SPARSE MATRICES

Intensive Computation

Annalisa Massini
2021-2022

Lecture 21

COMPACT STORAGE FORMAT

Most of the material is from:

L. Formaggia, F. Saleri, A. Veneziani **Solving Numerical PDEs: Problems, Applications, Exercises -** Appendix *The treatment of sparse matrices*

BSR format from:

https://software.intel.com/en-us/mkl-developer-reference-c-sparse-blas-bsr-matrix-storage-format

Storage Methods for Sparse Matrix

- A matrix is ***sparse*** if it contains a **large number** of zeros
- ***sparsity*** of the matrix =

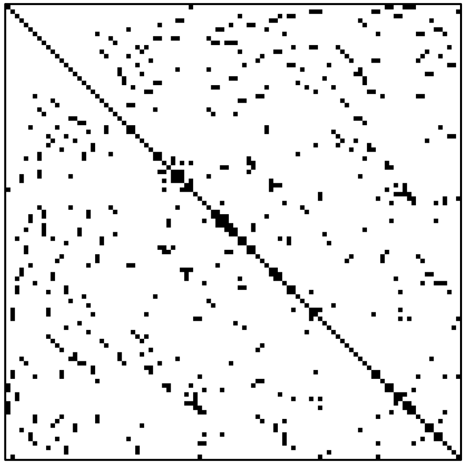
  number of zero-valued elements / total number of elements
- ***density* = 1 - *sparsity***
- A matrix is **sparse** if its sparsity is > 0.5
- **But** *sparsity is interesting* if in a matrix of size nxn

  → the number of non-zero entries is $O(n)$
- This means that the average number of non-zero entries in each row is bounded independently from *n*
- A non-sparse matrix is said **full** or **dense** if the number of non-zero elements is $O(n^2)$

Storage Methods for Sparse Matrix

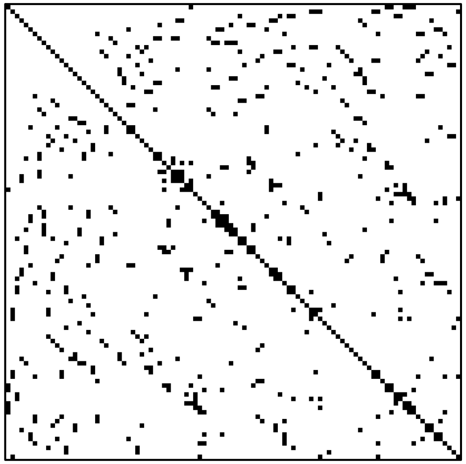
- If the location of the zero elements is known a-priori, we can avoid reserving storage for them

- The distribution of non-zero elements of a sparse matrix may be described by:
    - the **sparsity pattern**, defined as the set $\{(i,j): A_{ij} \neq 0\}$
    - the matrix graph, where nodes *i* and *j* are connected by an edge if and only if $A_{ij} \neq 0$
- In order to take advantage of the large number of zero elements, ***special schemes*** *are required to store sparse matrices*



Storage Methods for Sparse Matrix

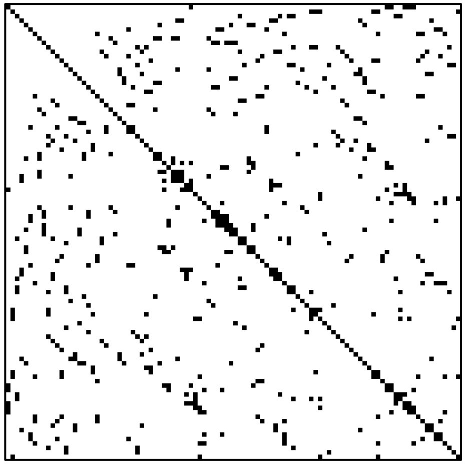
- The use of adequate storage techniques for sparse matrices is fundamental, especially with large-scale problems
- Large sparse matrices often appear in scientific or engineering applications when solving partial differential equations
- Example
  - Suppose we want to solve the Navier-Stokes equations on a two-dimensional grid formed by 10.000 vertexes with finite elements
  - The number of degrees of freedom is around 10^5 for the pressure and 4×10^5 for each component of the velocity
  - The associated matrix will then be 90000×90000
  - If we store all 8.1×10^9 coefficients, using double precision (8 bytes), around 60 Gigabytes are necessary!
  - ***This is too much and memory handle is very inefficient***



Storage Methods for Sparse Matrix

- In case of a **three-dimensional problem** the situation becomes even **worse**, since the number of degrees of freedom grows very rapidly as the grid gets finer
  - Nowadays it is common to deal with millions of degrees of freedom

- Therefore to store sparse matrices efficiently we need **data formats** that are **more compact** than the classical array



Storage Methods for Sparse Matrix

- The adoption of sparse formats may affect the ***speed of certain operations***

- For example, with a sparse format we **cannot access** or search for a **particular element** (or group of elements) directly, using the two indexes *i* and *j* to determine where entry A_{ij} is located in the memory
- On the other hand, even if the operation of accessing an entry of a matrix in sparse format turns out to be less efficient, by adopting a sparse format we will nevertheless **access only nonzero elements,** thus **executing only useful operations**

Storage Methods for Sparse Matrix

- Hence, in general, the sparse format is preferable in terms of storage as well as in terms of computing time, as long as the matrix is **sufficiently sparse**

- The main goal of sparse formats is:
  - to **represent only the nonzero elements**
  - to be able **to efficiently perform the common matrix operations**

Storage Methods for Sparse Matrix

- We can distinguish different kinds of **operations** on a matrix
- The most important operations are:

1. **accessing** a **generic element** (random access)
2. **accessing** the elements of a **whole row**: important when multiplying a matrix by a vector
3. **accessing** the elements of a **whole column**, or equivalently, of a row in the transpose matrix (relevant for operations such as symmetrizing the matrix after imposing Dirichlet conditions)
4. **adding a new element** to the matrix pattern: this is a critical issue if the pattern is not known beforehand or it can change throughout the computations
5. And, **multiplying a matrix and a vector** that is a very **common** intermediate **operation** used in many numerical methods

Storage Methods for Sparse Matrix

- It is important to characterize formats for sparse matrices by the computational cost of these operations and by how the latter depends on the matrix size

- Different formats for sparse matrices exist due to the fact that there is *no format that is simultaneously optimal for all the above operations*, and at the same time *efficient in terms of* ***storage capacity***

Storage Methods for Sparse Matrix

- In the following:
  - ***n*** is the matrix' size
  - ***nz*** *is* the number of non-zero entries
  - We adopt the convention of indexing entries of matrices and vectors (arrays) starting from 1 (as in Matlab)
  - *Aij* will denote the entry of the matrix A on row *i* and column *j*
- To estimate how much memory the matrix occupies we assume that:
  - an integer occupies 4 bytes
  - a real number (floating point repres.) 8 bytes (double precision)
  - For example, storing a square matrix having n = 12 would require $12 \times 12 \times 8 = 1152$ bytes

The Coordinate format: COO format

- The simplest storage scheme for sparse matrices is the format by **coordinate**

- The data structure consists of three arrays:
  - **A** - a real array containing all the real (or complex) values of the nonzero elements in **any order**
  - **I** - an integer array containing their row indices
  - **J** - a second integer array containing their column indices
  - I, J and A all have *nz* elements, as many as the number of non-zero elements of the matrix

The Coordinate format: COO format

Example

The matrix A

1.	0.	0.	**2.**	0.
3.	**4.**	0.	**5.**	0.
6.	0.	**7.**	**8.**	**9.**
0.	0.	**10.**	**11.**	0.
0.	0.	0.	0.	**12.**

is represented (*for example*) by

A	**12.**	**9.**	**7.**	**5.**	**1.**	**2.**	**11.**	**3.**	**6.**	**4.**	**8.**	**10.**
I	**5**	**3**	**3**	**2**	**1**	**1**	**4**	**2**	**3**	**2**	**3**	**4**
J	**5**	**5**	**3**	**4**	**1**	**4**	**4**	**1**	**1**	**2**	**4**	**3**

- Notice that elements are listed in an ***arbitrary order***

The Coordinate format: COO format

Example - *n*=12 and *nz*=58

101	102	0	103	0	0	0	0	0	0	0	0
104	105	106	107	108	0	0	0	0	0	0	0
0	109	110	0	111	112	0	0	0	0	0	0
113	114	0	115	116	0	117	0	0	0	0	0
0	118	119	120	121	122	123	124	0	0	0	0
0	0	125	0	126	127	0	128	129	0	0	0
0	0	0	130	131	0	132	133	0	134	0	0
0	0	0	0	135	136	137	138	139	140	141	0
0	0	0	0	0	142	0	143	144	0	145	146
0	0	0	0	0	0	147	148	0	149	150	0
0	0	0	0	0	0	0	151	152	153	154	155
0	0	0	0	0	0	0	0	156	0	157	158

The space occupied is:

- $8 \times n \times n$ =
  = 8 x 12 x 12 **= 1152** bytes

in full format

The Coordinate format: COO format

Example - n=12 and nz=58

101	**102**	0	**103**	0	0	0	0	0	0	0	0
104	**105**	**106**	**107**	**108**	0	0	0	0	0	0	0
0	**109**	**110**	0	**111**	**112**	0	0	0	0	0	0
113	**114**	0	**115**	**116**	0	**117**	0	0	0	0	0
0	**118**	**119**	**120**	**121**	**122**	**123**	**124**	0	0	0	0
0	0	**125**	0	**126**	**127**	0	**128**	**129**	0	0	0
0	0	0	**130**	**131**	0	**132**	**133**	0	**134**	0	0
0	0	0	0	**135**	**136**	**137**	**138**	**139**	**140**	**141**	0
0	0	0	0	0	**142**	0	**143**	**144**	0	**145**	**146**
0	0	0	0	0	0	**147**	**148**	0	**149**	**150**	0
0	0	0	0	0	0	0	**151**	**152**	**153**	**154**	**155**
0	0	0	0	0	0	0	0	**156**	0	**157**	**158**

The space occupied is:

- $8 \times n \times n$ = **1152** bytes **in full format**
- $(4+4+8) \times nz$ = 16 x 58 = **= 928** bytes **in COO format**

A

101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	...
...	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	...
...	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	

I

1	1	1	2	2	2	2	2	3	3	3	3	4	4	4	4	4	5	5	5	...
...	5	5	5	5	6	6	6	6	6	7	7	7	7	7	8	8	8	8	8	...
...	8	8	9	9	9	9	9	10	10	10	10	11	11	11	11	11	12	12	12	

J

1	2	4	1	2	3	4	5	2	3	5	6	1	2	4	5	7	2	3	4	...
...	5	6	7	8	3	5	6	8	9	4	5	7	8	10	5	6	7	8	9	...
...	10	11	6	8	9	11	12	7	8	10	11	8	9	10	11	12	9	11	12	

The Coordinate format: COO format

- COO format *does not guarantee rapid access to an element, nor to rows or columns*

- Finding the generic element of the matrix from the row and column indexes normally requires a number of operations proportional to *nz*
- In fact, it is necessary to go through all elements of I and J until one hits those indexes, using expensive comparison operations

- Using specific techniques to store the indexes in special search data structure, it is possible to reduce the cost to $O(\log_2(nz))$, but at a higher storing price

The Coordinate format: COO format

- The operation of **multiplying** a matrix A and a vector **x** can be done directly, by running through the elements of the three arrays

- A possible code for the product **y** = A**x** using MATLAB

101	102	0	103	0	0	0	0	0	0	0	0
104	105	106	107	108	0	0	0	0	0	0	0
0	109	110	0	111	112	0	0	0	0	0	0
113	114	0	115	116	0	117	0	0	0	0	0
0	118	119	120	121	122	123	124	0	0	0	0
0	0	125	0	126	127	0	128	129	0	0	0
0	0	0	130	131	0	132	133	0	134	0	0
0	0	0	0	135	136	137	138	139	140	141	0
0	0	0	0	0	142	0	143	144	0	145	146
0	0	0	0	0	0	147	148	0	149	150	0
0	0	0	0	0	0	0	151	152	153	154	155
0	0	0	0	0	0	0	0	156	0	157	158

```
y=zeros(nz,1);
for k=1:nz
   i=I(k);
   j=J(k);
   y(i)= y(i) + A(k)*x(j); % notice the use of i and j
end
```

101	102	103	104	105	106	107	108	109	110	111	...
1	1	1	2	2	2	2	2	3	3	3	...
1	2	4	1	2	3	4	5	2	3	5	...

The Coordinate format: COO format

Observations

- The additional cost of this operation (compared to the analogue for a full matrix) depends essentially on indirect addressing:
  - accessing **`y(i)`** requires first of all to access **`I(k)`**

- The access and update of arrays **`x`** and **`y`** does not proceed by consecutive elements → the possibility of optimizing the use of the processor's cache is greatly reduced

The Coordinate format: COO format

Observations

- Operations are performed only on non-zero elements and in general we have $nz << n^2$

- An advantage of this format is that:
  - It is easy to add a new element to the matrix
  - In fact, it is enough to add a new entry to the arrays I, J and A

- For this reason, COO is often used when the pattern is not known a priori

The *skyline* format

- The format called **skyline** is among the first used to store matrices arising from the method of finite elements
- The idea is to store the area formed by the **elements between the first and last non-zero coefficient**, on **each row**

101	102	**0**	103	0	0	0	0	0	0	0	0
104	105	106	107	108	0	0	0	0	0	0	0
0	109	110	**0**	111	112	0	0	0	0	0	0
113	114	**0**	115	116	**0**	117	0	0	0	0	0
0	118	119	120	121	122	123	124	0	0	0	0
0	0	125	**0**	126	127	**0**	128	129	0	0	0
0	0	0	130	131	**0**	132	133	**0**	134	0	0
0	0	0	0	135	136	137	138	139	140	141	0
0	0	0	0	0	142	**0**	143	144	**0**	145	146
0	0	0	0	0	0	147	148	**0**	149	150	0
0	0	0	0	0	0	0	151	152	153	154	155
0	0	0	0	0	0	0	0	156	**0**	157	158

- This forces to **store some null entries**

The *skyline* format

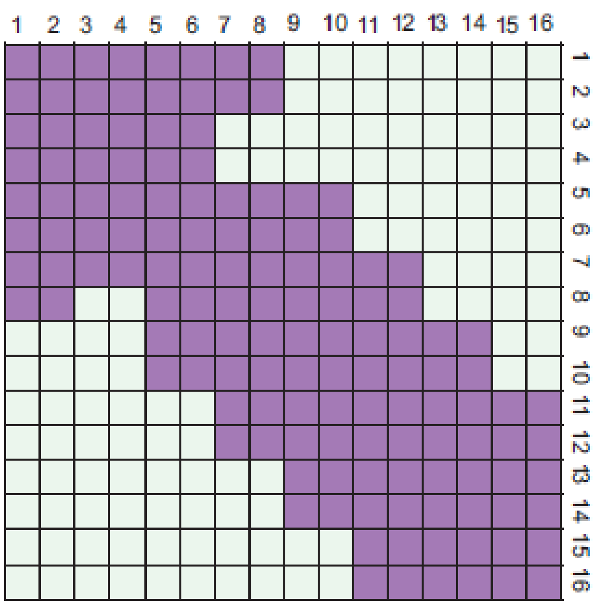
- This extra cost will be small if the matrix has non-zero entries clustered around the diagonal

101	102	0	103	0	0	0	0	0	0	0	0
104	105	106	107	108	0	0	0	0	0	0	0
0	109	110	0	111	112	0	0	0	0	0	0
113	114	0	115	116	0	117	0	0	0	0	0
0	118	119	120	121	122	123	124	0	0	0	0
0	0	125	0	126	127	0	128	129	0	0	0
0	0	0	130	131	0	132	133	0	134	0	0
0	0	0	0	135	136	137	138	139	140	141	0
0	0	0	0	0	142	0	143	144	0	145	146
0	0	0	0	0	0	147	148	0	149	150	0
0	0	0	0	0	0	0	151	152	153	154	155
0	0	0	0	0	0	0	0	156	0	157	158

- Indeed, algorithms have been developed to cluster non zero elements by permuting the rows and columns of the matrix (see, for example, the Cuthill-McKee algorithm)

Skyline for symmetric matrices

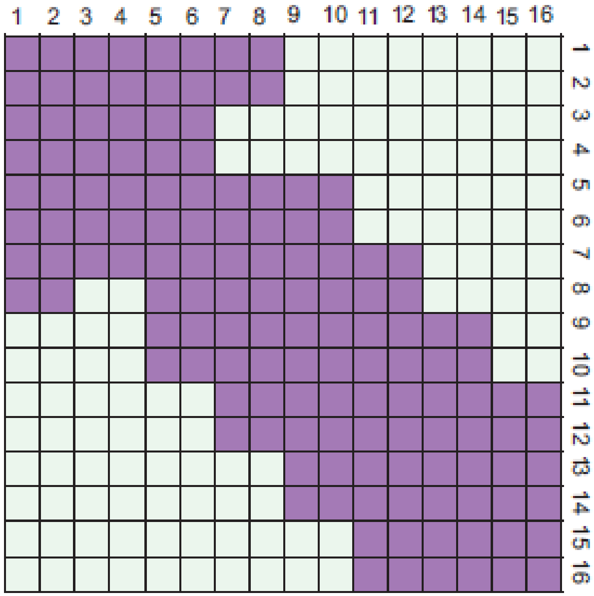
- If a matrix is **symmetric** we can store only:
  - Its **lower triangular part** (diagonal included)
  - **Or** we can store the **diagonal on an auxiliary array** and treat the **off-diagonal entries** separately, having the advantage of allowing the *direct access to the diagonal elements*



Skyline for symmetric matrices

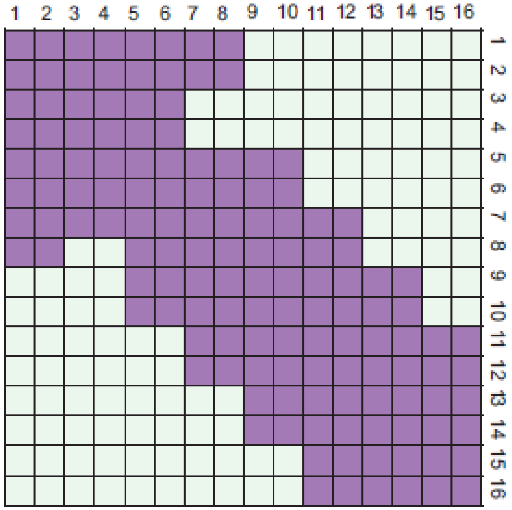
The ***skyline* format** with diagonal array is given by:

- **D** - real array storing diagonal entries
- **AL** - real array storing all *skyline* elements row-wise (except the diagonal)
  This can clearly include null coefficients
- **I** - integer array storing *pointers to rows* of matrix A
  - The *k*th component of array I points to the first element of row (k + 1) in AL



Skyline for symmetric matrices

- All elements of AL from position **`I(k)`** to **`I(k+1)-1`** are the off-diagonal elements belonging to row *k* + 1, in column order
- Notice that:
  - ***The first row is not stored***, since it only has the diagonal element
  - **`I(k)`** points to the first non-zero element on the (k+1)-th row
  - The difference **`I(k+1)- I(k)`** gives the number of the off-diagonal elements on row k + 1 belonging to the *skyline*



Skyline for symmetric matrices

Example

- We want to store the symmetric matrix obtained from the lower triangular part of matrix A (seen before) using the *skyline* format
- This matrix can be obtained with the Matlab instruction
  `tril(A)+ tril(A,-1)'`

101	104	0	113	0	0	0	0	0	0	0	0
104	105	109	114	118	0	0	0	0	0	0	0
0	109	110	0	119	125	0	0	0	0	0	0
113	114	0	115	120	0	130	0	0	0	0	0
0	118	119	120	121	126	131	135	0	0	0	0
0	0	125	0	126	127	0	136	142	0	0	0
0	0	0	130	131	0	132	137	0	147	0	0
0	0	0	0	135	136	137	138	143	148	151	0
0	0	0	0	0	142	0	143	144	0	152	156
0	0	0	0	0	0	147	148	0	149	153	0
0	0	0	0	0	0	0	151	152	153	154	157
0	0	0	0	0	0	0	0	156	0	157	158

Skyline for symmetric matrices

Example

- Diagonal **D**

101	105	110	115	120	121	127	132	138	144	149	154	158

- Pointer **I** and lower skyline elements **AL**

1	2	3	6	9	12	15	18	21	24	27	30

104	109	113	114	0	118	119	120	125	0	126	130	131	0	135	136	137	142	0	143	147	148	0	151	152	153	156	0	157

101	104	0	113	0	0	0	0	0	0	0	0
104	105	109	114	118	0	0	0	0	0	0	0
0	109	110	0	119	125	0	0	0	0	0	0
113	114	0	115	120	0	130	0	0	0	0	0
0	118	119	120	121	126	131	135	0	0	0	0
0	0	125	0	126	127	0	136	142	0	0	0
0	0	0	130	131	0	132	137	0	147	0	0
0	0	0	0	135	136	137	138	143	148	151	0
0	0	0	0	0	142	0	143	144	0	152	156
0	0	0	0	0	0	147	148	0	149	153	0
0	0	0	0	0	0	0	151	152	153	154	157
0	0	0	0	0	0	0	0	156	0	157	158

Skyline for symmetric matrices

Example

- Diagonal **D**

101	105	110	115	120	121	127	132	138	144	149	154	158

- Pointers **I** and lower skyline elements **AL**

1	2	3	6	9	12	15	18	21	24	27	30

104	109	113	114	0	118	119	120	125	0	126	130	131	0	135	136	137	142	0	143	147	148	0	151	152	153	156	0	157

- Note that in the *n*th place of the array **I** we have left a pointer at the beginning of an hypothetical position. In this way:
  - We can compute the number of skyline elements in the last row, that is `I(n) - I(n-1)`
  - `I(n)- 1` is the **total number of elements** in the skyline

Skyline for symmetric matrices

The product $\mathbf{y} = A\mathbf{x}$ following MATLAB syntax is given by:

```
y=D.*x;
for k=2:n
  nex = I(k)-I(k-1);
  ik = I(k-1):I(k)-1;
  jcol= k-nex:k-1;
  y(k) = y(k)+dot(AL(ik),x(jcol));
  y(jcol)= y(jcol)+AL(ik)*x(k);
end
```

- We ***operate symmetrically on rows and columns*** to exploit the fact that only the lower triangular part was stored in AL

Skyline for symmetric matrices

- The memory needed to store the matrix in this format depends on how effectively the skyline reproduces the actual pattern
- In our case:
  - The **full format** requires: 12 x 12 x 8 = **1152**
  - Array **AL** contains **29 real numbers** (including six 0s)
  - Array **D** of **fixed length *n*=12** containing reals
  - Array **I** of **fixed length *n*=12** containing integers
  - **Total**: (29 + 12) x 8 +n x 4 = **376**

- In general, we need $(n_{AL} + n)$ x 8 + n x 4
- Generally, *Skyline* is more convenient than the COO format if the coefficients are well clustered around the diagonal

Skyline for general matrices

- As for **non-symmetric matrices**, a reasonable way to proceed is to split A into:
  - The diagonal D
  - The strictly lower triangular part E
  - The strictly upper triangular part F

- Using the Matlab syntax, these matrices would be defined as:

```
D=diag(diag(A));
E=tril(A,-1);
F=triu(A,1);
```

Skyline for general matrices

- In general, we need two arrays of indexes: one for pointer to array E and one for pointers to array FT
- If the pattern of A is symmetric, the skyline of E coincides with that of FT, and the same array of pointers I is for both triangular parts
- Diagonal **D**

101	105	110	115	121	127	132	138	144	149	154	158

- Pointer **I**, lower *skyline* elements **E** and upper *skyline* elements **FT**

FT:

102	106	0	107	103	116	111	108	122	0	112	0	123	117	133	128	124	139	0	129	140	134	150	145	141	155	156	0	146

I:

1	2	3	6	9	12	15	18	21	24	27	30

E:

104	109	113	114	0	118	119	120	125	0	126	130	131	0	135	136	137	142	0	143	147	148	0	151	152	153	156	0	157

Skyline for general matrices

- The product matrix-vector $\mathbf{y} = \mathrm{A}\mathbf{x}$ now reads

```
y=D.*x;
for k=2:n
  nex = I(k)-I(k-1);
  ik = I(k-1):I(k)-1;
  jcol = k-nex:k-1;
  y(k) = y(k)+dot(E(ik),x(jcol));
  y(jcol)= y(jcol)+FT(ik)*x(k);
end
```

- **icol** and **ik** contain all indexes corresponding to the columns of row k, so the scalar product **dot(E(ik),x(jcol))** and the multiplication vector-constant **FT(ik)*x(k)** are optimized

Skyline for general matrices

- Notice that in this format the access to diagonal entries is direct
- Being able to access diagonal entries directly has certain advantages:
  - For instance there are methods that, to impose essential boundary condition, only need the access to diagonal elements
- The cost of extracting a row is independent of the matrix' size
- The fact that the data relative to a row are stored consecutively in the memory allows the system to optimize the processor's cache memory when multiplying a matrix by a vector
- The extraction of column is an **expensive** operation that requires many comparisons, and whose cost grows linearly in *n*

The Compressed Sparse Row (CSR) format

- The problem with the *skyline* format is that the memory used depends on the numeration of elements and is in general impossible to avoid the unnecessary storage of zero elements

- The CSR (Compressed Sparse Row) format can be seen as a compressed version of COO, and also as an improved *skyline*, that stores non-zero elements only

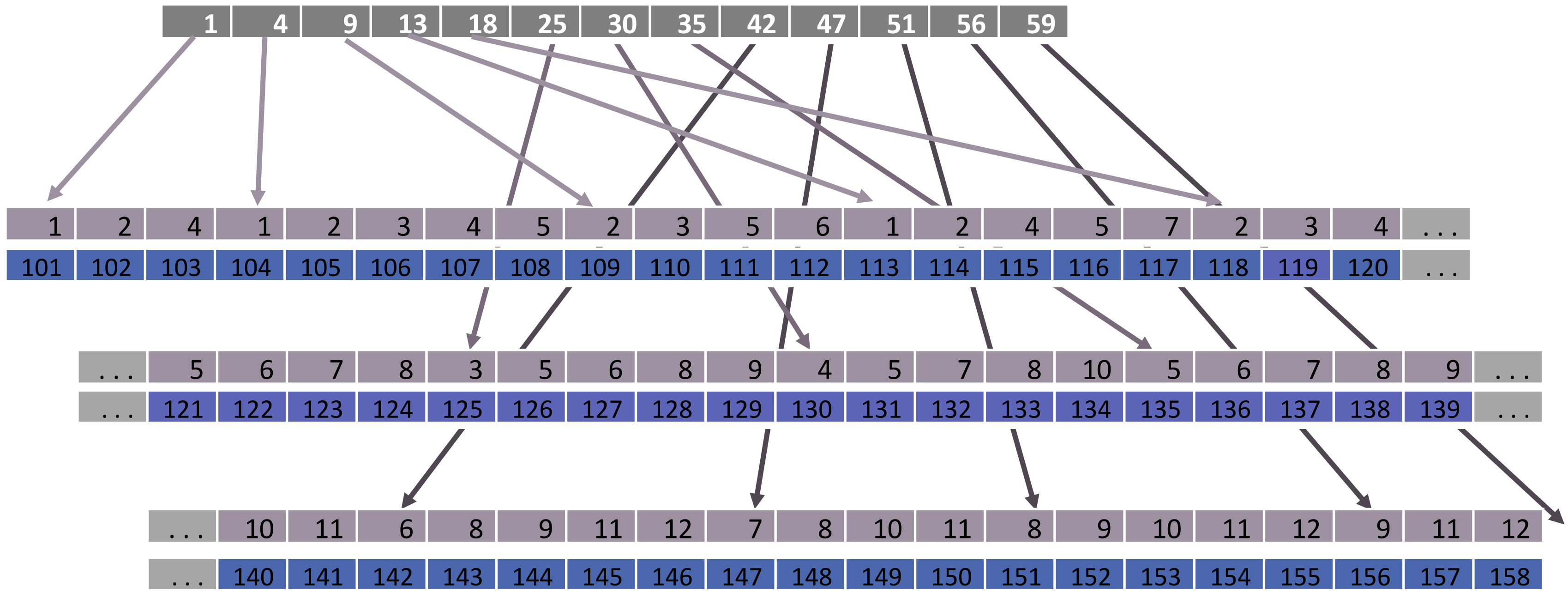
The Compressed Sparse Row (CSR) format

The CSR format uses three arrays:

- **A** - real array of length *nz* storing the non-zero entries of the matrix, ordered row-wise. It coincides with array A of the COO format
- **J** - integer array of length *nz*, whose entry J(*k*) indicates the column of the element A(*k*). It coincides with array J of the COO format
- **I** - integer array of length *n* containing *pointers* to the rows. Then `I(k)` gives the position where the *k*-th row in A and J begins

The Compressed Sparse Row (CSR) format

- Array I is usually of length *n* + 1, so that the number of non-zero entries on row *k* is always `I(k+1)-1-I(k)`
- To make this hold, the last element `I(n+1)` will contain *nz* + 1 and in this way we also have that `nz=I(n+1)-I(1)`



The Compressed Sparse Row (CSR) format

- The CSR format uses $8 \times nz + 4 \times (nz + n + 1)$ bytes
- CSR format suits square and rectangular matrices alike
- Operations:
  - quick **extraction of row *i*** → elements between **`I(i)`** and **`I(i+1)-1`**
  - **column extraction** requires localizing on *each row* the values of **`J`** corresponding to the wanted column
    - If we adopt no particular ordering, the cost operation is proportional to *nz*
    - If, instead, column indexes of each row in J are ordered in increasing order as in our example, with a binary-search algorithm the extraction cost for a column becomes proportional to $n \log_2(m)$, where m is the mean number of elements on each row
  - the **access to a generic element** has normally a cost proportional to m, yet if we order columns it reduces to $\log_2 m$

The Compressed Sparse Row (CSR) format

The matrix-vector product $\mathbf{y} = \mathrm{A}\mathbf{x}$ is given by

```
y=zeros(n,1);
  % y=A(I(1:n)).*x if the diagonal is stored first
for k=1:n
  ik=I(k):I(k+1)-1;
  % ik=I(k)+1:I(k+1)-1; if the diagonal is stored first
  jcol =J(ik); y(k)=y(k)+dot(A(ik),x(jcol));
end
```

The CSC (Compressed Sparse Column) format

- The **CSC (Compressed Sparse Column) format** stores matrices by ordering them column-wise
- It is easy to extract a column as opposed to rows
- The roles of vectors I and J is exchanged compared with the CSR format
- When performing matrix-vector multiplication with a sparse matrix in CSC format it is preferable to compute the result as a linear combination of the columns of the matrix
- Indeed, if $\mathbf{c}_i$ indicates the i-th column of matrix A, we have that $A\mathbf{x} = \Sigma_i \, x_i\mathbf{c}_i$

The CSC (Compressed Sparse Column) format

- Therefore, the matrix-vector product $\mathbf{y} = A\mathbf{x}$ on a CSC matrix may be computed as:

```
y=zeros(n,1);
for k=1:n
  xcoeff=x(k);
  jk=I(k):I(k+1)-1;
  ik=J(jk);
  y(ik)=y(ik) + xcoeff * A(jk)';
end
```

The MSR (Modified Sparse Row) format

- The **MSR (Modified Sparse Row)** format is a special version of CSR for square matrices exploiting the fact that:
  - The diagonal elements of many matrices are usually nonzero (matrices generated by finite elements)
  - The diagonal elements are accessed more often than the rest of the elements
- **Diagonal** entries can be stored in one single array, since their *indexes are implicitly known* from their position in the array
- As for the symmetric skyline, only off-diagonal elements are stored in a special fashion, i.e. through a format akin to CSR

The MSR (Modified Sparse Row) format

The MSR format uses two arrays:

- **V** - real array of values:
  - In the first *n* entries of V we store the diagonal
  - The place *n*+1 in V is left with ***no significant value*** (may sometimes carry some information concerning the matrix)
  - From place *n*+2 onwards off-diagonal elements are stored, row-wise
  - V has length *nz* + 1
- **B** - Bind
  - B has the same length as V → *nz* + 1
  - The first *n* + 1 point to where rows begin
  - From *n*+2 to *nz*+1 there are the column indexes of the elements stored in the corresponding places in V

The MSR (Modified Sparse Row) format

Example

101	102	0	103	0	0	0	0	0	0	0	0
104	105	106	107	108	0	0	0	0	0	0	0
0	109	110	0	111	112	0	0	0	0	0	0
113	114	0	115	116	0	117	0	0	0	0	0
0	118	119	120	121	122	123	124	0	0	0	0
0	0	125	0	126	127	0	128	129	0	0	0
0	0	0	130	131	0	132	133	0	134	0	0
0	0	0	0	135	136	137	138	139	140	141	0
0	0	0	0	0	142	0	143	144	0	145	146
0	0	0	0	0	0	147	148	0	149	150	0
0	0	0	0	0	0	0	151	152	153	154	155
0	0	0	0	0	0	0	0	156	0	157	158

- **Array B**

14	16	20	23	27	33	37	41	47	51	54	58	60	2	4	1	3	4	5	2	5	...

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

...	10	5	6	7	9	10	11	6	8	11	12	7	8	11	8	9	10	12	9	11

- **Array V**

101	105	110	115	121	127	132	138	144	149	154	158	*	102	103	104	106	107	108	109	...

...	111	112	113	114	116	117	118	119	120	122	123	124	125	126	128	129	130	131	133	...

...	134	135	136	137	139	140	141	142	143	145	146	147	148	150	151	152	153	155	156	157

The MSR (Modified Sparse Row) format

- The MSR format turns out to be **very efficient** in memory terms
- It is one of the most ***compact*** formats for sparse matrices
- It is used in several linear algebra libraries for large problems
- The *drawback* is that it ***only*** applies to *square matrices*
- The matrix-vector product is coded as:

```
y=V(1:n).*x;
for k=1:n
  ik=B(k):B(k+1)-1;
  jcol =B(ik);
  y(k)=y(k)+dot(A(ik),x(jcol));
end
```

BSR (Block Sparse Row) format

- The **BSR format** is a CSR with dense submatrices of fixed shape instead of scalar items
- The block size must evenly divide the shape of the matrix

101	102	0	103	0	0	0	0	0	0	0	0
104	105	106	107	108	0	0	0	0	0	0	0
0	109	110	0	111	112	0	0	0	0	0	0
113	114	0	115	116	0	117	0	0	0	0	0
0	118	119	120	121	122	123	124	0	0	0	0
0	0	125	0	126	127	0	128	129	0	0	0
0	0	0	130	131	0	132	133	0	134	0	0
0	0	0	0	135	136	137	138	139	140	141	0
0	0	0	0	0	142	0	143	144	0	145	146
0	0	0	0	0	0	147	148	0	149	150	0
0	0	0	0	0	0	0	151	152	153	154	155
0	0	0	0	0	0	0	0	156	0	157	158

A	B		
C	D	E	
	F	G	H
		I	L

- In this example the block size is 3 x 3

BSR (Block Sparse Row) format

- The BSR format store the **non-zero blocks** of the sparse matrix
- A **non-zero block** is the block that contains *at least one non-zero element*

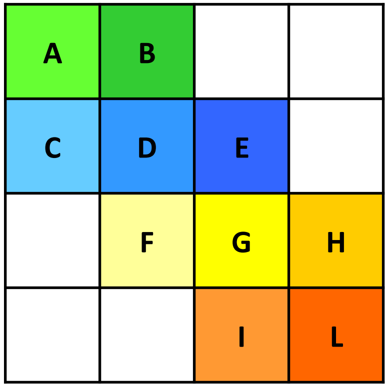
101	102	0	103	0	0	0	0	0	0	0	0
104	105	106	107	108	0	0	0	0	0	0	0
0	109	110	0	111	112	0	0	0	0	0	0
113	114	0	115	116	0	117	0	0	0	0	0
0	118	119	120	121	122	123	124	0	0	0	0
0	0	125	0	126	127	0	128	129	0	0	0
0	0	0	130	131	0	132	133	0	134	0	0
0	0	0	0	135	136	137	138	139	140	141	0
0	0	0	0	0	142	0	143	144	0	145	146
0	0	0	0	0	0	147	148	0	149	150	0
0	0	0	0	0	0	0	151	152	153	154	155
0	0	0	0	0	0	0	0	156	0	157	158

A	B		
C	D	E	
	F	G	H
		I	L

BSR (Block Sparse Row) format

The **BSR format** consists of four arrays:

- **Values** - real array containing the elements of the non-zero blocks of a sparse matrix
  - The elements are stored block-by-block in row-major order
  - All elements of non-zero blocks are stored, even if some of them are equal to zero
  - Within each non-zero block elements are stored in column-major order in the case of one-based indexing, and in row-major order in the case of the zero-based indexing



BSR (Block Sparse Row) format

The **BSR format** consists of four arrays:

- **Columns** - integer array where element *i* is the number of the column in the block matrix that contains the *i*-th non-zero block
- **PointerB** - integer array where element *j* gives the index of the element in the *columns* array that is first non-zero block in row *j* of the block matrix
- **PointerE** - integer array where element *j* gives the index of the element in the *columns* array that contains the last non-zero block in a row *j* of the block matrix plus 1

BSR (Block Sparse Row) format

Example

- Values

101	104	0	102	105	109	0	106	110	103	107	0	0	108	111	0	0	112	...	
...	113	0	0	114	118	0	0	119	125	115	120	0	116	121	126	0	122	127	...
...	117	123	0	0	124	128	0	0	129	130	0	0	131	135	0	0	136	142	...
...	132	137	0	133	138	143	0	139	144	134	140	0	0	141	145	0	0	146	...
...	147	0	0	148	151	0	0	152	156	149	153	0	150	154	157	0	155	158	

- Columns

1	2	1	2	3	2	3	4	3	4

- PointerB

1	3	6	9

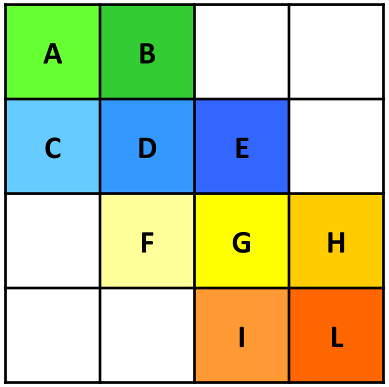
- PointerE

3	6	9	11

A	B		
C	D	E	
	F	G	H
		I	L

BSR (Block Sparse Row) format

- The length of the ***values*** array is equal to the number of all elements in the non-zero blocks
- The length of the ***columns*** array is equal to the number of non-zero blocks
- The length of the ***pointerB*** and ***pointerE*** arrays is equal to the number of block rows in the block matrix



Diagonal format

- Diagonally structured matrices are matrices whose nonzero elements are located along a small number of diagonals

The **diag format** consist of:

- **DIAG** - a rectangular real array storing the diagonals
  - DIAG has size n x Nd, where Nd is the number of diagonals
- **IOFF** - an integer array containing the offsets of each diagonal with respect to the main diagonal
  - IOFF has size Nd

Diagonal format

- The **order** in which the diagonals are stored in of DIAG is generally **unimportant**
- Since several more **operations** are performed with the **main diagonal**, storing it in the **first column** may be slightly advantageous

- Note that all the diagonals except the main diagonal have fewer than n elements, so there are positions in DIAG that will not be used

Diagonal format

Example

- Matrix

101	102	0	103	0	0	0	0	0	0	0	0
104	105	106	107	108	0	0	0	0	0	0	0
0	109	110	0	111	112	0	0	0	0	0	0
113	114	0	115	116	0	117	0	0	0	0	0
0	118	119	120	121	122	123	124	0	0	0	0
0	0	125	0	126	127	0	128	129	0	0	0
0	0	0	130	131	0	132	133	0	134	0	0
0	0	0	0	135	136	137	138	139	140	141	0
0	0	0	0	0	142	0	143	144	0	145	146
0	0	0	0	0	0	147	148	0	149	150	0
0	0	0	0	0	0	0	151	152	153	154	155
0	0	0	0	0	0	0	0	156	0	157	158

Element DIAG(i, j) is located in position $a_{i,i+ioff(j)}$ of the original matrix

- DIAG

113	0	104	101	102	0	103
118	114	109	105	106	107	108
125	119	0	110	0	111	112
130	0	120	115	116	0	117
135	131	126	121	122	123	124
142	136	0	127	0	128	129
147	0	137	132	133	0	134
151	148	143	138	139	140	141
156	152	0	144	0	145	146
0	0	153	149	150	0	0
0	0	157	154	155	0	0
0	0	0	158	0	0	0

IOFF

-3	-2	-1	0	1	2	3

Ellpack-Itpack format

- The **Ellpack-Itpack format** is a general scheme, popular on vector machines

- The Ellpack-Itpack format consists of two rectangular arrays:
  - **COEF** - real array (similar to DIAG) that contains the nonzero elements of A (completing the row by zeros as necessary)
  - **JCOEF** - integer array that contains the column positions of each entry in COEF
  - COEF and JCOEF have size ***n x Nd***, where *n* is the number of rows and *Nd* is the maximum number of nonzero elements per row, whith *Nd* small

Ellpack-Itpack format

Example

- Matrix

101	102	0	103	0	0	0	0	0	0	0	0
104	105	106	107	108	0	0	0	0	0	0	0
0	109	110	0	111	112	0	0	0	0	0	0
113	114	0	115	116	0	117	0	0	0	0	0
0	118	119	120	121	122	123	124	0	0	0	0
0	0	125	0	126	127	0	128	129	0	0	0
0	0	0	130	131	0	132	133	0	134	0	0
0	0	0	0	135	136	137	138	139	140	141	0
0	0	0	0	0	142	0	143	144	0	145	146
0	0	0	0	0	0	147	148	0	149	150	0
0	0	0	0	0	0	0	151	152	153	154	155
0	0	0	0	0	0	0	0	156	0	157	158

COEF

101	102	103	0	0	0	0
104	105	106	107	108	0	0
109	110	111	112	0	0	0
113	114	115	116	117	0	
118	119	120	121	122	123	124
125	126	127	128	129	0	0
130	131	132	133	134	0	0
135	136	137	138	139	140	141
142	143	144	145	146	0	0
147	148	149	150	0	0	0
151	152	153	154	155	0	0
156	157	158	0	0	0	0

JCOEF

1	2	4	0	0	0	0
1	2	3	4	5	0	0
2	3	5	6	0	0	0
1	2	4	5	7	0	
2	3	4	5	6	7	8
3	5	6	8	9	0	0
4	5	7	8	10	0	0
5	6	7	8	9	10	11
6	8	9	11	12	0	0
7	8	10	11	0	0	0
8	9	10	11	12	0	0
9	11	12	0	0	0	0

MATLAB AND SPARSE MATRICES

Material from:

https://it.mathworks.com/help/matlab/math/constructing-sparse-matrices.html

Matlab and Sparse Matrices

- MATLAB *never creates sparse matrices automatically*
- A representation of the pattern is given by the command **`spy`**

- You must determine if a matrix contains a large enough percentage of zeros to benefit from sparse techniques

- The **density** of a matrix is the ***number of nonzero elements divided by the total number of matrix elements***
- For matrix M, this would be

  `nnz(M)/prod(size(M))` or **`nnz(M) / numel(M)`**
- Matrices with very low density are often good candidates for use of the sparse format

Matlab and Sparse Matrices

Converting Full to Sparse

- You can convert a full matrix to sparse storage using the **`sparse`** function with a single argument

```
S = sparse(A)
```

- For example, given the matrix A:

```
A = [ 0 0 0 5
      0 2 0 0
      1 3 0 0
      0 0 4 0];
```

```
S = sparse(A)
```

produces:

```
(3,1)    1
(2,2)    2
(3,2)    3
(4,3)    4
(1,4)    5
```

- Output: nonzero elements of S, with their row and column indices
- The elements are sorted by columns

Matlab and Sparse Matrices

Converting Full to Sparse

- You can convert a sparse matrix to full storage using the `full` function, provided the matrix order is not too large
- For example `A = full(S)` reverses the example conversion

- Converting a full matrix to sparse storage is **not** the most frequent way of generating sparse matrices

- If the order of a matrix is small enough that full storage is possible, then *conversion to sparse storage rarely offers significant savings*

Matlab and Sparse Matrices

Creating Sparse Matrices Directly

- You can create a sparse matrix from a list of nonzero elements using the **sparse** function with five arguments

```
S = sparse(i,j,s,m,n)
```

  where
  - **i** and **j** are vectors of row and column indices, respectively, for the nonzero elements of the matrix
  - **s** is a vector of nonzero values whose indices are specified by the corresponding (i,j) pairs
  - **m** is the row dimension for the resulting matrix
  - **n** is the column dimension
- The matrix S of the previous example can be generated with:

```
S = sparse([3 2 3 4 1],[1 2 2 3 4],[1 2 3 4 5],4,4)
```

Matlab and Sparse Matrices

Creating Sparse Matrices Directly

- The matrix representation of the second difference operator is a tridiagonal matrix with -2s on the diagonal and 1s on the super- and sub-diagonal

- One way to generate it is:

```
D = sparse(1:n,1:n,-2*ones(1,n),n,n);
E = sparse(2:n,1:n-1,ones(1,n-1),n,n);
S = E+D+E'
```

Matlab and Sparse Matrices

Creating Sparse Matrices Directly

For n = 5, MATLAB responds with

```
S =
    (1,1)        -2
    (2,1)         1
    (1,2)         1
    (2,2)        -2
    (3,2)         1
    (2,3)         1
    (3,3)        -2
    (4,3)         1
    (3,4)         1
    (4,4)        -2
    (5,4)         1
    (4,5)         1
    (5,5)        -2
```

The full command

F = full(S)

displays the corresponding full matrix

```
F = full(S)

F =
    -2   1   0   0   0
     1  -2   1   0   0
     0   1  -2   1   0
     0   0   1  -2   1
     0   0   0   1  -2
```