Solution of Tridiagonal and Sparse Linear Equation Systems

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Topics

Solution of tridiagonal and sparse linear equation systems

- Optimal sequential algorithm
- Cyclic reduction
- Domain decomposition
- *LU* decomposition of sparse matrices
- Parallelisation

Optimal Sequential Algorithm

- As an extreme case of sparse equation systems we consider

$$Ax = b \qquad (1)$$

with $A \in \mathcal{R}^{N \times N}$ tridiagonal.

$$\begin{pmatrix} * & * & & & & \\ * & * & * & & & \\ & * & * & * & & \\ & & * & * & * & \\ & & & * & * & * \\ & & & & * & * \end{pmatrix}$$

- The optimal algorithm is the Gaussian elimination, sometimes also called Thomas algorithm.

Optimal Sequential Algorithm

- Gaussian elimination for tridiagonal systems

  // Forward elimination (here solution, not LU decomposition):
  for $(k = 0; k < N - 1; k++)$ {
  $l = a_{k+1,k}/a_{k,k}$;
  $a_{k+1,k+1} = a_{k+1,k+1} - l \cdot a_{k,k+1}$
  $b_{k+1} = b_{k+1} - l \cdot b_k$;
  } // $(N-1) \cdot 5$ fp operations
  // Backward substitution
  $x_{N-1} = b_{N-1}/a_{N-1,N-1}$;
  for $(k = N - 2; k \geq 0; k--)$ {
  $x_k = (b_k - a_{k,k+1} \cdot x_k + 1)/a_{k,k}$;
  } // $(N-1)3 + 1$ fp operations

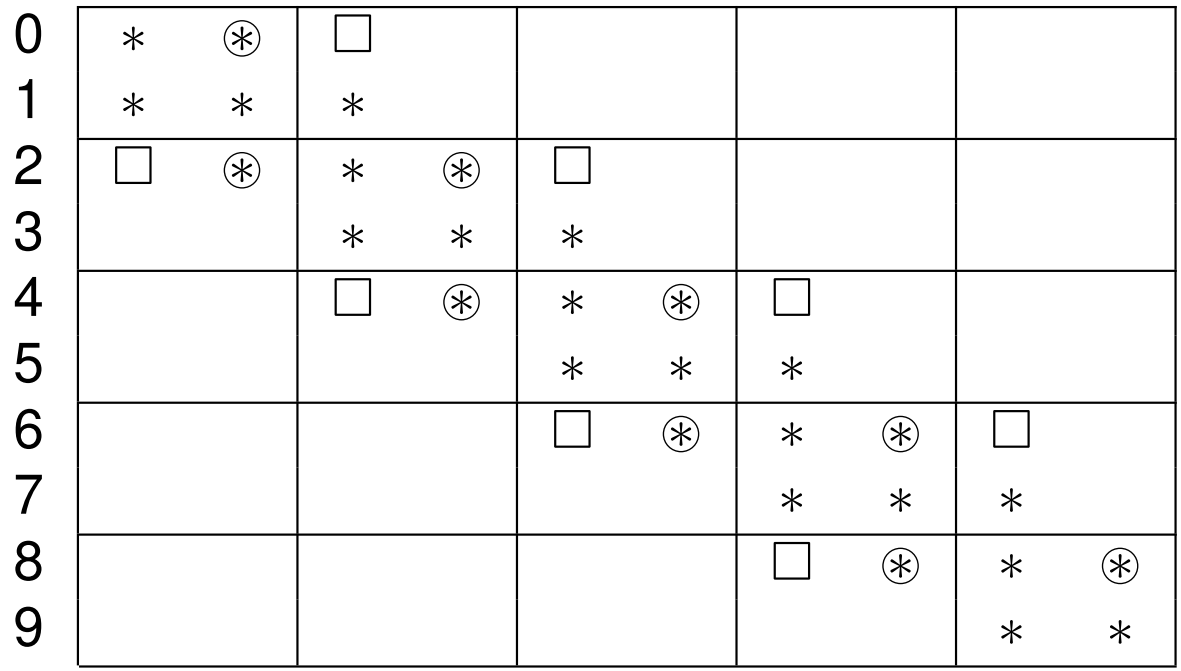
- The sequential complexity amounts to

$$T_S = 8Nt_f$$

  Obviously the algorithm is strictly sequential!

Cyclic Reduction

- Consider a tridiagonal matrix with $N = 2M$ (N even).
- *Idea:* Eliminate in each *even* row k the elements $a_{k-1,k}$ and $a_{k+1,k}$ with the help of the odd rows above resp. beneath.
- Each even row is therefore only coupled with the second previous and second next; since these are just even, the dimension has been reduced to $M = N/2$.
- The remaining system is again tridiagonal, and the idea can be applied recursively.



⊛ are removed, thereby fill-in (□) is generated.

Cyclic Reduction

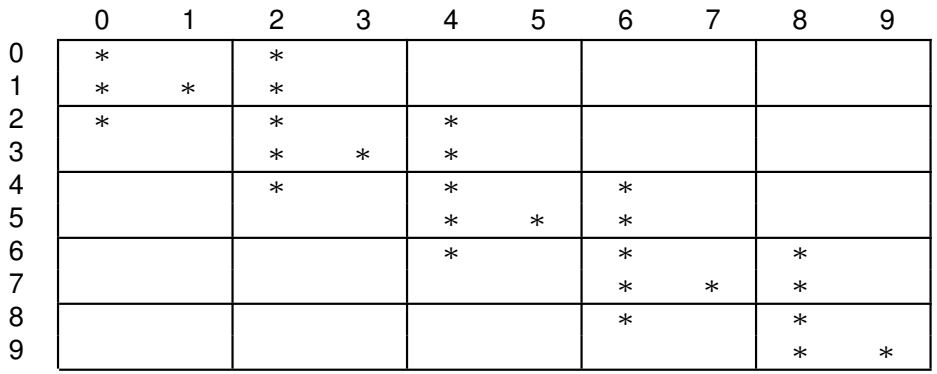
- Algorithm of cyclic reduction

  // Elimination of all odd unknowns in even rows:
  for $(k = 1; k < N; k \mathrel{+}= 2)$
  {
  // row k modifies row $k-1$
  $l = a_{k-1,k} / a_{k,k}$;
  $a_{k-1,k-1} = a_{k-1,k-1} - l \cdot a_{k,k-1}$;
  $a_{k-1,k+1} = -l \cdot a_{k,k+1}$; // fill-in
  $b_{k-1} = b_{k-1} - l \cdot b_k$;
  } // $\frac{N}{2} 6 t_f$
  for $(k = 2; k < N; k \mathrel{+}= 2)$;
  {
  // row $k-1$ modifies row k
  $l = a_{k,k-1} / a_{k-1,k-1}$;
  $a_{k,k-2} = l \cdot a_{k-1,k-2}$; // fill-in
  $a_{k,k} = l \cdot a_{k-1,k}$;
  } // $\frac{N}{2} 3 t_f$

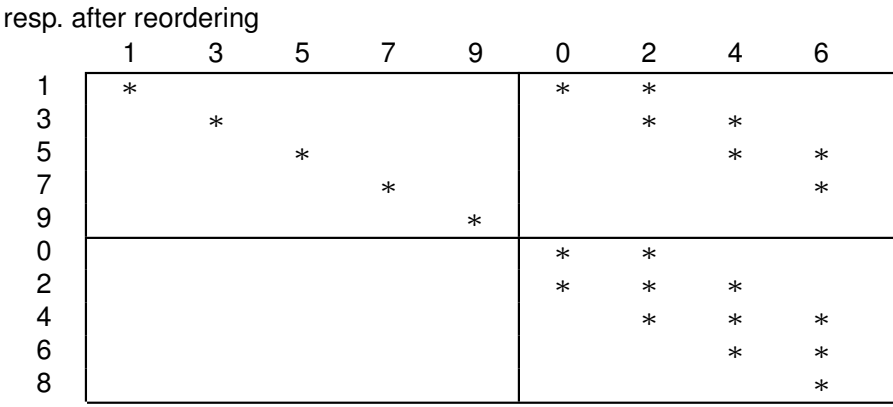
- All traversals of both loops can be processed in parallel (if we assume a machine with shared memory)!

Cyclic Reduction

- Result of this elimination is



resp. after reordering



- Are the x_{2k}, $k = 0, \ldots, M-1$, calculated, then the odd unknowns can be calculated with

  for $(k = 1; k < N-1; k \mathrel{+}= 2)$

  $$x_k = (b_k - a_{k,k-1} \cdot x_{k-1} - a_{k,k+1} \cdot x_{k+1}) / a_{k,k};$$

  // $\frac{N}{2} 5 t_f$

  $$x_{N-1} = (b_{N-1} - a_{N-1,N-2} \cdot x_{N-2}) / a_{N-1,N-1};$$

  completely in *parallel*.

Cyclic Reduction

- The *sequential* effort for the cyclic reduction is therefore

$$\begin{aligned} T_S(N) &= (6+3+5)t_f\left(\frac{N}{2}+\frac{N}{4}+\frac{N}{8}+\cdots+1\right) \\ &= 14Nt_f \end{aligned}$$

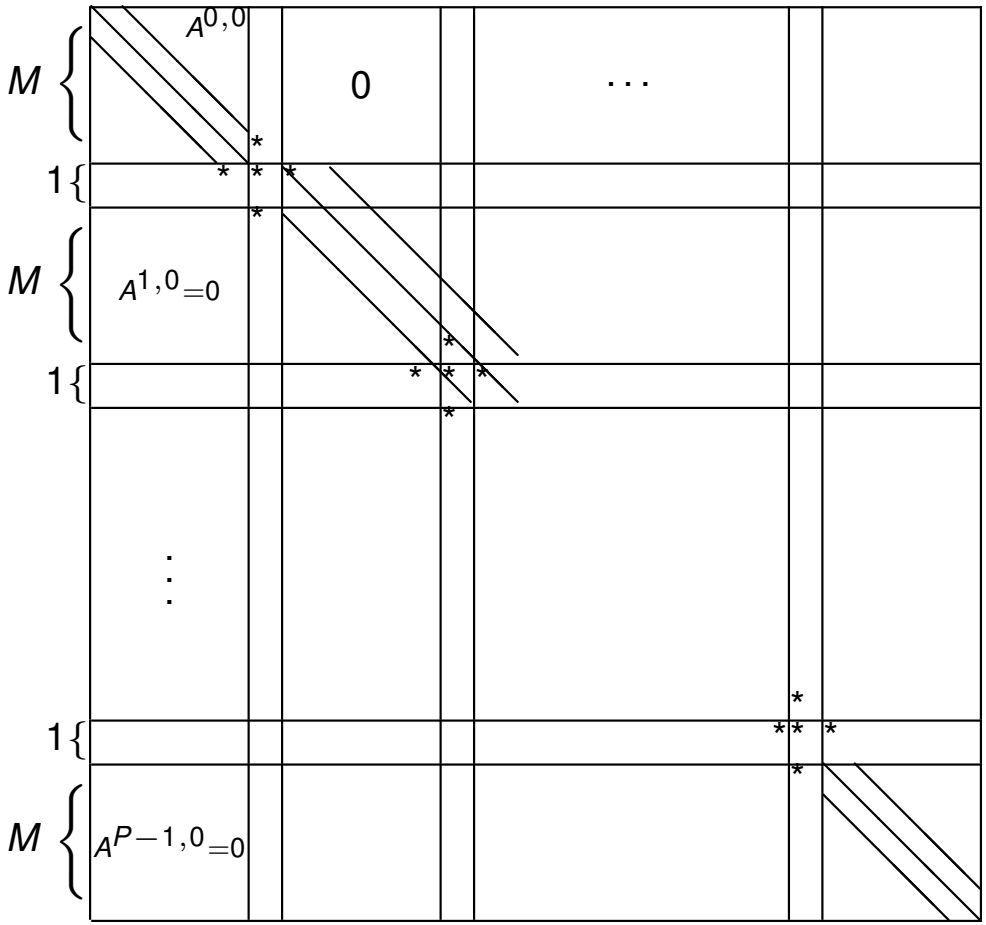
- This is nearly twice as much as the optimal sequential algorithm needs. Therefore the cyclic reduction can be parallelised. The maximal achievable efficiency is however

$$E_{\max} = \frac{8}{14} \approx 0.53,$$

where we have assumed, that all operations are executed optimally parallel and communication is for free (backward substitution needs only $\frac{N}{2}$ processors!). We have not taken into account that cyclic reduction neccesitates more index calculation!

Domain Decomposition Methods

- Another approach can be in principle be extended to more general problem formulations: domain decomposition methods
- Be P the number of processors and $N = MP + P - 1$ for a $M \in \mathbf{N}$. We subdivide then the $N \times N$ matrix A in P blocks à M rows with a single row between the blocks:



Domain Decomposition Methods

- The unknowns between the blocks form the *interface.* Each block is at most coupled to two interface unknowns.
- Now we sort rows and columns of the matrix such that the interface unknowns are moved to the end. This results in the following shape:

$$\left(\begin{array}{cccc|c} A^{0,0} & & & & A^{0,I} \\ & A^{1,1} & & & A^{1,I} \\ & & \ddots & & \vdots \\ & & & A^{P-1,P-1} & A^{P-1,I} \\ \hline A^{I,0} & A^{I,1} & \dots & A^{I,P-1} & A^{I,I} \end{array}\right),$$

where $A^{p,p}$ are the $M \times M$ tridiagonal partial matrices from A and $A^{I,I}$ is a $P-1 \times P-1$ diagonal matrix. The $A^{p,I}$ have the general form

$$A^{p,I} = \left(\begin{array}{c|c|c} \dots & \begin{array}{c} * \\ \\ * \end{array} & \dots \end{array}\right).$$

Domain Decomposition Methods

- Idea: Eliminate blocks $A^{I,*}$ in the block representation. Thereby $A^{I,I}$ is modified, more exact the following block representation is created:

$$\left(\begin{array}{cccc|c} A^{0,0} & & & & A^{0,I} \\ & A^{1,1} & & & A^{1,I} \\ & & \ddots & & \vdots \\ & & & A^{P-1,P-1} & A^{P-1,I} \\ \hline 0 & 0 & \dots & 0 & S \end{array}\right),$$

mit $S = A^{I,I} - \sum_{p=0}^{P-1} A^{I,p} \left(A^{p,p}\right)^{-1} A^{p,I}$.

- S is in general denoted as „Schurcomplement“. All eliminations in $\sum_{p=0}^{P-1}$ can be executed *parallel*.
- After solution of a system $Sy = d$ for the interface unknowns the inner unknowns can again be calculated in parallel.
- S has dimension $P-1 \times P-1$ and is itself sparse, as we can see soon.

Execution of the Plan

1. Transform $A^{p,p}$ to diagonal shape.
($a_{i,j}$ denotes $(A^{p,p})_{i,j}$, if not stated otherwise):

$\forall p$ parallel

for $(k = 0; k < M - 1; k++)$ // lower diagonal

{

$l = a_{k+1,k} / a_{k,k}$;

$a_{k+1,k+1} = a_{k+1,k+1} - l \cdot a_{k,k+1}$;

if $(p > 0)$ $a^{p,l}_{k+1,p-1} = a^{p,l}_{k+1,p-1} - l \cdot a_{k,p-1}$;

// fill-in left boundary

$b^p_{k+1} = b^p_{k+1} - l \cdot b^p_k$;

} // $(M-1)7t_f$

for $(k = M - 1; k > 0; k--)$ // upper diagonal

{

$l = a_{k-1,k} / a_{k,k}$;

$b^p_{k-1} = b^p_{k-1} - l \cdot b^p_k$;

if $(p > 0)$ $a^{p,l}_{k-1,p-1} = a^{p,l} - l \cdot a^{p,l}_{k,p-1}$; // left boundary

if $(p < P - 1)$ $a^{p,l}_{k-1,p} = a^{p,l}_{k-1,p} - l \cdot a^{p,l}_{k,p}$; // right boundary, fill-in

} // $(M-1)7t_f$

Execution of the Plan

2. Eliminate in $A^{I,*}$.

$\forall p$ parallel:

if $(p > 0)$

{

$I = a^{I,p}_{p-1,0} / a^{p,p}_{0,0}$;

$a^{I,I}_{p-1,p-1} = a^{I,I}_{p-1,p-1} - I \cdot a^{p,I}_{0,p-1}$; // diagonal in S

if $(p < P-1)$ $a^{I,I}_{p-1,p} = a^{I,I}_{p-1,p} - I \cdot a^{p,I}_{0,p}$; // upper diag. in S, fill-in

$b^{I}_{p-1} = b^{I}_{p-1} - I \cdot b^{p}_{0}$;

}

if $(p < P-1)$

{ // right boundary

$I = a^{I,p}_{p,M-1} / a^{p,p}_{M-1,M-1}$;

if $(p > 0)$ $a^{I,I}_{p,p-1} = a^{I,I}_{p,p-1} - I \cdot a^{p,I}_{M-1,p-1}$;

// fill-in lower diag of S

$a^{I,I}_{p,p} = a^{I,I}_{p,p} - I \cdot a^{p,I}_{M-1,p}$;

$b^{I}_{p} = b^{I}_{p} - I \cdot b^{p}_{M-1}$;

}

Execution of the Plan

3. Solve Schurcomplement.
S is *tridiagonal* with dimension $P-1 \times P-1$. Assume that $M \gg P$ and solve sequential. $\longrightarrow 8Pt_f$ effort.
4. Calculate inner unknowns.
Here, only one diagonal matrix has to be solved per processor.

$\forall p$ parallel:

for $(k = 0; k < M-1; k++)$

$x_k^p = (b_k^p - a_{k,p-1}^{p,l} \cdot x_{p-1}^l - a_{k,p}^{p,l} \cdot x_p^l)/a_{k,k}^{p,p};$

// $M5t_f$

Analysis

- Total effort parallel:

$$
\begin{aligned}
T_P(N,P) &= 14Mt_f + O(1)t_f + 8Pt_f + 5Mt_f = \\
&= 19Mt_f + 8Pt_f
\end{aligned}
$$

(without communication!)

$$
\begin{aligned}
E_{\max} &= \frac{8(MP+P-1)t_f}{(19Mt_f + 8Pt_f)\,P} \approx \\
&\underbrace{\approx}_{\text{für } P \ll M} \frac{1}{\frac{19}{8} + \frac{P}{M}} \leq \frac{8}{19} = 0.42
\end{aligned}
$$

- The algorithm needs additional memory for the fill-in. Cyclic reduction works with overwriting of old entries.

LU Decomposition of Sparse Matrices

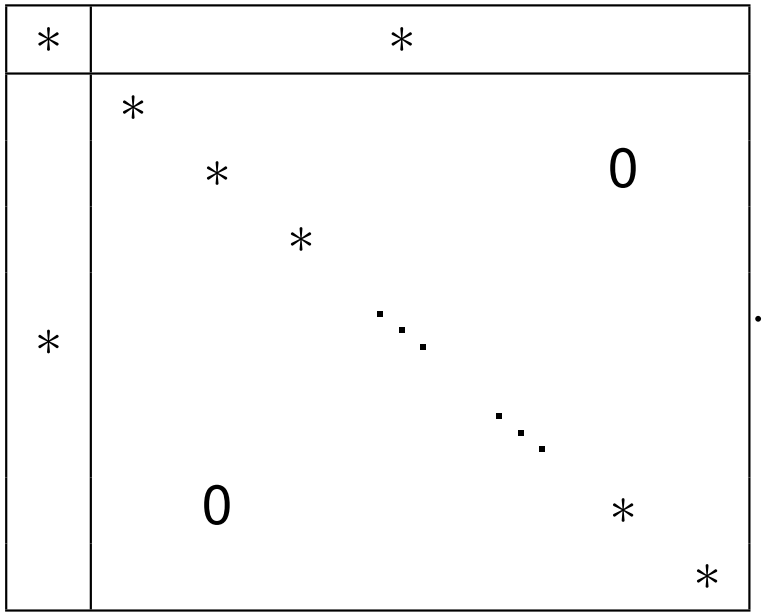
What is a sparse matrix

- In general one speaks of a sparse matrix, if it has in (nearly) each row only a constant number of non-zero elements.
- If $A \in \mathcal{R}^{N \times N}$, then A has only $O(N)$ instead of N^2 entries.
- For large enough N it is then advantegeous regarding computing time and memory not to process resp. to store this large number of zeros.

LU Decomposition of Sparse Matrices

Fill-in

- While *LU* decomposition elements, that initially have been zero, can get non-zero during the elimination process.
- On speaks then of *„Fill-in“*.
- This heavily depends on the structure of the matrix. As a extreme example consider the „arrow matrix“

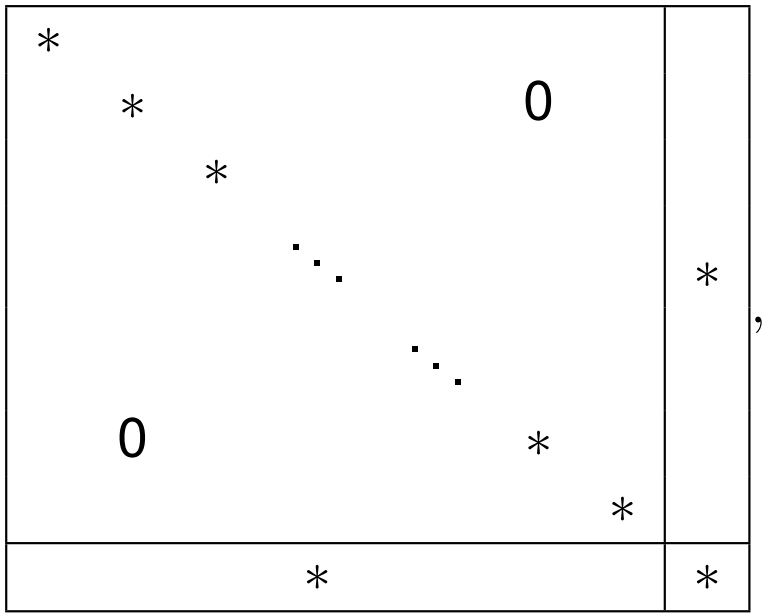


- During elimination in the natural sequence (without pivoting) the whole matrix is „filled-in“.

LU Decomposition of Sparse Matrices

Reordering of the matrix

- If we rearrange the matrix by row and column permutations to the form



,

- Obviously no fill-in is produced.
- An important point in the *LU* decomposition of sparse matrices is to find a matrix ordering such that the fill-in is minimised.
- Reordering is strongly coupled to pivoting.

Pivoting

- If the matrix A is symmetric positive definite (SPD), then the LU factorisation is always numerically stable, and *no* pivotng is necessary.

$\rightarrow$ The matrix can thus be reordered in advance, that the fill-in gets small.

- For a general, invertible matrix one will need to use pivoting.

$\rightarrow$ Then during elimination a compromise between numerical stability and fill-in has to be found dynamically.

- Therefore nearly all codes restrict to the symmetric positive case and determine an elimination sequence that minimizes the fill-in in advance.
- The exact solution of the minimization problem is $\mathcal{NP}$ complete.

$\rightarrow$ One therefore uses heuristical methods.

Graph of a Matrix

Matrix graph

- In the symmetric positive case fill-in can be investigated purely by the zero structure of the matrix.
- For an arbitrary, now not necessarily symmetric $A \in \mathcal{R}^{N \times N}$ we define an undirected graph $G(A) = (V_A, E_A)$ by

$$\begin{aligned} V_A &= \{0, \ldots, N-1\} \\ (i,j) \in E_A &\iff a_{ij} \neq 0 \vee a_{ji} \neq 0. \end{aligned}$$

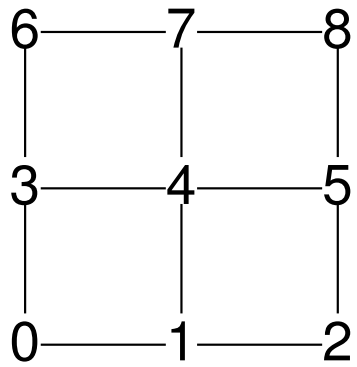
- This graph describes the direct dependencies of the unknowns beneath each other.

Graph of a Matrix

Example:

	0	1	2	3	4	5	6	7	8
0	∗	∗		∗					
1	∗	∗	∗		∗				
2		∗	∗			∗			
3	∗			∗	∗		∗		
4		∗		∗	∗	∗		∗	
5			∗		∗	∗			∗
6				∗			∗	∗	
7					∗		∗	∗	∗
8						∗		∗	∗

A

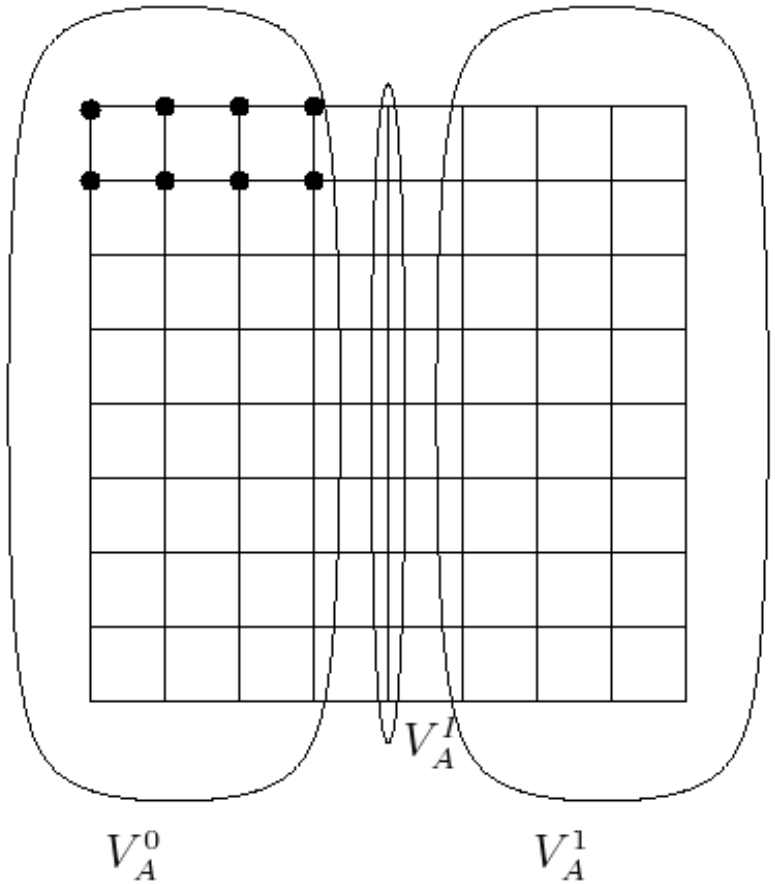


$G(A)$

Matrix Ordering Strategies

Nested Disection

- An important method to order SPD matrices for the purpose of fill-in minimisation is the *„nested disection“*.
- Example:
  The graph $G(A)$ of the matrix A be a quadratic grid



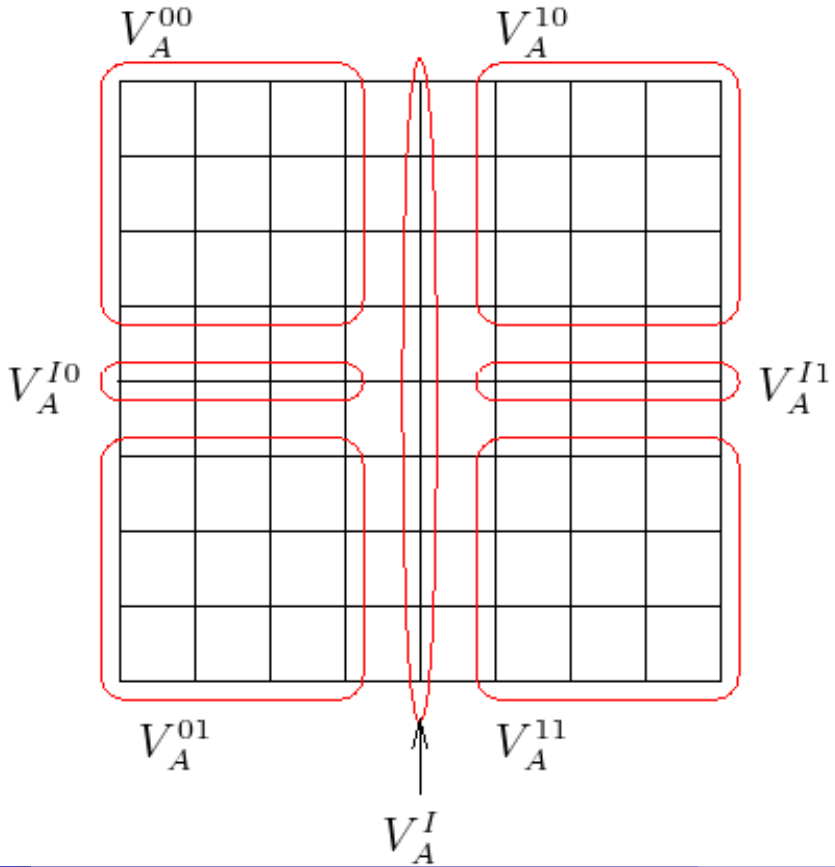
Matrix Ordering Strategies

Now we divide the node set V_A in three parts: V_A^0, V_A^1 and V_A^I, such that

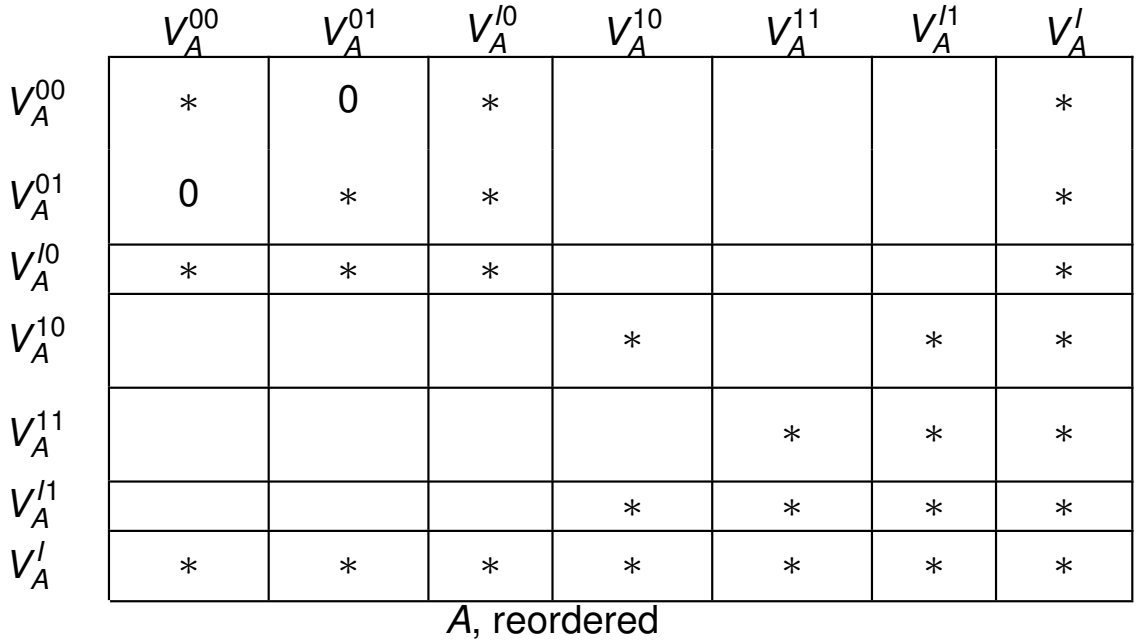
- V_A^0 and V_A^1 are as large as possible,
- V_A^I is a separator, this means when V_A^I is removed from the graph this is split into two parts. Thus there is *no* $(i, j) \in E_A$, such that $i \in V_A^0$ and $j \in V_A^1$.
- V_A^I is as small as possible,
- The figure shows a possibility for such a partitioning.

Matrix Ordering Strategies

- Now one reorders the rows and columns such that first the indices V_A^0 are present, then V_A^1 and finally V_A^I.
- Then we apply the method *recursively* to the partial graphs with the node sets V_A^0 and V_A^1.
- The method stops, if the graphs has reached a predefined size.
- Example graph after two steps:



Matrix Ordering Strategies



Complexity of the nested disection

- For the example above the nested disection numbering leads to a complexity of $O(N^{3/2})$ for the LU decomposition.
- For comparisoon one needs with lexicographic numbering (band matrix) $O(N^2)$ operations.

Data Structures for Sparse Matrices

- There are a series of data structures for storage of sparse matrices.
- Goal is an efficient implementation of algorithms.
- Thus one has to watch out for data locality and as few overhead as possible by additional index calculation.
- An often used data structure is *„compressed row storage“*
- If the $N \times N$ matrix has in total M non-zero elements, then one stores the matrix elements row-wise in an one-dimensional field:

  double $a[M]$;
- The management of index information happens via three arrays

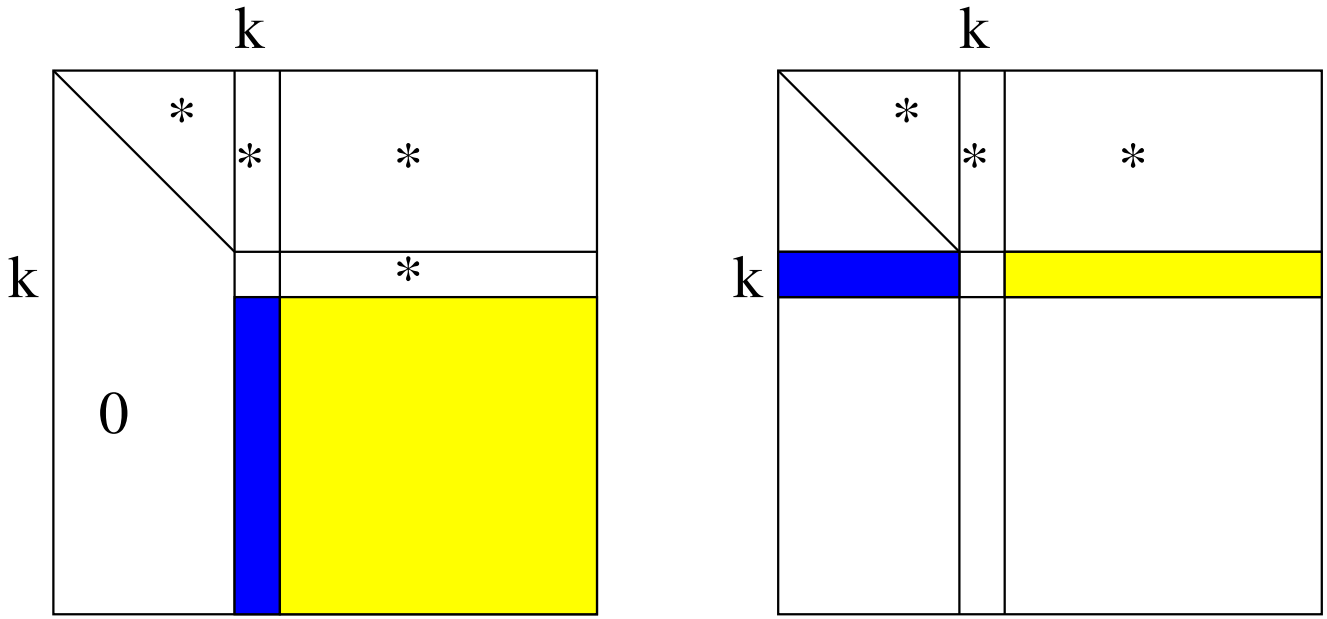
  int $s[N]$, $r[N]$, $j[M]$;
- Their meaning shows the realisation of the matrix-vector product $y = Ax$:

```
for (i = 0; i < N; i++) {
    y[i] = 0;
    for (k = r[i]; k < r[i] + s[i]; k++)
        y[i] += a[k] · x[j[k]];
}.
```

- r provides row start, s the row length, and j the column index.

Elimination Forms

- In the *LU* decomposition of dense matrices we have used the so-called *kij* form of the *LU* decomposition.



- Here in each step k all a_{ik} for $i > k$ are eliminated, which requires a modification of all a_{ij} with $i, j > k$.
- This situation is shown left.
- In the *kji* variant one eliminates in step k all a_{kj} with $j < k$.
- Here the a_{ki} with $i \geq k$ are modified. Wach out, that the a_{kj} have to be eliminated from left to right!
- For the following sequential *LU* decomposition for sparse matrices we are going to start from this *kji* variant.

Sequential Algorithm

- In the following we assume:
  - The matrix A can be factorized in the given ordering without pivoting. The ordering has been choosen in an appropriate way to minimize fill-in.
  - The data structure stores all elements a_{ij} with $(i,j) \in G(A)$. Because of the definiton of $G(A)$ applies:

$$(i,j) \notin G(A) \;\Rightarrow\; a_{ij} = 0 \wedge a_{ji} = 0.$$

    If $a_{ij} \neq 0$, then in every case also a_{ji} is stored, *also if this is zero.* The matrix does not have to be symmetric.
- The extension of the structure of A happens purely because of the information in $G(A)$. Thus also a a_{kj} is formally eliminated, if $(k,j) \in G(A)$ applies. This can possibly create a fill-in a_{ki}, albeit applies $a_{ki} = 0$.
- The now presented algorithm uses the sets $S_k \subset \{0,\ldots,k-1\}$, that contain in step k exactly the column indices, that have to be eliminated.

Sequential Algorithm

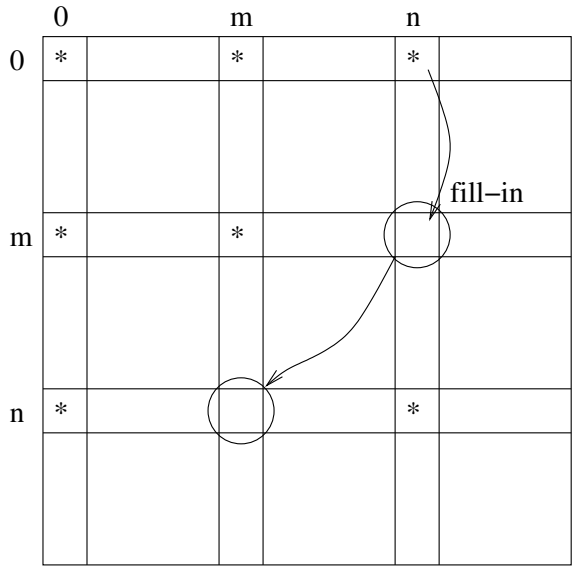
for $(k = 0; k < N; k++)\ S_k = \emptyset;$
for $(k = 0; k < N; k++)$
{
    // 1. extend matrix graph
    for $(j \in S_k)$
    {
        $G(A) = G(A) \cup \{(k, j)\};$
        for $(i = k; i < N; i++)$
            if $((j, i) \in G(A))$
                $G(A) = G(A) \cup \{(k, i)\};$
    }

    // 2. Eliminate
    for $(j \in S_k)$
    {   // eliminate $a_{k,j}$
        $a_{k,j} = a_{k,j} / a_{j,j};$ // L factor
        for $(i = j + 1; i < N; i++)$
            $a_{k,i} = a_{k,i} - a_{k,j} \cdot a_{j,i};$
    }

    // 3. update S_i for $i > k$, holds because of symmetry of E_A
    for $(i = k + 1; i < N; i++)$
        if $((k, i) \in G(A))$ // $\Rightarrow (i, k) \in G(A)$
            $S_i = S_i \cup \{k\};$
}

Sequential Algorithm

- We consider in an example, how the S_k are mapped.



- At start $G(A)$ shall contain the elements

$$G(A) = \{(0,0),(m,m),(n,n),(0,n),(n,0),(0,m),(m,0)\}$$

- For $k = 0$ is set in step 1 $S_m = \{0\}$ and $S_n = \{0\}$.
- Now, next for $k = m$ the $a_{m,0}$ is eliminated.
- This generates the fill-in (m, n), which again has in step 3 for $k = m$ as consequence the instruction $S_n = s_n \cup \{m\}$.
- Thus applies at start of traversal $k = n$ correctly $S_n = \{0, m\}$ and in step 1 the fill-in $a_{n,m}$ is correctly generated, *before* the elimination of $a_{n,\mathbf{0}}$ is performed. This is enabled because of the symmetry of G_A.

Parallelisation

LU decomposition of sparse matrices has the following possibilites for a parallelisation:

- *coarse granularity:* In all 2^d partial sets of indices, that has been created by nested disection of depth d, one can start in parallel with the elimination. First for the indices, that correspond to the separators, communication is necessary.
- *medium granularity:* Single rows can be processed in parallel, as soon as the according pivot row is locally available. This corresponds to the parallelisation of the dense *LU* decomposition.
- *fine granularity:* modifications of an individual row can be processed in parallel, as soon as the pivot line and the multiplicator are available. This is used for the two-dimensional data distribution in the dense case.

Parallelisation: Case $N = P$

Program (LU decomposition for sparse matrices and $N = P$)

```
parallel sparse-lu-1
{
    const int N = ...;
    process Π[int k ∈ {0, ..., N − 1}]
    {// (only pseudo code!)
        S = ∅;                                          // 1. set S
        for (j = 0; j < k; j++)
            if ((k, j) ∈ G(A)) S = S ∪ {j};             // the start
        for (j = 0; j < k; j++)                         // 2. process row k
            if (j ∈ S_k)
            {
                recv(Π_j, r);                           // wait, until Π_j sends the row j
                // extend pattern
                for (i = j + 1; i < N; i++)
                {
                    if (i < k ∧ (j, i) ∈ G(A))          // info is in r
                        S = S ∪ {i};                    // processor i will send row i
                    if ((j, i) ∈ G(A) ∪ {(k, i)})       // info is in r
                        G(A) = G(A) ∪ {(k, i)};
                }
                // eliminate a_{k,j} = a_{k,j} / a_{j,j};   // info is in r
                for (i = j + 1; i < N; i++)
                    a_{k,i} = a_{k,i} − a_{k,j} · a_{j,i};   // info is in r
            }
        for (i = k + 1; i < N; i++)                     // 3. send away
            if ((k, i) ∈ G(A))                          // local info!
                send row k at Π_i;                      // k knowns, that i needs row k.
    }
}
```

Parallelisation for $N \gg P$

For case $N \gg P$

- Each processor has now a complete block of rows. Three things have to happen:
- *Receive pivot rows* of other processors and store them in the set R.
- *Send finished rows* from the send buffer S to the target processors.
- *Local elimination*
  - choose a row j from the receive buffer R.
  - eliminate with this row locally all possible $a_{k,j}$.
  - if a row is going to be ready, put it into the send buffer (there may be several target processors).