SPARSE DIRECT METHODS

- *Building blocks for sparse direct solvers*
- *SPD case. Sparse Column Cholesky/*
- *Elimination Trees - Symbolic factorization*

Direct Sparse Matrix Methods

Problem addressed: Linear systems $Ax = b$

➤ We will consider mostly Cholesky –

➤ We will consider some implementation details and tricks used to develop efficient solvers

Basic principles:

- Separate computation of structure from rest [symbolic factorization]
- Do as much work as possible statically
- Take advantage of clique formation (supernodes, mass-elimination).

Sparse Column Cholesky

For $j = 1, \ldots, n$ Do:

$l(j:n, j) = a(j:n, j)$

For $k = 1, \ldots, j-1$ Do:

// cmod(k,j):

$l_{j:n,j} := l_{j:n,j} - l_{j,k} * l_{j:n,k}$

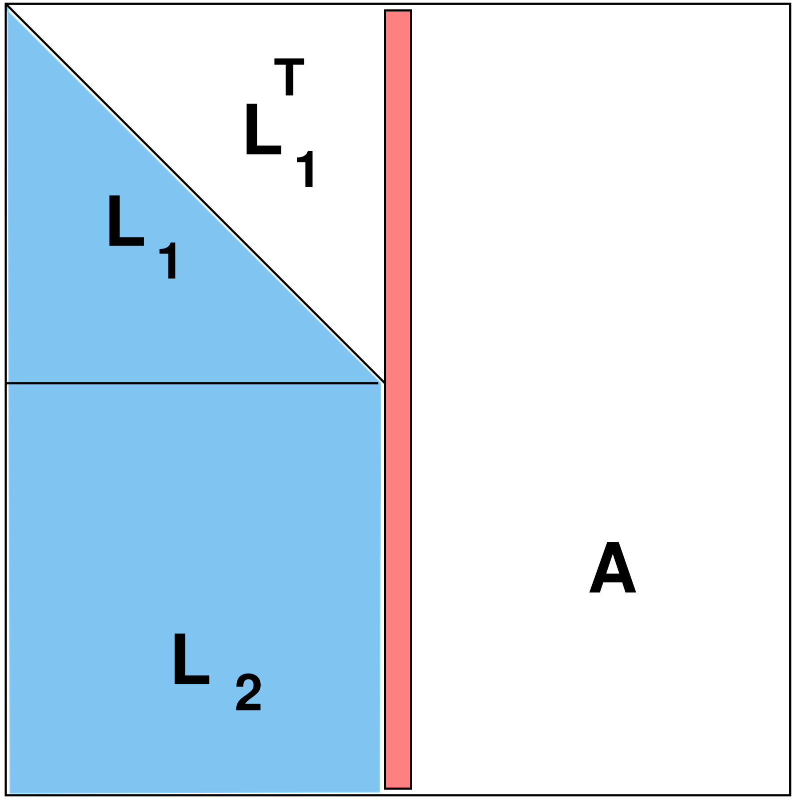
EndDo

// cdiv (j) [Scale]

$l_{j,j} = \sqrt{l_{j,j}}$

$l_{j+1:n,j} := l_{j+1:n,j} / l_{jj}$

EndDo



The four essential stages of a solve

1. Reordering: $A \quad \longrightarrow \quad A := PAP^T$

- Preprocessing: uses graph [Min. deg, AMD, Nested Dissection]

2. Symbolic Factorization: Build static data structure.

- Exploits 'elimination tree', uses graph only.
- Also: 'supernodes'

3. Numerical Factorization: Actual factorization $A = LL^T$

- Pattern of L known. Use static data structure. Exploit supernodes

4. Triangular solves: Solve $Ly = b$ then $L^T x = y$

ELIMINATION TREES

The notion of elimination tree

- Elimination trees are useful in many different ways [theory, symbolic factorization, etc..]

- For a matrix whose graph is a tree, parent of column $j < n$ is defined by

$$\boxed{Parent(j) = i, \text{ where } a_{ij} \neq 0 \text{ and } i{>}j}$$

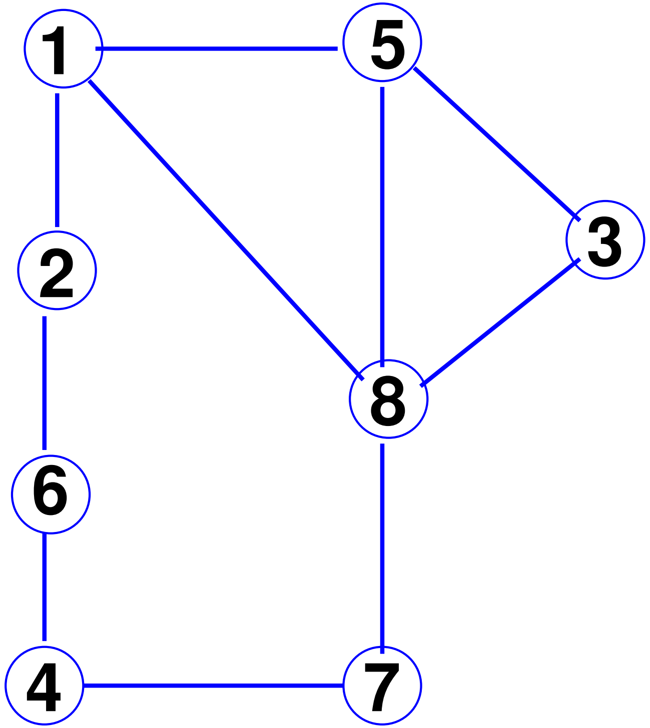
- For a general matrix matrix, consider $A = LL^T$, and G^F = 'filled' graph = graph of $L + L^T$. Then

$$\boxed{Parent(j) = \min(i) \ s.t. \ a_{ij} \neq 0 \text{ and } i{>}j}$$

- Defines a tree rooted at column n (Elimintion tree).

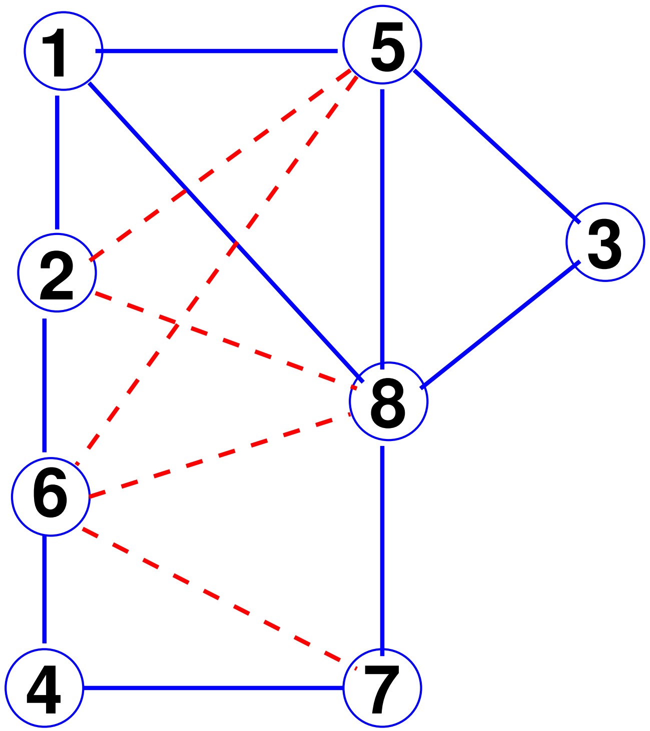
Example: Original matrix and Graph

$$\begin{bmatrix} 1 & \star & & & \star & & & \star \\ \star & 2 & & & & \star & & \\ & & 3 & & \star & & & \star \\ & & & 4 & & \star & \star & \\ \star & & \star & & 5 & & & \star \\ & \star & & \star & & 6 & & \\ & & & \star & & & 7 & \star \\ \star & & \star & & \star & & \star & 8 \end{bmatrix}$$

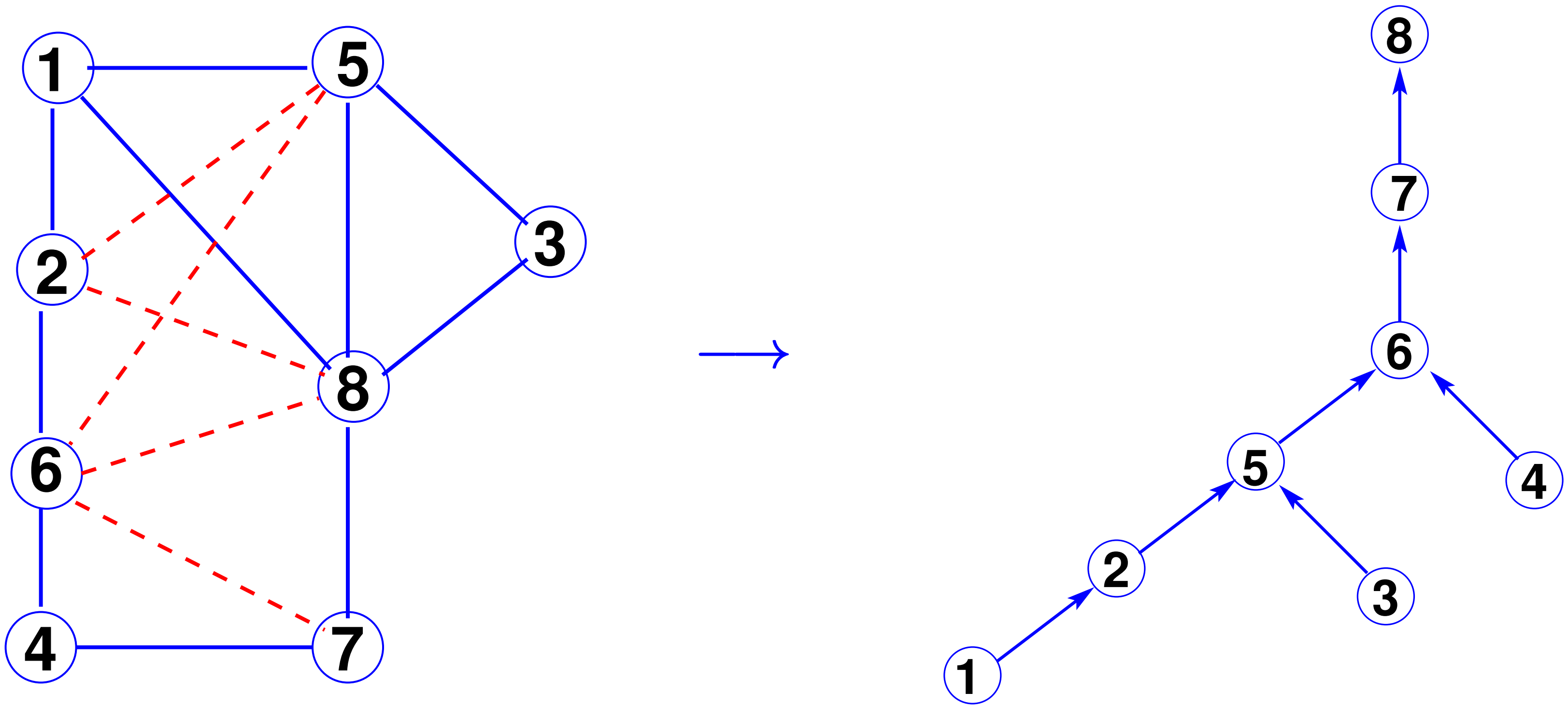


Filled matrix+graph

$$\begin{bmatrix}
1 & \star & & & \star & & & \star \\
\star & 2 & & & \blacksquare & \star & & \blacksquare \\
& & 3 & & \star & & & \star \\
& & & 4 & & \star & \star & \\
\star & \blacksquare & \star & & 5 & \blacksquare & & \star \\
& \star & & \star & \blacksquare & 6 & \blacksquare & \blacksquare \\
& & & \star & & \blacksquare & 7 & \star \\
\star & \blacksquare & \star & & \star & \blacksquare & \star & 8
\end{bmatrix}$$



Corresponding Elimination Tree

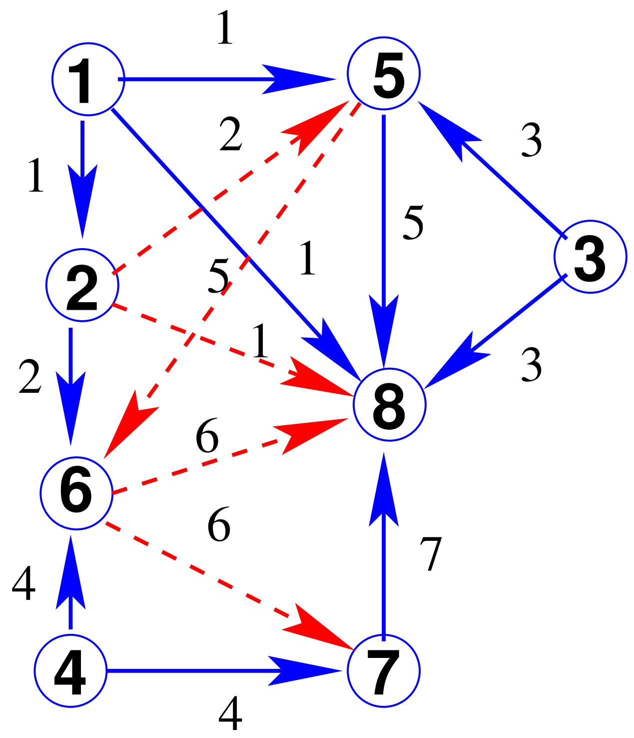


- Parent(i) = 'first nonzero entry in L(i+1:n,i)'
- Parent(i) = min $\{j > i \mid j \ \in \ Adj_{G^F}(i)\}$

Where does the elimination tree come from?

- Answer in the form of an excercise.

Consider the elimination steps for the previous example. A directed edge means a row (column) modification. It shows the task dependencies. There are unnecessary dependencies. For example: $1 \rightarrow 5$ can be removed because it is subsumed by the path $\mathbf{1 \rightarrow 2 \rightarrow 5}$.



To do: Remove all the redundant dependencies.. What is the result?

Facts about elimination trees

➤ Elimination Tree defines dependencies between columns.

➤ The root of a subtree cannot be used as pivot before any of its descendents is processed.

➤ Elimination tree depends on ordering;

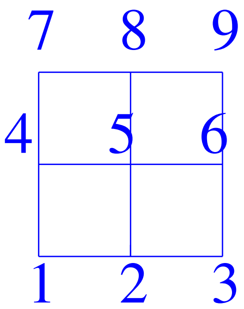
➤ Can be used to define 'parallel' tasks.

➤ For parallelism: flat and wide trees $\rightarrow$ good; thin and tall (e.g. of tridiagonal systems) $\rightarrow$ Bad.

➤ For parallel executions, Nested Dissection gives better trees than Minimun Degree ordering.

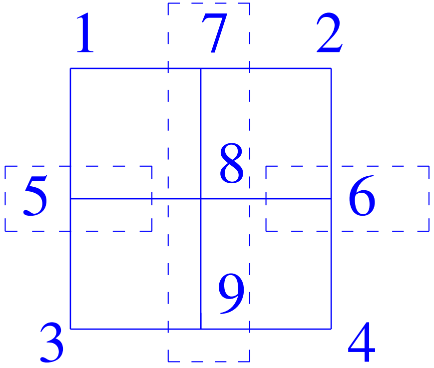
Elim. tree depends on ordering (Not just the graph)

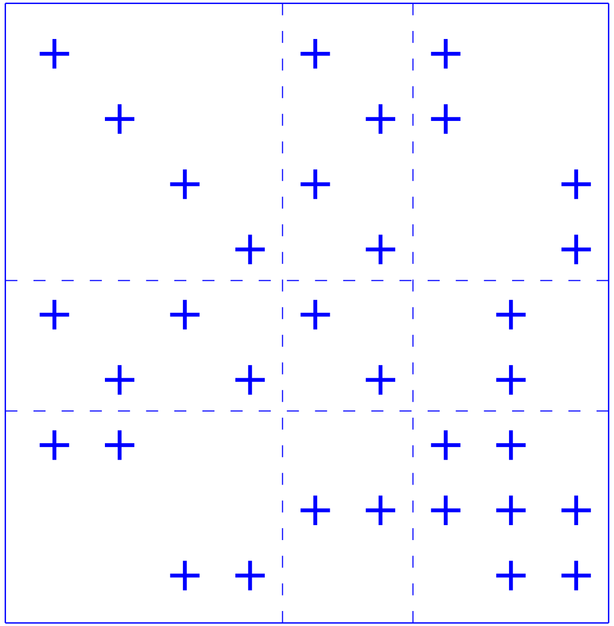
Example: 3×3 grid for 5-point stencil [natural ordering]

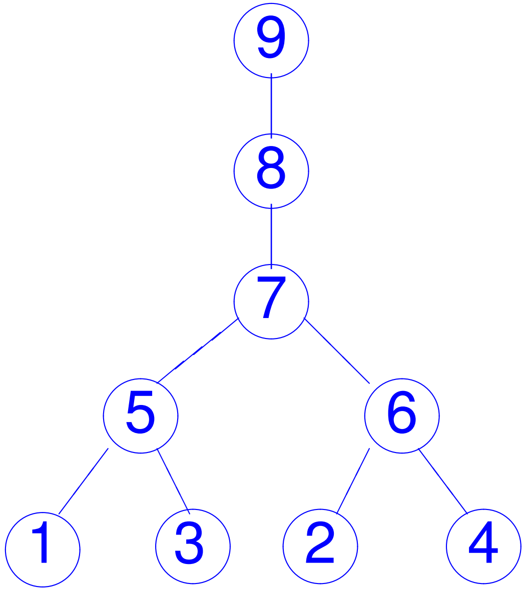


$$
\left[\begin{array}{ccc|ccc|ccc}
+ & + & & + & & & & & \\
+ & + & + & & + & & & & \\
& + & + & & & + & & & \\
\hline
+ & & & + & + & & + & & \\
& + & & + & + & + & & + & \\
& & + & & + & + & & & + \\
\hline
& & & + & & & + & + & \\
& & & & + & & + & + & + \\
& & & & & + & & + & +
\end{array}\right]
$$

➤ Same example with nested dissection ordering





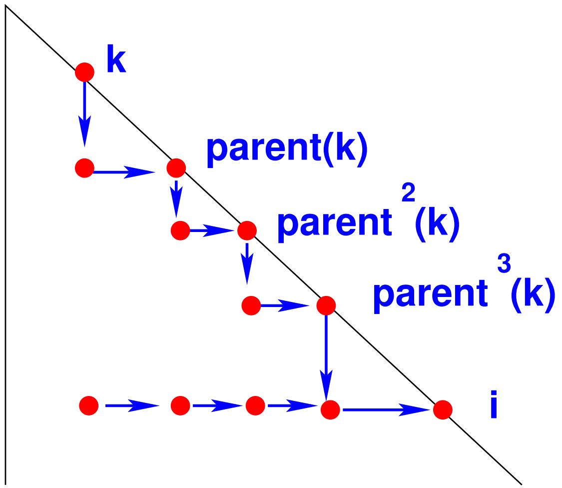


Properties

➤ The elimination tree is a spanning tree of the filled graph [a tree containing all vertices] - obtained by removing edges.

➤ If $l_{ik} \neq 0$ then i is an ancestor of k in the tree

✍1 In the previous example: follow the creation of the fill-in (6,8).



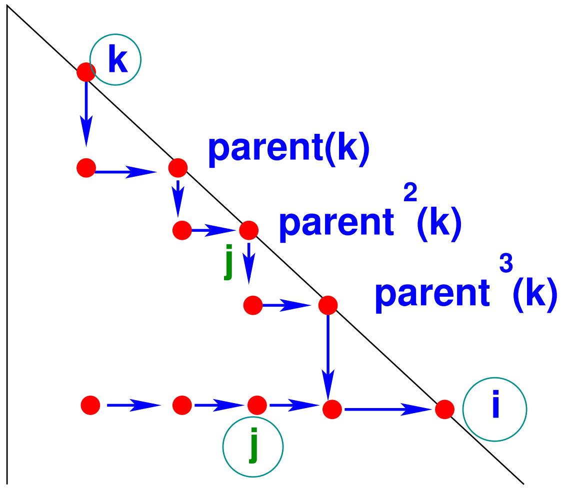
In particular: if $a_{ik} \neq 0, k < i$ then $i \rightsquigarrow k$

➤ Consequence: no fill-in between branches of the same subtree

Elimination trees and the pattern of L

➤ It is easy to determine the sparsity pattern of L because the pattern of a given column is “inherited” by the ancestors in the tree.

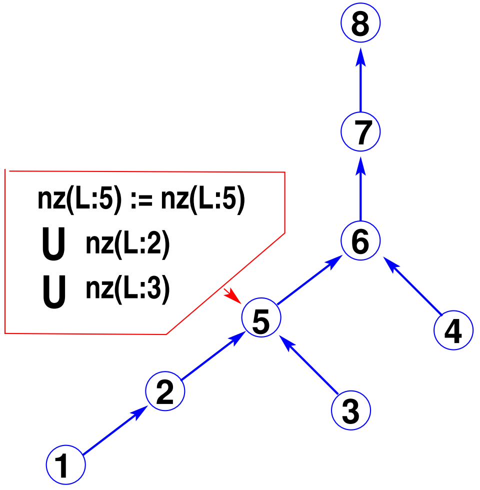
Theorem: For $i > j$, $l_{ij} \neq 0$ iff j is an ancestor of some $k \in Adj_A(i)$ in the elimination tree.



In other words:

$$\boxed{l_{ij} \neq 0, i > j \ \text{ iff } \ \exists k \in Adj_A(i) s.t. \ j \rightsquigarrow k}$$

In theory: To construct the pattern of L, go up the tree and accumulate the patterns of the columns. Initially L has the same pattern as $TRIL(A)$.



- However: Let us assume tree is not available ahead of time
- Solution: Parents can be obtained dynamically as the pattern is being built.
- This is the basis of symbolic factorization.

Notation :

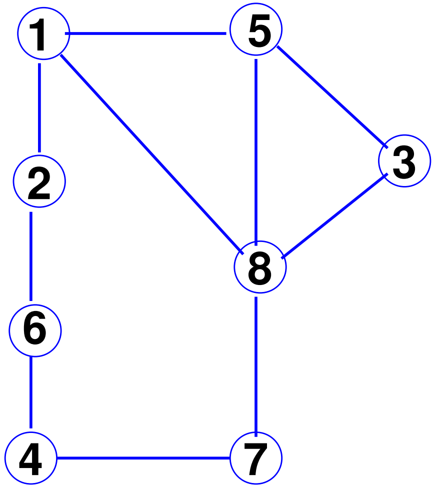
➤ $nz(X)$ is the pattern of X (matrix or column, or row). A set of pairs (i, j)

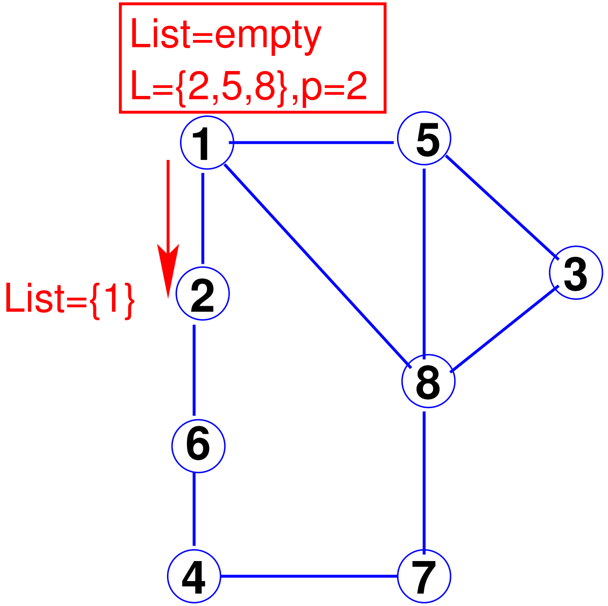
➤ $tril(X)$ = Lower triangular part of pattern [matlab notation] $\{(i, j) \in X \,|i > j\}$

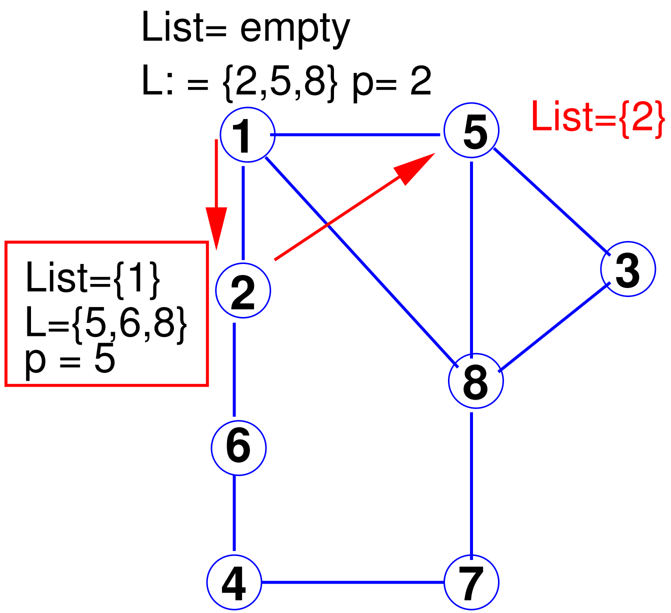
➤ Idea: dynamically create the list of nodes needed to update $L_{:,j}$.

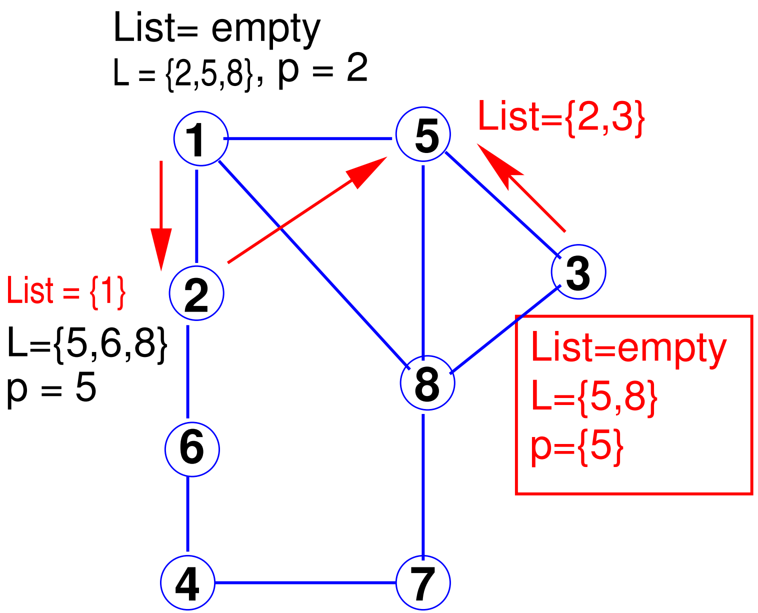
1. Set: $nz(L) = tril(nz(A))$,
2. Set: $list(j) = \emptyset, j = 1, \cdots, n$
3. For $j = 1 : n$
4.   for $k \in list(j)$ do
5. $nz(L_{:,j}) := nz(L_{:,j}) \cup nz(L_{:,k})$
6.   end
7. $p = \min\{i > j \mid L_{i,j} \neq 0\}$
8. $list(p) := list(p) \cup \{j\}$
9. End

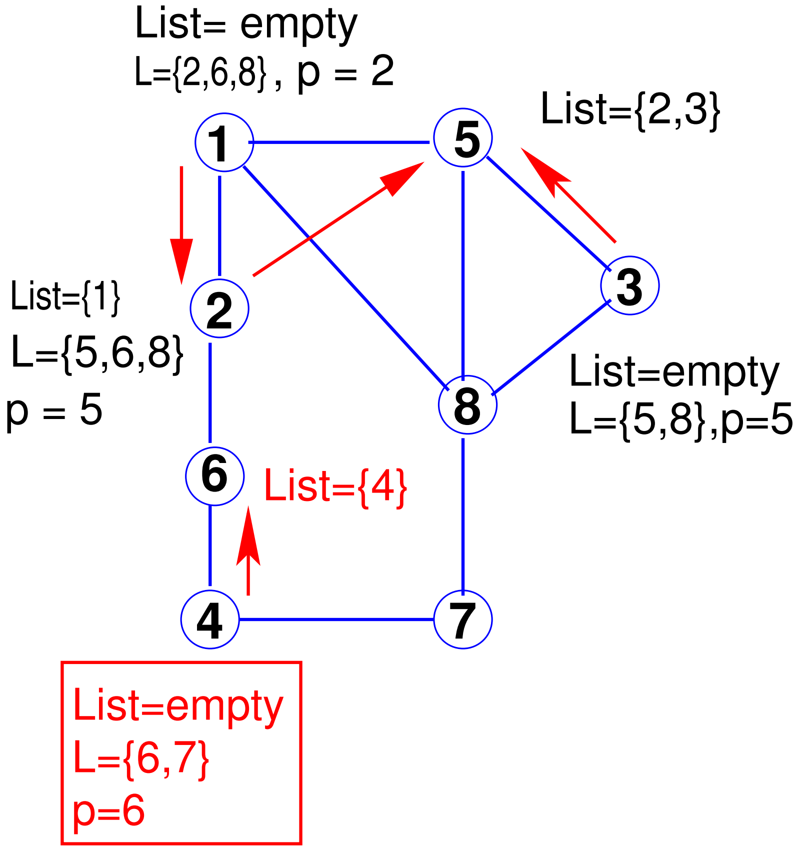
Example: Consider the earlier example:

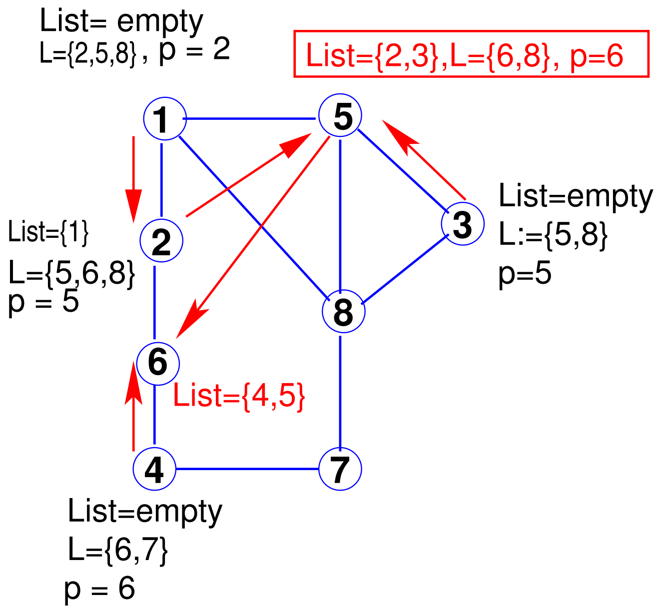


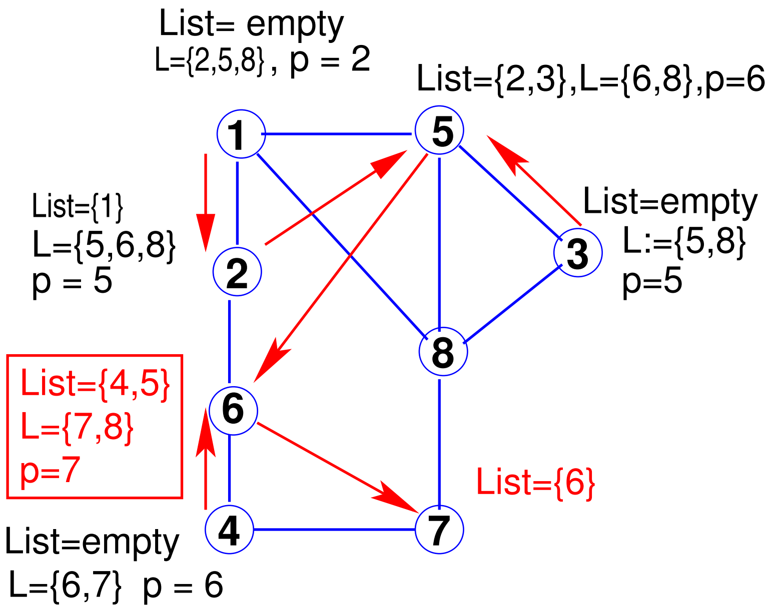





List= empty
L = {2,5,8}, p = 2
List={2,3}
List = {1}
L={5,6,8}
p = 5
List=empty
L={5,8}
p={5}
1
5
3
2
8
6
4
7


List= empty
L={2,6,8} , p = 2
List={2,3}
List={1}
L={5,6,8}
p = 5
List=empty
L={5,8},p=5
List={4}
List=empty
L={6,7}
p=6
1
5
2
3
8
6
4
7


List= empty
L={2,5,8} , p = 2
List={2,3},L={6,8}, p=6
1
5
List={1}
2
L={5,6,8}
p = 5
3
List=empty
L:={5,8}
p=5
8
6
List={4,5}
4
7
List=empty
L={6,7}
p = 6


List= empty
L={2,5,8} , p = 2
List={2,3},L={6,8},p=6
1
5
List={1}
L={5,6,8}
p = 5
2
List=empty
L:={5,8}
p=5
3
8
List={4,5}
L={7,8}
p=7
6
List={6}
4
7
List=empty
L={6,7} p = 6

Multifrontal methods

- Start with the frontal method.

- Recall: Finite element matrix:

$$\boldsymbol{A} = \sum \boldsymbol{A}^{[e]}$$

$\boldsymbol{A}^{[e]}$ = element matrix associated with element e.

- An old idea: Execute Gaussian elimination as the elements are being assembled

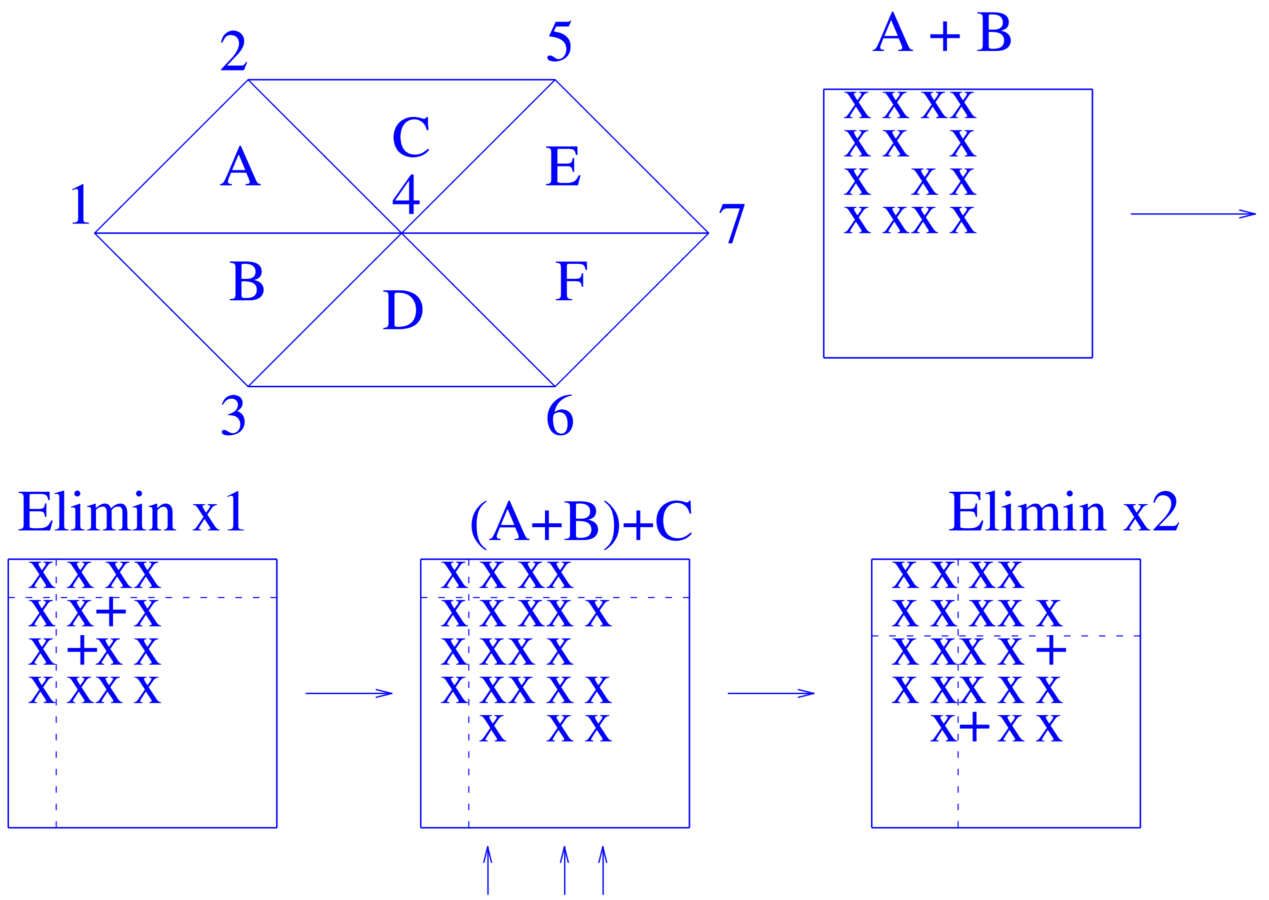
- Dependency: variabes $\leftrightarrow$ elements, creates an assembly tree.

- Method is called *the frontal method*

- Very popular among finite element users: saves storage

The origin: Frontal method (circa 1970s)

- Assemble $A + B$ then eliminate x_1
- Elimination of x_1 creates an update matrix

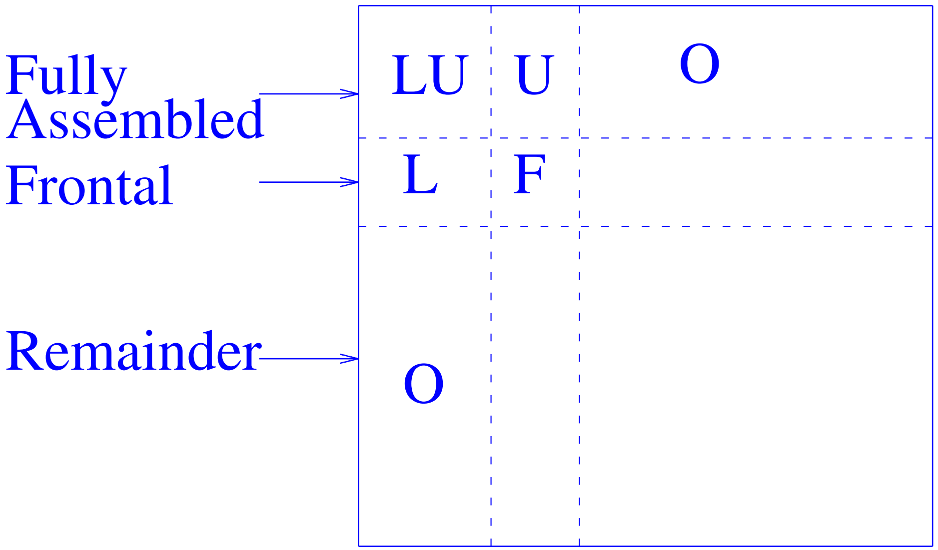


- Matrix has 3 parts:

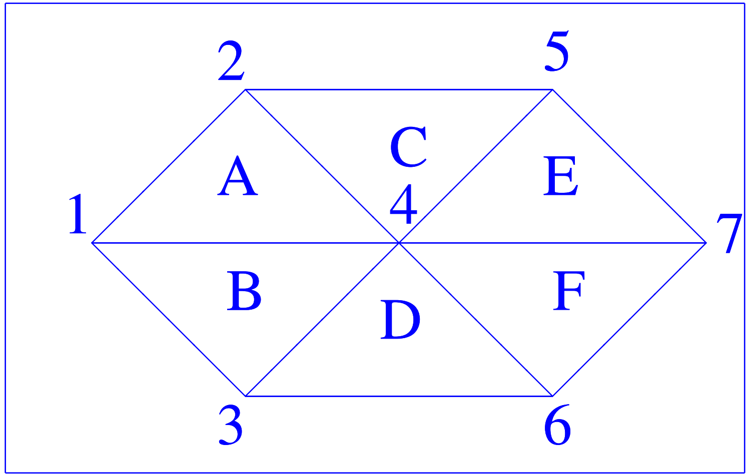
1) Fully assembled (no longer modified)

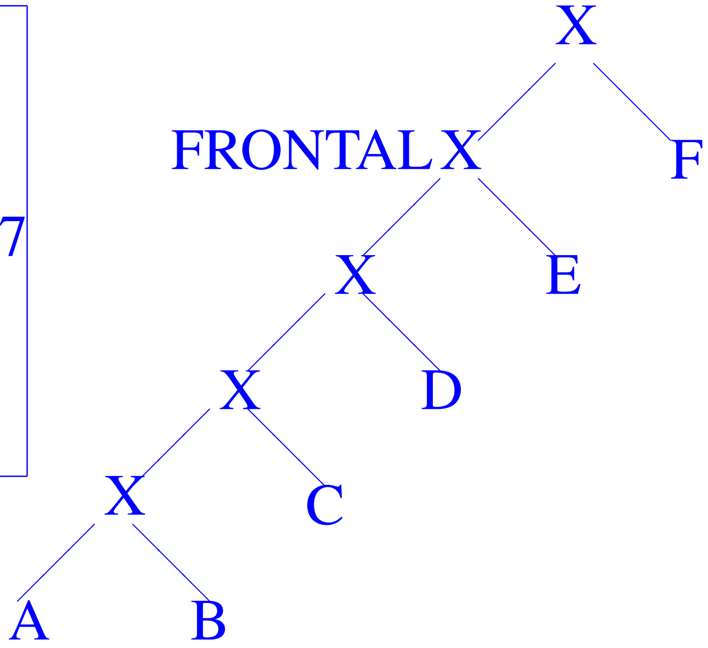
2) Frontal matrix: undergoes assembly + updates

3) Remainder: not accessed yet.



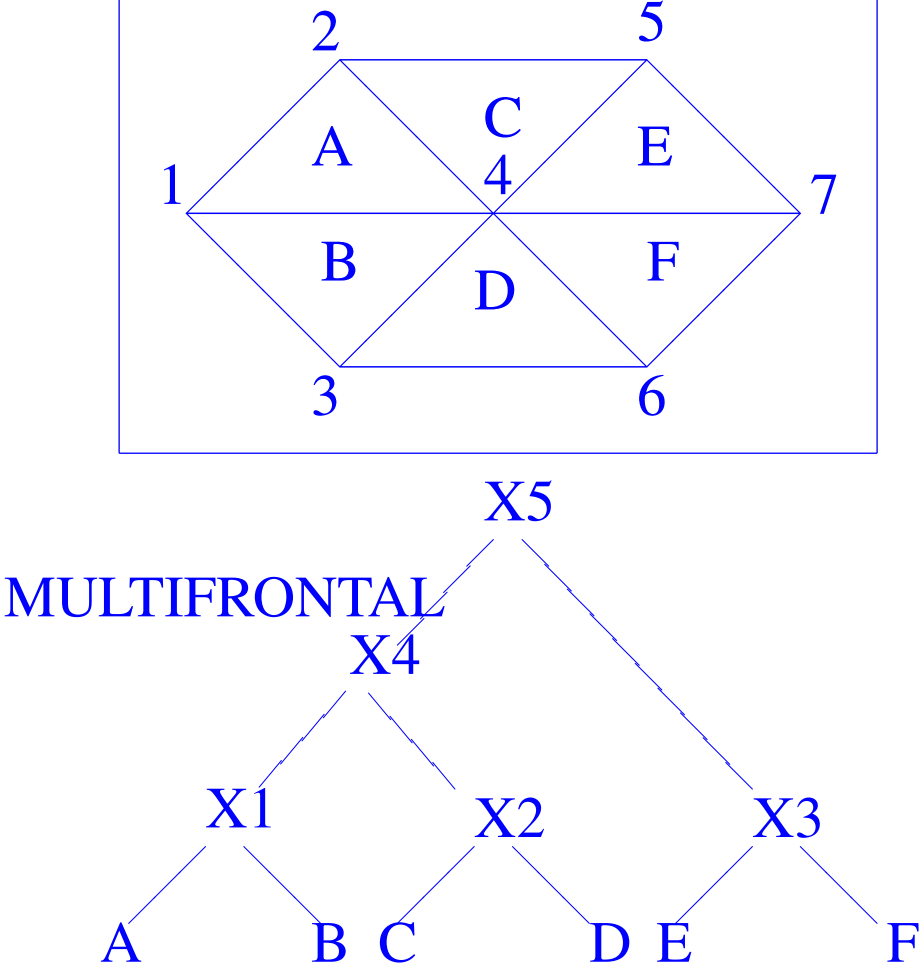
Assembly tree: - analogue to elimination tree





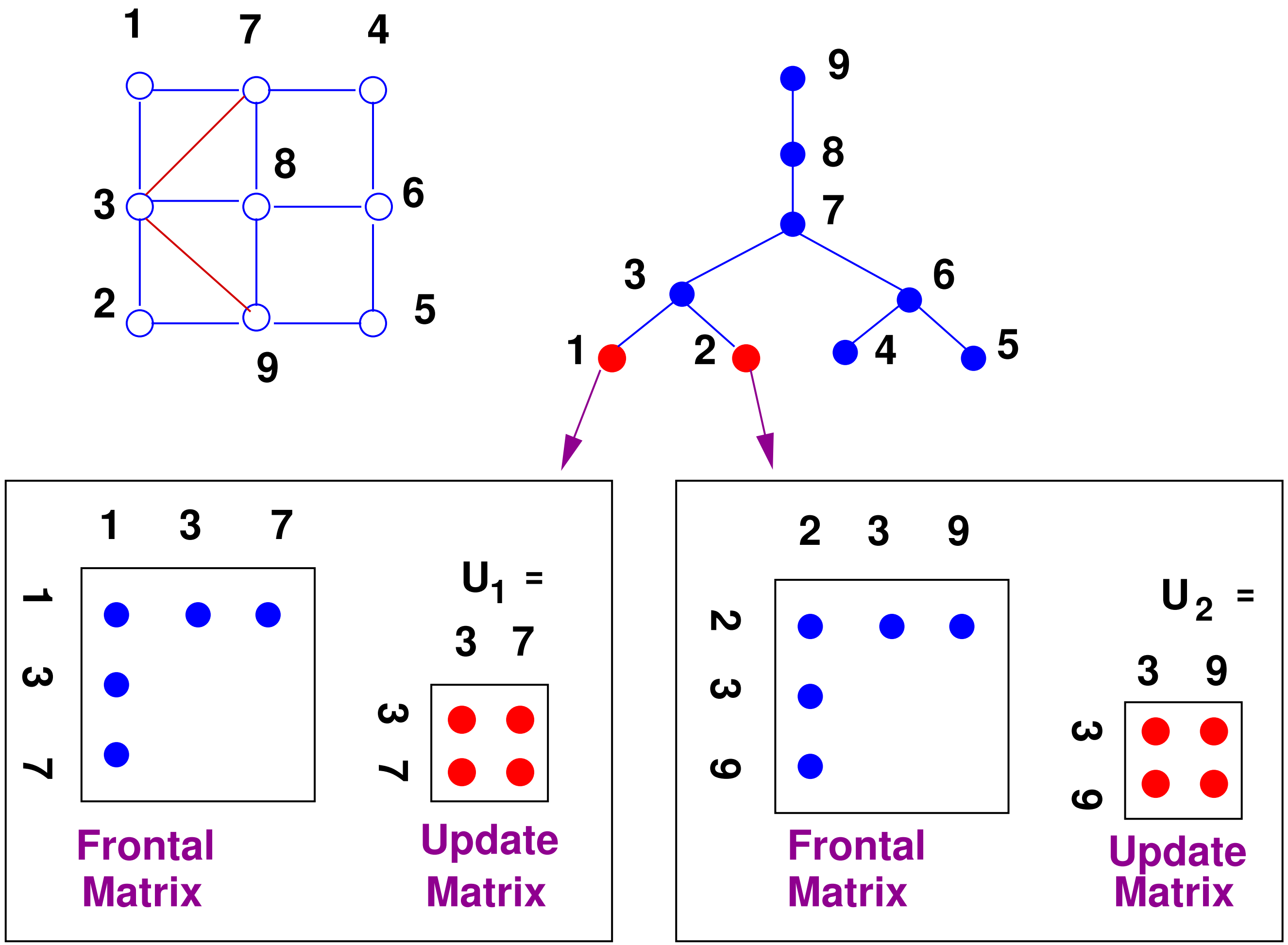
➤ Can proceed from several incoupled elements at the same time → multi-frontal technique [Duff & Reid, 1983]

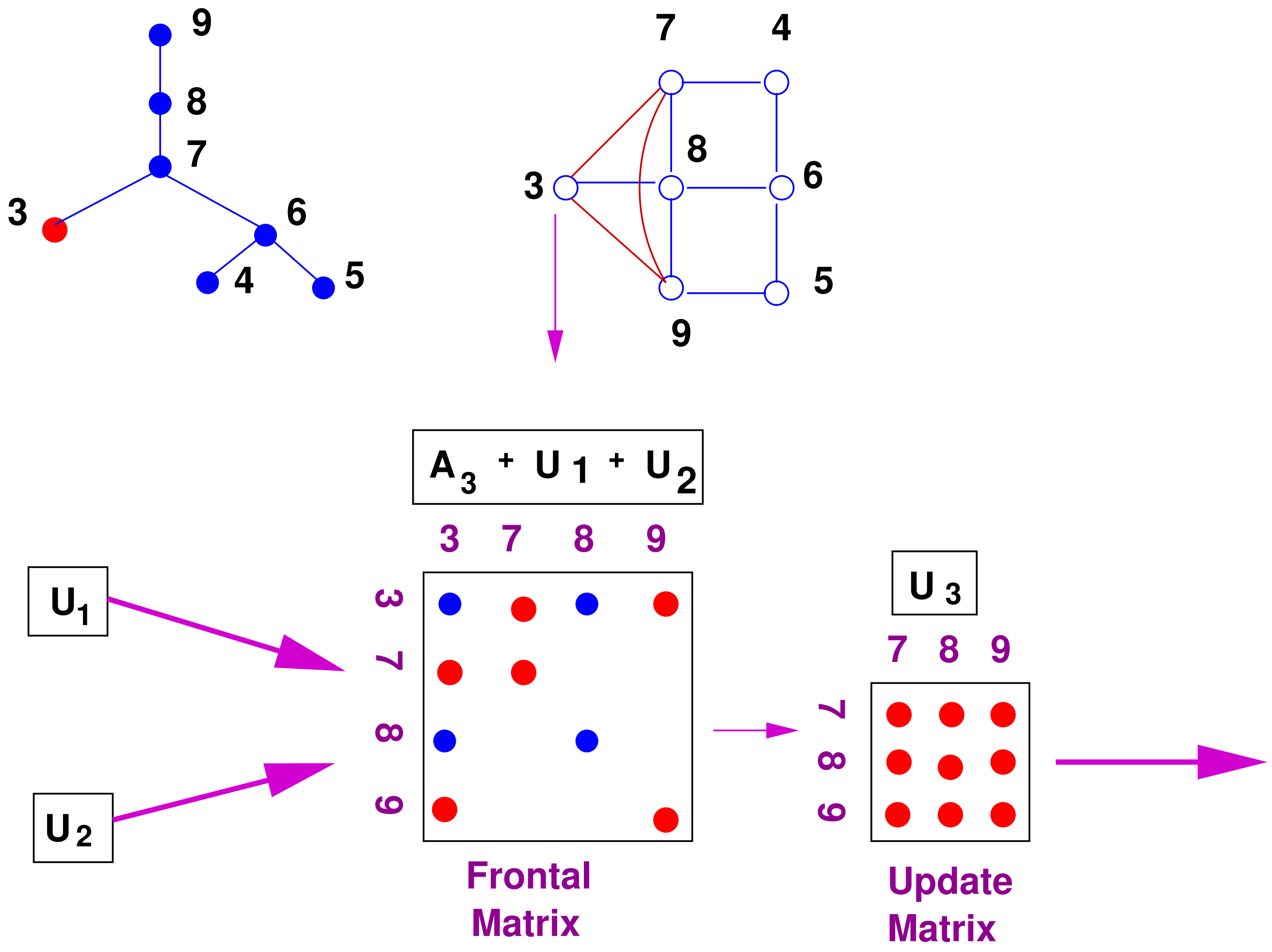
Assembly tree for Multifrontal Method



Multifrontal methods: extension to general matrices

- Elimination tree replaces assembly tree
- Proceed in post-order traversal of elimination tree in order not to violate task dependencies.
- When a node is eliminated an update matrix is created.
- This matrix is passed to the parent which adds it to its frontal matrix.
- Requires a stack of pending update matrices
- Update matrices popped out as they are needed
- Often implemented with nested dissection-type ordering
- More complex than a left-looking algorithm


1 7 4
8
3 6
2 5
9
9
8
7
3 6
1 2 4 5
1 3 7
U_1 =
3 7
Frontal Matrix
Update Matrix
2 3 9
U_2 =
3 9
Frontal Matrix
Update Matrix



9
8
7
3
6
4
5
7
4
8
3
6
5
9
A 3 + U 1 + U 2
3 7 8 9
U1
U2
3
7
8
9
U 3
7 8 9
7
8
9
Frontal
Matrix
Update
Matrix

Eliminating nodes 1 and 2: What happens on matrix

$$
\left[\begin{array}{c|c|c|ccc|c|c|c}
1 & & \star & & & & \star & & \\
\hline
 & 2 & \star & & & & & & \star \\
\hline
\star & \star & 3 & & & & \blacksquare & \star & \blacksquare \\
\hline
 & & & 4 & & \star & \star & & \\
 & & & & 5 & \star & & & \star \\
 & & & \star & \star & 6 & & \star & \\
\hline
\star & & \blacksquare & \star & & & 7 & \star & \\
\hline
 & & \star & & & \star & \star & 8 & \star \\
\hline
 & \star & \blacksquare & & \star & & & \star & 9
\end{array}\right]
\begin{array}{l}
\\
\\
\leftarrow U_1(3,:) \quad \leftarrow U_2(3,:) \\
\\
\\
\\
\leftarrow U_1(7,:) \\
\\
\qquad\qquad\quad \leftarrow U_2(9,:)
\end{array}
$$

Supernodes

Columns inherit patterns of the columns from which they are updated $\rightarrow$ Many columns with same sparsity pattern. Supernode = a set of contiguous columns in the Cholesky factor L that have the same sparsity pattern.

- The set $\{j, j+1, ..., j+s\}$ is a supernode if

$$NZ(L_{*,k}) = NZ(L_{*,k+1}) \bigcup \{k+1\} \quad j \le k < j+s$$

where $NZ(L_{*,k})$ is nonzero set of column k of L.

- Other terms used: Mass elimination, indistinguishible nodes, active variables in front, subscript compression,...

- Gain in performance due to savings in Gather-Scatter operations.

A few existing solvers (among many)

Code	Method	Scope	Developer
CHOLMOD	Left-Looking	SPD	T. Davis
MA67	Multifrontal	Symm	HSL
MA48	Right-Looking	UnSymm	HSL
SuperLU	Left-Looking	UnSymm	S. Li (LBL)
Pardiso	Left-Looking	Symm. Patt.	O. Schenk (Lugano)
MA41	Multifrontal	Symm Patt.	HSL
MUMPS	Multifrontal	Symm Patt.	Amestoy (Toulouse)
Pastix	Left+Right-Looking	Symm, symm. patt.	Labri (Bordeaux)
SuperLU_Dist	Right-Looking	UnSymm	S. Li (LBL)