Parallel Numerical Algorithms

Chapter 7 – Cholesky Factorization

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Outline

1. Cholesky Factorization
2. Parallel Dense Cholesky
3. Parallel Sparse Cholesky

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 $\boldsymbol{L}$ is 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

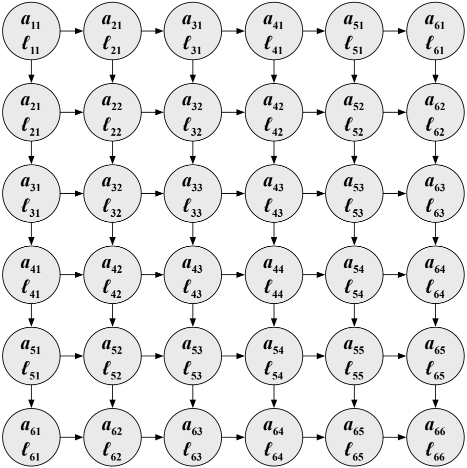
- For $i, j = 1, \ldots, n$, fine-grain task (i, j) stores a_{ij} and computes and stores

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

  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



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), $k = i + 1, \ldots, n$
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), $k = i + 1, \ldots, n$
else
  recv broadcast of a_{jj} from task (j, j)
  $a_{ij} = a_{ij} / a_{jj}$
  broadcast a_{ij} to tasks (i, k), $k = j + 1, \ldots, n$
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

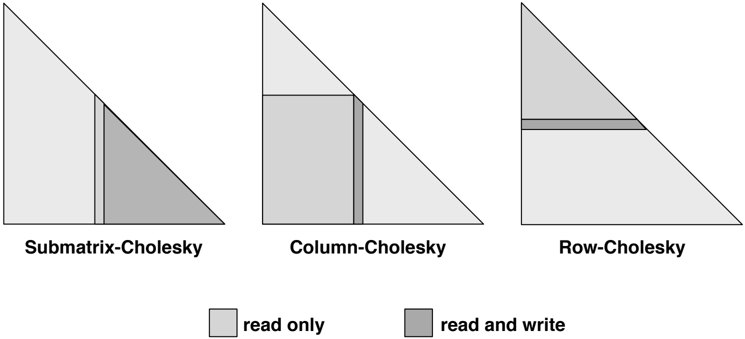
- Rather than repeat analyses for dense matrices, we focus instead on sparse matrices, for which column-oriented algorithms are typically used

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*: with k in outer loop, inner loops perform rank-1 update of remaining unreduced *submatrix* using current column
- *Column-Cholesky*: with j in outer loop, inner loops compute current *column* using matrix-vector product that accumulates effects of previous columns
- *Row-Cholesky*: 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
  $\quad a_{ij} = a_{ij}/a_{jj}$
  end

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

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

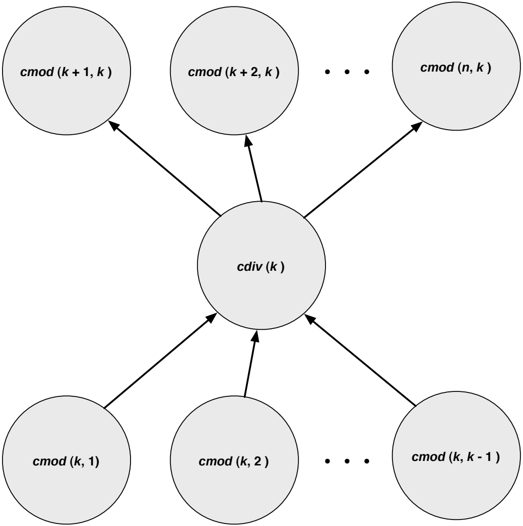
- right-looking
- immediate-update
- data-driven
- fan-out

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* $(k, *)$ 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* $(*, k)$ 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

Sparse Matrices

- Matrix is *sparse* if most of its entries are zero
- For efficiency, store and operate on only nonzero entries, e.g., *cmod*(j, 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, sparsity worth exploiting for family of matrices if there are $\Theta(n)$ nonzero entries, i.e., (small) constant number of nonzeros per row or column

Sparsity Structure

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

Sparse Cholesky Algorithms

Submatrix-Cholesky

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

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

Column-Cholesky

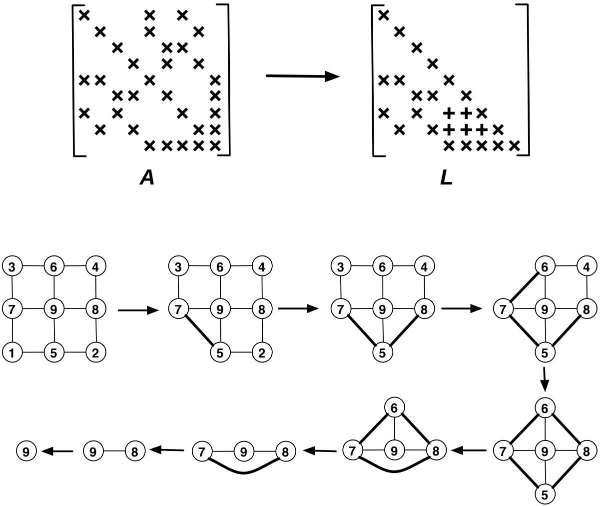
for $j = 1$ **to** n
  for $k \in$ *Struct* $(\boldsymbol{L}_{j*})$
    cmod (j, k)
  end
  cdiv (j)
end

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

Graph Model

- *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 $a_{ij} \neq 0$
- 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*

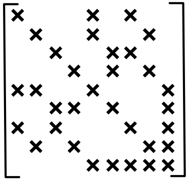
Example: Graph Model of Elimination



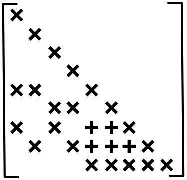
Elimination Tree

- *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



A



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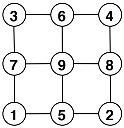
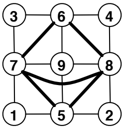
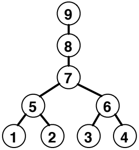


$G\,(A)$



$F\,(A)$



$T\,(A)$

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

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

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, numbering nodes in *separators* last

Symbolic Factorization

- For 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 solution*: 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 *leaf* nodes of elimination tree can be computed simultaneously

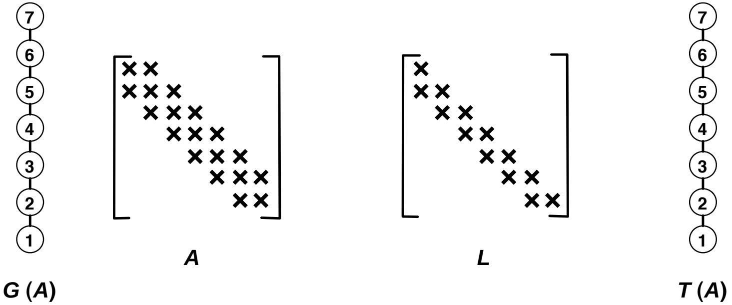
Parallel Sparse Cholesky

- *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



Example: Minimum Degree, 1-D Grid

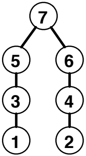
G **(*A*)**

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

A

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

L



T **(*A*)**

Example: Nested Dissection, 1-D Grid

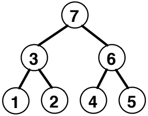
$G\,(A)$

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

A

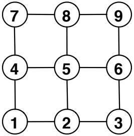
$$\begin{bmatrix} \times & & & & & & \\ & \times & & & & & \\ \times & \times & \times & & & & \\ & & & \times & & & \\ & & & & \times & & \\ & & & \times & \times & \times & \\ & \times & + & & \times & + & \times \end{bmatrix}$$

L



$T\,(A)$

Example: Band Ordering, 2-D Grid



$G\,(A)$

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

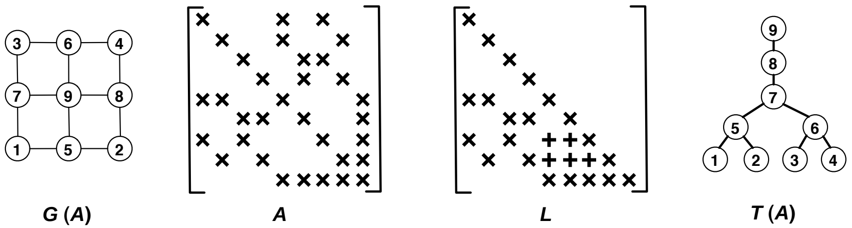
A

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

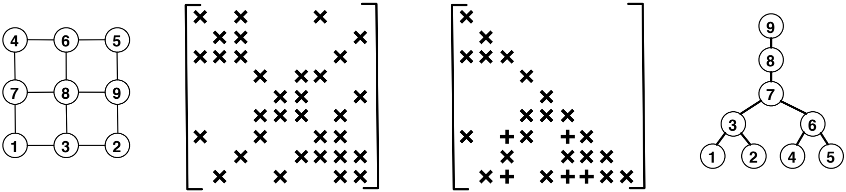
L

$T\,(A)$

Example: Minimum Degree, 2-D Grid



Example: Nested Dissection, 2-D Grid

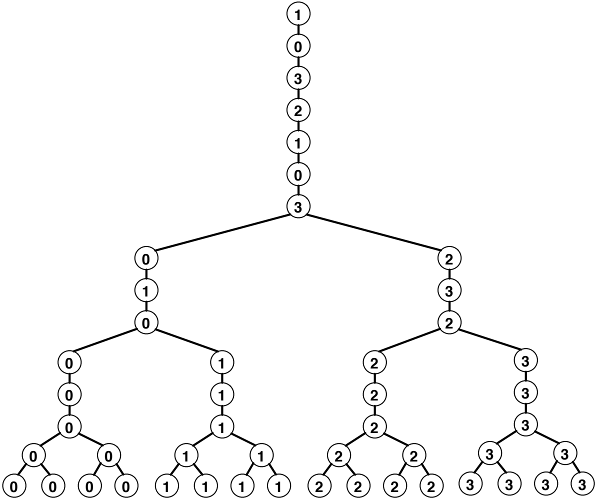


G (*A*) *A* *L* *T* (*A*)

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 ∈ mycols
    if j is leaf node in T(A) then
        cdiv(j)
        send L_{*j} to processes in map(Struct(L_{*j}))
        mycols = mycols − {j}
    end
end
while mycols ≠ ∅
    receive any column of L, say L_{*k}
    for j ∈ mycols ∩ Struct(L_{*k})
        cmod(j, k)
        if column j requires no more cmods then
            cdiv(j)
            send L_{*j} to processes in map(Struct(L_{*j}))
            mycols = mycols − {j}
        end
    end
end
```

Fan-In Sparse Cholesky

for $j = 1$ **to** n
  if $j \in$ *mycols* or *mycols* $\cap$ *Struct*$(\boldsymbol{L}_{j*}) \neq \emptyset$ **then**
    $u = 0$
    for $k \in$ *mycols* $\cap$ *Struct*$(\boldsymbol{L}_{j*})$
      $u = u + \ell_{jk}\, \boldsymbol{L}_{*k}$
    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 $\{i_1, \ldots, i_r\} = \textit{Struct}(\boldsymbol{L}_{*j})$

Let $$\boldsymbol{F}_j = \begin{bmatrix} a_{j,j} & a_{j,i_1} & \ldots & a_{j,i_r} \\ a_{i_1,j} & 0 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ a_{i_r,j} & 0 & \ldots & 0 \end{bmatrix}$$

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:

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

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 requires factorization of dense matrix of size $\Theta(\sqrt{n})$ for 2-D grid problem with n grid points, so isoefficiency function is at least $\Theta(p^3)$ for 1-D algorithm and $\Theta(p\sqrt{p})$ for 2-D algorithm
- Scalability analysis is difficult for arbitrary sparse problems, but best current parallel algorithms for sparse factorization can achieve isoefficienty $\Theta(p\sqrt{p})$ for important classes of problems

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