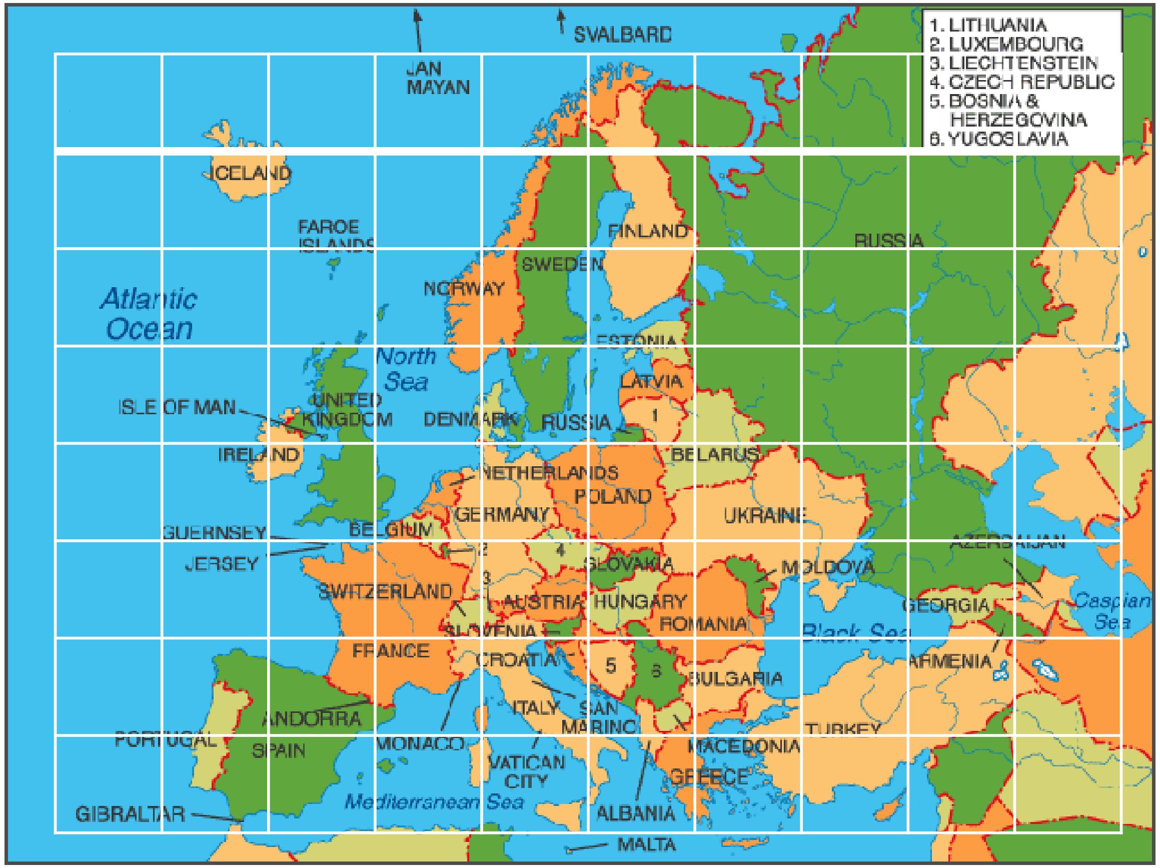
(Parallel) Sparse Matrix Computations

Sparse Matrices arise in

- Simulation of Physical/Chemical Phenomena
  - Modeled through particles/molecules/point clouds
- (Spatial) Database Applications
- Graph Computations
- Combinatorial Optimization

Example: Finite Differences



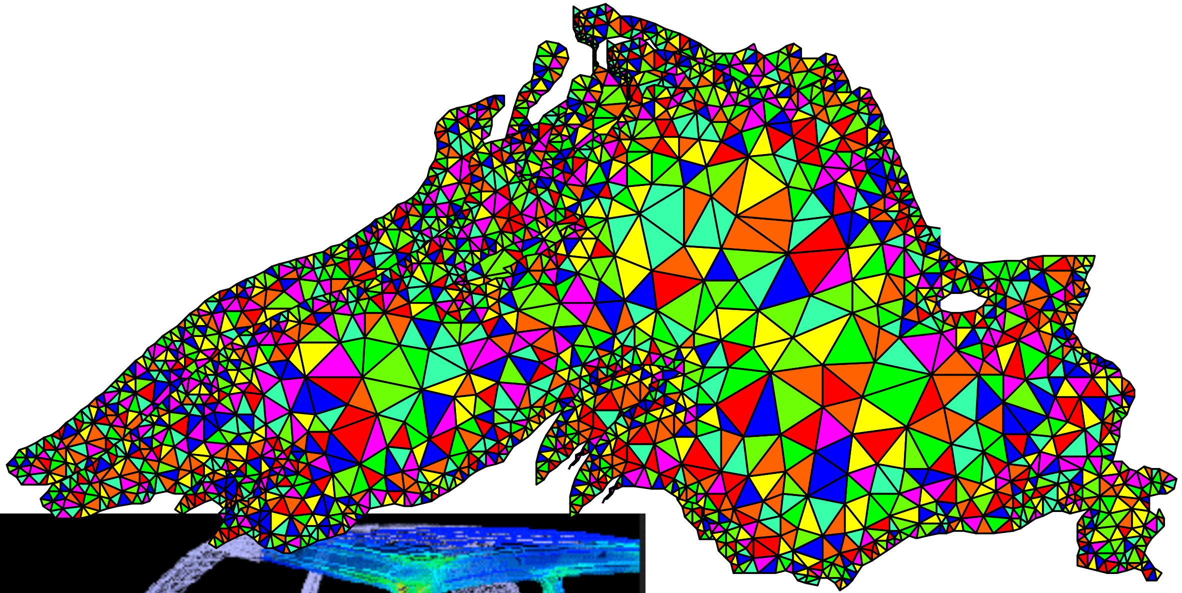
In case of a 5x5 grid this leads to 25 grid points and the following sparse matrix:

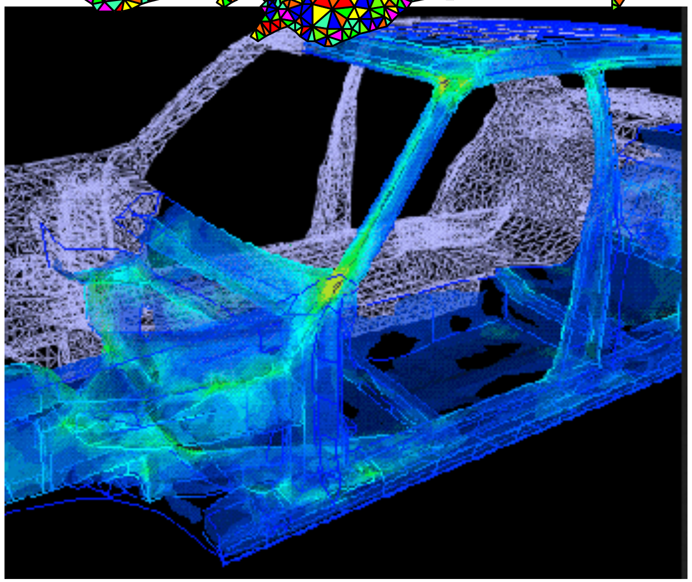
Number of grid points in the x direction

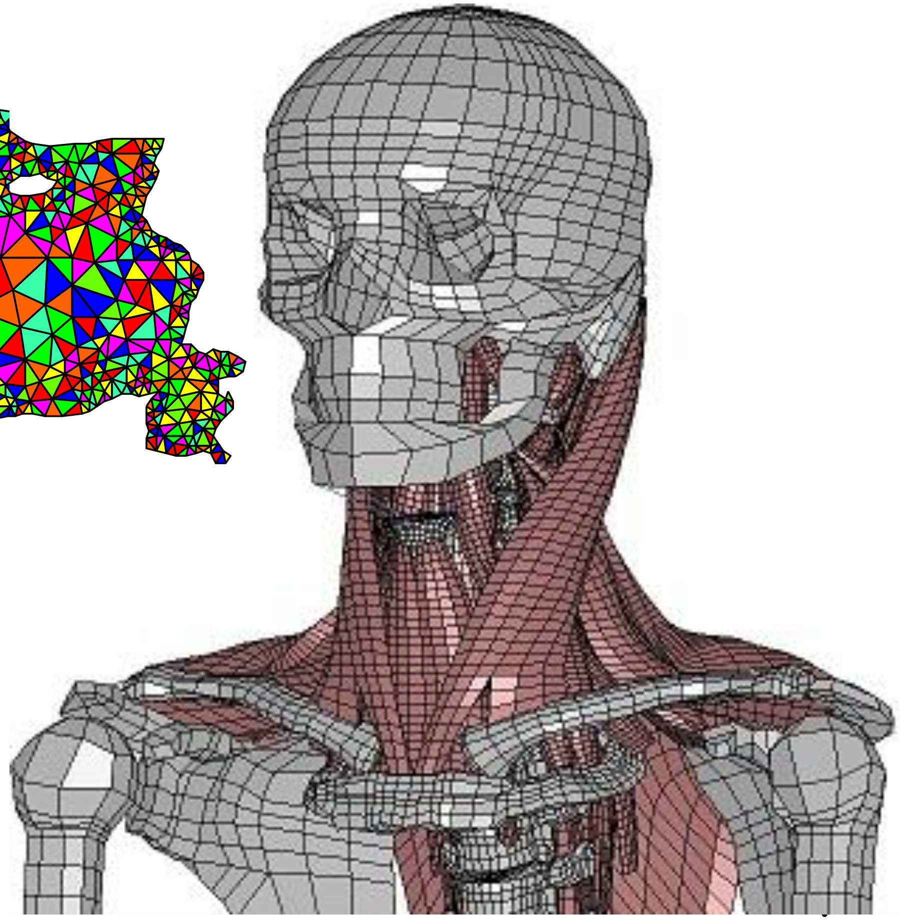
$$A = \begin{pmatrix}
x & x & 0. & 0. & x & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
x & x & x & 0. & 0. & x & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & x & x & x & 0. & 0. & x & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & 0. & x & x & x & 0. & 0. & x & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
x & 0. & 0. & x & x & x & 0. & 0. & x & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & x & 0. & 0. & x & x & x & 0. & 0. & x & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & 0. & x & 0. & 0. & x & x & x & 0. & 0. & x & 0. & 0. & 0. & 0. & 0. \\
0. & 0. & 0. & x & 0. & 0. & x & x & x & 0. & 0. & x & 0. & 0. & 0. & 0. \\
0. & 0. & 0. & 0. & x & 0. & 0. & x & x & x & 0. & 0. & x & 0. & 0. & 0. \\
0. & 0. & 0. & 0. & 0. & x & 0. & 0. & x & x & x & 0. & 0. & x & 0. & 0. \\
0. & 0. & 0. & 0. & 0. & 0. & x & 0. & 0. & x & x & x & 0. & 0. & x & 0. \\
0. & 0. & 0. & 0. & 0. & 0. & 0. & x & 0. & 0. & x & x & x & 0. & 0. & x \\
0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & x & 0. & 0. & x & x & x & 0. & 0. \\
0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & x & 0. & 0. & x & x & x & 0. \\
0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & x & 0. & 0. & x & x & x \\
0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & x & 0. & 0. & x & x
\end{pmatrix}$$

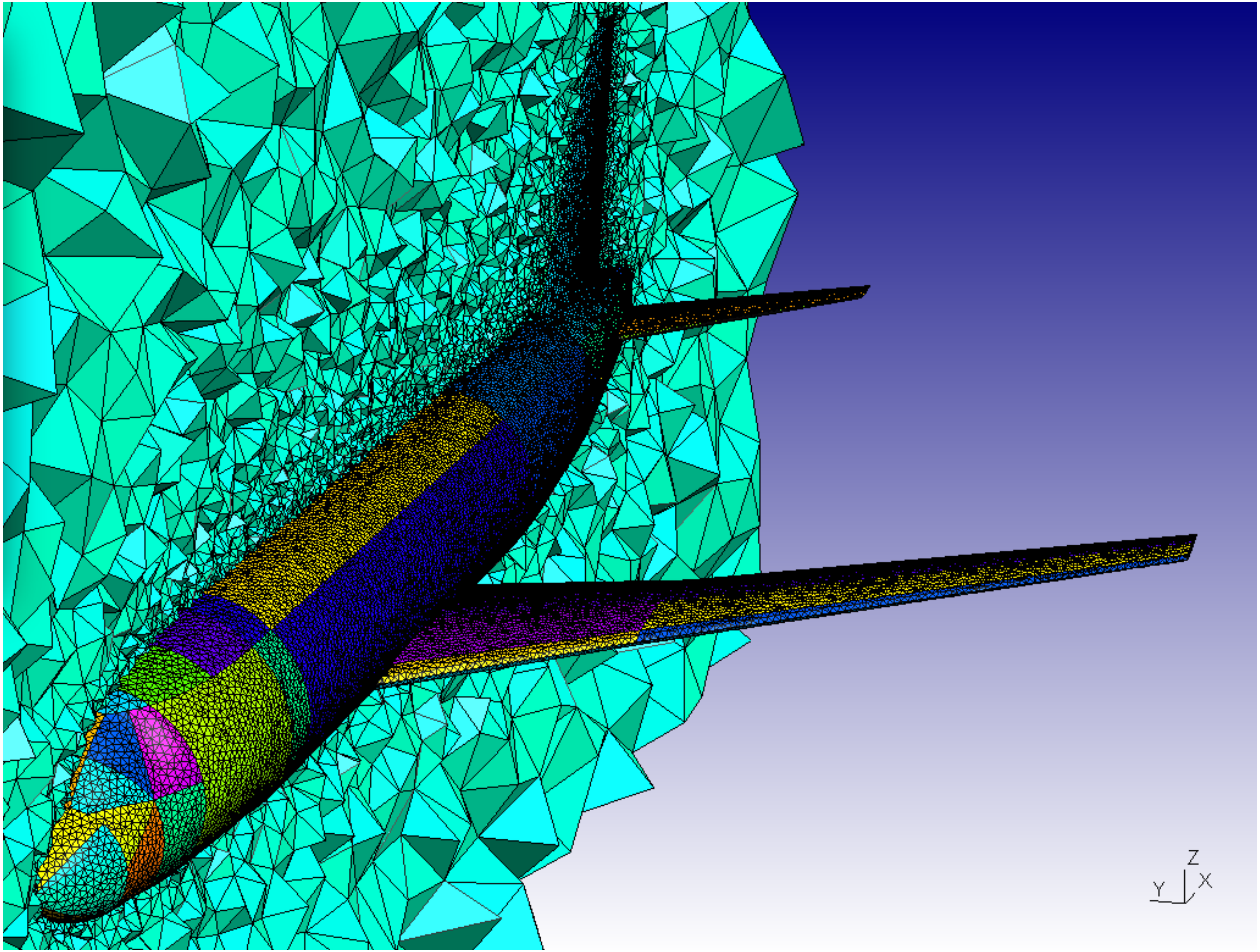
Number of grid points in the y direction

Example: Finite Elements for more complex geometries

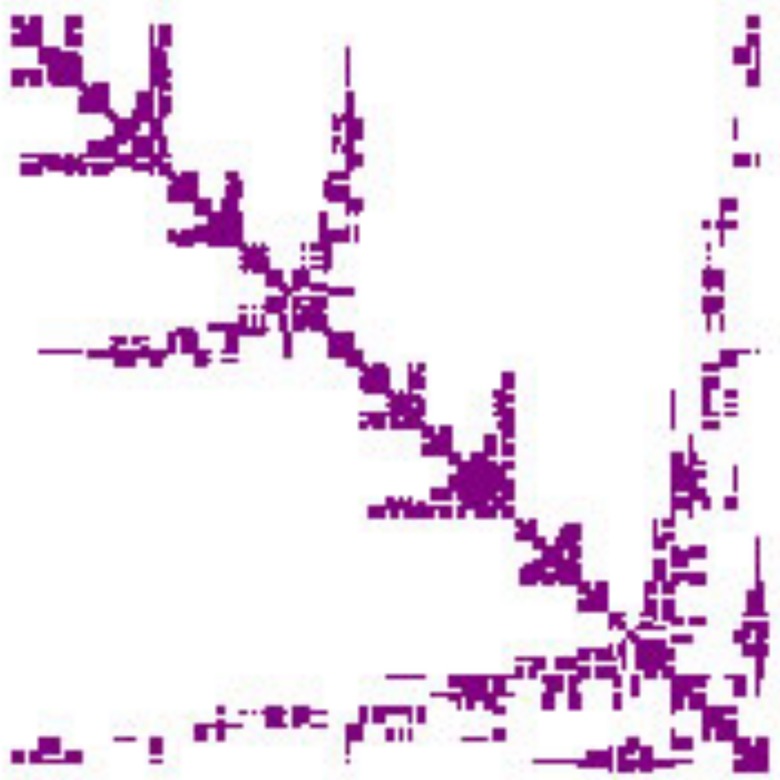


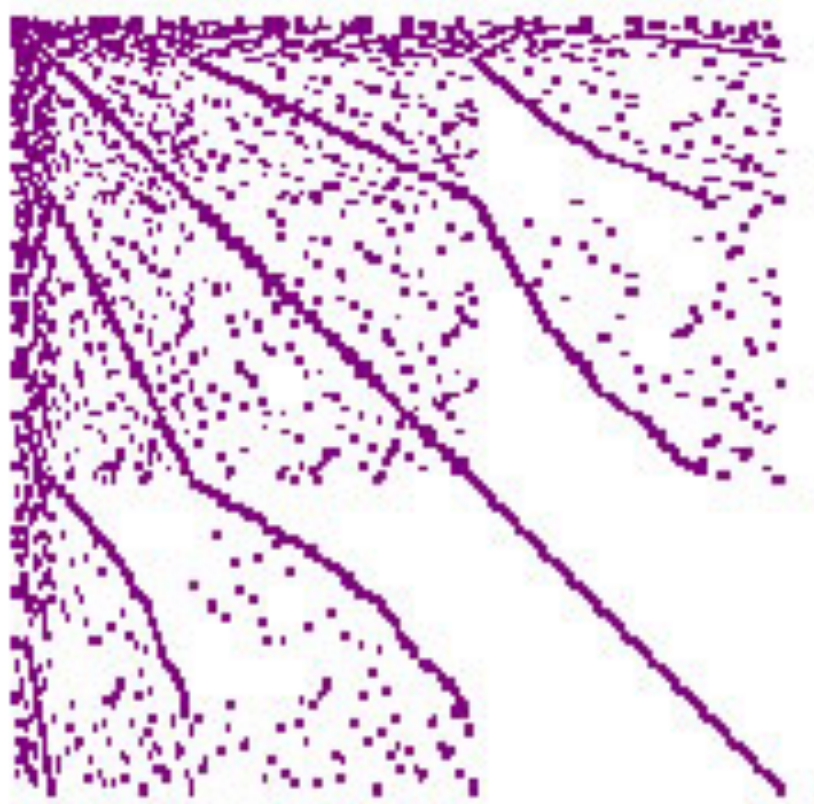





Z
Y
X

Leads to:

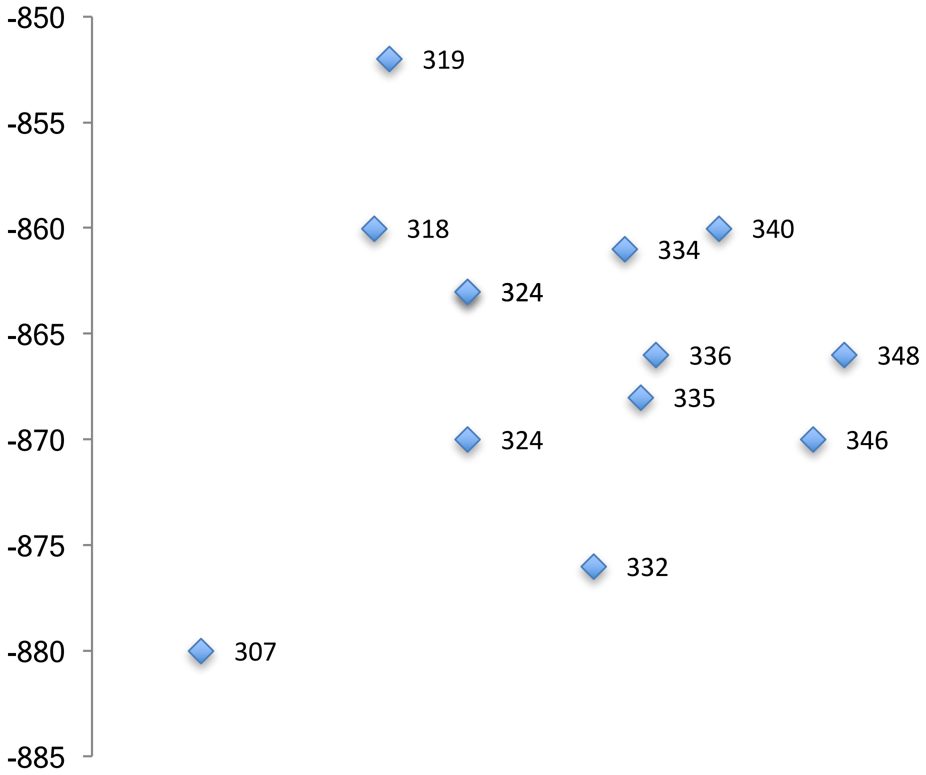




(Spatial) Databases Applications:

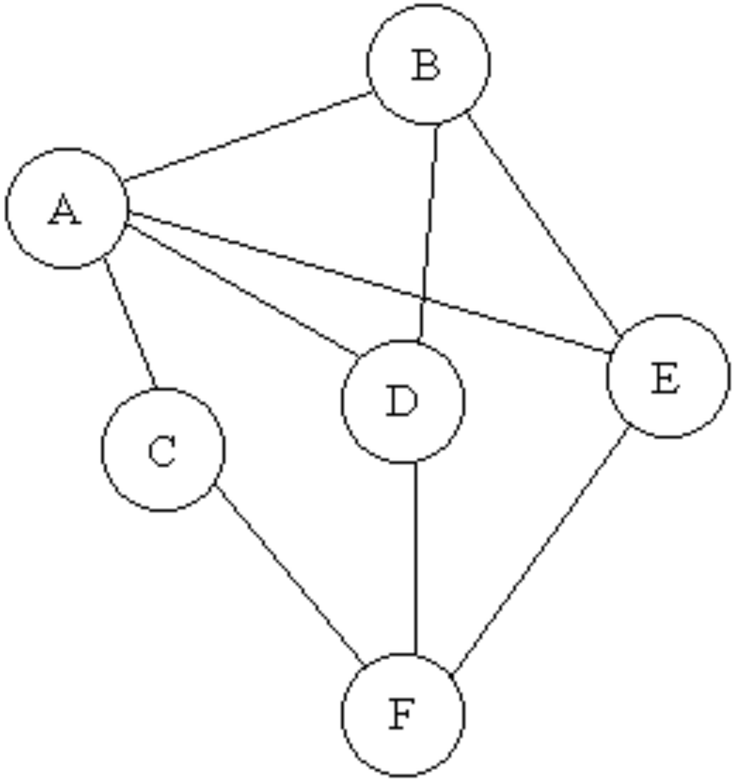
	City	State	ZipCode	Latitude	Longitude
1	Troy	AL	36081	31.809675	-85.972173
2	Mobile	AL	36685	30.686394	-88.053241
3	Trussville	AL	35173	33.621385	-86.602739
4	Montgomery	AL	36106	32.35351	-86.265837
5	Selma	AL	36701	32.41179	-87.022234
6	Talladega	AL	35161	33.43451	-86.102689
7	Tuscaloosa	AL	35402	33.209003	-87.571005
8	Huntsville	AL	35801	34.729135	-86.584979
9	Gadsden	AL	35901	34.014772	-86.007172
10	Birmingham	AL	35266	33.517467	-86.809484
11	Montgomery	AL	36124	32.38012	-86.300629
12	Decatur	AL	35602	34.60946	-86.977029
13	Eufaula	AL	36072	31.941565	-85.239689

Stored using longitude and latitude values, normalized x10

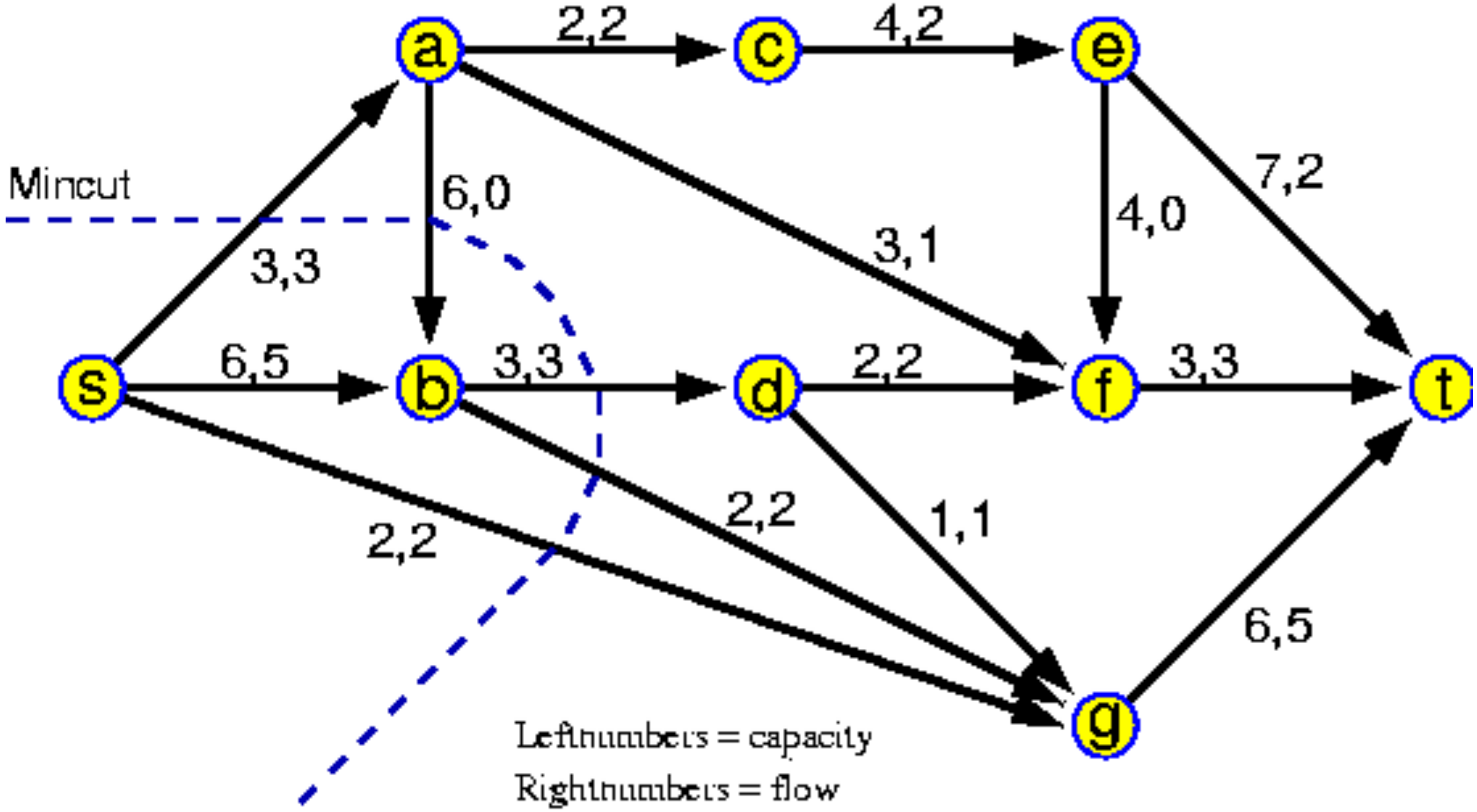


Example: Graph Algorithms

	A	B	C	D	E	F
A	-	1	1	1	1	
B	1	-		1	1	
C	1		-			1
D	1	1		-		1
E	1	1			-	1
F			1	1	1	-



Example: Combinatorial Optimization



Solving Ax = b, with sparse A

- Direct Methods
  - $A\,x = LU\,x = b$
- Iterative Methods
  - Write $Ax = b$ as

    $M\,x = (M\text{-}A)\,x + b$, for some matrix M
  - Solve each time:

    $M\,x_{k+1} = (M\text{-}A)\,x_k + b$
  - Until

    $||\,x_{k+1} - x_k\,|| < \varepsilon$, for some small ε

  Choose easy invertible M:
  - Diagonal part of A (Jacobi's)
  - Triangular part of A (Gauss Seidel)
  - Combination of the two (Successive Overrelaxation)
  - If $M = A$, then we have the direct method
  - Incomplete LU Factorization

Stability in direct methods

- Recapture Dense LU:

```
DO I = 1, N
   PIVOT = A(I, I)
   DO J = I+1, N
      MULT = A(J, I) / PIVOT
      A(J, I) = MULT
      DO K = I+1, N
         A(J, K) = A(J, K) - MULT * A(I, K)
      ENDDO
   ENDDO
ENDDO
```

- What if the PIVOT IS 0 (or very small) ?

Pivoting

$$\begin{pmatrix} 0 & 1 \\ 2 & 3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 4 \\ 5 \end{pmatrix}$$

- ➔ Whenever $a_{kk} = 0$ (or small) for some k. Look for a_{mk} which is not zero (or large)
- ➔ Permute row m to row k (exchange row m and row k)
- ➔ a_{mk} is now on the diagonal

$$\begin{pmatrix} 2 & 3 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 5 \\ 4 \end{pmatrix}$$

Numerical instability with small pivots

$$\begin{pmatrix} 0.001 & 2.42 \\ 1.00 & 1.58 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 5.20 \\ 4.57 \end{pmatrix}$$

If Gaussian elimination is performed with 3 decimal floating point arithmetic (0.123 E10), then (1.58 – 2420 = -2420 and 4.57-5200 = -5200)

$$\begin{pmatrix} 0.001 & 2.42 \\ 0 & -2420 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 5.20 \\ -5200 \end{pmatrix}$$

Which gives as result $\tilde{x} = \begin{pmatrix} -3.00 \\ 2.15 \end{pmatrix}$ ($0.001 * x_1 = 5.20 - 2.42 * 2.15 = -0.003$)

However 1.00*-3.00 + 1.58*2.15 = 0.397 ≠ 4.57

This is solved by partial pivoting (again).

➔ Ensure that the absolute value of all multipliers <= 1, or for all entries l_{ij} of L: $|l_{ij}| <= 1$

This is achieved by choosing only pivots $\boldsymbol{a_{kk}}$ such that

$$|\mathrm{a}_{kk}^{(k)}| >= |a_{ik}^{(k)}|, \; i > k$$

This is again achieved by row interchanges.

Example

$$A = \begin{bmatrix} 3 & 17 & 10 \\ 2 & 4 & -2 \\ 6 & 18 & -12 \end{bmatrix}$$

At the first step 6 is chosen as pivot.

So row 1 -> row 3, row 2 -> row 2, and row 3 -> row 1

This can be represented with permutation matrices:

$$P_1 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \text{ and } P_1 A = \begin{bmatrix} 6 & 18 & -12 \\ 2 & 4 & -2 \\ 3 & 17 & 10 \end{bmatrix}$$

The elimination step can be represented by:

$$E_1 = \begin{bmatrix} 1 & 0 & 0 \\ -1/3 & 1 & 0 \\ -1/2 & 0 & 1 \end{bmatrix}, \text{ so } E_1 P_1 A = \begin{bmatrix} 6 & 18 & -12 \\ 0 & -2 & 2 \\ 0 & 8 & 16 \end{bmatrix}$$

.

At the second step compute: $E_2 P_2 E_1 P_1 A$

With $P_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$ and

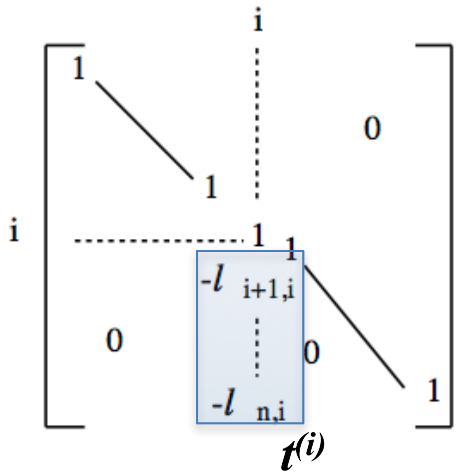
$$E_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1/4 & 1 \end{bmatrix} \text{ to yield } \begin{bmatrix} 6 & 18 & -12 \\ 0 & 8 & 16 \\ 0 & 0 & 6 \end{bmatrix} = U$$

In general all steps can be represented as:

$$E_{n-1} P_{n-1} \cdots E_2 P_2 E_1 P_1 A = U$$

with

$E_i =$



and

$$L(k+1:n, k) = P_{n-1} \cdots P_{k+1} \cdot t^{(k)}$$

Solution is obtained by

$$
\begin{aligned}
&1. \quad c = Pb \\
&2. \quad Ly = c \\
&3. \quad Ux = y
\end{aligned}
$$

with: $P = P_{n-1} P_{n-2} \ldots P_2 P_1$, $P A = L U$

$$Ax = b \Rightarrow PAx = Pb \Rightarrow LUx = Pb \Rightarrow L\,(\,Ux\,) = Pb$$

Complete Pivoting

With partial pivoting the growth of the entries in the lower triangular matrix can still be as large as 2^{n-1} (if pivot ≈ 1 at each step, then entries can double at each step)

➔Need for finding better pivots

Instead of

$$|a_{kk}^{(k)}| >= \mathbf{max}\ (|a_{ik}^{(k)}|,\ i > k\ )$$

choose

$$|a_{kk}^{(k)}| >= \mathbf{max}\ (|a_{ij}^{(k)}|,\ i\ ,j > k\ )$$

So with complete pivoting each step can be expressed as:

$$E_{n-1} P_{n-1} E_{n-2} P_{n-2} \dots E_1 P_1 A\, Q_1 Q_2 \dots Q_{n-1} = U.$$

So,

$$PAQ = LU$$

with $P = P_{n-1} P_{n-2} \dots P_2 P_1$, $Q = Q_1 Q_2 \dots Q_{n-2} Q_{n-1}$

So, the solution x can be obtained by

1. $c = Pb$
2. $Ly = c$
3. $Uz = y$
4. $Q^T x = z \quad (Q^T = Q^{-1})$

For many systems pivoting is not required

1. A is strictly diagonally dominant, if $|A_{ii}| > \sum_{j=1_{j \neq i}}^{n} |a_{ij}|$.

   Theorem 1 *If A^T is strictly diagonally dominant, then LU obtained with no pivoting has the property that $|L_{ij}| \leq 1$, for all i, j.*

2. A is symmetric, if $A_{ij} = A_{ji}$ for all i, j. A is positive definite, if for every $x \neq 0$

$$x^T A x > 0$$

   ($x^T Ax$ often reflects the energy of the underlying physical system and is therefore often positive.)

   Theorem 2 *If A is symmetric positive definite, then*

$$\varrho = \max_{i,j,k} |a_{ij}^{(k)}| \leq \max_{i,j} |a_{ij}|.$$

   In this case LU can be written as $A = L \cdot L^T$ (or LDL^T, avoiding the calculation of square roots). This is called **Choleski Factorization**.

Iterative Methods

$$Mx_{k+1} = (M\text{-}A)\, x_k + b$$

with M easy invertible, meaning that in most of the cases M^{-1} can be directly expressed by a single matrix $\mathcal{M}$

➔So, the solution can be obtained by simply performing (sparse) matrix multiplications

$$x_{k+1} = \mathcal{M}\,((M\text{-}A)\, x_k + b)$$

Implementation Issues

- **Data Storage**: Pointer structures, Linked lists, Linear Arrays
- **Pivot Search**: Multiple storage schemes
- **Masking Operations**: Gather/Scatter Operations
- **Garbage collection**: Fill-in, Explicit garbage collection
- **Permutation Issues**: Implicit and/or explicit

$$A = (a_{ij}) = \begin{pmatrix} 1. & 0. & 0. & -1. & 0. \\ 2. & 0. & -2. & 0. & 3. \\ 0. & -3. & 0. & 0. & 0. \\ 0. & 4. & 0. & -4. & 0. \\ 5. & 0. & -5. & 0. & 6. \end{pmatrix}$$

Coordinate Scheme Storage

```
int     IRN[11], JCN[11];
float  VAL[11];
```

	1	2	3	4	5	6	7	8	9	10	11
IRN	1	2	2	1	5	3	4	5	2	4	5
JCN	4	5	1	1	5	2	4	3	3	2	1
VAL	-1.	3.	2.	1.	6.	-3.	-4.	-5.	-2.	4.	5.

- No explicit order of the nonzero entries is enforced
- Fetching row/column requires the whole data structure to be searched
- Insertion and/or deletion of nonzero entries is simple

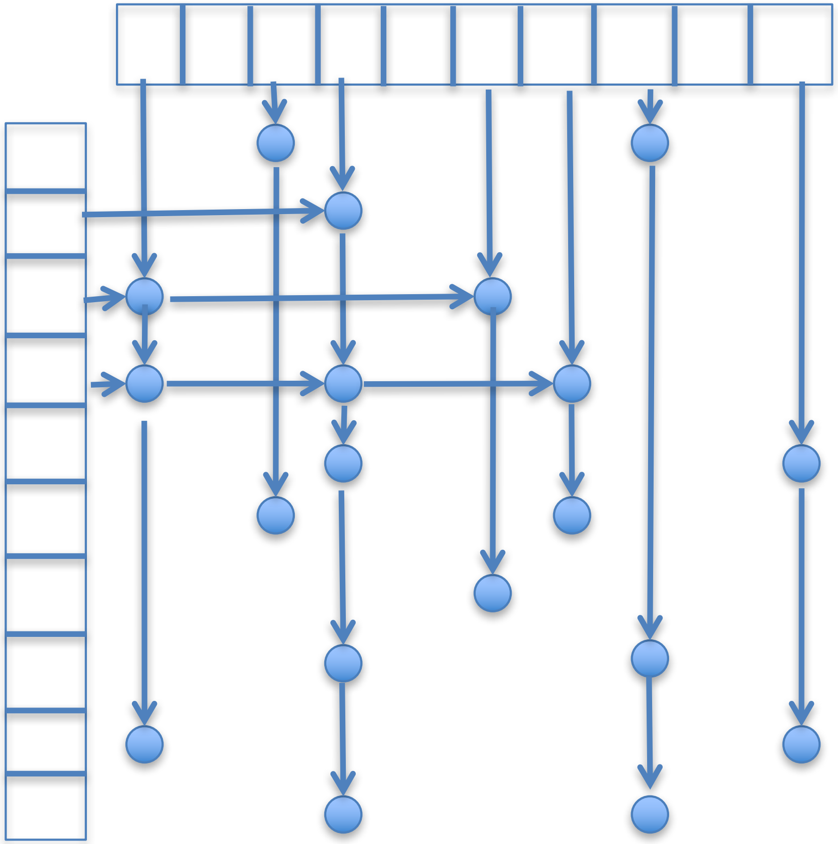
Sparse Compressed Row/Column Format

int LENROW[5], POINTER[5], ICN[11]
float VAL[11]

LENROW	2	3	1	2	3						
POINTER	1	3	6	7	9						
ICN	4	1	5	1	3	2	4	2	3	1	5
VAL	-1.	1.	3.	2.	-2.	-3.	-4.	4.	-5.	5.	6.

- LENCOL, POINTER, and IRN are used for compressed column format
- Fetching row or column is very easy in corresponding format
- Insertion of nonzero elements is a big problem – expanded row/column is put at the end, and the LENROW/LENCOL is updated correspondingly
- Instead of LENROW/LENCOL the last element in each row in ICN is negated

Linked List (Pointer) Implementations



- Very flexible
- Access to data very inefficient
  - Pointer chasing
  - Addresses not consecutive: bad spatial locality

ExtendedColumn/ITpack/JaggedDiagonal Format

Shift all nonzero entries to the beginning of each row

```
int    INDEX[5][max]
float  VALUE[5][max]
```

$$\text{INDEX:} \begin{pmatrix} 1 & 4 & 0 \\ 1 & 3 & 5 \\ 2 & 0 & 0 \\ 2 & 4 & 0 \\ 1 & 3 & 5 \end{pmatrix} \text{ and VALUE:} \begin{pmatrix} 1. & -1. & 0. \\ 2. & -2. & 3. \\ -3. & 0. & 0. \\ 4. & -4. & 0. \\ 5. & -5. & 6. \end{pmatrix}$$

- Especially suited for vector processing
- Commonly used in sparse matrix multiplication
- Very good use of spatial locality

Full Dense Format

float A[i][j]

- Seems wasteful
- Mostly restricted to sub-blocks of the matrix which contain many nonzero's
- Used to locally expand rows and/or columns
- Often used in hybrid storage schemes with other formats

Pivot Search

- When doing Gaussian Elimination: rows are added to other rows
- Compressed row storage seems to be the natural choice
- However, for partial pivoting for instance: each time all elements in a column need to be inspected

➔ Both row AND column compressed storage are required

Masking Operations (GATHER/SCATTER)

Adding one sparse row to another:

- Two incrementing pointers
- Scattering target row into a dense row, with a masking array indicating which position in the row are nonzero

```
DO J =  POINTER (K), POINTER (K+1) – 1                       |
     TARGET ( ICN (K) ) = VAL ( K )                          | SCATTER
     MASK ( ICN (K) ) = TRUE                                 |

DO J =  POINTER (I), POINTER (I+1) – 1
     TARGET ( ICN (J) ) = TARGET ( ICN (J) ) + PIV * VAL ( J )
     IF MASK (ICN(J)) = FALSE THEN MASK (ICN(J)) = True

DO J = 1, N
     IF ( MASK (ICN(J)) = TRUE ) THEN write TARGET (ICN(J)) back   | GATHER
```

Fill-in / Garbage Collection

- Note that the write back will cause problems in general
- Additional space is reserved to store the expanded columns or rows and the old location will have to be released at some point
- In direct solvers this is mostly explicitly controlled!!!!!
- In any case: it is extremely important to minimize the amount of fill-in

Fill-in Control (Markowitch counts)

$r^{(k)}_i$ = the number of nonzero elements in row i of the active $(n\text{-}k)x(n\text{-}k)$ sub-matrix

$c^{(k)}_j$ = the number of nonzero elements in column j of the active $(n\text{-}k)x(n\text{-}k)$ sub-matrix

➔ Instead of complete pivoting, choose pivot based on:

$|a_{ij}^{(k)}| \geq u.|$ values in column j of the active submatrix $|$
such that $(r_i^{(k)} - 1)(c_j^{(k)} - 1)$ is *minimized.*

u (0 < u <= 1) is thresshold parameter balancing between stability and fill-in control

Permutations

- If $Q = P^T$ then PAQ (= PAP^T) is a symmetric permutation
  - Diagonal elements stay on the diagonal
  - The associated (di)graph stays the same
- Permutations can be executed explicitly (beforehand), on the fly, or implicitly by referring each time to P(I) instead of I

Lab Assignment

Write a C-program which implements LU factorization with partial pivoting.

See course website for details.