i = j+1$ to $n$
        $a_{ij} = a_{ij}/a_{jj}$
    end
end
```

Column Operations

Column-oriented algorithms can be stated more compactly by introducing column operations

- *cdiv*$(\, j\,)$: column j is divided by square root of its diagonal entry

```
$a_{jj} = \sqrt{a_{jj}}$
for $i = j + 1$ to $n$
    $a_{ij} = a_{ij} / a_{jj}$
end
```

- *cmod*$(\, j, k)$: column j is modified by multiple of column k, with $k < j$

```
for $i = j$ to $n$
    $a_{ij} = a_{ij} - a_{ik}\, a_{jk}$
end
```

Column-Oriented Cholesky Algorithms

Submatrix-Cholesky

```
for $k = 1$ to $n$
    cdiv$(k)$
    for $j = k + 1$ to $n$
        cmod$(j, k)$
    end
end
```

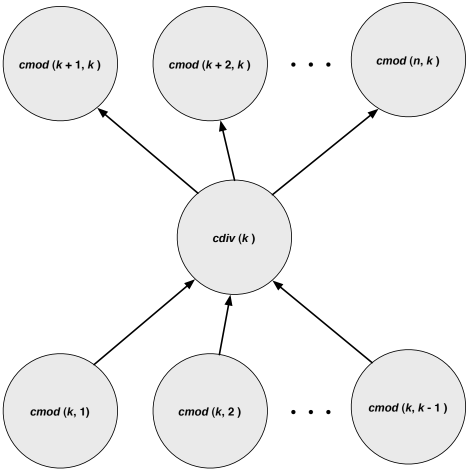
- right-looking
- immediate-update
- data-driven
- fan-out

Column-Cholesky

```
for $j = 1$ to $n$
    for $k = 1$ to $j - 1$
        cmod$(j, k)$
    end
    cdiv$(j)$
end
```

- left-looking
- delayed-update
- demand-driven
- fan-in

Data Dependences



Data Dependences

- *cmod* $(k, \star)$ operations along bottom can be done in any order, but they all have same target column, so updating must be coordinated to preserve data integrity
- *cmod* $(\star, k)$ operations along top can be done in any order, and they all have different target columns, so updating can be done simultaneously
- Performing *cmods* concurrently is most important source of parallelism in column-oriented factorization algorithms
- For dense matrix, each *cdiv* (k) depends on immediately preceding column, so *cdivs* must be done sequentially

Sparsity Structure

- For sparse matrix $\boldsymbol{M}$, let $\boldsymbol{M}_{i\star}$ denote its ith row and $\boldsymbol{M}_{\star j}$ its jth column
- Define *Struct*$(\boldsymbol{M}_{i\star}) = \{k < i \mid m_{ik} \neq 0\}$, nonzero structure of row i of strict lower triangle of $\boldsymbol{M}$
- Define *Struct*$(\boldsymbol{M}_{\star j}) = \{k > j \mid m_{kj} \neq 0\}$, nonzero structure of column j of strict lower triangle of $\boldsymbol{M}$

Sparse Cholesky Algorithms

Submatrix-Cholesky

```
for $k = 1$ to $n$
    cdiv( $k$ )
    for $j \in$ Struct($\boldsymbol{L}_{\star k}$)
        cmod( $j, k$ )
    end
end
```

- right-looking
- immediate-update
- data-driven
- fan-out

Column-Cholesky

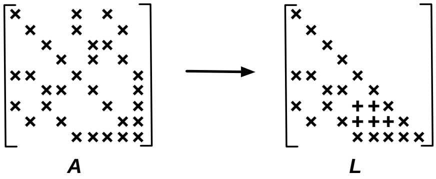
```
for $j = 1$ to $n$
    for $k \in$ Struct($\boldsymbol{L}_{j \star}$)
        cmod( $j, k$ )
    end
    cdiv( $j$ )
end
```

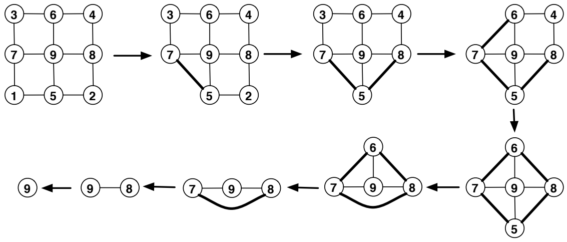
- left-looking
- delayed-update
- demand-driven
- fan-in

Graph Model

- Recall that adjacency graph $G(\boldsymbol{A})$ of symmetric $n \times n$ matrix $\boldsymbol{A}$ is undirected graph with edge between vertices i and j if $a_{ij} \neq 0$
- At each step of Cholesky factorization algorithm, corresponding vertex is eliminated from graph
  - Neighbors of eliminated vertex in previous graph become *clique* (fully connected subgraph) in modified graph
  - Entries of $\boldsymbol{A}$ that were initially zero may become nonzero entries, called *fill*

Example: Graph Model of Elimination





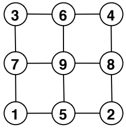
Elimination Tree

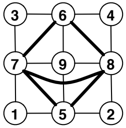
- *parent*(j) is row index of first offdiagonal nonzero in column j of $\boldsymbol{L}$, if any, and j otherwise
- *Elimination tree* $T(\boldsymbol{A})$ is graph having n vertices, with edge between vertices i and j, for $i > j$, if $i =$ *parent*(j)
- If matrix is irreducible, then elimination tree is single tree with root at vertex n; otherwise, it is more accurately termed *elimination forest*
- $T(\boldsymbol{A})$ is spanning tree for *filled graph*, $F(\boldsymbol{A})$, which is $G(\boldsymbol{A})$ with all fill edges added
- Each column of Cholesky factor $\boldsymbol{L}$ depends only on its descendants in elimination tree

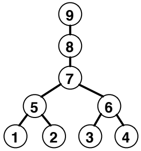
Example: Elimination Tree

$$
\begin{bmatrix}
\times & & & & \times & & \times & & \\
& \times & & & \times & & & \times & \\
& & \times & & & \times & \times & & \\
& & & \times & & \times & & \times & \\
\times & \times & & & \times & & & & \times \\
& & \times & \times & & \times & & & \times \\
\times & & \times & & & & \times & & \times \\
& \times & & \times & & & & \times & \times \\
& & & & \times & \times & \times & \times & \times
\end{bmatrix}
\qquad
\begin{bmatrix}
\times & & & & & & & & \\
& \times & & & & & & & \\
& & \times & & & & & & \\
& & & \times & & & & & \\
\times & \times & & & \times & & & & \\
& & \times & \times & & \times & & & \\
\times & & \times & & + & + & \times & & \\
& \times & & \times & + & + & + & \times & \\
& & & & \times & \times & \times & \times & \times
\end{bmatrix}
$$

A $\qquad$ L


$G\,(A)$


$F\,(A)$


$T\,(A)$

Effect of Matrix Ordering

- Amount of fill depends on order in which variables are eliminated
- Example: “arrow” matrix — if first row and column are dense, then factor fills in completely, but if last row and column are dense, then they cause no fill

$$
\begin{bmatrix}
\times & \times & \times & \times & \times & \times & \times & \times & \times \\
\times & \times & & & & & & & \\
\times & & \times & & & & & & \\
\times & & & \times & & & & & \\
\times & & & & \times & & & & \\
\times & & & & & \times & & & \\
\times & & & & & & \times & & \\
\times & & & & & & & \times & \\
\times & & & & & & & & \times
\end{bmatrix}
\qquad
\begin{bmatrix}
\times & & & & & & & & \times \\
& \times & & & & & & & \times \\
& & \times & & & & & & \times \\
& & & \times & & & & & \times \\
& & & & \times & & & & \times \\
& & & & & \times & & & \times \\
& & & & & & \times & & \times \\
& & & & & & & \times & \times \\
\times & \times & \times & \times & \times & \times & \times & \times & \times
\end{bmatrix}
$$

Ordering Heuristics

General problem of finding ordering that minimizes fill is NP-complete, but there are relatively cheap heuristics that limit fill effectively

- *Bandwidth or profile reduction*: reduce distance of nonzero diagonals from main diagonal (e.g., RCM)
- *Minimum degree*: eliminate node having fewest neighbors first
- *Nested dissection*: recursively split graph into pieces using a *vertex separator*, numbering separator vertices last

Symbolic Factorization

- For symmetric positive definite (SPD) matrices, ordering can be determined in advance of numeric factorization
- Only locations of nonzeros matter, not their numerical values, since pivoting is not required for numerical stability
- Once ordering is selected, locations of all fill entries in $\boldsymbol{L}$ can be anticipated and efficient static data structure set up to accommodate them prior to numeric factorization
- Structure of column j of $\boldsymbol{L}$ is given by union of structures of lower triangular portion of column j of $\boldsymbol{A}$ and prior columns of $\boldsymbol{L}$ whose first nonzero below diagonal is in row j

Solving Sparse SPD Systems

Basic steps in solving sparse SPD systems by Cholesky factorization

1. *Ordering*: Symmetrically reorder rows and columns of matrix so Cholesky factor suffers relatively little fill
2. *Symbolic factorization*: Determine locations of all fill entries and allocate data structures in advance to accommodate them
3. *Numeric factorization*: Compute numeric values of entries of Cholesky factor
4. *Triangular solve*: Compute solution by forward- and back-substitution

Parallel Sparse Cholesky

- In sparse submatrix- or column-Cholesky, if $a_{jk} = 0$, then *cmod*(j,k) is omitted
- Sparse factorization thus has additional source of parallelism, since “missing” *cmods* may permit multiple *cdivs* to be done simultaneously
- Elimination tree shows data dependences among columns of Cholesky factor $\boldsymbol{L}$, and hence identifies potential parallelism
- At any point in factorization process, all factor columns corresponding to *leaves* in the elimination tree can be computed simultaneously

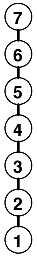
Parallel Sparse Cholesky

- *Height* of elimination tree determines longest serial path through computation, and hence parallel execution time
- *Width* of elimination tree determines degree of parallelism available
- Short, wide, well-balanced elimination tree desirable for parallel factorization
- Structure of elimination tree depends on ordering of matrix
- So ordering should be chosen *both* to preserve sparsity and to enhance parallelism

Levels of Parallelism in Sparse Cholesky

- *Fine-grain*
    - Task is one multiply-add pair
    - Available in either dense or sparse case
    - Difficult to exploit effectively in practice
- *Medium-grain*
    - Task is one *cmod* or *cdiv*
    - Available in either dense or sparse case
    - Accounts for most of speedup in dense case
- *Large-grain*
    - Task computes entire set of columns in subtree of elimination tree
    - Available only in sparse case

Example: Band Ordering, 1-D Grid



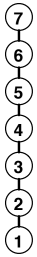
G (A)

$$\begin{bmatrix} \times & \times & & & & & \\ \times & \times & \times & & & & \\ & \times & \times & \times & & & \\ & & \times & \times & \times & & \\ & & & \times & \times & \times & \\ & & & & \times & \times & \times \\ & & & & & \times & \times \end{bmatrix}$$

A

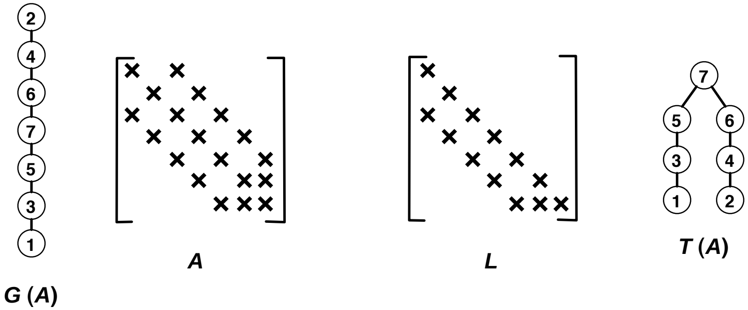
$$\begin{bmatrix} \times & & & & & & \\ \times & \times & & & & & \\ & \times & \times & & & & \\ & & \times & \times & & & \\ & & & \times & \times & & \\ & & & & \times & \times & \\ & & & & & \times & \times \end{bmatrix}$$

L

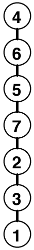


T (A)

Example: Minimum Degree, 1-D Grid



Example: Nested Dissection, 1-D Grid



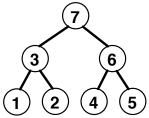
***G* (*A*)**

$$\begin{bmatrix} \times & & \times & & & & \\ & \times & \times & & & & \times \\ \times & \times & \times & & & & \\ & & & \times & & \times & \\ & & & & \times & \times & \times \\ & & & \times & \times & \times & \\ & \times & & & \times & & \times \end{bmatrix}$$

A

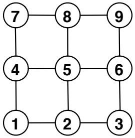
$$\begin{bmatrix} \times & & & & & & \\ & \times & & & & & \\ \times & \times & \times & & & & \\ & & & \times & & & \\ & & & & \times & & \\ & & & \times & \times & \times & \\ & \times & + & & \times & + & \times \end{bmatrix}$$

L

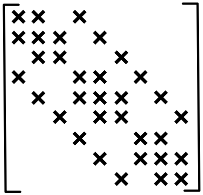


***T* (*A*)**

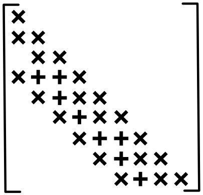
Example: Band Ordering, 2-D Grid



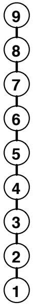
G (*A*)



A

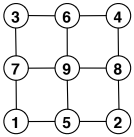


L



T (*A*)

Example: Minimum Degree, 2-D Grid



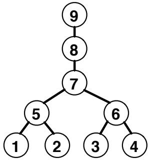
***G* (*A*)**

$$\begin{bmatrix}
\times & & & & \times & & \times & & \\
& \times & & & \times & & & \times & \\
& & \times & & & \times & \times & & \\
& & & \times & & \times & & \times & \\
\times & \times & & & \times & & & & \times \\
& & \times & \times & & \times & & & \times \\
\times & & \times & & & & \times & & \times \\
& \times & & \times & & & & \times & \times \\
& & & & \times & \times & \times & \times & \times
\end{bmatrix}$$

A

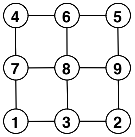
$$\begin{bmatrix}
\times & & & & & & & & \\
& \times & & & & & & & \\
& & \times & & & & & & \\
& & & \times & & & & & \\
\times & \times & & & \times & & & & \\
& & \times & \times & & \times & & & \\
\times & & \times & & + & + & \times & & \\
& \times & & \times & + & + & + & \times & \\
& & & & \times & \times & \times & \times & \times
\end{bmatrix}$$

L



***T* (*A*)**

Example: Nested Dissection, 2-D Grid



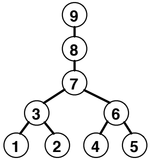
***G* (*A*)**

$$\begin{bmatrix} \times & & \times & & & & \times & & \\ & \times & \times & & & & & & \times \\ \times & \times & \times & & & & & \times & \\ & & & \times & & \times & \times & & \\ & & & & \times & \times & & & \times \\ & & & \times & \times & \times & & \times & \\ \times & & & \times & & & \times & \times & \\ & & \times & & & \times & \times & \times & \times \\ & \times & & & \times & & & \times & \times \end{bmatrix}$$

A

$$\begin{bmatrix} \times & & & & & & & & \\ & \times & & & & & & & \\ \times & \times & \times & & & & & & \\ & & & \times & & & & & \\ & & & & \times & & & & \\ & & & \times & \times & \times & & & \\ \times & & + & \times & & + & \times & & \\ & & \times & & & \times & \times & \times & \\ & \times & + & & \times & + & + & \times & \times \end{bmatrix}$$

L

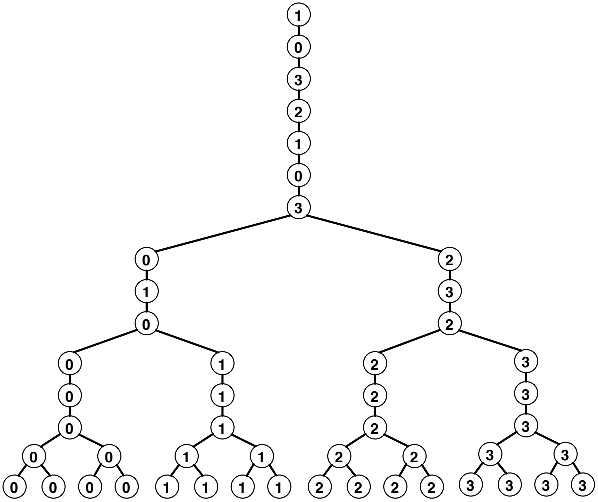


***T* (*A*)**

Mapping

- Cyclic mapping of columns to processors works well for dense problems, because it balances load and communication is global anyway
- To exploit locality in communication for sparse factorization, better approach is to map columns in *subtree* of elimination tree onto *local subset* of processors
- Still use cyclic mapping within dense submatrices (“supernodes”)

Example: Subtree Mapping



Fan-Out Sparse Cholesky

```
for $j \in$ *mycols*
    if $j$ is leaf node in $T(\boldsymbol{A})$ then
        *cdiv*$(\,j)$
        send $\boldsymbol{L}_{\star j}$ to processes in *map*(*Struct*($\boldsymbol{L}_{\star j}$))
        *mycols* $=$ *mycols* $- \{\,j\,\}$
    end
end
while *mycols* $\neq \emptyset$
    receive any column of $\boldsymbol{L}$, say $\boldsymbol{L}_{\star k}$
    for $j \in$ *mycols* $\cap$ *Struct*($\boldsymbol{L}_{\star k}$)
        *cmod*$(\,j, k)$
        if column $j$ requires no more *cmods* then
            *cdiv*$(\,j)$
            send $\boldsymbol{L}_{\star j}$ to processes in *map*(*Struct*($\boldsymbol{L}_{\star j}$))
            *mycols* $=$ *mycols* $- \{\,j\,\}$
        end
    end
end
```

Fan-In Sparse Cholesky

```
for $j = 1$ to $n$
    if $j \in$ *mycols* or *mycols* $\cap$ *Struct*$(\boldsymbol{L}_{j\star}) \neq \emptyset$ then
        $u = 0$
        for $k \in$ *mycols* $\cap$ *Struct*$(\boldsymbol{L}_{j\star})$
            $u = u + \ell_{jk}\, \boldsymbol{L}_{\star k}$
        if $j \in$ *mycols* then
            incorporate $u$ into factor column $j$
            while any aggregated update column
                for column $j$ remains, receive one
                and incorporate it into factor column $j$
            end
            *cdiv*$(j)$
        else
            send $u$ to process *map*$(j)$
        end
    end
end
```

Multifrontal Sparse Cholesky

- Multifrontal algorithm operates recursively, starting from root of elimination tree for $\boldsymbol{A}$
- Dense frontal matrix $\boldsymbol{F}_j$ is initialized to have nonzero entries from corresponding row and column of $\boldsymbol{A}$ as its first row and column, and zeros elsewhere
- $\boldsymbol{F}_j$ is then updated by *extend_add* operations with update matrices from its children in elimination tree
- *extend_add* operation, denoted by $\oplus$, merges matrices by taking union of their subscript sets and summing entries for any common subscripts
- After updating of $\boldsymbol{F}_j$ is complete, its partial Cholesky factorization is computed, producing corresponding row and column of $\boldsymbol{L}$ as well as update matrix $\boldsymbol{U}_j$

Example: *extend_add*

$$\begin{bmatrix} a_{11} & a_{13} & a_{15} & a_{18} \\ a_{31} & a_{33} & a_{35} & a_{38} \\ a_{51} & a_{53} & a_{55} & a_{58} \\ a_{81} & a_{83} & a_{85} & a_{88} \end{bmatrix} \oplus \begin{bmatrix} b_{11} & b_{12} & b_{15} & b_{17} \\ b_{21} & b_{22} & b_{25} & b_{27} \\ b_{51} & b_{52} & b_{55} & b_{57} \\ b_{71} & b_{72} & b_{75} & b_{77} \end{bmatrix}$$

$$= \begin{bmatrix} a_{11}+b_{11} & b_{12} & a_{13} & a_{15}+b_{15} & b_{17} & a_{18} \\ b_{21} & b_{22} & 0 & b_{25} & b_{27} & 0 \\ a_{31} & 0 & a_{33} & a_{35} & 0 & a_{38} \\ a_{51}+b_{51} & b_{52} & a_{53} & a_{55}+b_{55} & b_{57} & a_{58} \\ b_{71} & b_{72} & 0 & b_{75} & b_{77} & 0 \\ a_{81} & 0 & a_{83} & a_{85} & 0 & a_{88} \end{bmatrix}$$

Multifrontal Sparse Cholesky

```
Factor( $j$)
    Let $\{i_1, \dots, i_r\} = \textit{Struct}(\boldsymbol{L}_{\star j})$
    Let $\boldsymbol{F}_j = \begin{bmatrix} a_{j,j} & a_{j,i_1} & \dots & a_{j,i_r} \\ a_{i_1,j} & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ a_{i_r,j} & 0 & \dots & 0 \end{bmatrix}$
    for each child $i$ of $j$ in elimination tree
        Factor($i$)
        $\boldsymbol{F}_j = \boldsymbol{F}_j \oplus \boldsymbol{U}_i$
    end
    Perform one step of dense Cholesky:
```

$$\boldsymbol{F}_j = \begin{bmatrix} \ell_{j,j} & \boldsymbol{0} \\ \ell_{i_1,j} & \\ \vdots & \boldsymbol{I} \\ \ell_{i_r,j} & \end{bmatrix} \begin{bmatrix} 1 & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{U}_j \end{bmatrix} \begin{bmatrix} \ell_{j,j} & \ell_{i_1,j} & \dots & \ell_{i_r,j} \\ \boldsymbol{0} & & \boldsymbol{I} & \end{bmatrix}$$

Advantages of Multifrontal Method

- Most arithmetic operations performed on dense matrices, which reduces indexing overhead and indirect addressing
- Can take advantage of loop unrolling, vectorization, and optimized BLAS to run at near peak speed on many types of processors
- Data locality good for memory hierarchies, such as cache, virtual memory with paging, or explicit out-of-core solvers
- Naturally adaptable to parallel implementation by processing multiple independent fronts simultaneously on different processors
- Parallelism can also be exploited in dense matrix computations within each front

Summary for Parallel Sparse Cholesky

Principal ingredients in efficient parallel algorithm for sparse Cholesky factorization

- Reordering matrix to obtain relatively short and well balanced elimination tree while also limiting fill
- Multifrontal or supernodal approach to exploit dense subproblems effectively
- Subtree mapping to localize communication
- Cyclic mapping of dense subproblems to achieve good load balance
- 2-D algorithm for dense subproblems to enhance scalability

Scalability of Sparse Cholesky

- Performance and scalability of sparse Cholesky depend on sparsity structure of particular matrix
- Sparse factorization with nested dissection requires factorization of dense matrix of dimension $\Theta(\sqrt{n}\,)$ for 2-D grid problem with n grid points ($\sqrt{n}$ is the size of the root vertex separator), for which unconditional weak scalability is possible
- However, efficiency often deteriorates as a result of the rest of the sparse factorization taking more time

References – Dense Cholesky

- G. Ballard, J. Demmel, O. Holtz, and O. Schwartz, Communication-optimal parallel and sequential Cholesky decomposition, *SIAM J. Sci. Comput.* 32:3495-3523, 2010
- J. W. Demmel, M. T. Heath, and H. A. van der Vorst, Parallel numerical linear algebra, *Acta Numerica* 2:111-197, 1993
- D. O'Leary and G. W. Stewart, Data-flow algorithms for parallel matrix computations, *Comm. ACM* 28:840-853, 1985
- D. O'Leary and G. W. Stewart, Assignment and scheduling in parallel matrix factorization, *Linear Algebra Appl.* 77:275-299, 1986

References – Sparse Cholesky

- M. T. Heath, Parallel direct methods for sparse linear systems, D. E. Keyes, A. Sameh, and V. Venkatakrishnan, eds., *Parallel Numerical Algorithms*, pp. 55-90, Kluwer, 1997
- M. T. Heath, E. Ng and B. W. Peyton, Parallel algorithms for sparse linear systems, *SIAM Review* 33:420-460, 1991
- J. Liu, Computational models and task scheduling for parallel sparse Cholesky factorization, *Parallel Computing* 3:327-342, 1986
- J. Liu, Reordering sparse matrices for parallel elimination, *Parallel Computing* 11:73-91, 1989
- J. Liu, The role of elimination trees in sparse factorization, *SIAM J. Matrix Anal. Appl.* 11:134-172, 1990

References – Multifrontal Methods

- I. S. Duff, Parallel implementation of multifrontal schemes, *Parallel Computing* 3:193-204, 1986
- A. Gupta, Parallel sparse direct methods: a short tutorial, IBM Research Report RC 25076, November 2010
- J. Liu, The multifrontal method for sparse matrix solution: theory and practice, *SIAM Review* 34:82-109, 1992
- J. A. Scott, Parallel frontal solvers for large sparse linear systems, *ACM Trans. Math. Software* 29:395-417, 2003

References – Scalability

- A. George, J. Lui, and E. Ng, Communication results for parallel sparse Cholesky factorization on a hypercube, *Parallel Computing* 10:287-298, 1989
- A. Gupta, G. Karypis, and V. Kumar, Highly scalable parallel algorithms for sparse matrix factorization, *IEEE Trans. Parallel Distrib. Systems* 8:502-520, 1997
- T. Rauber, G. Runger, and C. Scholtes, Scalability of sparse Cholesky factorization, *Internat. J. High Speed Computing* 10:19-52, 1999
- R. Schreiber, Scalability of sparse direct solvers, A. George, J. R. Gilbert, and J. Liu, eds., *Graph Theory and Sparse Matrix Computation*, pp. 191-209, Springer-Verlag, 1993

References – Nonsymmetric Sparse Systems

- I. S. Duff and J. A. Scott, A parallel direct solver for large sparse highly unsymmetric linear systems, *ACM Trans. Math. Software* 30:95-117, 2004
- A. Gupta, A shared- and distributed-memory parallel general sparse direct solver, *Appl. Algebra Engrg. Commun. Comput.*, 18(3):263-277, 2007
- X. S. Li and J. W. Demmel, SuperLU_Dist: A scalable distributed-memory sparse direct solver for unsymmetric linear systems, *ACM Trans. Math. Software* 29:110-140, 2003
- K. Shen, T. Yang, and X. Jiao, S+: Efficient 2D sparse LU factorization on parallel machines, *SIAM J. Matrix Anal. Appl.* 22:282-305, 2000