Ingénieurs
Mathématiques appliquées
et Calcul Scientifique

**Spécialité MACS 3ème année**

# Calcul Haute Performance

## Notes de cours

**L. Halpern**

# Table des matières


**1 Classical methods** **5**

1.1 Direct methods . . . 6
1.1.1 Gauss method . . . 6
1.1.2 Codes . . . 7
1.1.3 Theoretical results . . . 7
1.1.4 Symmetric definite matrices : Cholewski decomposition 8
1.1.5 Elimination with Givens rotations . . . 8
1.2 Sparse and banded matrices . . . 10
1.3 Stationary iterative methods . . . 13
1.3.1 Classical methods . . . 14
1.3.2 Fundamentals tools . . . 14
1.4 Non-Stationary iterative methods. Symmetric definite positive matrices . . . 16
1.4.1 Definition of the iterative methods . . . 17
1.4.2 Comparison of the iterative methods . . . 19
1.4.3 Condition number and error . . . 19
1.5 Preconditioning . . . 23
1.6 Krylov methods for non symmetric matrices, Arnoldi algorithm 27
1.6.1 Gram-Schmidt orthogonalization and $QR$ decomposition 27
1.6.2 Arnoldi algorithm . . . 28
1.6.3 Full orthogonalization method or FOM . . . 29
1.6.4 GMRES algorithm . . . 30

**2 Multigrid methods** **37**

2.1 The V- cycle process . . . 37
2.1.1 The Smoother . . . 38
2.1.2 Projection on the coarse grid . . . 38
2.1.3 Coarse resolution . . . 39
2.1.4 Projection on the fine grid . . . 39
2.1.5 Result of the coarse walk . . . 39
2.1.6 Postsmoothing . . . 41
2.1.7 Spectral analysis . . . 41
2.1.8 Number of elementary operations . . . 44
2.2 The finite elements multigrid algorithm . . . 44
2.2.1 Preliminaries . . . 44
2.2.2 Discrete norm . . . 46
2.2.3 Definition of the multigrid algorithm . . . 47

2.2.4 Convergence property of the multigrid algorithm . . . . 48
2.3 Multigrid Preconditioner . . . . . 51

**3 Fast methods using Fast Fourier Transform** **53**
3.1 Presentation of the method . . . . . 53
3.2 Discrete and Fast Fourier Transform . . . . . 57
3.3 The algorithm . . . . . 61

**4 Substructuring methods** **65**
4.1 The Schur Complement method . . . . . 65
4.2 Direct method for the resolution of the interface problem . . . 68
4.3 The conjugate gradient algorithm . . . . . 69
4.4 The Dirichlet Neumann algorithm . . . . . 70
4.4.1 Presentation of the algorithm . . . . . 71
4.4.2 Convergence analysis in one dimension . . . . . 71
4.5 Appendix : `matlab` scripts in 1-D . . . . . 73

# Chapitre 1

# Classical methods

## Contents


**1.1 Direct methods . . . . . 6**

1.1.1 Gauss method . . . . . 6

1.1.2 Codes . . . . . 7

1.1.3 Theoretical results . . . . . 7

1.1.4 Symmetric definite matrices : Cholewski decomposition . . . . . 8

1.1.5 Elimination with Givens rotations . . . . . 8

**1.2 Sparse and banded matrices . . . . . 10**

**1.3 Stationary iterative methods . . . . . 13**

1.3.1 Classical methods . . . . . 14

1.3.2 Fundamentals tools . . . . . 14

**1.4 Non-Stationary iterative methods. Symmetric definite positive matrices . . . . . 16**

1.4.1 Definition of the iterative methods . . . . . 17

1.4.2 Comparison of the iterative methods . . . . . 19

1.4.3 Condition number and error . . . . . 19

**1.5 Preconditioning . . . . . 23**

**1.6 Krylov methods for non symmetric matrices, Arnoldi algorithm . . . . . 27**

1.6.1 Gram-Schmidt orthogonalization and $QR$ decomposition . . . . . 27

1.6.2 Arnoldi algorithm . . . . . 28

1.6.3 Full orthogonalization method or FOM . . . . . 29

1.6.4 GMRES algorithm . . . . . 30


**Purpose** : Solve $Ax = b$, where $A$ is a squared matrix and $b$ is a given righthand side, or a family of given righthand sides.

## 1.1 Direct methods

### 1.1.1 Gauss method

**Example**

$$\underbrace{\begin{pmatrix} 1 & 3 & 1 \\ 1 & 1 & -1 \\ 3 & 11 & 6 \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} 9 \\ 1 \\ 36 \end{pmatrix}}_{x} = \underbrace{\begin{pmatrix} 9 \\ 1 \\ 36 \end{pmatrix}}_{b}$$

Take the $3 \times 4$ matrix $\bar{A} = [A \,|\, b]$. Define

$$M_1 = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -3 & 0 & 1 \end{pmatrix}$$

and multiply on the left by $M_1$ to put zeros under the diagonal in the first column :

$$M_1[A \,|\, b] = \left(\begin{array}{ccc|c} 1 & 3 & 1 & 9 \\ 0 & -2 & -2 & -8 \\ 0 & 2 & 3 & 9 \end{array}\right).$$

Multiply now on the left by $M_2$ to put zeros under the diagonal in the second column :

$$M_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix}$$

$$M_2\, M_1[A \,|\, b] = \left(\begin{array}{ccc|c} 1 & 3 & 1 & 9 \\ 0 & -2 & -2 & -8 \\ 0 & 0 & 1 & 1 \end{array}\right)$$

Define $M = M_2 M_1$. Then the column $j$ of $M$ is the column $j$ of $M_j$ :

$$M = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -3 & 1 & 1 \end{pmatrix}.$$

$$M[A \,|\, b] = [MA \,|\, Mb].$$

$$Ax = b \iff MAx = Mb : M \text{ is a } \textbf{preconditioner}.$$

The matrix $U = MA$ is upper triangular, and solving $Ux = Mb$ is simpler than solving $Ax = b$. Define $L = M^{-1}$. In the column $j$, the entries below the diagonal are those of $M$ with a change of signe.

$$L := M^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 3 & -1 & 1 \end{pmatrix}.$$

$$U = MA \iff A = LU, Ax = b \iff LUx = b \iff \begin{cases} Ly = b \\ Ux = y \end{cases}$$

Solving $Ax = b$ is then equivalent to performing the $LU$ decomposition, and solving two triangular systems. Counting of operations :

1. $LU$ decomposition $\mathcal{O}(\frac{2n^3}{3})$ elementary operations.
2. Solve $Ly = b$ $\mathcal{O}(n^2)$ elementary operations.
3. Solve $Ux = y$ $\mathcal{O}(n^2)$ elementary operations.

For $P$ values of the righthand side, $N_{op} \sim \frac{2n^3}{3} + P \times 2n^2$.

### 1.1.2 Codes

```
function x=BackSubstitution(U,b)
% BACKSUBSTITUTION solves by backsubstitution a linear system
% x=BackSubstitution(U,b) solves Ux=b, U upper triangular by
% backsubstitution
n=length(b);
for k=n:-1:1
s=b(k);
for j=k+1:n
s=s-U(k,j)*x(j);
end
x(k)=s/U(k,k);
end
x=x(:);
```

```
function x=Elimination(A,b)
% ELIMINATION solves a linear system by Gaussian elimination
% x=Elimination(A,b) solves the linear system Ax=b using Gaussian
% Elimination with partial pivoting. Uses the function
% BackSubstitution
n=length(b);
norma=norm(A,1);
A=[A,b]; % augmented matrix
for i=1:n
[maximum,kmax]=max(abs(A(i:n,i))); % look for Pivot A(kmax,i)
kmax=kmax+i-1;
if maximum < 1e-14*norma; % only small pivots
error('matrix is singular')
end
if i ~= kmax % interchange rows
h=A(kmax,:); A(kmax,:)=A(i,:); A(i,:)=h;
end
A(i+1:n,i)=A(i+1:n,i)/A(i,i); % elimination step
A(i+1:n,i+1:n+1)=A(i+1:n,i+1:n+1)-A(i+1:n,i)*A(i,i+1:n+1);
end
x=BackSubstitution(A,A(:,n+1));
```

### 1.1.3 Theoretical results

**Theorem 1.1 (Regular case)** *Let $A$ be an invertible matrix, with all principal minors $\neq 0$. Then there exists a unique matrix $L$ lower triangular with $l_{ii} = 1$ for all $i$, and a unique matrix $U$ upper triangular, such that $A = LU$. Furthermore $\det(A) = \prod_{i=1}^{n} u_{ii}$.*

**Theorem 1.2 (Partial pivoting)** *Let $A$ be an invertible matrix. There exist a permutation matrix $P$, a matrix $L$ lower triangular with $l_{ii} = 1$ for all $i$, and a matrix $U$ upper triangular, such that*

$$PA = LU$$

### 1.1.4 Symmetric definite matrices : Cholewski decomposition

**Theorem 1.3** *If $A$ is symmetric definite positive, there exists a unique lower triangular matrix $R$ with positive entries on the diagonal, such that $A = RR^T$.*

### 1.1.5 Elimination with Givens rotations

This is meant to avoid pivoting. It is used often in connection with the resolution of least-square problems. In the $i$ step of the Gauss algorithm, we need to eliminate $x_i$ in equations $i+1$ to $n$ of the reduced system :

$$\begin{array}{rccccccc}
(i): & a_{ii}x_i & +\cdots & + & a_{in}x_n & = & b_i \\
 & \vdots & \vdots & & & & \\
(k): & a_{ki}x_i & +\cdots & + & a_{kn}x_n & = & b_k \\
 & \vdots & \vdots & & & & \\
(i): & a_{ni}x_i & +\cdots & + & a_{nn}x_n & = & b_n
\end{array}$$

If $a_{ki} = 0$, nothing needs to be done. If $a_{ki} \neq 0$, we multiply equation$(i)$ with $\sin\alpha$ and equation $(k)$ with $\cos\alpha$ and add. This leads to replacing equation $(k)$ by the linear combination

$$(k)_{new} = -\sin\alpha \cdot (i) + \cos\alpha \cdot (k).$$

The idea is to choose $\alpha$ such that the first coefficient in the line vanishes, *i.e.*

$$-\sin\alpha \cdot a_{ii} + \cos\alpha \cdot a_{ki} = 0.$$

Since $a_{ki} \neq 0$, this defines $\mathrm{cotg}\alpha_{ki}$, that is $\alpha_{ki}$ modulo $\pi$. For stability reasons, line $(i)$ is also modified, end we end up with

$$\begin{array}{rcll}
(i)_{new} & = & \cos\alpha \cdot (i) & +\sin\alpha \cdot (k) \\
(k)_{new} & = & -\sin\alpha \cdot (i) & +\cos\alpha \cdot (k)
\end{array}$$

From which the sine and cosine of $\alpha_{ki}$ are obtained through well-known trigonometric formulas

$$\sin\alpha_{ki} = 1/\sqrt{1+\mathrm{cotg}^2\alpha_{ki}}, \quad \cos\alpha_{ki} = \sin\alpha_{ki}\,\mathrm{cotg}\alpha_{ki}.$$

$$\begin{array}{rcll}
A_{ij_{new}} & = & \cos\alpha_{ki} \cdot A_{ij} & +\sin\alpha_{ki} \cdot A_{kj} \\
A_{kj_{new}} & = & -\sin\alpha_{ki} \cdot A_{ij} & +\cos\alpha_{ki} \cdot A_{kj}
\end{array}$$

```
function x=BackSubstitutionSAXPY(U,b)
% BACKSUBSTITUTIONSAXPY solves linear system by backsubstitution
% x=BackSubstitutionSAXPY(U,b) solves Ux=b by backsubstitution by
% modifying the right hand side (SAXPY variant)n=length(b);
n=length(b);
for i=n:-1:1
x(i)=b(i)/U(i,i);
b(1:i-1)=b(1:i-1)-x(i)*U(1:i-1,i);
end
x=x(:);
```

```
function x=EliminationGivens(A,b);
% ELIMINATIONGIVENS solves a linear system using Givens-rotations
% x=EliminationGivens(A,b) solves Ax=b using Givens-rotations. Uses
% the function BackSubstitutionSAXPY.
n=length(A);
for i= 1:n
for k=i+1:n
if A(k,i)~=0
cot=A(i,i)/A(k,i); % rotation angle
si=1/sqrt(1+cot^2); co=si*cot;
A(i,i)=A(i,i)*co+A(k,i)*si; % rotate rows
h=A(i,i+1:n)*co+A(k,i+1:n)*si;
A(k,i+1:n)=-A(i,i+1:n)*si+A(k,i+1:n)*co;
A(i,i+1:n)=h;
h=b(i)*co+b(k)*si; % rotate right hand side
b(k)=-b(i)*si+b(k)*co; b(i)=h;
end
end;
if A(i,i)==0
error('Matrix is singular');
end;
end
x=BackSubstitutionSAXPY(A,b);
```

Note $G^{ik}$ which differs from identity only on the rows $i$ and $k$ where

$$g_{ii} = g_{kk} = \cos\alpha, \quad g_{ik} = -g_{ki} = \sin\alpha$$

Example for $n = 5$,

$$G^{24} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & \cos\alpha & 0 & \sin\alpha & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & -\sin\alpha & 0 & \cos\alpha & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Multipliying a vector $b$ by $G^{ik}$ changes only the components $i$ and $k$,

$$G^{ik}\begin{pmatrix}\vdots\\ b_i\\ \vdots\\ b_k\\ \vdots\end{pmatrix}=\begin{pmatrix}\vdots\\ \cos\alpha\cdot b_i \quad +\sin\alpha\cdot b_k\\ \vdots\\ -\sin\alpha\cdot b_i \quad +\cos\alpha\cdot b_k\\ \vdots\end{pmatrix}$$

$$G^{ik}\boldsymbol{e}_i=\cos\alpha\,\boldsymbol{e}_i-\sin\alpha\,\boldsymbol{e}_k,\quad G^{ik}\boldsymbol{e}_k=\sin\alpha\,\boldsymbol{e}_i+\cos\alpha\,\boldsymbol{e}_k.$$

$G^{ik}$ represents the rotation of angle $\alpha$ in the plane generated by $\boldsymbol{e}_i$ and $\boldsymbol{e}_k$. $(G^{ik}(\alpha))^*=G^{ik}(-\alpha)$, $(G^{ik}(\alpha))^*G^{ik}(\alpha)=I$. Thus it is an orthogonal matrix. By applying successively $G_{21},\ldots,G_{n1}$ whereever $a_{k1}$ is not zero, we put zeros under the diagonal in the first column. We continue the process until the triangular matrix $R$ is obtained. Then there are orthogonal matrices $G_1,\cdots,G_N$ such that Then

$$Q^*=G_N\ldots G_1,\quad QA=R.$$

Q is an orthogonal matrix,

$$Q^*Q=G_N\ldots G_1G_1^*\ldots G_N^*=I.$$

then

$$A=QR,$$

we have reached the $QR$ decomposition of the matrix $A$.

## 1.2 Sparse and banded matrices

Example : a banded matrix, with upper bandwidth $p=3$ and lower bandwidth $q=2$, in total $p+q+1$ nonzero diagonals.

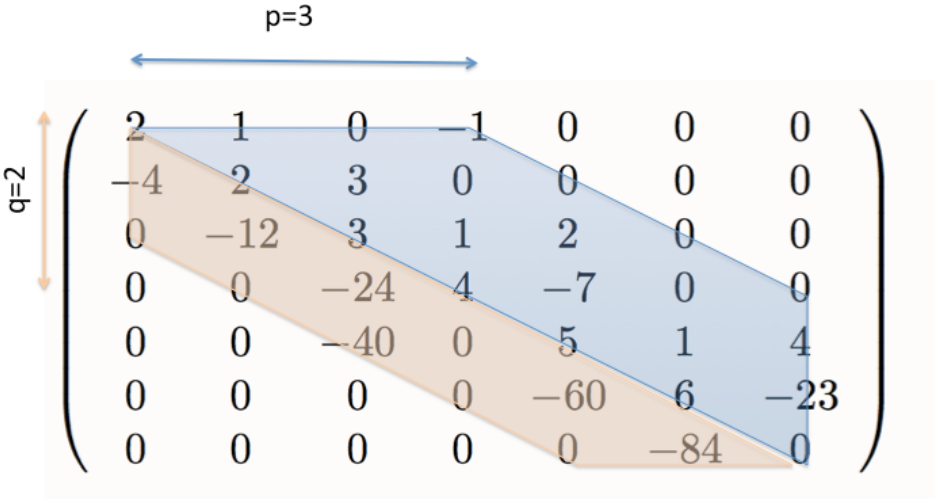



FIGURE 1.1 – A bandmatrix

Then $L$ is lowerbanded with $q = 2$, and $U$is upperbanded with $p = 3$.

$$U = \begin{pmatrix} 2 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 4 & 3 & -2 & 0 & 0 & 0 \\ 0 & 0 & 12 & -5 & 2 & 0 & 0 \\ 0 & 0 & 0 & -6 & -3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 20 & 1 & 4 \\ 0 & 0 & 0 & 0 & 0 & 9 & -11 \\ 0 & 0 & 0 & 0 & 0 & 0 & -102.7 \end{pmatrix}$$

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -3 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & -3.3 & 2.81 & 0 & 0 & \\ 0 & 0 & 0 & 0 & -3 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -9.3 & 1 \end{pmatrix}$$

FIGURE 1.2 – LU decomposition

It is not the case anymore, when pivoting is used :

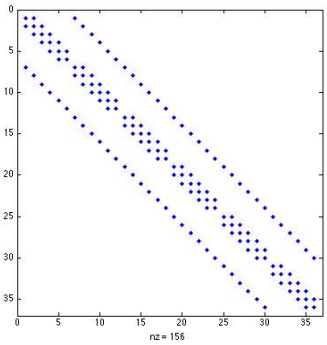
$$L = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.6 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ -0.5 & -0.17 & -0.05 & -0.21 & 0.025 & 0.0027 & 1 \end{pmatrix}$$

$$U = \begin{pmatrix} -4 & 2 & 3 & 0 & 0 & 0 & 0 \\ 0 & -12 & 3 & 1 & 2 & 0 & 0 \\ 0 & 0 & -40 & 0 & 5 & 1 & 4 \\ 0 & 0 & 0 & 4 & -10 & -0.6 & -2.4 \\ 0 & 0 & 0 & 0 & -60 & 6 & -23 \\ 0 & 0 & 0 & 0 & 0 & -84 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.275 \end{pmatrix}$$

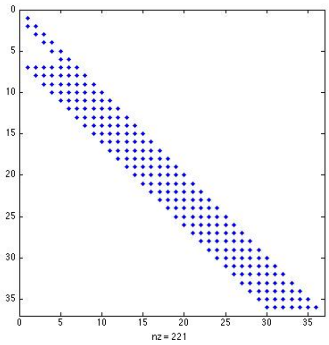
Here the permutation matrix is

$$P = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

In the Cholewsky decomposition, Note that if $A$ is banded, $R$ is banded with the same lower bandwidth, but it may be less sparse, in the sense that it can have more zeros. Consider as an example the $36 \times 36$ sparse matrix of $2-D$ finite differences in a square. With the command `spy` de matlab, the nonzero terms appear in blue :




A bandmatrix sparse matrix




Corresponding Cholewski

Even though $R$ has the same bandwidth as $A$, nonzero diagonals appear.

EXERCISE Write the Gauss and Givens algorithms for a tridiagonal matrix $A = diag(c,-1) + diag(d,0) + diag(e,1)$.

**LU factorization** : verify that

$$c_k = l_k\, u_k,\ \ d_{k+1} = l_k\, f_k + u_{k+1},\ \ e_k = f_k.$$

then it is not necessary to compute $f_k$, and only recursively

$$c_k = l_k\, u_k, \quad u_{k+1} = d_{k+1} - l_k\, e_k.$$

```
n=length(d);
for k=1:n-1 % LU-decomposition with no pivoting
        c(k)=c(k)/d(k);
        d(k+1)=d(k+1)-c(k)*e(k);
end
for k=2:n % forward substitution
        b(k)=b(k)-c(k-1)*b(k-1);
end
b(n)=b(n)/d(n); % backward substitution
for k=n-1:-1:1
```

```
        b(k)=(b(k)-e(k)*b(k+1))/d(k);
end
```

**Givens** : verify that the process inserts an extra updiagonal.

```
n=length(d);
e(n)=0;
for i=1: n-1 % elimination
        if c(i)~=0
                t=d(i)/c(i); si=1/sqrt(1+t*t); co=t*si;
                d(i)=d(i)*co+c(i)*si; h=e(i);
                e(i)=h*co+d(i+1)*si; d(i+1)=-h*si+d(i+1)*co;
                c(i)=e(i+1)*si; e(i+1)=e(i+1)*co;
                h=b(i); b(i)=h*co+b(i+1)*si;
                b(i+1)=-h*si+b(i+1)*co;
        end;
end;
b(n)=b(n)/d(n); % backsubstitution
b(n-1)=(b(n-1)-e(n-1)*b(n))/d(n-1);
for i=n-2:-1:1,
        b(i)=(b(i)-e(i)*b(i+1)-c(i)*b(i+2))/d(i);
end;
```

## 1.3 Stationary iterative methods

For any splitting $A = M - N$, write $Mx = Nx + b$,

Define the sequence $Mx^{m+1} = Nx^m + b$.

$$\begin{aligned} Mx^{m+1} = Nx^m + b &\iff Mx^{m+1} = (M-A)x^m + b \\ &\iff x^{m+1} = (I - M^{-1}A)x^m + M^{-1}b \\ &\iff x^{m+1} = x^m - M^{-1}Ax^m + M^{-1}b \\ &\iff \text{fixed point algorithm to solve } x - M^{-1}Ax + M^{-1}b = x \\ &\iff \text{fixed point algorithm to solve } M^{-1}Ax = M^{-1}b. \end{aligned}$$

Again, $M$ is a preconditioner.

**Definition 1.1**

- $e^m := x - x^m$ *is the error at step* $m$.
- $r^m := b - Ax^m = Ae^m$ *is the residual at step* $m$.
- $R = M^{-1}N = I - M^{-1}A$ *is the iteration matrix.*

Then the sequence of the errors satisfies

$$Me^{m+1} = Ne^m, \quad e^{m+1} = M^{-1}Ne^m$$

**Stopping criterion** Usually, one stops if $\frac{\|r^m\|}{\|b\|} < \varepsilon$.

### 1.3.1 Classical methods

Use $A = D - E - F$ .

| | | |
|---|---|---|
| Jacobi | $M = D$ | $R := J = I - D^{-1}A$ |
| Relaxed Jacobi | $M = \frac{1}{\omega}D$ | $R = I - \omega D^{-1}A$ |
| Gauss-Seidel | $M = D - E$ | $R := \mathcal{L}_1 = I - D^{-1}A$ |
| SOR | $M = \frac{1}{\omega}D - E$, | $R := \mathcal{L}_\omega = (D - \omega E)^{-1}((1-\omega)D + \omega F)$ |
| Richardson | $M = \frac{1}{\rho}I$ | $R = I - \rho A$ |

The relaxed methods are obtained as follows : define $\hat{x}^m$ as an application of Jacobi or Gauss-Seidel, then take the centroid of $\hat{x}^m$ and $x^m$ as $x^{m+1} = \omega\hat{x}^m + (1-\omega)x^m$.
For symmetric positive definite matrices $A$, RIchardson is a gradient method with fixed parameter. There is an optimal value for this parameter, given by $\rho_{opt} = \frac{2}{\lambda_1+\lambda_n}$ where the $\lambda_j$ are the eigenvaues of $A$.

### 1.3.2 Fundamentals tools

Define the sequence

$$e^{m+1} = Re^m,\ R = M^{-1}N.$$

Then $e^m = R^m e_0$, and for any norm

$$\|e^{m+1}\| \leq \|R\|\|e^m\|, \quad \|e^m\| \leq \|R^m\|\|e^0\|.$$

**Definition 1.2**

- $\rho(R) = \max\{|\lambda|, \lambda \textit{ eigenvalue of } R\}$ *is the spectral radius of* $R$.
- $\rho_m(R) = \|R^m\|^{1/m}$ *is the mean convergence factor of* $R$.
- $\rho_\infty(R) = \lim_{m\to\infty}\|R^m\|^{1/m}$ *is the asymptotic convergence factor of* $R$.

**Theorem 1.4**

- *For any matrix* $R$*, for any norm, for any* $m$, $\rho_m(R) \geq \rho(R)$*. The sequence* $\rho_m(R)$ *has a limit, called the asymptotic convergence factor of* $R$ *and denoted by* $\rho_\infty(R)$.
- *The sequence* $x^m$ *is convergent for any* $x^0$ *if and only if* $\rho(R) < 1$.

To reduce the initial error by a factor $\varepsilon$, we need $m$ iterations, defined by

$$\frac{\|e^m\|}{\|e^0\|} \leq (\rho_m(R))^m \sim \varepsilon.$$

So $m \sim \dfrac{\log\varepsilon}{\log\rho_m(R)}$. It is easier to use the asymptotic value relation, $m \sim \dfrac{\log\varepsilon}{\log\rho_\infty(R)}$. Then to obtain another decimal digit in the solution, one needs to choose $\varepsilon = 10^{-1}$, then $\bar{m} \sim -\dfrac{\ln(10)}{\ln(\rho(R))}$.

**Definition 1.3** *The asymptotic convergence rate is* $F = -\ln(\rho(R))$.

### Diagonally dominant matrices

**Theorem 1.5**

- *If $A$ is a matrix, either strictly diagonally dominant, or irreducible and strongly diagonally dominant, then the Jacobi algorithm converges.*
- *If $A$ is a matrix, either strictly diagonally dominant, or irreducible and strongly diagonally dominant, then for $0 < \omega \leq 1$, the SOR algorithm converges.*

### $M$- matrices

**Definition 1.4** *$A \in \mathbb{R}^{n\times n}$ is a $M$-matrix if*

1. *$a_{ii} > 0$ for $i = 1, \ldots, n$,*
2. *$a_{ij} \leq 0$ for $i \neq j$, $i, j = 1, \ldots, n$,*
3. *$A$ is invertible,*
4. *$A^{-1} \geq 0$.*

**Theorem 1.6** *If $A$ is a $M$-matrix and $A = M - N$ is a regular splitting ($M$ is invertible and both $M^{-1}$ and $N$ are nonnegative), then the stationary method converges.*

### Symmetric positive definite matrices

**Theorem 1.7 (Householder-John)** *Suppose $A$ is positive. If $M + M^T - A$ is positive definite, then $\rho(R) < 1$.*

**Corollary 1.1**

1. *If $D + E + F$ is positive definite, then Jacobi converges.*
2. *If $\omega \in (0, 2)$, then SOR converges.*

### Tridiagonale matrices

**Theorem 1.8**

1. *$\rho(\mathcal{L}_1) = (\rho(J))^2$ : Jacobi Gauss-Seidel converge or diverge simultaneously. If convergent, Gauss-Seidel is twice as fast.*
2. *Suppose the eigenvalues of $J$ are real. Then Jacobi and SOR converge or diverge simultaneously for $\omega \in ]0, 2[$.*
3. *Same assumptions, SOR has an optimal parameter $\omega^* = \dfrac{2}{1 + \sqrt{1 - (\rho(J))^2}}$, and then $\rho(\mathcal{L}_{\omega^*}) = \omega^* - 1$.*

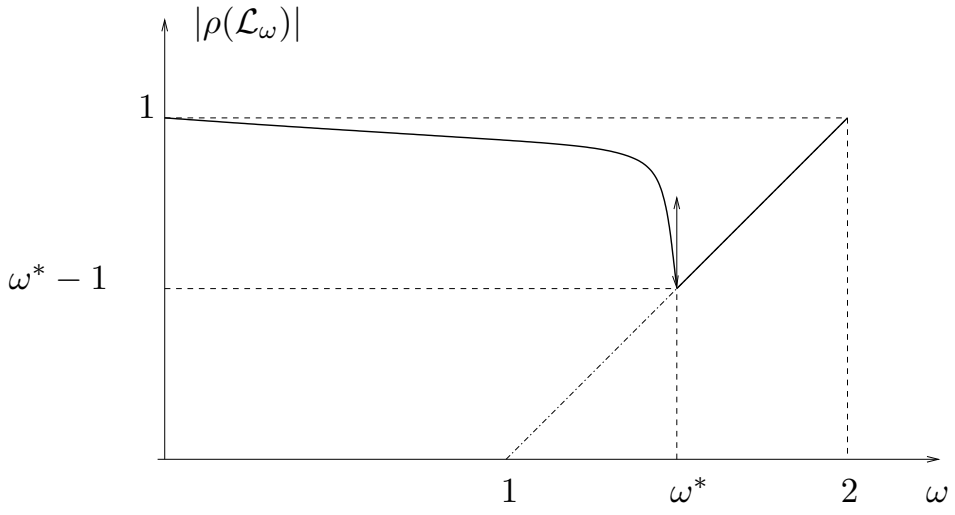



FIGURE 1.3 – Variations of $\rho(\mathcal{L}_\omega)$ as a fonction of $\omega$

## 1.4 Non-Stationary iterative methods. Symmetric definite positive matrices

**Descent methods**

### 1.4.1 Definition of the iterative methods

Suppose the descent directions $p_m$ are given beforehand. Define

$$x^{m+1} = x^m + \alpha_m p^m, \quad e^{m+1} = e^m - \alpha_m p^m, \quad r^{m+1} = r^m - \alpha_m A p^m.$$

Define the $A$ norm : $\|y\|_A^2 = (Ay, y)$.

**Theorem 1.9** *$x$ is the solution of $Ax = b$ $\iff$ it minimizes over $\mathbb{R}^N$ the functional $J(y) = \frac{1}{2}(Ay, y) - (b, y)$.*

This is equivalent to minimizing $G(y) = \frac{1}{2}(A(y-x), y-x) = \frac{1}{2}\|y-x\|_A^2$. At step $m$, $\alpha_m$ is defined such as to minimize $J$ in the direction of $p_m$. Define the quadratic function of $\alpha$

$$\varphi_m(\alpha) = J(x^m + \alpha p^m) = J(x^m) - \alpha(r^m, p^m) + \frac{1}{2}\alpha^2(Ap^m, p^m).$$

Minimizing $\varphi_m$ leads to

$$\alpha_m = \frac{(p^m, r^m)}{(Ap^m, p^m)}, \quad (p^m, r^{m+1}) = 0$$

$$G(x^{m+1}) = G(x^m)(1 - \mu_m), \quad \mu_m = \frac{(r^m, p^m)^2}{(Ap^m, p^m)(A^{-1}r^m, r^m)}$$

- **Steepest descent (gradient à pas optimal)** $p^m = r^m$.

$$x^{m+1} = x^m + \alpha_m r^m, \quad e^{m+1} = e^m - \alpha_m r^m, \quad r^{m+1} = (I - \alpha_m A)p^m.$$

$$\alpha_m = \frac{\|r^m\|^2}{(Ar^m, r^m)}, \quad (r^m, r^{m+1}) = 0$$

$$G(x^{m+1}) = G(x^m)\left(1 - \frac{\|r^m\|^4}{(Ar^m, r^m)(A^{-1}r^m, r^m)}\right) \leq \left(\frac{\kappa(A) - 1}{\kappa(A) + 1}\right)^2 G(x^m)$$

- **Conjugate gradient**

$$x^{m+1} = x^m + \alpha_m p^m, \quad \alpha_m = \frac{(p^m, r^m)}{(Ap^m, p^m)}, \quad (r^m, p^{m-1}) = 0.$$

Search $p^m$ as $p^m = r^m + \beta_m p^{m-1}$

$$G(x^{m+1}) = G(x^m)(1 - \mu_m)$$

$$\mu_m = \frac{(r^m, p^m)^2}{(Ap^m, p^m)(A^{-1}r^m, r^m)} = \frac{\|r^m\|^4}{(Ap^m, p^m)(A^{-1}r^m, r^m)}$$

Maximize $\mu_m$, or minimize

$$(Ap^m, p^m) = \beta_m^2 (Ap^{m-1}, p^{m-1}) + 2\beta_m (Ap^{m-1}, r^m) + (Ar^m, r^m)$$

$$\beta_m = -\frac{(Ap^{m-1}, r^m)}{(Ap^{m-1}, p^{m-1})} \quad \Rightarrow (Ap^{m-1}, p^m) = 0$$

$$(r^m, r^{m+1}) = 0, \quad \beta_m = \frac{\|r^m\|^2}{\|r^{m-1}\|^2}.$$

**Properties of the conjugate gradient** Choose $p^0 = r^0$. Then $\forall m \geq 1$, if $r^i \neq 0$ for $i < m$.

1. $(r^m, p^i) = 0$ for $i \leq m-1$.
2. $\text{vec}(r^0, \ldots, r^m) = \text{vec}(r^0, Ar^0, \ldots, A^m r^0)$.
3. $\text{vec}(p^0, \ldots, p^m) = \text{vec}(r^0, Ar^0, \ldots, A^m r^0)$.
4. $(p^m, Ap^i) = 0$ for $i \leq m-1$.
5. $(r^m, r^i) = 0$ for $i \leq m-1$.

**Definition 1.5** *Krylov space* $\mathcal{K}_m = vec(r^0, Ar^0, \ldots, A^{m-1} r^0)$.

**Theorem 1.10 (optimality of CG)** *A symétrique définie positive,*

$$\|x^m - x\|_A = \inf_{y \in x^0 + \mathcal{K}_m} \|y - x\|_A, \quad \|x\|_A = \sqrt{x^T A x}.$$

**Theorem 1.11** *Convergence in at most $N$ steps (size of the matrix). Furthermore*

$$G(x^m) \leq 4 \left( \frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^2 G(x^{m-1})$$

**The conjugate gradient algorithm**

$$x^0 \text{chosen}, \quad p^0 = r^0 = b - Ax^0.$$

while $m < Niter$ or $\|r^m\| \geq tol$, do

$$\begin{aligned}
\alpha_m &= \frac{\|r^m\|^2}{(Ap^m, p^m)}, \\
x^{m+1} &= x^m + \alpha_m p^m, \\
r^{m+1} &= r^m - \alpha_m A p^m, \\
\beta_{m+1} &= \frac{\|r^{m+1}\|^2}{\|r^m\|^2}, \\
p^{m+1} &= r^{m+1} - \beta_{m+1} p^m.
\end{aligned}$$

end.

### 1.4.2 Comparison of the iterative methods

**Basic example :**. 1-D Poisson equation $-u'' = f$ on $(0,1)$, with Dirichlet boundary conditions $u(0) = g_g,\ u(1) = g_d$. Introduce the second order finite difference stencil.

$$(0,1) = \cup(x_j, x_{j+1}), \quad x_{j+1} - x_j = h = \frac{1}{n+1}, \quad j = 0, \ldots, n.$$

$$-\frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2} \sim f(x_i), \quad i = 1, \ldots n$$

$$u_0 = g_g, \quad u_{n+1} = g_d.$$

$$|u_i - u(x_i)| \leq h^2 \ \frac{\sup_{x\in[a,b]} |u^{(4)}(x)|}{12}$$

.

The vector of discrete unknowns is $u =^t (u_1, \ldots, u_n)$.

$$A = \frac{1}{h^2}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & 0 \\ & \ddots & \ddots & \ddots & \\ & 0 & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \quad b = \begin{pmatrix} f_1 - \frac{g_g}{h^2} \\ f_2 \\ \vdots \\ f_{n-1} \\ f_n - \frac{g_d}{h^2} \end{pmatrix}$$

The matrix $A$ is symmetric definite positive.

The discrete problem to be solved is

$$Au = b$$

### 1.4.3 Condition number and error

$$Ax = b, \quad A\hat{x} = \hat{b}$$

Define $\kappa(A) = \|A\|_2\|A^{-1}\|_2$. If $A$ is symmetric $> 0$, $\kappa(A) = \frac{\max \lambda_i}{\min \lambda_i}$.

**Theorem 1.12**

$$\frac{\|\hat{x} - x\|_2}{\|x\|_2} \leq \kappa(A)\frac{\|\hat{b} - b\|_2}{\|b\|_2}$$

*and there is a $b$ such that it is equal.*

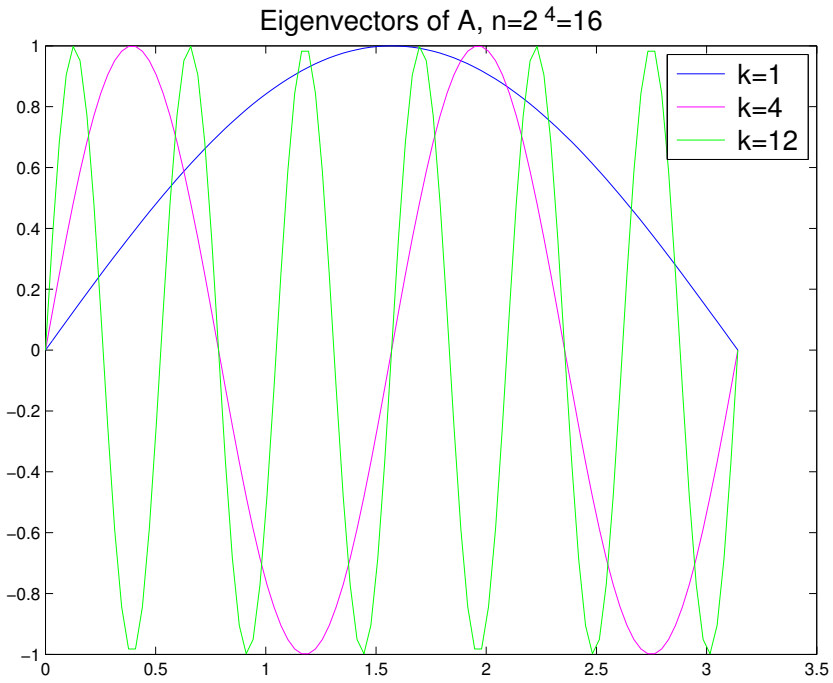



FIGURE 1.4 – Eigenvectors of $A$

Eigenvalues and eigenvectors of $A$ ($h \times (n+1) = 1$).

$$\mu_k = \frac{4}{h^2} \sin^2 \frac{k\pi h}{2}, \quad \Phi^{(k)} = \left( \sin \frac{jk\pi}{n+1} \right)_{1 \leq j \leq n},$$

$$\kappa(A) = \frac{\sin^2 \frac{n\pi h}{2}}{\sin^2 \frac{\pi h}{2}} = \frac{\cos^2 \frac{\pi h}{2}}{\sin^2 \frac{\pi h}{2}} \sim \frac{4}{\pi^2 h^2}$$

For any iterative method, the eigenfunctions of the iteration matrix are equal to those of $A$.

| **Algorithm** | **Eigenvalues of the iteration matrix** $R$ |
|---|---|
| Jacobi | $\lambda_k(J) = 1 - \frac{h^2}{2}\mu_k = cos(k\pi h)$ |
| Gauss-Seidel | $\lambda_k(\mathcal{L}_1) = (\lambda_k(J))^2 = cos^2(k\pi h)$ |
| SOR | $\eta = \lambda_k(\mathcal{L}_\omega)$ solution of $(\eta + \omega - 1)^2 = \eta\omega(\lambda_k(J))^2$. |

TABLE 1.1 – Eigenvalues of the iteration matrix

| **Algorithm** | **Convergence factor** | $n = 5$ | $n = 30$ | $n = 60$ |
|---|---|---|---|---|
| Jacobi | $\cos \pi h$ | 0.81 | 0.99 | 0.9987 |
| Gauss-Seidel | $\cos^2 \pi h$ | 0.65 | 0.981 | 0.9973 |
| SOR | $\dfrac{1-\sin \pi h}{1+\sin \pi h}$ | 0.26 | 0.74 | 0.9021 |
| steepest descent | $\dfrac{K(A)-1}{K(A)+1} = \cos \pi h$ | 0.81 | 0.99 | 0.9987 |
| conjugate gradient | $\dfrac{\sqrt{K(A)}-1}{\sqrt{K(A)}+1} = \dfrac{\cos \pi h - \sin \pi h}{\cos \pi h + \sin \pi h}$ | 0.51 | 0.86 | 0.9020 |

TABLE 1.2 – Convergence factor

| Algorithm | convergence factor $\rho_\infty$ | convergence rate $F$ |
|---|---|---|
| Jacobi | $1 - \frac{\varepsilon^2}{2}$ | $\frac{\varepsilon^2}{2}$ |
| Gauss-Seidel | $1 - \varepsilon^2$ | $\varepsilon^2$ |
| SOR | $1 - 2\varepsilon$ | $2\varepsilon$ |
| Steepest descent | $1 - \varepsilon^2$ | $1\varepsilon^2$ |
| conjugate gradient | $1 - 2\varepsilon$ | $2\varepsilon$ |

TABLE 1.3 – Asymptotic behavior in function of $\varepsilon = \pi h$

| $n$ | Jacobi and steepest descent | Gauss-Seidel | SOR | conjugate gradient |
|---|---|---|---|---|
| 10 | 56 | 28 | 4 | 4 |
| 100 | 4760 | 2380 | 38 | 37 |

TABLE 1.4 – Reduction factor for one digit $M \sim -\dfrac{\ln(10)}{F}$

| | |
|---|---|
| Gauss elimination | $n^2$ |
| optimal overrelaxation | $n^{3/2}$ |
| FFT | $n \ln_2(n)$ |
| conjugate gradient | $n^{5/4}$ |
| multigrid | $n$ |

TABLE 1.5 – Asymptotic order of the number of elementary operations needed to solve the $1-D$ problem as a function of the number of grid points

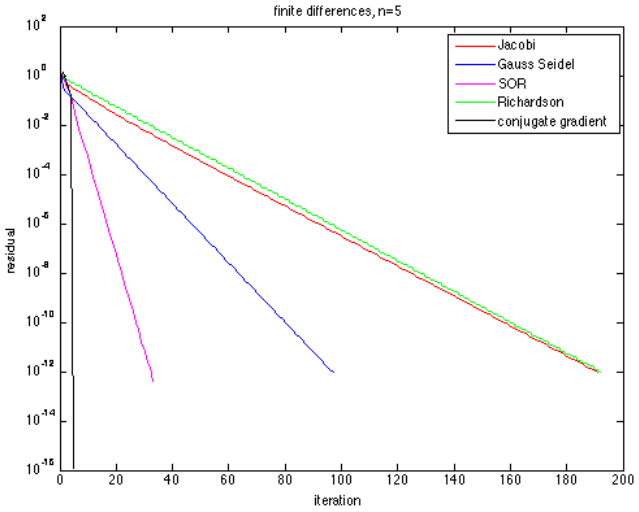



FIGURE 1.5 – Convergence history, $n = 5$

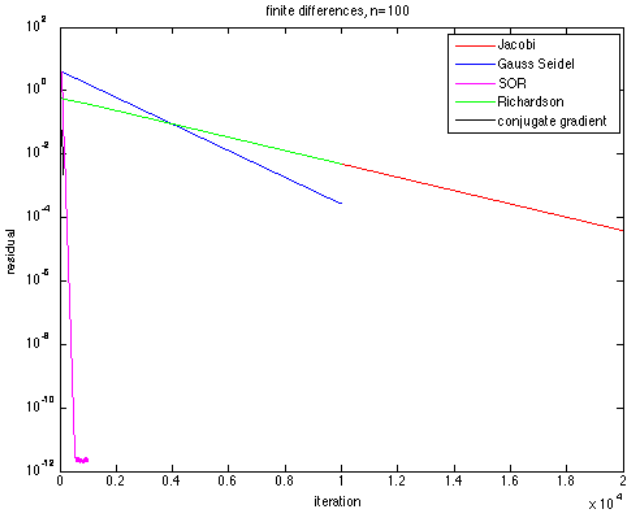



FIGURE 1.6 – Convergence history, $n = 100$

Not only the conjugate gradient is better, but the convergence rate being $\mathcal{O}(h^{1/2})$, the number of iterations necessary to increases the precision of one digit is multiplied by $\sqrt{10}$ when the mesh size is divided by 10, whereas for the Jacobi or Gauss-Seidel it is divided

by 100. The miracle of multigrids, is that the convergence rate is independent of the mesh size.

## 1.5 Preconditioning

**Preconditioning : purpose**

Take the system $AX = b$, with $A$ symmetric definite positive, and the conjugate gradient algorithm. The speed of convergence of the algorithm deteriorates when $\kappa(A)$ increases. The purpose is to replace the problem by another system, better conditioned. Let $M$ be a symmetric regular matrix. Multiply the system on the left by $M^{-1}$.

$$AX = b \iff M^{-1}AX = M^{-1}b \iff (M^{-1}AM^{-1})MX = M^{-1}b$$

Define

$$\tilde{A} = M^{-1}AM^{-1}, \quad \tilde{X} = MX, \quad \tilde{b} = M^{-1}b,$$

and the new problem to solve $\tilde{A}\tilde{X} = \tilde{b}$. Since $M$ is symmetric, $\tilde{A}$ is symmetric definite positive. Write the conjugate gradient algorithm for this "tilde" problem.

**The algorithm for $\tilde{A}$**

$$\tilde{X}^0 \text{ given}, \quad \tilde{p}^0 = \tilde{r}^0 = \tilde{b} - \tilde{A}\tilde{X}^0.$$

While $m < Niter$ or $\|\tilde{r}^m\| \geq tol$, do

$$\begin{aligned}
\alpha_m &= \frac{\|\tilde{r}^m\|^2}{(\tilde{A}\tilde{p}^m, \tilde{p}^m)}, \\
\tilde{X}^{m+1} &= \tilde{X}^m + \alpha_m \tilde{p}^m, \\
\tilde{r}^{m+1} &= \tilde{r}^m - \alpha_m \tilde{A}\tilde{p}^m, \\
\beta_{m+1} &= \frac{\|\tilde{r}^{m+1}\|^2}{\|\tilde{r}^m\|^2}, \\
\tilde{p}^{m+1} &= \tilde{r}^{m+1} - \beta_{m+1}\tilde{p}^m.
\end{aligned}$$

Now define

$$p^m = M^{-1}\tilde{p}^m, \quad X^m = M^{-1}\tilde{X}^m, \quad r^m = M\tilde{r}^m,$$

and replace in the algorithme above.

**The algorithm for $A$**

$$Mp^0 = M^{-1}r^0 = M^{-1}b - M^{-1}AM^{-1}MX^0 \iff \begin{cases} p^0 = M^{-2}r^0, \\ r^0 = b - AX^0. \end{cases}$$

$$\|\tilde{r}^m\|^2 = (M^{-1}r^m, M^{-1}r^m) = (M^{-2}r^m, r^m)$$

Define $\boxed{z^m = M^{-2}r^m}$. Then $\boxed{\beta_{m+1} = \frac{(z^{m+1}, r^{m+1})}{(z^m, r^m)}}$.

$$(\tilde{A}\tilde{p}^m, \tilde{p}^m) = (M^{-1}AM^{-1}Mp^m, Mp^m) = (Ap^m, p^m)$$

$$\Rightarrow \boxed{\alpha_m = \frac{(z^m, r^m)}{(Ap^m, p^m)}}.$$

$$MX^{m+1} = MX^m + \alpha_m Mp^m \iff \boxed{X^{m+1} = X^m + \alpha_m p^m}.$$

$$M^{-1}r^{m+1} = M^{-1}r^m - \alpha_m M^{-1}AM^{-1}Mp^m \iff \boxed{r^{m+1} = r^m - \alpha_m Ap^m}.$$

$$Mp^{m+1} = M^{-1}r^{m+1} - \beta_{m+1}Mp^m \iff \boxed{p^{m+1} = z^{m+1} - \beta_{m+1}p^m}.$$

**The algorithm for $A$**

Define $C = M^2$.

$$X^0 \text{ given}, \quad r^0 = b - AX^0, \quad \text{solve } Cz^0 = r^0, \quad p^0 = z^0.$$

While $m < Niter$ or $\|r^m\| \geq tol$, do

$$\begin{aligned} \alpha_m &= \frac{(z^m, r^m)}{(Ap^m, p^m)}, \\ X^{m+1} &= X^m + \alpha_m p^m, \\ r^{m+1} &= r^m - \alpha_m A p^m, \\ \text{solve } Cz^{m+1} &= r^{m+1}, \\ \beta_{m+1} &= \frac{(z^{m+1}, r^{m+1})}{(z^m, r^m)}, \\ p^{m+1} &= z^{m+1} - \beta_{m+1} p^m. \end{aligned}$$

**How to choose $C$**

$C$ must be chosen such that

1. $\tilde{A}$ is better conditioned than $A$,
2. $C$ is easy to invert.

Use an iterative method such that $A = C - N$ with symmetric $C$. For instance it can be a symmetrized version of SOR, named SSOR, defined for $\omega \in (0, 2)$ by

$$C = \frac{1}{\omega(2-\omega)}(D - \omega E)D^{-1}(D - \omega F).$$

Notice that if $A$ is symmetric definite positive, so is $D$ and its coefficients are positive, then its square root $\sqrt{D}$ is defined naturally as the diagonal matrix of the square roots of the coefficients. Then $C$ can be rewritten as

$$C = SS^T, \quad \text{with } S = \frac{1}{\sqrt{\omega(2-\omega)}}(D - \omega E)D^{-1/2},$$

yielding a natural Cholewski decomposition of $C$.

Another possibility is to use an incomplete Cholewski decomposition of $A$. Even if $A$ is sparse, that is has many zeros, the process of LU or Cholewski decomposition is very expensive, since it creates non zero values.

**Example : Matrix of finite differences in a square**

Poisson equation

$$-(\Delta_h u)_{i,j} = -\frac{1}{h^2}(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) - \frac{1}{h^2}(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}) = f_{i,j},$$
$$1 \leq i \leq M, 1 \leq j \leq M$$

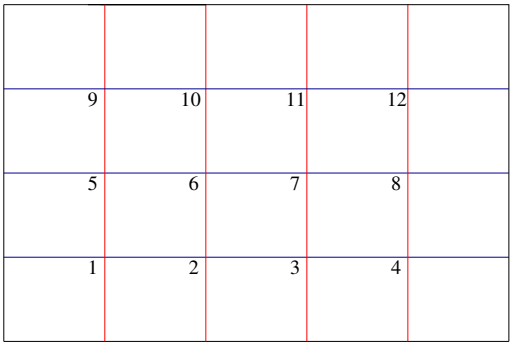



FIGURE 1.7 – Numbering by line

The point $(x_i, y_j)$ has for number $i+(j-1)M$. A vector of all unknowns $X$ is created :

$$Z = (u_{1,1}, u_{2,1}, u_{M,1}), (u_{1,2}, u_{2,2}, u_{M,2}), \cdots (u_{1,M}, u_{2,M}, u_{M,M})$$

with $Z_{i+(j-1)*M} = u_{i,j}$.
If the equations are numbered the same way (equation $\#k$ is the equation at point $k$), the matrix is block-tridiagonal :

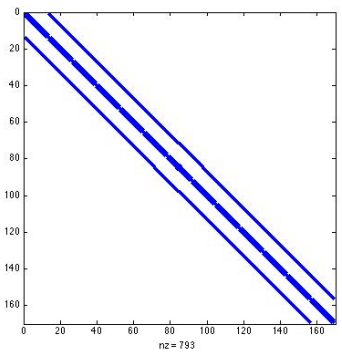
$$A = \frac{1}{h^2} \begin{pmatrix} B & -C & & 0_M & \\ -C & B & -C & & \\ & \ddots & \ddots & \ddots & \\ & & -C & B & -C \\ & 0_M & & -C & B \end{pmatrix} \tag{1.1}$$

$$C = I_M, \quad B = \begin{pmatrix} 4 & -1 & & 0 & \\ -1 & 4 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 4 & -1 \\ & 0 & & -1 & 4 \end{pmatrix}$$

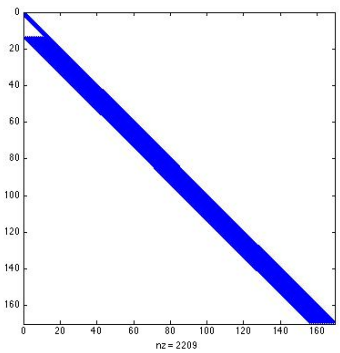
The righthand side is $b_{i+(j-1)*M} = f_{i,j}$, and the system takes the form $AZ = b$.

**Cholewski decomposition of $A$**

The block-Cholewski decomposition of $A$, $A = RR^T$, is block-bidiagonale, but the blocks are not tridiagonale as in $A$, as the `spy` command of matlab can show, in the case where $M = 15$.




spy(A)




spy(R)

However, if we look closely to the values of $R$ between the main diagonales where $A$ was non zero, we see that where the coefficients of $A$ are zero, the coefficients of $R$ are small. Therefore the incomplete Cholewski preconditioning computes only the values of $R$ where the coefficient of $A$ is not zero, and gains a lot of computational time.

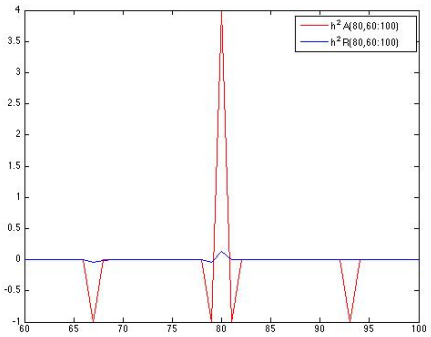



FIGURE 1.8 – Variation of the coefficients of Cholewski in the line 80 for $M = 15$

The matlab codes are as follows ([3])

**Cholewski**

```
Ch=tril(A);
for k=1:nn
    Ch(k,k)=sqrt(Ch(k,k));
    Ch(k+1:nn,k)=Ch(k+1:nn,k)/Ch(k,
        k);
    for j=k+1:nn
        Ch(j:nn,j)=Ch(j:nn,j)-Ch(j:
            nn,k)*Ch(j,k);
    end
end
```

**Incomplete Cholewski**

```
ChI=tril(A);
for k=1:nn
    ChI(k,k)=sqrt(ChI(k,k));
    for j=k+1:nn
        if ChI(j,k) ~= 0
            ChI(j,k)=ChI(j,k)/ChI(k
                ,k);
        end
    end
    for j=k+1:nn
        for i=j:n
            if ChI(i,j) ~= 0
                ChI(i,j)=ChI(i,j)-
                    ChI(i,k)*ChI(j,k
                    );
            end
        end
    end
end
```

Then use $C = R * R^T$.

**Comparison** For the 2-D finite differences matrix and $n = 25$ internal points in each direction, we compare the convergence of the conjugate gradient and various preconditioning : Gauss-Seidel, SSOR with optimal parameter, and incomplete Cholewski. The gain even with $\omega = 1$ is striking. Furthermore Gauss-Seidel is comparable with Incomplete Cholewski.

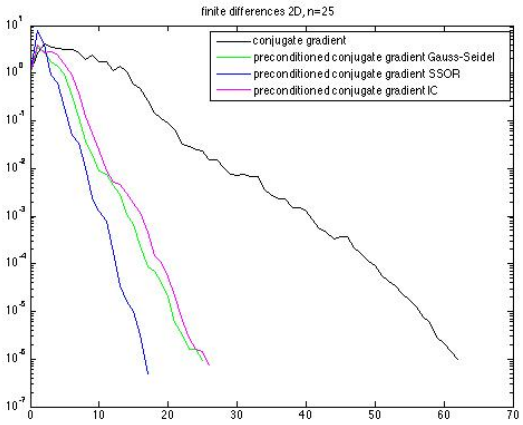



FIGURE 1.9 – Convergence history, influence of preconditioning

## 1.6 Krylov methods for non symmetric matrices, Arnoldi algorithm

### 1.6.1 Gram-Schmidt orthogonalization and $QR$ decomposition

Starting with a free family $(v_1, \cdots, v_m, \cdots)$ in a vector space $E$, the process builds an orthonormal family $(w_1, \cdots, w_m, \cdots)$ recursively.

•. Define $w_1 = \dfrac{v_1}{\|v_1\|}$.

•. Note $r_{1,2} = (v_2, w_1)$, and define $u_2 = v_2 - r_{1,2}w_1$. By construction $u_2$ is orthogonal to $w_1$. It only remains to make it of norm 1 by defining $r_{2,2} = \|u_2\|$, $w_2 = \dfrac{u_2}{r_{2,2}}$.

•. Suppose we have built $(w_1, \cdots, w_j)$ orthonormal. Define $r_{i,j+1} = (v_{j+1}, w_i)$ for $1 \leq i \leq j$, and

$$u_{j+1} = v_{j+1} - \sum_{i=1}^{j} r_{i,j+1}w_i, \quad r_{j+1,j+1} = \|u_{j+1}\|, \quad w_{j+1} = \frac{u_{j+1}}{r_{j+1,j+1}}.$$

Then $(w_1, \cdots, w_j)$ is orthonormal. Furthermore, we can rewrite the previous equality as

$$v_{j+1} = r_{j+1,j+1}w_{j+1} + \sum_{i=1}^{j} r_{i,j+1}w_i,$$

which gives for each $j$ ;

$$v_j = \sum_{i=1}^{j} r_{i,j}w_i\,. \tag{1.2}$$

Define the matrix $K$ whose columns are the $v_j$, the matrix $Q$ whose columns are the $w_j$, and the upper triangular matrix $R$ whose coefficients are $r_{i,j}$ for $i \leq j$, and 0 otherwise. Then (1.2) takes the matrix form

$$K = QR \tag{1.3}$$

The matrix $Q$ is orthogonal, so this is exactly the so-called $QR$ decomposition of the matrix $K$. Note that the matrix K DOES NOT NEED TO BE SQUARE, nor the matrix $Q$, but the matrix $R$ has size $m \times m$.

### 1.6.2 Arnoldi algorithm

The purpose is to build recursively a orthonormal basis of the Krylov space $\mathcal{K}_m = vect(r, Ar, \cdots, A^{m-1}r)$. We will take advantage of the special form of the generating family to proceed a slight modification of Gram Schmidt.

•. Define $q_1 = \dfrac{r}{\|r\|}$.

•. Now we must orthogonalize $q_1$ and $Ar$, or equivalently $q_1$ and $Aq_1$ :

$$h_{1,1} = (Aq_1, q_1), \quad u_2 = Aq_1 - h_{1,1}q_1, \quad h_{2,1} = \|u_2\|, \quad q_2 = \frac{u_2}{h_{2,1}}.$$

Then $q_2 \in Vec(q_1, Aq_1) = Vec(r, Ar) = \mathcal{K}_2$ and $(q_1, q_2)$ is an orthonormal basis. All this can be rewritten as

$$Aq_1 = h_{1,1}q_1 + h_{2,1}q_2.$$

Then $\mathcal{K}_3 = Vec(q_1, q_2, A^2r) = Vec(q_1, q_2, Aq_2)$. Therefore, instead of orthonormalizing with the new vector $A^2r$, we can do it with the new vector $Aq_2$. Define

$$u_3 = Aq_2 - h_{1,2}q_1 - h_{2,2}q_2, \quad h_{2,2} = (Aq_2, q_2), \quad h_{1,2} = (Aq_2, q_1), \quad h_{3,2} = \|u_3\|, \; q_3 = \frac{u_3}{h_{3,2}}.$$

This generalizes in building an orthonormal basis of $\mathcal{K}_{j+1}$ by

$$u_{j+1} = Aq_j - \sum_{i=1}^{j} h_{i,j}q_i \ , \quad h_{i,j} = (Aq_j, q_i), \quad h_{j+1,j} = \|u_{j+1}\|, \; q_{j+1} = \frac{u_{j+1}}{h_{j+1,j}}.$$

**Theorem 1.13** *If the algorithm goes through $m$, then $(q_1, \ldots, q_m)$ is a basis of $\mathcal{K}_m$.*

Below is the matlab script

```
for j=1:m do
                h(i,j)=(A*v(j,:),v(i,:)) , i=1:i
       w(j,:)=A*v(j,:)−sum(h(i,j)v(i,:)
       h(j+1,j)=norm(w(j,:),2)
       If h(j+1,j) == 0 stop
       v(j+1,:)= w(j,:)/h(j+1,j)
```

The definition of the $q_j$ above can be rewritten as

$$Aq_j = \sum_{i=1}^{j+1} h_{i,j}q_i \tag{1.4}$$

Define the Hessenberg matrix $\widetilde{H}_m$ as the matrix of the $h_{i,j}$ for $i \leq j+1$, and 0 otherwise. $\widetilde{H}_m$ is a matrix of size $(m+1) \times m$.

$$\widetilde{H}_m = \begin{pmatrix} h_{1,1} & & \cdots & & h_{1,m} \\ h_{2,1} & h_{2,2} & & \cdots & h_{2,m} \\ 0 & h_{3,2} & \ddots & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & h_{m,m-1} & h_{m,m} \\ 0 & 0 & 0 & 0 & h_{m+1,m} \end{pmatrix}$$

Define $V_m = [q_1, \cdots, q_m]$. $H_m$ is the $m \times m$ matrix obtained from the $(m+1) \times m$ matrix $\widetilde{H}_m$ by deleting the last row.

**Proposition 1.1**

$$AV_m = V_{m+1}\widetilde{H}_m, \quad AV_m = V_{m+1}\widetilde{H}_m = V_m H_m + h_{m+1,m}q_{m+1}e_m^T, \quad V_m^T AV_m = H_m. \tag{1.5}$$

Proof The first identity is just rewriting (1.4). As for the second one, rewrite the first one in blocks as

$$V_{m+1}\widetilde{H}_m = [V_m, q_{m+1}]\begin{bmatrix} H_m \\ h_{m+1,m}e_m^T \end{bmatrix} = V_m H_m + h_{m+1,m}q_{m+1}e_m^T.$$

Use this now in the first equality to obtain

$$AV_m = V_m H_m + h_{m+1,m}q_{m+1}e_m^T.$$

Multiply on the left by $V_m^T$. Since $V_m$ is orthogonal, and $V_m^T q_{m+1} = [(q_1, q_{m+1}), \cdots, (q_m, q_{m+1})]^T = 0$, we obtain

$$V_m^T AV_m = H_m.$$

■

### 1.6.3 Full orthogonalization method or FOM

Search for an approximate solution in $x_0 + \mathcal{K}_m(A, r_0)$ in the form $x_m = x_0 + V_m y$, and impose $r_m \perp \mathcal{K}_m(A, r_0)$. This is equivalent to $V_m^T r_m = 0$, which by

$$r_m = b - A(x_0 + V_m y) = r_0 - AV_m y$$

can be written by (1.5) as

$$V_m^T AV_m y = V_m^T r_0 \text{ or } H_m y = \|r_0\|e_1.$$

The small Hessenberg system

$$H_m y = \|r_0\|e_1 \tag{1.6}$$

can be solved at each step using a direct method : suppose all the principal minors of $H_m$ are nonzero. Due to the special structure of $H_m$, the $LU$ factorization of $H_m$ has the form

$$L = \begin{pmatrix} 1 & & \cdots & & 0 \\ l_1 & 1 & & \cdots & 0 \\ 0 & l_2 & \ddots & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & l_{m-1} & 1 \end{pmatrix}, \quad U = \begin{pmatrix} u_{11} & & \cdots & & u_{1m} \\ 0 & u_{22} & & \cdots & u_{2m} \\ 0 & 0 & \ddots & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & u_{mm} \end{pmatrix}$$

The following matlab code gives the $LU$ factorization

```
u(1,:)=h(1,:);
for i=1:m-1
l(i)=h(i+1,i)/u(i,i);
 for j=i+1:n
u(i+1,j)=h(i+1,j)-l(i)*u(i,j)
end
end
```

```
u(1,:)=h(1,:);
for i=1:m-1
l(i)=h(i+1,i)/u(i,i);
       for j=i+1:n
       u(i+1,j)=h(i+1,j)-l(i)*u(i,j)
       end
end
```

The computational cost is $m^2 + 2m - 1$ operations.

**Theorem 1.14** *At each step $m$, $r_m$ is parallel to $q_{m+1}$.*

Proof

$$r_m = r_0 - AV_m y = r_0 - (V_m H_m + h_{m+1,m} q_{m+1} e_m^T) y = r_0 - V_m H_m y - h_{m+1,m} y_m q_{m+1}.$$

But $H_m y = \|r_0\| e_1$, therefore $r_0 - V_m H_m y = r_0 - \|r_0\| V_m e_1 = r_0 - \|r_0\| q_1 = 0$. Therefore $r_m = -h_{m+1,m} y_m q_{m+1}$ is parallel to $q_{m+1}$.

■

```
function [X,R,H,Q]=FOM(A,b,x0);
% FOM full orthogonalization method
% [X,R,H,Q]=FOM(A,b,x0) computes the decomposition A=QHQ?, Q
    orthogonal
% and H upper Hessenberg, Q(:,1)=r/norm(r), using Arnoldi in order to
% solve the system Ax=b with the full orthogonalization method. X
    contains
% the iterates and R the residuals
n=length(A); X=x0;
r=b-A*x0; R=r; r0norm=norm(r);
Q(:,1)=r/r0norm;
for k=1:n
    v =A*Q(:,k);
    for j=1:k
        H(j,k)=Q(:,j)'*v; v=v-H(j,k)*Q(:,j);
    end
    e0=zeros(k,1); e0(1)=r0norm; % solve system
    y=H\e0; x= x0+Q*y;
    X=[X x];
    R=[R b-A*x];
    if k<n
        H(k+1,k)=norm(v); Q(:,k+1)=v/H(k+1,k);
    end
end
```

### 1.6.4 GMRES algorithm

Here we minimize at each step the residual $r_m$ in $\mathcal{K}_m(A, r_0)$, which is equivalent to the minimization of $J(y) = \|r_0 - AV_m y\|_2$ for $y$ in $\mathbb{R}^m$, Use the Proposition to write

$$r_0 - AV_m y = \|r_0\| q_1 - V_{m+1} \widetilde{H}_m y = V_{m+1}(\|r_0\| e_1 - \widetilde{H}_m y).$$

Since $V_{m+1}$ is orthogonal, then

$$\|r_0 - AV_m y\| = \|\|r_0\| e_1 - \widetilde{H}_m y\|.$$

So in FOM we solve EXACTLY the square system $H_m y = \|r_0\| e_1$, while in GMRES we solve the LEAST SQUARE problem $\inf \|\|r_0\| e_1 - \widetilde{H}_m y\|$. This small minimization problem has a special form with a upper Hessenberg form, and is best solved by the Givens reflection method. Let us consider the case of $m = 3$ ($\sigma_0 = \|r_0\|$).

$$z = \widetilde{H}_3 y - \sigma_0 e_1 = \begin{pmatrix} h_{1,1} & h_{1,2} & h_{1,3} \\ h_{2,1} & h_{2,2} & h_{2,3} \\ 0 & h_{3,2} & h_{3,3} \\ 0 & 0 & h_{4,3} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} - \begin{pmatrix} \sigma_0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Multiply successively by the three $(m+1)\times(m+1)$ Givens matrices

$$Q_1 = \begin{pmatrix} c_1 & s_1 & 0 & 0 \\ -s_1 & c_1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad Q_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & c_2 & s_2 & 0 \\ 0 & -s_2 & c_2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad Q_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & c_3 & s_3 \\ 0 & 0 & -s_3 & c_3 \end{pmatrix},$$

to make the system triangular, and even better

$$Q_3Q_2Q_1z = \left(\begin{array}{ccc} \tilde{h}_{1,1} & \tilde{h}_{1,2} & \tilde{h}_{1,3} \\ 0 & \tilde{h}_{2,2} & \tilde{h}_{2,3} \\ 0 & 0 & \tilde{h}_{3,3} \\ \hline 0 & 0 & 0 \end{array}\right) \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} - \left(\begin{array}{c} c_1 \\ c_2 \\ c_3 \\ \hline c_4 \end{array}\right)$$

Therefore

$$\|z\|^2 = \|Q_3Q_2Q_1z\|^2 = \|Ry - c^I\|^2 + (c_4)^2$$

where $R$ is the upperblock of the matrix, and $c^I$ the upperblock of the vector. Now we have a regular system, and $y$ is THE solution of

$$Ry = c^I,$$

which is now an upper triangular system.

```
function [x,iter,resvec] = GMRES(A,b,restart,tol,maxit)
%GMRES  Generalized Minimum Residual Method for Schwarz methods
%   [x,iter]=GMRES(A,b,RESTART,TOL,MAXIT) uses gmres to solve a
    system
%   Ax=b where A is defined as the procedure 'A'.
%   This is an adapted copy of Matlabs GMRES.

n = length(b);

n2b = norm(b);                  % Norm of rhs vector, b

% x0=rand(n,1);
% x0 = ones(n,1);
f=1;                            % all frequencies to initialize
x0 = sin((1:n/2)'/(n/2+1)*pi*f); x0=[x0; x0];
for f=2:n/2,
  x0 = x0+[sin((1:n/2)'/(n/2+1)*pi*f); sin((1:n/2)'/(n/2+1)*pi*f)];
end;

x = x0;

% Set up for the method
flag = 1;
xmin = x;                       % Iterate which has minimal residual
    so far
imin = 0;                       % Outer iteration at which xmin was
    computed
jmin = 0;                       % Inner iteration at which xmin was
    computed
tolb = tol * n2b;               % Relative tolerance
if tolb==0,
```

```
28    tolb=tol;                     % use absolute error to find zero
          solution
29  end;
30  r = b - feval(A,x);             % Zero-th residual
31  normr = norm(r);                % Norm of residual
32
33  if normr <= tolb                % Initial guess is a good enough
        solution
34    flag = 0;
35    relres = normr / n2b;
36    iter = 0;
37    resvec = normr;
38    os = sprintf(['The initial guess has relative residual %0.2g' ...
39                  ' which is within\nthe desired tolerance %0.2g' ...
40                  ' so GMRES returned it without iterating.'], ...
41                 relres,tol);
42    disp(os);
43    return;
44  end
45
46
47  resvec = zeros(restart*maxit+1,1); % Preallocate vector for norm of
        residuals
48  resvec(1) = normr;              % resvec(1) = norm(b-A*x0)
49  normrmin = normr;               % Norm of residual from xmin
50  rho = 1;
51  stag = 0;                       % stagnation of the method
52
53  % loop over maxit outer iterations (unless convergence or failure)
54
55  for i = 1 : maxit
56    V = zeros(n,restart+1);       % Arnoldi vectors
57    h = zeros(restart+1,1);       % upper Hessenberg st A*V = V*H
          ...
58    QT = zeros(restart+1,restart+1); % orthogonal factor st QT*H = R
59    R = zeros(restart,restart);   % upper triangular factor st H = Q
          *R
60    f = zeros(restart,1);         % y = R\f => x = x0 + V*y
61    W = zeros(n,restart);         % W = V*inv(R)
62    j = 0;                        % inner iteration counter
63
64    vh = r;
65    h(1) = norm(vh);
66    V(:,1) = vh / h(1);
67    QT(1,1) = 1;
68    phibar = h(1);
69
70    for j = 1 : restart
71      j
72  %   MapU(x,sqrt(n),sqrt(n));
```

```
73
74      u = feval(A,V(:,j));          % matrix multiply
75      for k = 1 : j
76        h(k) = V(:,k)' * u;
77        u = u - h(k) * V(:,k);
78      end
79      h(j+1) = norm(u);
80      V(:,j+1) = u / h(j+1);
81      R(1:j,j) = QT(1:j,1:j) * h(1:j);
82      rt = R(j,j);
83
84  % find cos(theta) and sin(theta) of Givens rotation
85      if h(j+1) == 0
86        c = 1.0;                      % theta = 0
87        s = 0.0;
88      elseif abs(h(j+1)) > abs(rt)
89        temp = rt / h(j+1);
90        s = 1.0 / sqrt(1.0 + temp^2); % pi/4 < theta < 3pi/4
91        c = - temp * s;
92      else
93        temp = h(j+1) / rt;
94        c = 1.0 / sqrt(1.0 + temp^2); % -pi/4 <= theta < 0 < theta <=
              pi/4
95        s = - temp * c;
96      end
97
98      R(j,j) = c * rt - s * h(j+1);
99  %   zero = s * rt + c * h(j+1);
100
101     q = QT(j,1:j);
102     QT(j,1:j) = c * q;
103     QT(j+1,1:j) = s * q;
104     QT(j,j+1) = -s;
105     QT(j+1,j+1) = c;
106     f(j) = c * phibar;
107     phibar = s * phibar;
108
109     if j < restart
110       if f(j) == 0                  % stagnation of the method
111         stag = 1;
112       end
113       W(:,j) = (V(:,j) - W(:,1:j-1) * R(1:j-1,j))/ R(j,j);
114 % Check for stagnation of the method
115       if stag == 0
116         stagtest = zeros(n,1);
117         ind = (x ~= 0);
118         if ~(i==1 & j==1)
119           stagtest(ind) = W(ind,j) ./ x(ind);
120           stagtest(~ind & W(:,j) ~= 0) = Inf;
121           if abs(f(j))*norm(stagtest,inf) < eps
```

```
            stag = 1;
          end
        end
      end
      x = x + f(j) * W(:,j);       % form the new inner iterate
    else % j == restart
      vrf = V(:,1:j)*(R(1:j,1:j)\f(1:j));
% Check for stagnation of the method
      if stag == 0
        stagtest = zeros(n,1);
        ind = (x0 ~= 0);
        stagtest(ind) = vrf(ind) ./ x0(ind);
        stagtest(~ind & vrf ~= 0) = Inf;
        if norm(stagtest,inf) < eps
          stag = 1;
        end
      end
      x = x0 + vrf;                % form the new outer iterate
    end
    normr = norm(b-feval(A,x));
    resvec((i-1)*restart+j+1) = normr;

    if normr <= tolb               % check for convergence
      if j < restart
        y = R(1:j,1:j) \ f(1:j);
        x = x0 + V(:,1:j) * y;     % more accurate computation of xj
        r = b - feval(A,x);
        normr = norm(r);
        resvec((i-1)*restart+j+1) = normr;
      end
      if normr <= tolb             % check using more accurate xj
        flag = 0;
        iter = [i j];
        break;
      end
    end

    if stag == 1
      flag = 3;
      break;
    end

    if normr < normrmin            % update minimal norm quantities
      normrmin = normr;
      xmin = x;
      imin = i;
      jmin = j;
    end
  end                              % for j = 1 : restart

```

```
172   if flag == 1
173     x0 = x;                         % save for the next outer
          iteration
174     r = b - feval(A,x0);
175   else
176     break;
177   end
178
179 end                                 % for i = 1 : maxit
180
181 % returned solution is that with minimum residual
182
183 if n2b==0,
184   n2b=1;          % here we solved for the zero solution and thus show
185 end;              % the absolute residual !
186
187 if flag == 0
188   relres = normr / n2b;
189 else
190   x = xmin;
191   iter = [imin jmin];
192   relres = normrmin / n2b;
193 end
194
195 % truncate the zeros from resvec
196 if flag <= 1 | flag == 3
197   resvec = resvec(1:(i-1)*restart+j+1);
198 else
199   if j == 0
200     resvec = resvec(1:(i-1)*restart+1);
201   else
202     resvec = resvec(1:(i-1)*restart+j);
203   end
204 end
205
206
207 % only display a message if the output flag is not used
208 switch(flag)
209     case 0,
210       os = sprintf(['GMRES(%d) converged at iteration %d(%d) to a'
            ...
211                     ' solution with relative residual %0.2g'], ...
212                     restart,iter(1),iter(2),relres);
213
214     case 1,
215       os = sprintf(['GMRES(%d) stopped after the maximum %d
            iterations' ...
216                     ' without converging to the desired tolerance
                          %0.2g' ...
217                     '\n         The iterate returned (number %d(%d))'
```

```
                    ...
218                 ' has relative residual %0.2g'], ...
219                 restart,maxit,tol,iter(1),iter(2),relres);
220
221     case 2,
222       os = sprintf(['GMRES(%d) stopped at iteration %d(%d)' ...
223                 ' without converging to the desired tolerance
                      %0.2g' ...
224                 '\n         because the system involving the' ...
225                 ' preconditioner was ill conditioned.' ...
226                 '\n         The iterate returned (number %d(%d))'
                      ...
227                 ' has relative residual %0.2g'], ...
228                 restart,i,j,tol,iter(1),iter(2),relres);
229
230     case 3,
231       os = sprintf(['GMRES(%d) stopped at iteration %d(%d)' ...
232                 ' without converging to the\n         desired'
                      ...
233                 ' tolerance %0.2g because the method stagnated.'
                      ...
234                 '\n         The iterate returned (number %d(%d))'
                      ...
235                 ' has relative residual %0.2g'], ...
236                 restart,i,j,tol,iter(1),iter(2),relres);
237
238 end                              % switch(flag)
239 if flag == 0
240   disp(os);
241 else
242   warning(os);
243 end
244
245 semilogy(0:length(resvec)-1,resvec);
```

**Remark** If $A$ is symmetric, $H_m$ is tridiagonale.

**Restarted GMRES** For reasons of storage cost, the GMRES algorithm is mostly used by restarting every $M$ steps :

Compute $x_1, \cdots, x_M$.

If $r_M$ is small enough, stop,

else restart with $x_0 = x_M$.

# Chapitre 2

# Multigrid methods

## Contents


**2.1 The V- cycle process . . . . . 37**

2.1.1 The Smoother . . . . . 38

2.1.2 Projection on the coarse grid . . . . . 38

2.1.3 Coarse resolution . . . . . 39

2.1.4 Projection on the fine grid . . . . . 39

2.1.5 Result of the coarse walk . . . . . 39

2.1.6 Postsmoothing . . . . . 41

2.1.7 Spectral analysis . . . . . 41

2.1.8 Number of elementary operations . . . . . 44

**2.2 The finite elements multigrid algorithm . . . . . 44**

2.2.1 Preliminaries . . . . . 44

2.2.2 Discrete norm . . . . . 46

2.2.3 Definition of the multigrid algorithm . . . . . 47

2.2.4 Convergence property of the multigrid algorithm . 48

**2.3 Multigrid Preconditioner . . . . . 51**


Multigrid methods are a prime source of important advances in algorithmic efficiency , finding a rapidly increasing number of users. Unlike other known methods, multigrid offers the possibility of solving problems with N unknowns with O(N) work and storage, not just for special cases, but for large classes of problems. It relies on the use of several nested grids. For the modal presentation of the method, we refer to [7],[2], [5]. For the finite element part, we refer to [1].

## 2.1 The V- cycle process

One cycle of the multigrid method is given as follows. Suppose we want to solve $A^h\bar{U}^h = b^h$. We take an initial guess $U^h$, and define $MG(A^h, b, U^h)$ to be

**Step 1 : smoothing** $N_1$ iterations of the smoother, with initial guess $U^h$.

$$U^{h,1} = \mathcal{S}^h(A^h, b, U^h, N_1), \quad e^{h,1} = \bar{U}^h - U^{h,1}.$$

The residual is $r^{h,1} = b^h - A^h U^{h,1} = A^h e^{h,1}$.
It is projected on the coarse grid

$$r^{2h} = P_h^{2h} r^{h,1}$$

**Step 2 : Coarse resolution** The system $A^{2h}\tilde{U}^{2h} = r^{2h}$ is solved approximately by $p$ iterations of the multigrid solver on the coarse grid

$$U^{2h,r} = MG(A^{2h}, r^{2h}, U^{2h,r-1}), \quad U^{2h,0} = 0, 1 \leq r \leq p.$$

It is projected on the fine grid

$$U^{h,2} = U^{h,1} + P_{2h}^h U^{2h,r}, \quad e^{h,2} = e^{h,1} - P_{2h}^h U^{2h,r}$$

**Step 3 : Smoothing again** $N_2$ iterations of the smoother

$$U^{h,3} = \mathcal{S}^h(A^h, b^h, U^{h,2}, N_2).$$

We will describe the process in the simple case where the coarse problem is solved exactly, *i.e.*

$$U^{h,2} = U^{h,1} - P_{2h}^h \tilde{U}^{2h}$$

Define $Df2(p)$ the $p \times p$ matrix of $1 - D$ finite differences on a grid of mesh 1 :

$$Df_2(p) = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & 0 \\ & \ddots & \ddots & \ddots & \\ & 0 & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}, \quad (Df_2(p)U)_j = -U_{j-1} + 2U_j - U_{j+1}.$$

Then $A^h = \frac{1}{h^2} Df_2(n-1)$ and $A^{2h} = \frac{1}{4h^2} Df_2(2n-1)$.

### 2.1.1 The Smoother

If $S$ is the iteration matrix of the smoother, the result of the smoothing is

$$e^{h,1} = S^{N_1} e^0, \quad r^{h,1} = A^h e^{h,1}. \tag{2.1}$$

### 2.1.2 Projection on the coarse grid

The fine grid is $(\frac{k}{2n})$ for $1 \leq k \leq 2n-1$. The coarse grid is $(\frac{k}{n})$ for $1 \leq k \leq n-1$. Define $h = 1/2n$.

$$P_h^{2h} : \mathbb{R}^{2n-1} \to R^{n-1}, \quad (P_h^{2h} U^h)_j = \frac{1}{4}(U_{2j-1}^h + 2U_{2j}^h + U_{2j+1}^h).$$

The matrix of $P_h^{2h}$ is

$$P_h^{2h} = \begin{pmatrix} \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & 0 & 0 & \dots & \dots & \dots & \dots \\ 0 & 0 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & 0 & 0 & \dots & \dots \\ 0 & 0 & 0 & 0 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & \dots & \dots \\ & & & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & & \dots & & 0 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \end{pmatrix}$$

Define now

$$r^{2h} := P_h^{2h} r^h = P_h^{2h} A^h e^{h,1}.$$

### 2.1.3 Coarse resolution

Suppose the coarse grid problem is solved exactly.

$$A^{2h} \tilde{U}^{2h} = r^{2h}$$

.

### 2.1.4 Projection on the fine grid

We define the projection operator as :

$$P_{2h}^h : \mathbb{R}^{n-1} \to R^{2n-1}, \quad \begin{cases} (P_{2h}^h U^{2h})_{2j} = U_j^{2h} \\ (P_{2h}^h U^{2h})_{2j+1} = \frac{1}{2}(U_j^{2h} + U_{j+1}^{2h}) \end{cases}$$

The matrix is

$$P_{2h}^h = \begin{pmatrix} \frac{1}{2} & 0 & 0 & \dots & 0 \\ 1 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \vdots & & & & \\ \vdots & & & & \\ 0 & 0 & \dots & 0 & \frac{1}{2} \end{pmatrix}$$

### 2.1.5 Result of the coarse walk

$$e^{h,2} = (I - P_{2h}^h (A^{2h})^{-1} P_h^{2h} A^h) e^{h,1}$$

**Lemma 2.1**

$$\mathcal{K}er\, P_h^{2h} A^h = \{V \in \mathbb{R}^{2n-1},\, V_{2j} = 0,\, j = 1 \cdots, n-1\}, \tag{2.2}$$

$$\mathcal{K}er\, P_h^{2h} A^h \oplus \mathcal{I}m P_{2h}^h = \mathbb{R}^{2n-1}, \tag{2.3}$$

$$\forall V \in \mathbb{R}^{2n-1}, \forall j, (A^h P_{2h}^h V)_{2j+1} = 0, \tag{2.4}$$

$$P_h^{2h} A^h P_{2h}^h = A^{2h}. \tag{2.5}$$

Proof It is easy to compute

$$\begin{array}{rcl} (P_h^{2h} A^h U)_j & = & \frac{1}{4}((A^h U)_{2j-1} + 2(A^h U)_{2j} - (A^h U)_{2j+1}) \\ & = & \frac{1}{4h^2}(-U_{2j-2} + 2U_{2j-1} - U_{2j} + 2(-U_{2j-1} + 2U_{2j} - U_{2j+1}) - U_{2j} + 2U_{2j+1} - U_{2j+2}) \\ & = & \frac{1}{4h^2}(-U_{2j-2} + 2U_{2j} - U_{2j+2}) \\ & = & A^{2h} \begin{pmatrix} U_2 \\ \vdots \\ U_{2n-2} \end{pmatrix} \end{array}$$

Denoting by $U^e$ the vector of the even coordinates of $U$, we have proved that for any vector $U \in \mathbb{R}^{2n-1}$,

$$P_h^{2h} A^h U = U^e.$$

Therefore the kernel of $P_h^{2h} A^h$ is equal to the space of $U$ such that $U^e = 0$, which proves (2.2).

Now by the rank theorem,

$$\dim \mathcal{K}\mathrm{er} P_h^{2h} + \dim \mathcal{I}\mathrm{m} P_h^{2h} = 2n-1.$$

Since $A^h$ is an isomorphism in $\mathbb{R}^{2n-1}$, $\dim \mathcal{K}\mathrm{er} P_h^{2h} = \dim \mathcal{K}\mathrm{er} P_h^{2h} A^h$. Then

$$\dim \mathcal{K}\mathrm{er} P_h^{2h} A^h + \mathrm{rg} P_h^{2h} = 2n-1.$$

Since $P_h^{2h} = \frac{1}{2}(P_{2h}^h)^T$, they have the same rank, and therefore

$$\dim \mathcal{K}\mathrm{er} P_h^{2h} A^h + \mathrm{rg} P_{2h}^h = 2n-1.$$

Furthermore, any $U$ in $\mathcal{K}\mathrm{er} P_h^{2h} A^h \cap \mathcal{I}\mathrm{m} P_{2h}^h$ is equal to $P_{2h}^h w$, and $v_{2j} = 0$. Since $(P_{2h}^h w)_{2j} = w_j$, this proves that $w = 0$. Hence (2.3) is proved.

We now can prove in the same way, first that for $V$ in $\mathbb{R}^{n-1}$,

$$(A^h P_{2h}^h V)_{2j+1} = 0, \quad (A^h P_{2h}^h V)_{2j} = \frac{1}{2h^2}(-v_{j-1} + 2v_j - v_{j+1}) = 2(A^{2h} v)_j.$$

Then

$$(P_h^{2h} A^h P_{2h}^h V)_j = (A^{2h} v)_j.$$

■

**Lemma 2.2**

$$e^{h,1} = d^h + P_{2h}^h e^{2h},$$

*with*

$$d_{2j}^h = 0, \quad d_{2j+1}^h = \frac{h^2}{2}(A^h e^{h,1})_{2j+1}, \quad e_j^{2h} = e^{h,1})_{2j}$$

Proof By (2.3), we can expand $e^{h,1}$ as

$$e^{h,1} = d^h + P_{2h}^h e^{2h},$$

with $d^h \in Ker P_h^{2h} A^h$. By (2.2), $d_{2j}^h = 0$, and

$$e_{2j}^{h,1} = (P_{2h}^h e^{2h})_{2j} = e_j^{2h},$$

which determines the components of $e^{2h}$. Compute now the odd components,

$$e_{2j+1}^{h,1} = d_{2j+1}^h + (P_{2h}^h e^{2h})_{2j+1} = d_{2j+1}^h + \frac{1}{2}(e_j^{2h} + e_{j+1}^{2h}) = d_{2j+1}^h + \frac{1}{2}(e_{2j}^{h,1} + e_{2j+2}^h)$$

Therefore

$$d_{2j+1}^h = \frac{1}{2}(2e_{2j+1}^{h,1} - e_{2j}^{h,1} - e_{2j+2}^h) = \frac{h^2}{2}(A^h e^{h,1})_{2j+1}.$$

■

Apply the lemma to compute $e^{h,2}$.

$$P_{2h}^h (A^{2h})^{-1} P_h^{2h} A^h e^{h,1} = P_{2h}^h (A^{2h})^{-1} P_h^{2h} A^h (d^h + P_{2h}^h e^{2h}) = P_{2h}^h (A^{2h})^{-1} \underbrace{P_h^{2h} A^h P_{2h}^h}_{A^{2h}} e^{2h} = P_{2h}^h e^{2h}.$$

Therefore

$$e^{h,2} = e^{h,1} - P_{2h}^h e^{2h} = d^h,$$

which implies the elegant formula

$$e_{2j}^{h,2} = 0, \quad e_{2j+1}^{h,2} = \frac{h^2}{2}(A^h e^{h,1})_{2j+1} = \frac{h^2}{2} r_{2j+1}^{h,1}.$$

the even components have disappeared.

### 2.1.6 Postsmoothing

$$e^{h,3} = S^{N_2} e^{h,2}.$$

$$\boxed{e^{h,3} = S^{N_2} \Pi_o \frac{h^2}{2} A^h S^{N_1} e^h}$$

### 2.1.7 Spectral analysis

The smoothing matrix $S$ has eigenvalues $\lambda_k$, and eigenvectors $\Phi^{(k)}$. For relaxed Jacobi or the Gauss-Seidel algorithm, the eigenvalues are

$$\begin{aligned} \lambda_k^J(\omega) &= 1 - 2\omega \sin^2\left(\frac{k\pi h}{2}\right) && \text{for } 1 \le k \le 2n-1, \\ \lambda_k^{GS} &= \cos^2 k\pi h && \text{for } 1 \le k \le 2n-1, \end{aligned}$$

Figure 2.1 shows the eigenvalues as a function of $k$ for $n = 16$.

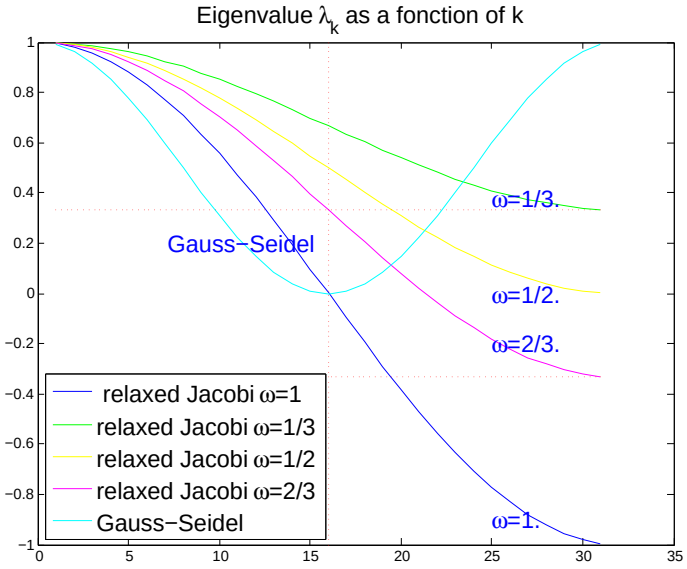



FIGURE 2.1 – Eigenvalues of the relaxed Jacobi iteration matrix as a function of $k$ for several values of $\omega$ together with Gauss-Seidel

* For small $k$, $\lambda_k^J(\omega) \sim 1 - \omega \frac{k^2\pi^2 h^2}{2}$.
* For $\omega = 2/3$, $n \le k \le 2n-1 \Rightarrow |\lambda_k^J(\omega)| \le \underbrace{1/3}_{\text{smoothing factor}}$
* For other modes. $|\lambda_k^J(\omega)| \in (1/3, 1 - \frac{4}{3}\sin^2(\frac{\pi h}{2}))$

When using Gauss-Seidel as a smoother, one can observe that the eigenvalues are small when $k \sim n : \lambda_k \le 1/2$ for $n/2 \le k \le 3n/2$..

For an initial error $e^h = \Phi^{(k)}$, the error and residual after $N_1$ iterations is

$$e^{h,1} = \lambda_k^{N_1} \Phi^{(k)}, \quad r^{h,1} = \mu_k \lambda_k^{N_1} \Phi^{(k)}.$$

From

$$e_{2j}^{h,2} = 0, \quad e_{2j+1}^{h,2} = \frac{h^2}{2} r_{2j+1}^{h,1}$$

we obtain

$$e^{h,2} = \frac{h^2}{2}\mu_k \lambda_k^{N_1} \Phi_{2j+1}^k.$$

If the same smoother is applied in postprocessing,

$$e^{h,3} = \lambda_k^{N_2} e^{h,2},$$

and finally,

$$e_{2j}^{h,3} = 0, \quad e_{2j+1}^{h,3} = \frac{h^2}{2}\mu_k \lambda_k^{N_1+N_2} \Phi_{2j+1}^k.$$

We can see now that even the low frequencies are damped. Choose relaxed Jacobi with $\omega = 2/3$. For $n \leq k \leq 2n-1$, we have, with $N = N_1 + N_2$,

$$|e_{2j+1}^{h,3}| \leq (\frac{2}{3})^N |\Phi_{2j+1}^k|,$$

and for $1 \leq k \leq n-1$,

$$|e_{2j+1}^{h,3}| \leq \sup_{x\in(0,1)} (x(1-\omega x)^N)|\Phi_{2j+1}^k| \leq \frac{1}{\omega(N+1)} \left(\frac{N}{N+1}\right)^N |\Phi_{2j+1}^k|$$

**For three iterations of the smoother (N=3), the low frequencies have been damped by a factor** 0.1582**, and the high frequencies by a factor 0.2963!!** The figures below show the result of one cycle of the above described algorithm, compared to three iterations of relaxed Jacobi, or Gauss-Seidel, for several inital guesses. $n = 10$.

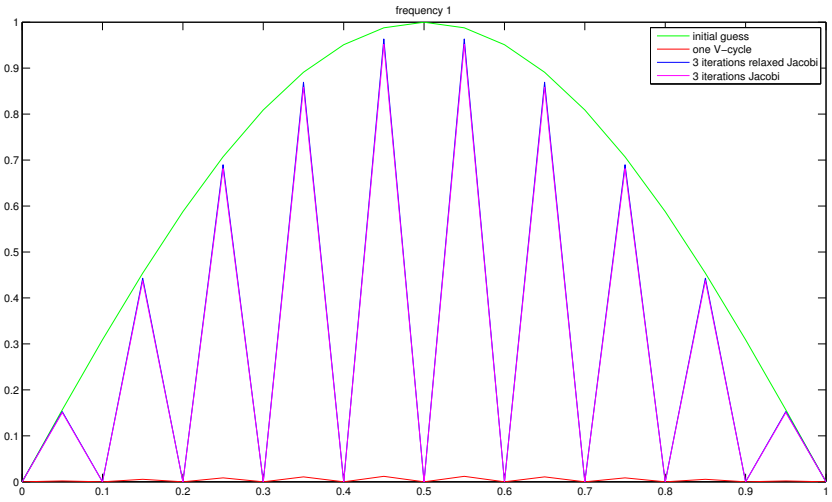



FIGURE 2.2 – Comparison of the iterative methods. Initial guess $\sin \pi x$

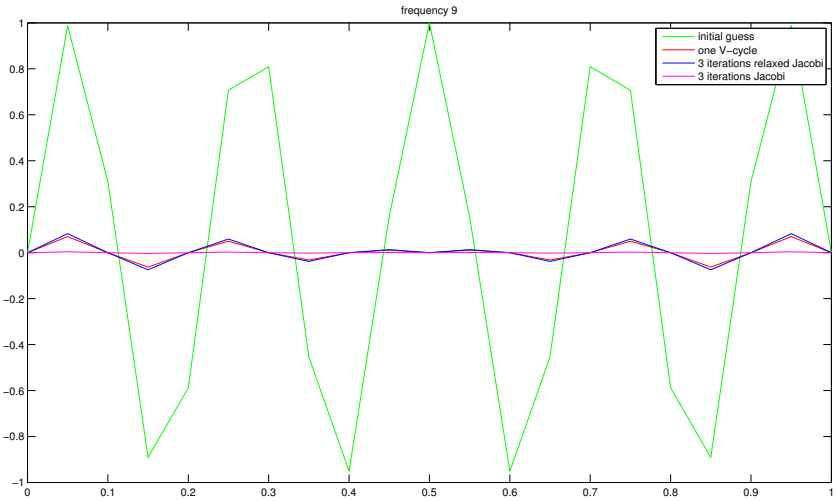



FIGURE 2.3 – Comparison of the iterative methods. Initial guess $\sin(n-1)\pi x$.

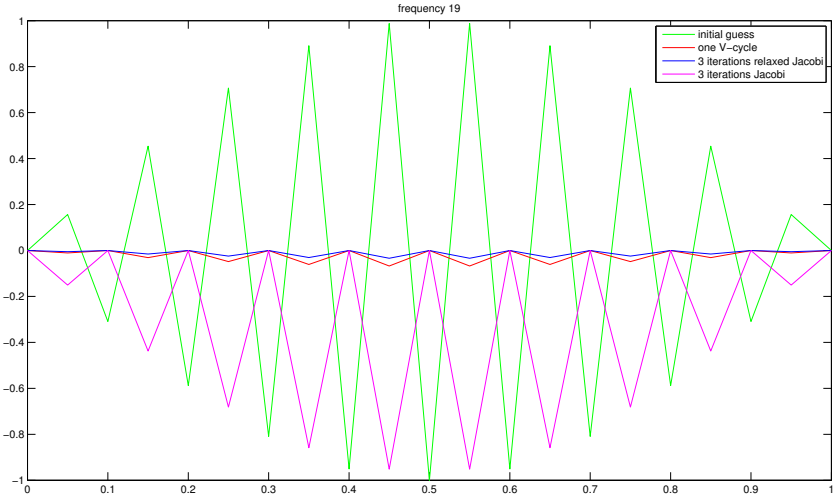
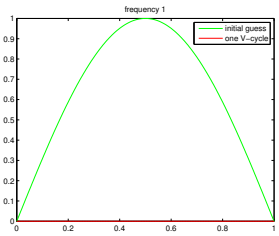
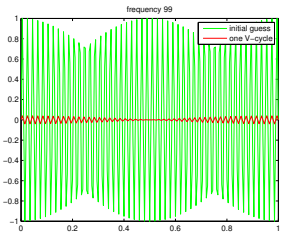


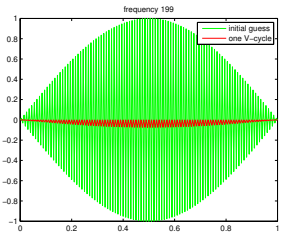

FIGURE 2.4 – Comparison of the iterative methods. Initial guess $\sin(2n-1)\pi x$.




Initial guess $\sin \pi x$




Initial guess $\sin(n-1)\pi x$




Initial guess $\sin(2n-1)\pi x$.

TABLE 2.1 – The effect of one V-cycle on one single mode for $n = 100$.

The $N_2$ last smoothing steps helps to reduce the high frequencies by a factor $(\frac{2}{3})^{N_2}$.

### 2.1.8 Number of elementary operations

| method | number of operations |
|---|---|
| Gauss elimination | $n^2$ |
| optimal overrelaxation | $n^{3/2}$ |
| preconditionned conjugate gradient | $n^{5/4}$ |
| FFT | $n \ln_2(n)$ |
| multigrid | $n$ |

TABLE 2.2 – Asymptotic order of the number of elementary operations as a function of the number of grid points in one dimension for the Laplace equation (sparse matrix)

## 2.2 The finite elements multigrid algorithm

Details on finite elements can be found in [4][6] and.[1].

We consider here an elliptic problem in $V = H_0^1(\Omega)$, where $\Omega$ is a convex polygone. If $\alpha_1 \leq a_{ij} \leq \alpha_2$ *a.e.* in $\Omega$, ,

$$a(u,v) = \sum_{i,j=1}^{2} \int_\Omega (a_{ij}(x)\nabla u(x)\nabla v(x) + a_0(x)u(x)v(x))\, dx$$

is an elliptic bilinear form. It therefore defines a norm, which is equivalent to the $H^1$ norme, that we call the energy norm

$$\|v\|_E = \sqrt{a(v,v)}$$

The variational problem is, to find $u \in V$ such that

$$\forall v \in V, a(u,v) = (f,v) \tag{2.6}$$

We know that there is a unique solution in $V$ which, furthermore, belongs to $H^2(\Omega)$.and $\|u\|_{H^2(\Omega)} \leq C\|f\|_{L^2(\Omega)}$.

### 2.2.1 Preliminaries

Let $\mathcal{T}_k$ be a sequence of triangulations of $\Omega$. $h_k$ is the longest measure of the side of the triangles in $\mathcal{T}_k$. $\mathcal{T}_k$ is obtaind from $\mathcal{T}_{k-1}$ by dividing each triangle into four triangles.

Let $(N^T, N^E, N)$ be the number of triangles outside the boundary of $\Omega$, edges and vertices respectively. There is a recursion relation :

$$N_{k+1}^T = 4N_k^T,\ N_{k+1} = N_k + N_k^E,\ N_{k+1}^E = 2N_k^E + 3N_k^T$$

which provides the total number of each, starting with the triangulation $\mathcal{T}_1$ in Figure 2.5 : $(N^T, N^E, N) = (N_1, N_1, 1)$.

$$N_{k+1}^T = 2^{2k}N_1,\ N_{k+1} = 2^{k-1}(2^k - 1)N_1,\ N_{k+1}^E = 2^{k-1}(2^{k+2} - 1)N_1$$

We have asymptotically

$$N_k \sim 2^{2k-1}N_1 \tag{2.7}$$

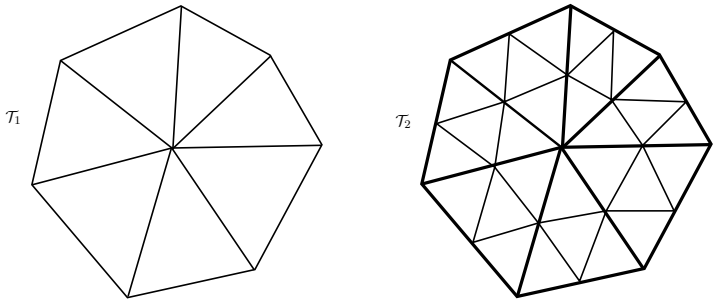



FIGURE 2.5 – Recursive triangulation

For each $k$, the diameter of the triangulation $h_k$ is the largest length of edge, therefore $h_{k+1} = h_k/2$. Then the triangulation is quasi-uniform (cf [1]), in the sense that there exists $\rho > 0$ such that

$$\inf_{T \in \mathcal{T}_k} \text{diam} B_T \geq \rho h_k$$

where $B_T$ is the largest ball contained in $T$. Its diameter is given by $\frac{4|T|}{length(T)}$ with $|T| := area(T) = \frac{1}{2}(AB)\dot{(}AC)\sin(\widehat{BAC})$, and $length(T)$ is the perimeter of $T$.

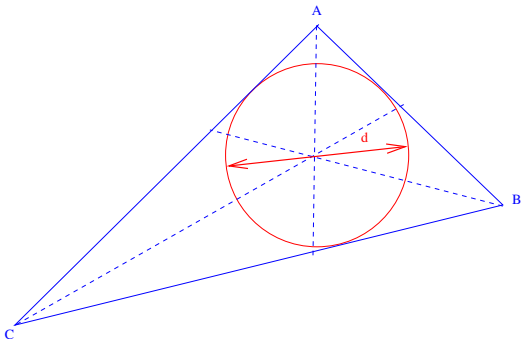



FIGURE 2.6 – triangle

It is easy to see that, after a refinement, the diameter is divided by 2, and so is $h$, therefore it suffices to define $\rho = \frac{1}{h_1} \inf_{T \in \mathcal{T}_1} \text{diam} B_T$.

$$V_k = \{v \in V \cap \mathcal{C}^0(\bar{\Omega}), \forall\, T \in \mathcal{T}_k, v|_T \in \mathbb{P}_1\}$$

This defines a sequence of finite-dimensional spaces, of dimension $N_k$, with $V_k \subset V_{k+1}$. We define the variational problem in $V_k$, to find $u_k \in V_k$ such that

$$\forall v \in V_k, a(u_k, v) = (f, v) \tag{2.8}$$

Classical finite element results assert that this problem has a unique solution, and the following error estimate holds :

$$\|u - u_k\|_{H^1(\Omega)} \leq C h_k \|u\|_{H^2(\Omega)}$$

We denote by $P_k$ the projection operator on $V_k$, defined for any $w$ in V by

$$\forall v \in V_k, a(P_k w, v) = a(w, v) \tag{2.9}$$

For $w$ in $V$, we introduce the solution $z$ of problem (2.6), and $z_h$ the solution of the discrete problem (2.8), both with data $w - P_h w$. Elementary algebra shows that

$$\|w - P_k w\|^2_{L^2(\Omega)} = a(w - P_k w, z - z_h)$$

It follows that there exists a constant independent of $h_k$ such that

$$\forall w \in V, \|w - P_k w\|_{L^2(\Omega)} \leq C h_k \|w - P_k w\|_{H^1(\Omega)} \tag{2.10}$$

We obtain the estimate on the error in $L^2(\Omega)$ by using the same argument (duality argument), replacing $w - P_k w$ by $u - u_k$.

$$\|u - u_k\|_{L^2(\Omega)} \leq C h_k \|u - u_k\|_{H^1(\Omega)} \leq C h_k^2 |u|_{H^2(\Omega)}$$

**Theorem 2.1 (Inverse estimate)**

$$\forall v \in V_k, \|v\|_{H^1} \leq \frac{C}{h_k} \|v\|_{L^2}$$

For a proof see [6], [1].

The goal of the multigrid method is to compute an approximate value $U_k$ of $u_k$ in $\mathcal{O}(N_k)$ operations, and such that

$$\|U_k - u_k\|_{H^s(\Omega)} \leq C h_k^{2-s} |u|_{H^2(\Omega)}$$

### 2.2.2 Discrete norm

Note globally $S_1, \cdots, S_{N_k}$ the vertices. Define a scalar product on $V_k$ by

$$(v, w)_k = h_k^2 \sum_{i=1}^{N_k} v(S_i) w(S_i) \tag{2.11}$$

**Theorem 2.2** *It is equivalent to the $L^2$ scalar product on $V_k$.*

Proof Use the exact integration formula in dimension 2 : denoting by $M_\alpha$ the mid-points of the edge in the triangle, we have for any $v \in \mathbb{P}_1$,

$$\|v\|^2_{L^2(T)} = \frac{|T|}{3} \sum_{\alpha=1}^{3} v^2(M_\alpha)$$

Now since $v$ is affine, the values at point $M_\alpha$ are the half-sum of values at points $S_\alpha$.

$$\sum_{\alpha=1}^{3} v^2(M_\alpha) = \frac{1}{4} \sum_{\alpha=1}^{3} (v(M_\beta) + v(M_\gamma))^2$$

But

$$(x+y)^2 + (y+z)^2 + (z+x)^2 = x^2 + y^2 + z^2 + (x+y+z)^2$$

therefore

$$\sum_{\alpha=1}^{3} (v(M_\alpha))^2 \leq \sum_{\alpha=1}^{3} (v(M_\beta) + v(M_\gamma))^2 \leq 4 \sum_{\alpha=1}^{3} (v(M_\alpha))^2,$$

$$\frac{|T|}{12} \sum_{\alpha=1}^{3} v^2(M_\alpha) \leq \|v\|^2_{L^2(T)} \leq \frac{|T|}{3} \sum_{\alpha=1}^{3} v^2(M_\alpha),$$

and the result follows by summing over all the triangles. ■

We define the operator $A_k$ by

$$\forall v, w \in V_k, (A_k v, w)_k = a(v, w) \tag{2.12}$$

and $f_k \in V_k$ by $(f_k, v) = (f, v)_k$ for all $v$ in $V_k$. Solve the discrete problem amounts to solving the $N_k$dimensional system of equations

$$A_k u_k = f_k$$

The operator $A_k$ is obviously symmetric positive definite wih respect to $(\cdot, \cdot)_k$. We define mesh-dependent norms as

$$|||v|||_{s,k} = \sqrt{(A_k^s v, v)_k}$$

Theorem 2.2 asserts that $|||\cdot|||_{0,k}$ is equivalent to the $L^2$ norm in $V_k$. As to the norm for $s = 1$, it coincides with the energy norm thanks to (2.12). We now estimate the spectral radius of $A_k$ :

**Lemma 2.3**

$$\rho(A_k) \leq \frac{C}{h_k^2}$$

Proof Let $\lambda$ be a (positive) eigenvalue, with eigenvector $v$.

$$a(v, v) = \lambda |||v|||_{0,k}^2$$

$$\lambda \leq b \frac{\|v\|_{H^1}^2}{\|v\|_{L^2}^2} \leq \frac{C^2}{h_k^2}$$

by the inverse inequality in Theorem 2.1. ■

### 2.2.3 Definition of the multigrid algorithm

In order to pass from one grid to the finer or coarser grid, we need to define transfer operators, which are mutually dual

$$\begin{gathered} \mathcal{I}_k \colon V_{k-1} \to V_k, \\ \forall v \in V_{k-1}, \mathcal{I}_k v \colon = v; \\ \\ \mathcal{R}_k \colon V_k \to V_{k-1}, \\ \forall v \in V_k, (\mathcal{R}_k v, w)_{k-1} := (\mathcal{I}_k w, v)_k = (w, v)_k; \end{gathered} \tag{2.13}$$

For any $k$ and initial guess $z_0 \in V_k$, and right-hand side $g \in V_k$, the $k-$th level iteration is an approximate solution $MG(A^k, z_0, g)$ in $V_k$ of

$$A_k z = g \tag{2.14}$$

defined as follows :

For k=1, there is only one grid to deal with, and $MG(A^1, z_0, g)$ is obtained by a direct method.

For $k > 1$, $z$ is obtained in three steps

**1 Presmoothing on the fine grid** : $m_1$ steps of a gradient algorithm

$$z_{l+1} = z_l - \mu_k (A_k z_l - g), \ 0 \leq l \leq m_1 - 1$$

**2 Error correction on the coarse grid** The residual $g - A_k z_{m_1}$ is transferred on the grid $\mathcal{T}_{k-1}$,

$$G = \mathcal{R}_k (g - A_k z_{m_1}). \tag{2.15}$$

Now we compute an approximate solution of the residual equation

$$A_{k-1}q = G \tag{2.16}$$

by performing $p$ steps of the multigrid algorithm on $\mathcal{T}_{k-1}$ :

$$q_0 = 0, q_l = MG(A^{k-1}, q_{l-1}, G),\ 1 \leq l \leq p$$

Then we project on the fine grid again

$$z_{m_1+1} := z_{m_1} + \mathcal{I}_k q_p$$

**3 Smoothing on the fine grid** we perform again a few steps of the gradient algorithm

$$z_{l+1} = z_l - \mu_k(A_k z_l - g),\ m_1 + 1 \leq l \leq m_1 + m_2$$

$$MG(k, z_0, g) = z_{m_1+m_2}$$

$m_1$ and $m_2$ are positive integers, p=1 is a V-cycle, p=2 is a W-cycle. Usually one uses $m_1 = 3$ and $m_2 = 1$.

The full-multigrid algorithm to solve $A_k f = f_k$ is therefore

$$\begin{array}{l} U_1 = A_1^{-1} f_1, \\ U_k : = MG(A_k, \mathcal{I}_k U_{k-1}, f_k) \end{array}$$

### 2.2.4 Convergence property of the multigrid algorithm

We suppose here for simplicity that there is no postsmoothing, *i.e.* $m_2 = 0$, we note $m := m_1$, and we consider a W-cycle, *i.e.* $p = 2$.

**Theorem 2.3** *If the relaxation coefficient $\mu_k$ satisfies*

$$\rho_k \leq \frac{1}{\mu_k} \leq \frac{C}{h_k^2} \tag{2.17}$$

*the one-sided W-cycle is convergent, and the following estimate holds :*

$$\|U_k - u_k\|_E \leq C h_k |u|_{H^2(\Omega)}$$

Proof The total error is

$$u_k - U_k = u_k - MG(A_k, \mathcal{I}_k U_{k-1}, f_k)$$

First, for $z$ in $V_k$ solution of (2.14), we must estimate $z - MG(A^k, z_0, g)$. It is equal to $z_{m_1} + \mathcal{I}_k q_2$. We rewrite the error as :

$$z - (z_{m_1} + \mathcal{I}_k q_2) = z - (z_{m_1} + \mathcal{I}_k q) + \mathcal{I}_k(q - q_2).$$

We start with the estimate of the first part :

**Lemma 2.4** *Let $q \in V_{k-1}$ the solution of (2.16), then $q = P_{k-1}(z - z_m)$.*

Proof We should show that for any $v \in V_{k-1}$,

$$a(q, v) = a(z - z_m, v)$$

We have successively

$$\begin{aligned} a(q, v) &= (A_{k-1}q, v)_{k-1} \text{ by definition of } A_{k-1} \text{ in (2.12)} \\ &= (G, v)_{k-1} \text{ by definition of } q \text{ in (2.16)} \\ &= (\mathcal{R}_k(g - A_k z_m), v)_{k-1} \text{by definition of } G \text{ in (2.15)} \\ &= (g - A_k z_{m_1}, v)_k \text{ by definition of } \mathcal{R}_k \text{ in (2.13)} \\ &= (A_k(z - z_{m_1}), v)_k \text{ by definition of } z \text{ in (2.14)} \\ &= a(z - z_{m_1}, v) \text{ by definition of } A_k \text{ in (2.12)} \end{aligned}$$

■

We can now write

$$z - (z_{m_1} + q) = z - z_{m_1} - P_{k-1}(z - z_{m_1}) = (I - P_{k-1})(z - z_{m_1}).$$

Since

$$z - z_m = (I - \mu_k A_k)^m (z - z_0)$$

so

$$z - (z_m + \mathcal{I}_k q) = (I - P_{k-1})(I - \mu_k A_k)^m (z - z_0). \tag{2.18}$$

We have to estimate the projection first :

**Lemma 2.5**

$$\forall v \in V_k, \|v - P_{k-1}v\|_E \leq C h_k \|A_k v\|_k$$

**Proof**

$$\begin{aligned}
\|v - P_{k-1}v\|_E^2 &= a(v - P_{k-1}v, v) \text{ by the definition of } P_{k-1}, \\
&= (v - \mathcal{I}_k P_{k-1} v, A_k v)_k, \text{ by definition of } A_k \text{ in (2.12)} \\
&\leq \|v - \mathcal{I}_k P_{k-1} v\|_k \|A_k v\|_k, \\
&\leq C \|v - P_{k-1}v\|_{L^2(\Omega)} \|A_k v\|_k \text{ by the equivalence of norms,} \\
&\leq C \|v - P_{k-1}v\|_{L^2(\Omega)} \|A_k v\|_k \\
&\leq C h_k \|v - P_{k-1}v\|_{H^1(\Omega)} \|A_k v\|_k \text{ by (2.10)} \\
&\leq C h_k \|v - P_{k-1}v\|_E \|A_k v\|_k \text{ by the equivalence of norms.}
\end{aligned}$$

■

We now study the relaxation operator

$$\mathcal{S}_k = I - \mu_k A_k$$

**Lemma 2.6** *For any $v$ in $V_k$,*

$$\|\mathcal{S}_k v\|_E \leq \|v\|_E$$

*Furthermore, there exists $C > 0$ such that, for any $k$, for any $v$ in $V_k$,*

$$\|A_k \mathcal{S}_k^m v\|_k \leq C h_k^{-1} m^{-1/2} \|v\|_{H^1(\Omega)}.$$

**Proof** we expand $v$ on the orthonormal eigenfunctions (with respect to the scalar product $()_k$) of the positive definite operator $A_k$, called $(\psi_1, \cdots, \psi_{N_k})$ associated to $(\lambda_1, \cdots, \lambda_{N_k})$ , $v = \sum_{j=1}^{N_k} v_j \psi_j$.

$$a(v, v) = (A_k v, v)_k = (\sum_{j=1}^{N_k} \lambda_j v_j \psi_j, \sum_{j=1}^{N_k} v_j \psi_j)_k = \sum_{j=1}^{N_k} \lambda_j v_j^2$$

$$\mathcal{S}_k v = \sum_{j=1}^{N_k} (1 - \mu_k \lambda_j) v_j \psi_j$$

$$a(\mathcal{S}_k v, \mathcal{S}_k v) = \sum_{j=1}^{N_k} \lambda_j (1 - \mu_k \lambda_j)^2 v_j^2$$

by the assumptions on $\mu_k$, we have $0 \leq \mu_k \lambda_j \leq 1$, and

$$a(\mathcal{S}_k v, \mathcal{S}_k v) \leq a(v, v)$$

$$\begin{aligned}\|A_k\mathcal{S}_k^m v\|_k &= \sum_{j=1}^{N_k} \lambda_j(1-\mu_k\lambda_j)^{2m} v_j^2 \\ &\leq \frac{1}{\mu_k} \sup_{x\in(0,1)} (x(1-x)^{2m}) \sum_{j=1}^{N_k} v_j^2 \\ &\leq \frac{1}{\mu_k}\frac{1}{2m}\|v\|_k^2 \\ &\leq C\frac{1}{mh_k^2}\|v\|_k^2 \leq C\frac{1}{mh_k^2}\|v\|_{L^2(\Omega)}^2 \leq C\frac{1}{mh_k^2}\|v\|_{H^1(\Omega)}^2.\end{aligned}$$

We return to the error in (2.18)

$$\begin{aligned}\|z-(z_m+\mathcal{I}_k q)\|_{H^1(\Omega)} &\leq Ch_k\|A_k\mathcal{S}_k^m(z-z_0)\|_k \\ &\leq \frac{C}{\sqrt{m}}\|z-z_0\|_{H^1(\Omega)}\end{aligned}$$

■

**Lemma 2.7** *For any $\gamma$, $0<\gamma<1$, we can choose $m$ such that*

$$\forall k \geq 1, \|z - MG(A^k, z_0, g)\|_E \leq \gamma\|z-z_0\|_E$$

The convergence rate in W-cycle is **independent of the mesh size** $h_k$

Proof The proof goes by recursion.

For $k=1$, $z = MG(A^k, z_0, g)$.

Suppose for any $j<k$, $\|z-MG(A^j,z_0,g)\|_E \leq \gamma\|z-z_0\|_E$ with $A^j z = g$. we now have $z - MG(A^k,z_0,g) = z-(z_m+\mathcal{I}_k q)+\mathcal{I}_k(q-q_2)$. By the recursion relation

$$\begin{aligned}\|q-q_2\|_E \leq \gamma^2\|q\|_E &\leq \gamma^2\|z-z_m\|_E \\ &\leq \gamma^2\|\mathcal{S}^m(z-z_0)\|_E \\ &\leq \gamma^2\|z-z_0\|_E\end{aligned}$$

and

$$\|z-MG(k,z_0,g)\|_E \leq (\frac{C}{\sqrt{m}}+\gamma^2)\|z-z_0\|_E$$

Choosing $m > (\frac{C}{\gamma-\gamma^2})^2$, we get the result. ■

We can now conclude the proof of the theorem :

$$\begin{aligned}\|u_k - U_k\|_E &\leq \gamma\|u_k - U_{k-1}\|_E \\ &\leq \gamma(\|u_k-u_{k-1}\|_E + \|u_{k-1}-U_{k-1}\|_E) \\ &\leq \gamma(C(h_k+h_{k-1})|u|_{H^2(\Omega)} + \|u_{k-1}-U_{k-1}\|_E) \\ &\leq \gamma(3Ch_k|u|_{H^2(\Omega)} + \|u_{k-1}-U_{k-1}\|_E)\end{aligned}$$

Since the error at step 1 vanishes, we see by recursion that

$$\|u_k - U_k\|_E \leq 3C\gamma|u|_{H^2(\Omega)}\sum_{j=2}^{k-2}\gamma^j h_{k-j}$$

Now we can choose $\gamma < 1/2$, and we obtain

$$\|u_k-U_k\|_E \leq h_k\frac{3C\gamma}{1-2\gamma}|u|_{H^2(\Omega)}$$

which concludes the proof of the theorem. ■

**Proposition 2.1** *For a number of cycles $p<4$, the work involved in the full multigrid method is $\mathcal{O}(N_k)$.*

Proof

* We call $d$ the maximum number of neighbours of a vertex ($d \sim 15$ for a general construction). Then the matrix $A^k$ has at most $d$ non zero elements in each line. The average number of elementary operations $(+, -, \times, :)$ to make the product of $A^k$ by a vector is $2d \times N_k$. The number of operations involved in one step of the gradient is $(2d+3) \times N_k$. All smoothings therefore require

$$(2d+3)(m_1+m_2) \times N_k \text{ elementary operations.}$$

* As for the projection of the residual, $G$ is defined by

$$G(S_i^{k-1}) = \frac{1}{4} \sum_{\text{neighbours of } S_i \text{ in } \mathcal{T}_k} r_m(S_j^k)$$

where $S_i^k$ are the vertices in $\mathcal{T}_k$. Therefore the number of operations in the projection step is also

$$d \times N_k \text{ elementary operations.}$$

Let us call $n_k$ the number of operations needed to run one cycle of the multigrid algorithm. We have the recursion relation

$$n_k = (2d+3) \times N_k + p n_{k-1}$$

and $n_k$ can be estimated asymptotically

$$n_k \sim p^{k-1} n_1 + (2d+3) N_k \sum_{j=1} k - 2 \left(\frac{p}{4}\right)^j$$

and if $p < 4$, we can write

$$n_k \sim (\frac{n_1}{N_1} + \frac{4\alpha}{3}) N_k$$

* For the full multigrid, the number of operations $\tilde{n}_k$ can also be estimated recursively by

$$\tilde{n}_k = n_k + \tilde{n}_{k-1}$$

which we solve as

$$\tilde{n}_k \sim \tilde{n}_1 + \sum_{j=2}^{k} n_j,$$

which altogether produces the result in the Proposition.

■

## 2.3 Multigrid Preconditioner

# Chapitre 3

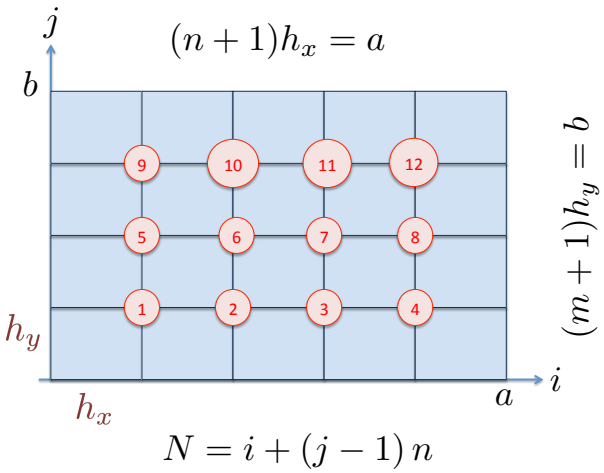
# Fast methods using Fast Fourier Transform

## Contents


3.1 Presentation of the method . . . . . 53
3.2 Discrete and Fast Fourier Transform . . . . . 57
3.3 The algorithm . . . . . 61


## 3.1 Presentation of the method

We'll work with the finite difference approximation of the Laplace equation in dimension 2.




$$A = \begin{pmatrix} B & C & 0 \\ C & B & C \\ 0 & C & B \end{pmatrix}$$

FIGURE 3.1 – Pavage de $[0, a] \times [0, b]$, $n = 4$ and $m = 3$

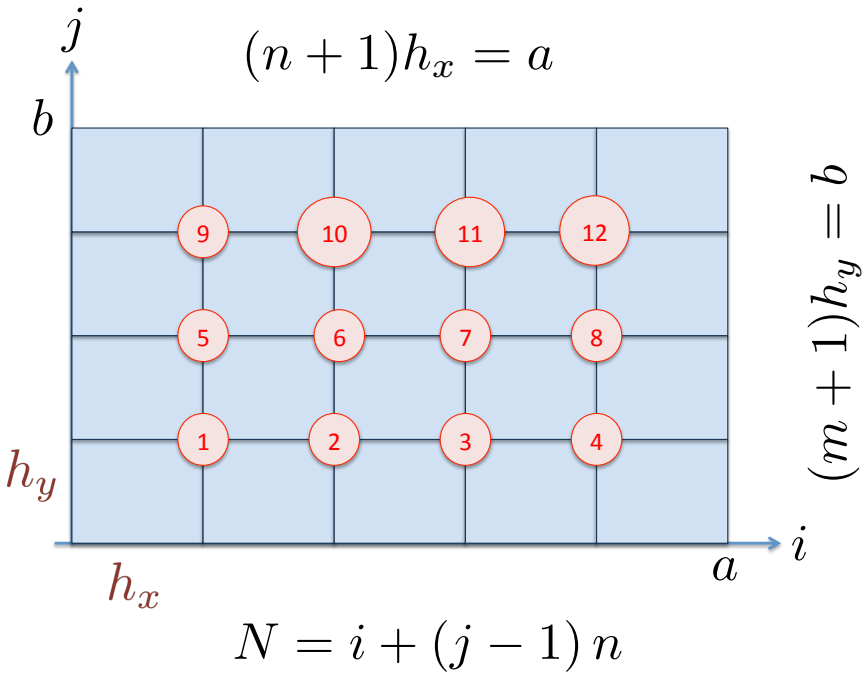



FIGURE 3.2 – Pavage de $[0, a] \times [0, b]$, $n = 4$ and $m = 3$

$$\left(\begin{array}{cccc|cccc|cccc}
\frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & 0 & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & 0 & 0 \\
\hline
-\frac{1}{h_y^2} & 0 & 0 & 0 & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & 0 \\
0 & -\frac{1}{h_y^2} & 0 & 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 \\
0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 & 0 & -\frac{1}{h_y^2} & 0 \\
0 & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & 0 & 0 & 0 & -\frac{1}{h_y^2} \\
\hline
0 & 0 & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & 0 & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{h_y^2} & 0 & 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2}
\end{array}\right)$$

$$A = \begin{pmatrix} B & C & 0 \\ C & B & C \\ 0 & C & B \end{pmatrix}$$

$$B = \begin{pmatrix} \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 & 0 \\ -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} & 0 \\ 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{1}{h_x^2} \\ 0 & 0 & -\frac{1}{h_x^2} & \frac{2}{h_x^2}+\frac{2}{h_y^2} \end{pmatrix} = A_1(h_x)+\frac{2}{h_y^2}\, I_n$$

$$C = -\begin{pmatrix} \frac{1}{h_y^2} & 0 & 0 & 0 \\ 0 & \frac{1}{h_y^2} & 0 & 0 \\ 0 & 0 & \frac{1}{h_y^2} & 0 \\ 0 & 0 & 0 & \frac{1}{h_y^2} \end{pmatrix} = -\frac{1}{h_y^2}\, I_n.$$

Consider now the general problem $Ax = b$, where $A$ is a $nm \times nm$ symmetric matrix $A$, block tridiagonal in the form

$$A = A(B,C) = \begin{pmatrix} B & C & & 0 \\ C & B & C & \\ & \ddots & \ddots & \ddots \\ & & C & B & C \\ & 0 & & C & B \end{pmatrix}. \tag{3.1}$$

Each block is a $n \times n$ matrix. The vectors $\boldsymbol{b}$ and $\boldsymbol{x}$ can be split by block of size $n$ as well, $x^j$ is the sought solution on the ligne $j$.

$$\boldsymbol{b} = \begin{pmatrix} \boldsymbol{b}^1 \\ \vdots \\ \boldsymbol{b}^m \end{pmatrix}, \quad \boldsymbol{x} = \begin{pmatrix} \boldsymbol{x}^1 \\ \vdots \\ \boldsymbol{x}^m \end{pmatrix}$$

The system can be rewritten as

$$\begin{pmatrix} B & C & & 0 \\ C & B & C & \\ & \ddots & \ddots & \ddots \\ & & C & B & C \\ & 0 & & C & B \end{pmatrix} \begin{pmatrix} \boldsymbol{x}^1 \\ \boldsymbol{x}^2 \\ \vdots \\ \boldsymbol{x}^{m-1} \\ \boldsymbol{x}^m \end{pmatrix} = \begin{pmatrix} \boldsymbol{b}^1 \\ \boldsymbol{b}^2 \\ \vdots \\ \boldsymbol{b}^{m-1} \\ \boldsymbol{b}^m \end{pmatrix}$$

which is a system of $m$ systems of dimension $n$ :

$$\begin{aligned} B\boldsymbol{x}^1 + C\boldsymbol{x}^2 &= \boldsymbol{b}^1 \\ \ddots & \\ C\boldsymbol{x}^{i-1} + B\boldsymbol{x}^i + C\boldsymbol{x}^{i+1} &= \boldsymbol{b}^i \\ \ddots & \\ C\boldsymbol{x}^{m-1} + B\boldsymbol{x}^m &= \boldsymbol{b}^m \end{aligned}$$

Suppose $B$ and $C$ are symmetric, and diagonalise in the same orthonormal basis $(\boldsymbol{q}^1, \ldots, \boldsymbol{q}^n)$. This is the case for our previous example. Denote by $Q$ the corresponding orthogonal matrix $Q = [\boldsymbol{q}^1, \ldots, \boldsymbol{q}^n]$. There exist two diagonal matrices $D^1$ and $D^2$ such that

$$B = QD^1Q^T, \quad C = QD^2Q^T.$$

Take for example the first equation

$$B\boldsymbol{x}^1 + C\boldsymbol{x}^2 = \boldsymbol{b}^1$$

and replace $B$ and $C$ :

$$QD^1Q^T\boldsymbol{x}^1 + QD^2Q^T\boldsymbol{x}^2 = \boldsymbol{b}^1$$

Multiply by $Q^T$ :

$$D^1Q^T\boldsymbol{x}^1 + D^2Q^T\boldsymbol{x}^2 = Q^T\boldsymbol{b}^1$$

Denote by $(\boldsymbol{c}^i, \boldsymbol{y}^i)$ the coordinates of $(\boldsymbol{b}^i, \boldsymbol{x}^i)$ in the new basis :

$$Q^T\boldsymbol{b}^i = \boldsymbol{c}^i, \quad Q^T\boldsymbol{x}^i = \boldsymbol{y}^i, \quad 1 \leq i \leq m.$$

Then the problem takes the form

$$\begin{aligned} D^1\boldsymbol{y}^1 + D^2\boldsymbol{y}^2 &= \boldsymbol{c}^1 \\ \ddots & \\ D^2\boldsymbol{y}^{i-1} + D^1\boldsymbol{y}^i + D^2\boldsymbol{y}^{i+1} &= \boldsymbol{c}^i \\ \ddots & \\ D^2\boldsymbol{y}^{m-1} + D^1\boldsymbol{y}^m &= \boldsymbol{c}^m \end{aligned}$$

These are all diagonal systems. Take the component number $j$ in each block of the previous system, for $1 \leq j \leq n$ :

$$\begin{aligned} D^1_j y^1_j + D^2_j y^2_j &= c^1_j \\ \ddots & = \\ D^2_j y^{i-1}_j + D^1_j y^i_j + D^2_j y^{i+1}_j &= c^i_j \\ \ddots & \\ D^2_j y^{m-1}_j + D^1_j y^m_j &= c^m_j \end{aligned}$$

which is written in matrix form as

$$\begin{pmatrix} D^1_j & D^2_j & & 0 & \\ D^2_j & D^1_j & D^2_j & & \\ & \ddots & \ddots & \ddots & \\ & & D^2_j & D^1_j & D^2_j \\ & 0 & & D^2_j & D^1_j \end{pmatrix} \begin{pmatrix} y^1_j \\ y^2_j \\ \vdots \\ y^{m-1}_j \\ y^m_j \end{pmatrix} = \begin{pmatrix} c^1_j \\ c^2_j \\ \vdots \\ c^{m-1}_j \\ c^m_j \end{pmatrix}$$

For each $j$, $1 \le j \le n$, define the tridiagonal $m \times m$ matrix

$$T_j = \begin{pmatrix} D_j^1 & D_j^2 & & 0 & \\ D_j^2 & D_j^1 & D_j^2 & & \\ & \ddots & \ddots & \ddots & \\ & & D_j^2 & D_j^1 & D_j^2 \\ & 0 & & D_j^2 & D_j^1 \end{pmatrix}$$

and 2 vectors in $\mathbb{R}^m$

$$\boldsymbol{d}^j = \begin{pmatrix} c_j^1 \\ \vdots \\ c_j^m \end{pmatrix}, \quad \boldsymbol{z}^j = \begin{pmatrix} y_j^1 \\ \vdots \\ y_j^m \end{pmatrix}$$

We have now $n$ tridiagonal systems of size $m$,

$$T_j \boldsymbol{z}^j = \boldsymbol{d}^j, \quad 1 \le j \le n.$$

which can be solved in parallel with a $LU$ decomposition for instance. For the 2D Laplace equation with equidistant grid, the computation of the $c^j$ and the reconstruction of $x$ can be done by Fast Fourier transform.

We have to compute for each $j$, $\boldsymbol{x}^j = Q\boldsymbol{y}^j$. The matrice $C$ is $-\dfrac{1}{h_y^2} I_n$, the matrix $B$ is $A_1(h_x) + \frac{2}{h_y^2} I_n$. The eigenvalues of $B$ are those of $A_1 + \frac{2}{h_y^2}$, which are $\frac{2}{h_y^2} + \frac{4}{h_x^2} \sin^2 \frac{k\pi h_x}{2}$, the eigenvectors of $B$ and $C$ are those of $A_1$, given by (after orthonormalisation)

$$\Phi_j^{(k)} = \sqrt{\frac{2}{n+1}} \sin \frac{jk\pi}{n+1}, \quad 1 \le j \le n,$$

Define the matrix $Q$ as the matrix of eigenvectors

$$Q = [\boldsymbol{\Phi}^{(1)}, \cdots, \boldsymbol{\Phi}^{(n)}].$$

By

$$Q\boldsymbol{v} = \sum_{k=1}^{n} v_k \boldsymbol{\Phi}^{(k)},$$

we obtain

$$(Q\boldsymbol{v})_j = (Q^T \boldsymbol{v})_j = \sqrt{\frac{2}{n+1}} \sum_{k=1}^{n} v_k \sin \frac{kj\pi}{n+1}.$$

Note that the sum can be extended to $k = 0$ and $k = n+1$ since the sinus vanishes.

$$(Q\boldsymbol{v})_j = (Q^T \boldsymbol{v})_j = \sqrt{\frac{2}{n+1}} \sum_{k=1}^{n+1} v_k \sin \frac{kj\pi}{n+1}. \tag{3.2}$$

The next section is occupied with the FFT, we'll come back to the algorithm later.

## 3.2 Discrete and Fast Fourier Transform

Let $n' = n + 1$. The Discrete Fourier Transform of length $n'$ is defined by

$$w_j = \sum_{k=1}^{n'} v_k \, e^{-2i \frac{kj\pi}{n'}}, \quad j = 1, \cdots, n'.$$

Define $r = e^{2i\frac{\pi}{n'}}$ the basic root of unity, then we rewrite the formula above as

$$w_j = \sum_{k=1}^{n'} v_k \, r^{-kj}, \quad j = 1, \cdots, n'. \tag{3.3}$$

**Lemma 3.1 (Inverse DFT)** *If $w = (w_j)_{1\leq j\leq n'}$ is the discrete Fourier transform of $v = (v_j)_{1\leq j\leq n'}$ from (3.3), then the inverse discrete Fourier transform is given by*

$$v_j = \frac{1}{n'} \sum_{k=1}^{n'} w_k \, r^{kj}, \quad j = 1, \cdots, n'. \tag{3.4}$$

Proof Just replace

$$\sum_{k=1}^{n'} \left( \frac{1}{n'} \sum_{p=1}^{n'} w_p \, r^{kp} \right) r^{-kj} \quad = \quad \frac{1}{n'} \sum_{p=1}^{n'} w_p \sum_{k=1}^{n'} r^{k(p-j)}$$

Since $z = r^{p-j}$ is a $n'-$ root of unity,

$$\begin{cases} \text{for } z \neq 1, & \sum_{k=1}^{n'} z^k = 0, \\ \text{for } z = 1, & \sum_{k=1}^{n'} z^k = n'. \end{cases}$$

Therefore

$$\frac{1}{n'} \sum_{p=1}^{n'} w_p \sum_{k=1}^{n'} r^{k(p-j)} = w_j$$

and the lemma is proven. ■

We now suppose that $n' = 2p$. We need to specify more $r$, that we call $r_{n'}$. Note for further use that $r_{n'}^{n'} = 1$ and $r_{n'}^{p} = -1$. Split the sum above into even $(k = 2\ell, \ell = 1 : p)$ and odd terms $(k = 2\ell - 1, \ell = 1 : p)$. For $j = 1, \cdots, 2p$,

$$\begin{aligned} w_j &= \sum_{k=1}^{n'} v_k \, r_{n'}^{-kj} \\ w_j &= \sum_{\ell=1}^{p} v_{2\ell} \, r_{n'}^{-2\ell j} + \sum_{\ell=1}^{p} v_{2\ell-1} \, r_{n'}^{-(2\ell-1)j} \\ &= \sum_{\ell=1}^{p} v_{2\ell} \, r_{n'}^{-2\ell j} + r^j \sum_{\ell=1}^{p} v_{2\ell-1} \, r_{n'}^{-2\ell j}. \end{aligned}$$

Defining for $j = 1, \cdots, 2p$,

$$u_j = \sum_{\ell=1}^{p} v_{2\ell} \, r_{n'}^{-2\ell j}, \quad t_j = \sum_{\ell=1}^{p} v_{2\ell-1} \, r_{n'}^{-2\ell j}.$$

Then

$$w_j = u_j + r_{n'}^j t_j.$$

We verify that for each $j$, $u_{j+p} = u_j$ and $t_{j+p} = t_j$ :

$$u_{j+p} = \sum_{\ell=1}^{p} v_{2\ell} \, r_{n'}^{-2\ell(j+p)} = r_{n'}^{-2\ell p} u_j = u_j.$$

This implies that we only need to compute $(u_j, t_j)$ for $1 \leq j \leq p$. Furthermore

$$w_{j+p} = u_{j+p} + r_{n'}^{j+p} t_{j+p} = u_j + r_{n'}^j r_{n'}^p t_j = u_j - r_{n'}^j t_j.$$

To compute $u_j$ and $t_j$ note that

$$\sum_{\ell=1}^{p} v_{2\ell}\, r_{n'}^{-2\ell j} = \sum_{\ell=1}^{p} v_{2\ell}\, (r_{n'}^2)^{-\ell j}$$

But $r_{n'}^2 = (e^{-\frac{2i\pi}{2p}})^2 = e^{-\frac{2i\pi}{p}} : r_{n'}^2 = r_p$. Therefore

$$u_j = \sum_{\ell=1}^{p} v_{2\ell}\, r_p^{-\ell j}, \quad t_j = \sum_{\ell=1}^{p} v_{2\ell-1}\, r_p^{-\ell j}.$$

The sums above are similar sums as that defining $w_j$, but with $p = n'/2$. This is the starting point for a dyadic computation of the $w_j$ : the Fast Fourier Transform.

To obtain $\{w_j\}_{1\leq j\leq 2p}$ from $\{v_j\}_{1\leq j\leq 2p}$, do

Compute $r_{n'}^j$ $\qquad j = 1, \cdots, p$

Compute $u_j = \sum_{\ell=1}^{p} v_{2\ell}\, r_p^{-\ell j}, \quad t_j = \sum_{\ell=1}^{p} v_{2\ell-1}\, r_p^{-\ell j}$ $\qquad j = 1, \cdots, p$

Compute $w_j = u_j + r_{n'}^j t_j, \quad w_{j+p} = u_j - r_{n'}^j t_j$ $\qquad j = 1, \cdots, p.$

$$r = e^{2i\frac{\pi}{n'}}, w_j = \sum_{k=1}^{n'} v_k\, r^{-kj}, \quad j = 1, \cdots, n'.$$

$n' = 2$, $r = -1$, initialization $w_1 = -v_1 + v_2, \quad w_2 = v_1 + v_2$.

```
function w=myFFT(v)
% MYFFT fast Fourier transform
% w=myFFT(v); computes recursively the Fourier tranform of
% the vector v whose length must be a power of 2.
n=length(v);
if n==2,
        w=[-v(1)+v(2);v(1)+v(2)];
else
        rp=exp(2i*pi/n*(1:n/2)');
        t=myFFT(v(1:2:n-1));
        u=myFFT(v(2:2:n));
        w=[u+rp.*t; u-rp.*t];
end;
```

$$r = e^{2i\frac{\pi}{n'}}, w_j = \sum_{k=1}^{n'} v_k\, r^{-kj}, \quad j = 1, \cdots, n'.$$

$n' = 2$, $r = -1$, initialization $w_1 = -v_1 + v_2, \quad w_2 = v_1 + v_2$.

```
function w=myFFT(v)
% MYFFT fast Fourier transform
% w=myFFT(v); computes recursively the Fourier tranform of
% the vector v whose length must be a power of 2.
n=length(v);
if n==2,
        w=[-v(1)+v(2);v(1)+v(2)];
else
        rp=exp(2i*pi/n*(1:n/2)');
        t=myFFT(v(1:2:n-1));
        u=myFFT(v(2:2:n));
        w=[u+rp.*t; u-rp.*t];
end;
```

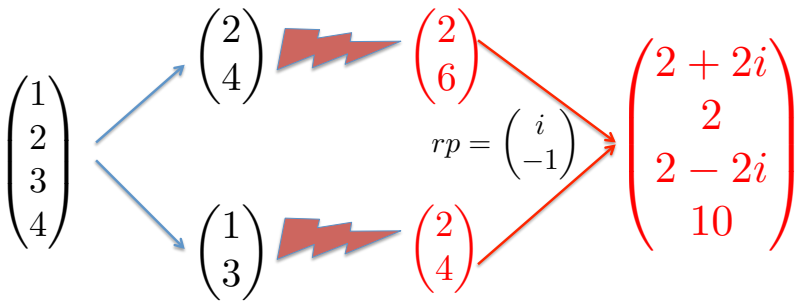



FIGURE 3.3 – FFT for $n' = 4$

It is easy to count the number of operations in the algorithm to be $\mathcal{O}(n \log_2(n))$, which is much better than *blockLU*.

## 3.3 The algorithm

We now show how to obtain the computation of $Qv$ in (3.2) with FFT.

$$
\begin{array}{ll}
\boldsymbol{v} \in \mathbb{R}^n, \ n' = n+1 \text{ EVEN} & \\
Q\boldsymbol{v} = \sqrt{\frac{2}{n+1}}\ \boldsymbol{z} \in \mathbb{R}^n, & z_j = \sum_{k=1}^{n} v_k \sin\frac{kj\pi}{n'} \quad 1 \le j \le n, \\
\tilde{\boldsymbol{v}} = [v;0] \in \mathbb{R}^{n'}, & \\
DFT(\tilde{\boldsymbol{v}}) = \boldsymbol{w} \in \mathbb{R}^{n'}, & w_j = \sum_{k=1}^{n'} \tilde{v}_k\, e^{-2i\frac{kj\pi}{n'}} \quad 1 \le j \le n'
\end{array}
$$

Note first that $z_j = \sum_{k=1}^{n'} \tilde{v}_k \sin\frac{kj\pi}{n'}$ as well. Consider first the even indices $z_2, \cdots, z_{n-1}$ :

$$
z_{2\ell} = \sum_{k=1}^{n'} \tilde{v}_k \sin\frac{2\ell k\pi}{n'} = -\mathcal{I}\mathrm{m} w_\ell, \quad \ell = 1, \cdots, \frac{n-1}{2}.
$$

Consider now the odd indices, $z_1, \cdots, z_n$

$$
\begin{array}{rcl}
z_{2\ell-1} & = & -\mathcal{I}\mathrm{m} \sum_{k=1}^{n'} \tilde{v}_k e^{-i\frac{k(2\ell-1)\pi}{n'}} = -\mathcal{I}\mathrm{m} \sum_{k=1}^{n'} (\tilde{v}_k e^{i\frac{k\pi}{n'}}) e^{-2i\frac{k\ell\pi}{n'}} \\
& = & -\mathcal{I}\mathrm{m}(DFT(\{\tilde{v}_k e^{i\frac{k\pi}{n'}}\}_k))_\ell, \quad \ell = 1, \cdots, \frac{n+1}{2}.
\end{array}
$$

Resuming with matlab notations

QFFT

$$
\begin{array}{rcll}
\boldsymbol{r_0} & = & e^{i\frac{\pi}{n'}} & \\
(Q\boldsymbol{v})_{2\ell} & = & -\sqrt{\frac{2}{n+1}}\ \mathcal{I}\mathrm{m}(FFT(\tilde{\boldsymbol{v}}))_\ell, & \ell = 1, \cdots, \frac{n-1}{2} \\
(Q\boldsymbol{v})_{2\ell-1} & = & -\sqrt{\frac{2}{n+1}}\ \mathcal{I}\mathrm{m}(FFT(\tilde{\boldsymbol{v}} \cdot * \boldsymbol{r_0}^{(1:n')'}))_\ell, & \ell = 1, \cdots, \frac{n+1}{2}
\end{array}
\tag{3.5}
$$

Summarizing the solution of

$$
\begin{pmatrix}
B & C & & 0 & \\
C & B & C & & \\
 & \ddots & \ddots & \ddots & \\
 & & C & B & C \\
 & 0 & & C & B
\end{pmatrix}
\begin{pmatrix}
\boldsymbol{x}^1 \\ \boldsymbol{x}^2 \\ \vdots \\ \boldsymbol{x}^{m-1} \\ \boldsymbol{x}^m
\end{pmatrix}
=
\begin{pmatrix}
\boldsymbol{b}^1 \\ \boldsymbol{b}^2 \\ \vdots \\ \boldsymbol{b}^{m-1} \\ \boldsymbol{b}^m
\end{pmatrix}
$$

**Step 1 : FFT** Compute $\boldsymbol{c}^j = Q^T \boldsymbol{b}^j$ by (3.5) for $1 \le j \le m$.

**Step 2 : Sort** $\{\boldsymbol{c}^1, \cdots, \boldsymbol{c}^m\}$ The righthand side has been build by rows in the mesh : $\boldsymbol{b}^j$ is the vector of the values of the forcing term on the line $y = j * h_y$.

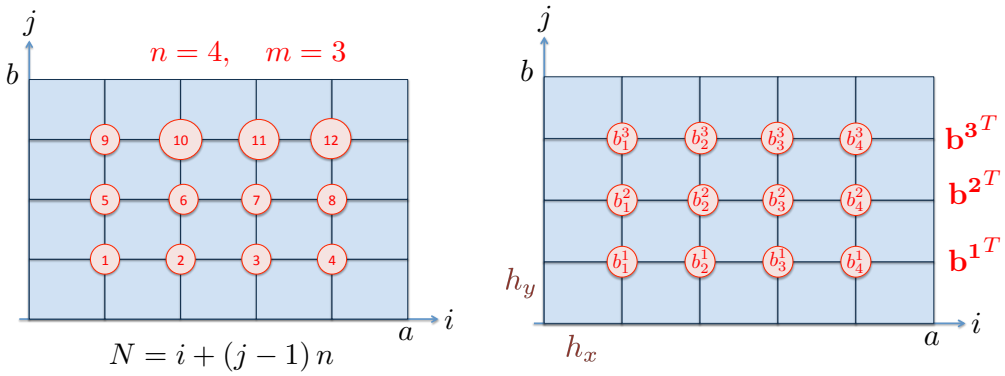



FIGURE 3.4 – Numbering

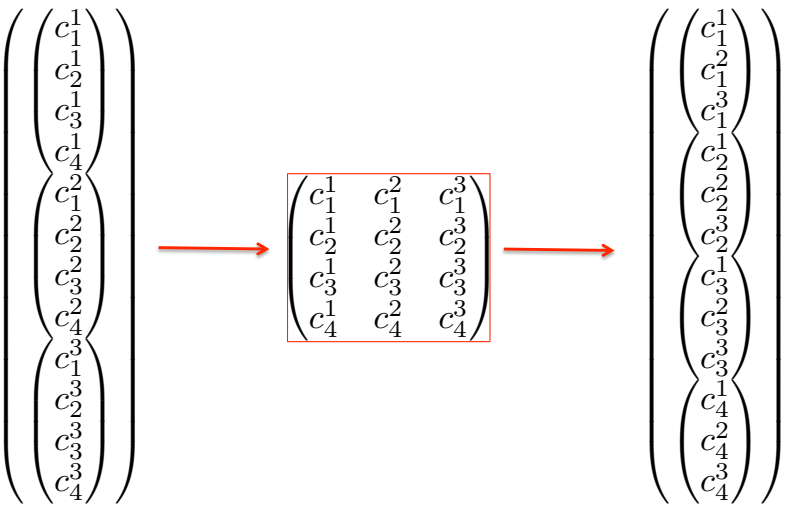


FIGURE 3.5 – Renumbering

The total vector $\boldsymbol{\sigma}$ is numbered from 1 to $nm$, with $N = i + (j-1) * n$. The matrix $C$ is built as follows

$$\begin{aligned} \boldsymbol{\sigma}(1:n) &\to C(:,1) \\ \boldsymbol{\sigma}(n+1:2n) &\to C(:,2) \\ &\vdots \\ \boldsymbol{\sigma}((m-1)n+1:mn) &\to C(:,m) \end{aligned}$$

```
for j=1:m
        C(:,j)=sig((j−1)∗n+1:j∗n )
end
```

and then instead of reading the columns, we read the rows.

**Step 3 : Solving the $n$ tridiagonal systems** of size $m$,

$$T_j \boldsymbol{z}^j = \boldsymbol{d}^j, \quad 1 \le j \le n.$$

with $\boldsymbol{d}^j = C(j,:)$, and

$$T_j = \begin{pmatrix} D_j^1 & D_j^2 & & 0 & \\ D_j^2 & D_j^1 & D_j^2 & & \\ & \ddots & \ddots & \ddots & \\ & & D_j^2 & D_j^1 & D_j^2 \\ & 0 & & D_j^2 & D_j^1 \end{pmatrix},$$

$$D_j^2 = -\frac{1}{h_y^2}, \quad D_j^1 = \frac{2}{h_y^2} + \frac{4}{h_x^2}\sin^2\frac{j\pi h}{2(n+1)}.$$

**Step 4 : Reordering the $\boldsymbol{z}^j$** into $\boldsymbol{y}^j$

**Step 5 : Recovering $\boldsymbol{x}^j$** $= Q\boldsymbol{y}^j$ by (3.5).

For this method, we talk about FFT preconditioning, since the system $A\boldsymbol{u} = \boldsymbol{b}$ is premultiplied by the block-diagonal matrix

$$\mathcal{Q} = \begin{pmatrix} Q^T & & & \\ & Q^T & 0 & \\ & & \ddots & \\ & 0 & & Q^T \end{pmatrix}$$

That is we write

$$\mathcal{Q}A\mathcal{Q}^T\mathcal{Q}\boldsymbol{u} = \mathcal{Q}\boldsymbol{b}.$$

# Chapitre 4

# Substructuring methods

## Contents


**4.1 The Schur Complement method . . . . . 65**
**4.2 Direct method for the resolution of the interface problem . . . . . 68**
**4.3 The conjugate gradient algorithm . . . . . 69**
**4.4 The Dirichlet Neumann algorithm . . . . . 70**
4.4.1 Presentation of the algorithm . . . . . 71
4.4.2 Convergence analysis in one dimension . . . . . 71
**4.5 Appendix : `matlab` scripts in 1-D . . . . . 73**


Principle
- Split the domain into sub-domains,
- solve iteratively a "condensed interface problem" : at each iteration , solve independantly local problems in the subdomains (using a direct or an iterative method).

Advantages :
These methods are :
• More robust than classical iterative ones and cheaper than direct methods.
• Better adapted to distributed parallel computing with message passing programming :
→ one sub-domain per processor
→ interface data update by message passing .
• Use of sequential legacy codes for local problems, modular approach to parallelism.

## 4.1 The Schur Complement method

Consider the problem

$$\left\{\begin{array}{rcll} -\Delta u & = & f & \text{dans } \Omega, \quad \eta \geq 0 \\ u & = & 0 & \text{sur } \partial\Omega \end{array}\right.$$

We write a variational formulation in $V = H_0^1(\Omega)$ :

$$\forall v \in V, \quad a(u,v) = (f,v)$$
$$\text{with } a(u,v) = \int_\Omega \nabla u \nabla v dx$$

We introduce a triangulation $\mathcal{T}_h = \cup K$ with vertices $S_i$, $1 \leq i \leq N$,

$$V_h = \{v \in V, \forall K \in \mathcal{T}_h, v_h|_K \in \mathbb{P}_1\}.$$

where $\mathbb{P}_n$ is the space of polynomials of degree lower than $n$ in two variables. $\varphi_i$ is the basis function associated to $S_i$, as described in Figure 4.1. We write the linear system $KU = F$. The entries of the matrix $K$ are the $a(\varphi_i, \varphi_j)$. The components of $U$ are the degrees of freedom, $U_i = u_h(S_i)$, and $F_i = (f, \varphi_i)$..

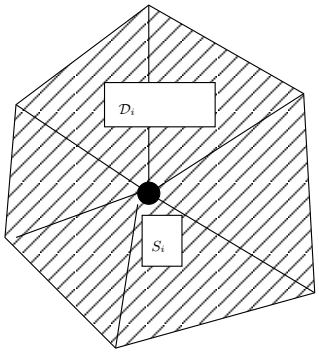



FIGURE 4.1 – $\mathcal{D}_i$, support of the basis function $\varphi_i$

The domain $\Omega$ is split into two nonoverlapping subdomains $\Omega_1$ and $\Omega_2$, and $\Gamma$ is the common boundary.

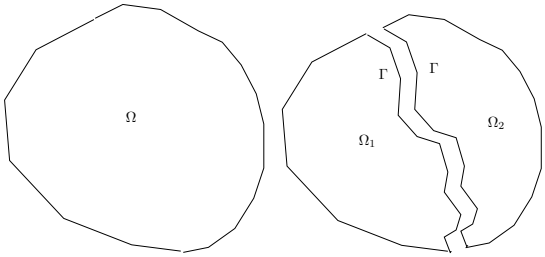



FIGURE 4.2 – Domain Decomposition

$$u_h = \sum_{S_j \in \Omega_1} u_h(S_j)\varphi_j + \sum_{S_j \in \Omega_2} u_h(S_j)\varphi_j + \sum_{S_j \in \Gamma} u_h(S_j)\varphi_j$$

$$a(u_h, \varphi_l) = \sum_{S_j \in \Omega_1} u_h(S_j)a(\varphi_j, \varphi_l) + \sum_{S_j \in \Omega_2} u_h(S_j)a(\varphi_j, \varphi_l) + \sum_{S_j \in \Gamma} u_h(S_j)a(\varphi_j, \varphi_l)$$

For $S_l \in \Omega_1$, the second sum vanishes, since the supports of $S_j \in \Omega_2$ and $S_l \in \Omega_1$ do not intersect. For $S_l \in \Omega_2$, the first sum vanishes. For $S_l \in \Gamma$, all sums contribute, but for the last one, the support of $S_l$ is split according to Figure 4.1.

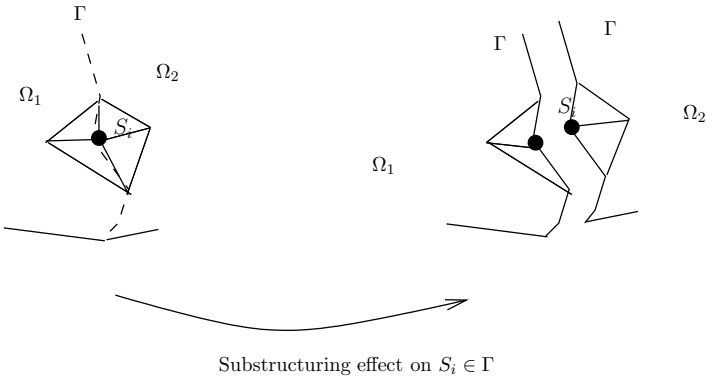



FIGURE 4.3 – Decomposition of the support of $\varphi_j \in \Gamma$

If $S_l \in \Gamma$ and $S_j \in \Gamma$ are neighbours,

$$\int_{\mathcal{D}_l \cap \mathcal{D}_j} \nabla\varphi_j \cdot \nabla\varphi_l \, dx = \int_{\mathcal{D}_l \cap \mathcal{D}_j \cap \Omega_1} \nabla\varphi_j \cdot \nabla\varphi_l \, dx + \int_{\mathcal{D}_l \cap \mathcal{D}_j \cap \Omega_2} \nabla\varphi_j \cdot \nabla\varphi_l \, dx$$

and the same for the computation of $(f, \varphi_l)$. The unknown $U$ is split into three blocks : $U_1$ is the block of the unknowns in the open domain $\Omega_1$, $U_2$ is the block of the unknowns in the open domain $\Omega_2$, $U_3$ is the block of the unknowns on the boundary $\Gamma$. The matrix $K$ is split according to the previous formula. We shall write

$$\begin{bmatrix} K_{11} & 0 & K_{13} \\ 0 & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix} = \begin{bmatrix} F_1 \\ F_2 \\ F_3 \end{bmatrix} \tag{4.1}$$

with $K_{33} = K_{33}^1 + K_{33}^2$ and $F_3 = F_3^1 + F_3^2$. We rewrite as a system of three systems.

$$\begin{cases} K_{11}U_1 & & +K_{13}U_3 & = & F_1 \\ & K_{22}U_2 & +K_{23}U_3 & = & F_2 \\ K_{31}U_1 & +K_{32}U_2 & +K_{33}U_3 & = & F_3 \end{cases} \tag{4.2}$$

Note that $K_{11}$ is the matrix of the Laplace problem in $\Omega_1$ with homogeneous Dirichlet boundary conditions on $\partial\Omega_1$, and is therefore invertible. Solving the first equation in (4.2) amounts to solving the Laplace equation in $\Omega_1$ with homogeneous Dirichlet boundary conditions on $\partial\Omega_1 - \Gamma$, and Dirichlet data $U_3$ on $\Gamma$. The first two problems can be solved in $U_1, U_2$ knowing $U_3$ as

$$U_1 = (K_{11})^{-1}(F_1 - K_{13}U_3), \quad U_2 = (K_{22})^{-1}(F_2 - K_{23}U_3)$$

Carrying these values into the first equation gives

$$SU_3 = (K_{33} - K_{31}K_{11}^{-1}K_{13} - K_{32}K_{22}^{-1}K_{23})U_3 = G_3$$
$$\text{with } G_3 = F_3 - K_{31}K_{11}^{-1}F_1 - K_{32}K_{22}^{-1}F_2$$

**Definition 4.1** *The matrix $S = K_{33} - K_{31}K_{11}^{-1}K_{13} - K_{32}K_{22}^{-1}K_{23}$ is the Schur Complement matrix.*

**Theorem 4.1** *The matrix $S$ est symmetric, positive, definite.*

It will be computed in parallel as

$$S = S^1 + S^2$$

with

$$S^i = K_{33}^i - K_{3i}K_{ii}^{-1}K_{i3}$$

Then the interface problem will be solved with direct or parallel methods. It is important to keep in mind that multiplying $S$ by $U_3$ amounts to solving Dirichlet problems in $\Omega_1$ and $\Omega_2$.

The first two equations in (4.2) is the resolution of Laplace equations. But what is the third one ? Suppose $w$ is a "regular" solution of $-\Delta w = f$ in $\Omega_1$. By the Green formula we have for any $v$ in $H^{1/2}(\Gamma)$,

$$< \frac{\partial w}{\partial n_1}, v >_{\partial\Omega} = (\nabla w, \nabla v) + (\Delta w, v) = (\nabla w, \nabla v) - (f, v)$$

We apply this to $w = (u_1)_h$, and $v = \varphi_i$, with $S_i \in \Gamma$, and obtain

$$(< \frac{\partial (u_1)_h}{\partial n_1}, \varphi_i >_\Gamma)_i = K_{31}U_1 + K_{33}^1 U_3 - F_3^1 = S^1 U_3 - F_3^1$$

We can now understand $S^i$ as the operator which, in the finite elements formulation, maps the value of $(u_1)_h$ on $\Gamma$ to its normal derivative. The last equation can now be written as

$$\forall S_i \in \Gamma, < \frac{\partial (u_1)_h}{\partial n_1} + \frac{\partial (u_2)_h}{\partial n_2}, \varphi_i >_\Gamma = 0$$

The full substructuring method can now be understood as the finite element discretization of : find $g$ defined on the interface $\Gamma$ such that, defining $u_1$ and $u_2$ as the solutions of

$$-\Delta u_j = f \text{ in } \Omega_j,$$
$$u_j = 0 \text{ on } \partial\Omega_j - \Gamma,$$
$$u_j = g \text{ on } \Gamma$$

then

$$\frac{\partial u_1}{\partial n_1} + \frac{\partial u_2}{\partial n_2} = 0 \text{ on } \Gamma.$$

The resolution of the interface problem can be solved either by a direct method, or by a Krylov method.

## 4.2 Direct method for the resolution of the interface problem

We work on system (4.1), and write a block-LU decomposition of $K$ as follows

$$\left(\begin{array}{c|c|c} K_{11} & 0 & K_{13} \\ \hline 0 & K_{22} & K_{23} \\ \hline K_{31} & K_{32} & K_{33} \end{array}\right) = \left(\begin{array}{c|c|c} L_{11} & 0 & 0 \\ \hline 0 & L_{22} & 0 \\ \hline L_{31} & L_{32} & L_{33} \end{array}\right) \left(\begin{array}{c|c|c} U_{11} & 0 & U_{13} \\ \hline 0 & U_{22} & U_{23} \\ \hline 0 & 0 & U_{33} \end{array}\right) \tag{4.3}$$

We identify

$$K_{11} = L_{11}U_{11}; K_{13} = L_{11}U_{13},$$

$$K_{22} = L_{22}U_{22}; K_{23} = L_{22}U_{23},$$

$$K_{31} = L_{31}U_{11}; K_{32} = L_{32}U_{22}; K_{33} = L_{31}U_{13} + L_{32}U_{23} + L_{33}U_{33}$$

Notice that $L_{3i}U_{i3} = K_{3i}K_{ii}^{-1}K_{i3}$, therefore $K_{33} - L_{31}U_{13} - L_{32}U_{23} = S$, and $S = L_{33}U_{33}$. The computations are made in parallel on two processors :

| PROCESSOR $(i)$ |
|---|
| Decomposition $L_{ii}U_{ii}$ de $K_{ii}$, |
| Computation of $U_{i3}, L_{3i}$, |
| Computation of $S^i = K_{33}^i - L_{3i}U_{i3}$ |
| Computation of $F^i$ and $F_3^i$ |
| ASSEMBLING |
| Computation of $S = S^1 + S^2$ and $F_3 = F_3^1 + F_3^2$, |
| Decomposition $L_{33}U_{33}$ of $S$. |

We then solve the triangular problems

$$\left(\begin{array}{c|c|c} L_{11} & 0 & 0 \\ \hline 0 & L_{22} & 0 \\ \hline L_{31} & L_{32} & L_{33} \end{array}\right)\left(\begin{array}{c} Z_1 \\ Z_2 \\ Z_3 \end{array}\right) = \left(\begin{array}{c} F_1 \\ F_2 \\ F_3 \end{array}\right)$$

$$\left(\begin{array}{c|c|c} U_{11} & 0 & U_{13} \\ \hline 0 & U_{22} & U_{23} \\ \hline 0 & 0 & U_{33} \end{array}\right)\left(\begin{array}{c} X_1 \\ X_2 \\ X_3 \end{array}\right) = \left(\begin{array}{c} Z_1 \\ Z_2 \\ Z_3 \end{array}\right)$$

| PROCESSEUR $(i)$ |
|---|
| Computation of $F_i$, $F_3^i$, |
| $L_{ii}z_i = F_i$, $G_3^i = F_3^i - L_{3i}Z_i$ |
| ASSEMBLING |
| $L_{33}Z_3 = G_3^1 + G_3^2$ |
| $U_{33}X_3 = Z_3$ |
| PROCESSOR $(i)$ |
| $U_{ii}X_i = Z_i - U_{i3}X_3$ |

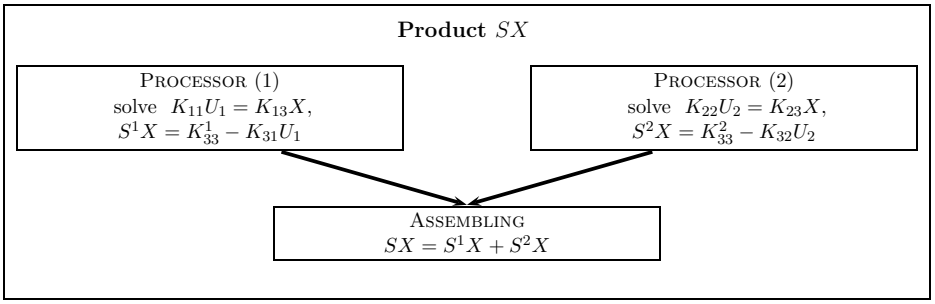
## 4.3 The conjugate gradient algorithm

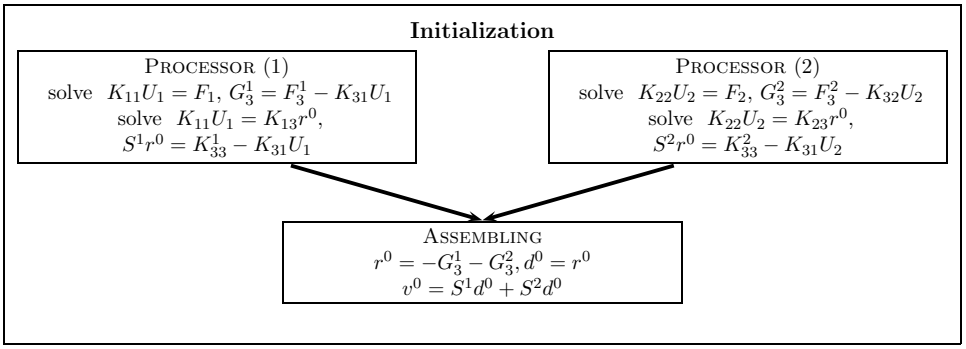
$S$ is a symmetric positive definite matrix. The conjugate gradient algorithm reduces to a descent method,defined by the initial guess $U_3^0$,the initial descent direction $d^0 = r^0 = SU_3^0 - G_3$. Let $r^k$ be the residual a step $k$. The next step will be

$$\begin{array}{c} v^k = Sd^k \\ \rho^k = \frac{\|r^k\|^2}{(v^k, d^k)} \\ U_3^{k+1} = U_3^k - \rho^k d^k \\ r^{k+1} = r^k - \rho^k v^k \\ d^{k+1} = r^{k+1} + \frac{\|r^{k+1}\|^2}{\|r^k\|^2} d^k \end{array}$$

All the products have to be made in parallel. Let us go into details.
For the initialization choose $U_3^0 = 0$, thus $r^0 = -G_3 = -F_3 + K_{31}K_{11}^{-1}F_1 + K_{32}K_{22}^{-1}F_2$.

We define a special box for the product $SX$ :




**Iteration**

$$v^k = Sd^k$$

$$\rho^k = \frac{\|r^k\|^2}{(v^k, d^k)}$$

$$U_3^{k+1} = U_3^k - \rho^k d^k$$

$$r^{k+1} = r^k - \rho^k v^k$$

$$d^{k+1} = r^{k+1} + \frac{\|r^{k+1}\|^2}{\|r^k\|^2} d^k$$

Note that the scalar products can also be done partly in parallel.

## 4.4 The Dirichlet Neumann algorithm

The purpose of the algorithm is to solve the coupling problem

$$\mathcal{L}u = f \text{ on } \Omega,$$
$$u = 0 \text{ on } \partial\Omega$$

by splitting $\Omega$ into two subdomains with interface $\Gamma$, and solving iteratively with an initial guess $g_0$,

### 4.4.1 Presentation of the algorithm

$$\begin{cases} \mathcal{L}u_1^n = f \text{ in } \Omega_1, \\ u_1^n = 0 \text{ on } \partial\Omega \cup \overline{\Omega_1}, \quad u_1^n = g^n \text{ on } \Gamma. \end{cases}$$

$$\begin{cases} \mathcal{L}u_2^n = f \text{ in } \Omega_2, \\ u_2^n = 0 \text{ on } \partial\Omega \cup \overline{\Omega_2}, \quad \dfrac{\partial u_2^n}{\partial \nu} = \dfrac{\partial u_1^n}{\partial \nu} \text{ on } \Gamma. \end{cases}$$

where $\dfrac{\partial}{\partial \nu}$ in $\Omega_2$ is the normal derivative, with $\nu$ the exterior normal to $\Omega_2$.

$$g^{n+1} = \theta u_2^n + (1-\theta) g^n.$$

The choice of the parameter is crucial and unfortunately depends on the position of the interface. If the subdomains and the problems are symmetric, the choice $\theta = \frac{1}{2}$ is optimal.

### 4.4.2 Convergence analysis in one dimension

Let $\mathcal{L} = \eta - d_x^2$, $\Omega = (a,b)$. Take $c$ in $(a,b)$. Then we have $\dfrac{\partial}{\partial \nu} = -\dfrac{d}{dx}$ on the interface at point $c$.

Define the error in the subdomain, $e_j^n = u_j^n - u$, and $h^n = g^n - u(c)$. The algorithm for the error is

$$\begin{cases} \mathcal{L}e_1^n = 0 \text{ in } \Omega_1, \\ e_1^n = 0 \text{ on } \partial\Omega \cup \overline{\Omega_1}, \quad e_1^n = h^n \text{ on } \Gamma. \end{cases}$$

$$\begin{cases} \mathcal{L}e_2^n = 0 \text{ in } \Omega_2, \\ e_2^n = 0 \text{ on } \partial\Omega \cup \overline{\Omega_2}, \quad \dfrac{\partial e_2^n}{\partial \nu} = \dfrac{\partial e_1^n}{\partial \nu} \text{ on } \Gamma. \end{cases}$$

$$h^{n+1} = \theta e_2^n(c) + (1-\theta) h^n.$$

This can be solved as

$$e_1^n = h^n \frac{\mathrm{sh}(\sqrt{\eta}(x-a))}{\mathrm{sh}(\sqrt{\eta}(c-a))}, \quad e_2^n = \beta^n \mathrm{sh}(\sqrt{\eta}(b-x)).$$

The coefficient $\beta^n$ is determined by the transmission condition $d_x e_2^n(c) = d_x e_1^n(c)$, that gives

$$-\beta^n \mathrm{ch}(\sqrt{\eta}(b-c) = h^n \frac{\mathrm{ch}(\sqrt{\eta}(c-a))}{\mathrm{sh}(\sqrt{\eta}(c-a))}$$

$$h^{n+1} = \underbrace{(-\theta \frac{\mathrm{sh}(\sqrt{\eta}(b-c))\mathrm{ch}(\sqrt{\eta}(c-a))}{\mathrm{sh}(\sqrt{\eta}(c-a))\mathrm{ch}(\sqrt{\eta}(b-c))} + (1-\theta))}_{\text{Convergence factor } \rho} h^n.$$

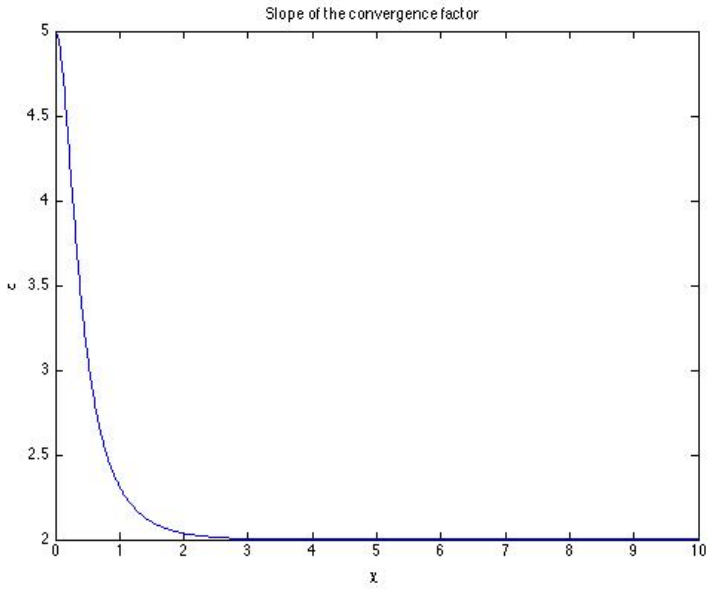
If the geometry is symmetric, that is if $b-c = c-a$, then the convergence factor reduces to

$$\rho = 1 - 2\theta,$$

that is small than 1 for $\theta \in (0,1)$, and vanishes for $\theta = 1/2$. Suppose now that $(c-a) = (b-a)/5$. Then defining $\chi = \sqrt{\eta}/5$, then

$$\rho = 1 - \theta(\frac{\tanh(4\chi)}{\tanh(\chi)} + 1).$$

It is a linear function of $\theta$, with a slope $\alpha = -(\frac{\tanh(4\chi)}{\tanh(\chi)} + 1) \in (-5, -2)$.




Therefore $\rho$ is an decreasing function of $\theta$, and it is equal to 1 for $\theta = \theta_0$, with

$$\theta_0 = \frac{2}{\frac{\tanh(4\chi)}{\tanh(\chi)} + 1} \in (\frac{2}{5}, 1).$$

Then the algorithm is convergent if and only if $\theta \leq \theta_0$.

## 4.5 Appendix : matlab scripts in 1-D

```
function u=SolveDD(f,eta,a,b,ga,gb)
% SOLVEDD solves eta-Delta in 1d using finite differences
%   u=SolveDD(f,eta,a,b,ga,gb,n) solves the one dimensional equation
%   (eta-Delta)u=f on the domain Omega=(a,b) with Dirichlet boundary
%   conditions u=ga at x=a and u=gb at x=b using a finite
%   difference approximation with length(f) interior grid points

J=length(f);
h=(b-a)/(J+1);
% construct 1d finite difference operator
e=ones(J,1);
A=spdiags([-e/h^2 (eta+2/h^2)*e -e/h^2],[-1 0 1],J,J);
f(1)=f(1)+ga/h^2;          % add boundary conditions into rhs
f(end)=f(end)+gb/h^2;
u=A\f;
u=[ga;u;gb];               % add boundary values to solution
```

```
function u=SolveND(f,eta,a,b,ga,gb)
% SOLVEND solves eta-Delta in 1d using finite differences
%   u=SolveND(f,eta,a,b,ga,gb) solves the one dimensional equation
%   (eta-Delta)u=f on the domain Omega=(a,b) with Neumann boundary
%   condition u'=ga at x=a and Dirichlet boundary
%   condition u=gb at x=b using a finite
%   difference approximation.
%   note the second order appproximation of the derivative

J=length(f);
h=(b-a)/J;
% construct 1d finite difference operator
e=ones(J,1);
A=spdiags([-e/h^2 (eta+2/h^2)*e -e/h^2],[-1 0 1],J,J);
A(1,2)=2*A(1,2);  %% Neumann boundary condition
% construct 1d finite difference operator
f(1)=f(1)-2*ga/h;          % add boundary conditions into rhs
f(end)=f(end)+gb/h^2;
u=A\f;
u=[u;gb];              % add boundary value to solution on the right
```

```
function [g,u1,u2]=algoDN(f,eta,a,b,step,ga,gb,g1,Nc,Imax,t)
% algoDN solves the Laplace equation by the Dirichlet-Neumann algorithm
%[g,u1,u2]=algoDN(f,eta,a,b,step,ga,gb,g,Nc,Imax,t)
%solves the Laplace equation eta u -Delta u = f in (a,b)
% by the Dirichlet-Neumann algorithm on (a+Nc*step) and (Nc*step,c)
% note the second order reconstruction of   u_1'(c)
 g=zeros(1,Imax);
g(1)=g1;
c=a+Nc*step;
x=(a:step:b);x1=(a:step:c); x2=(c:step:b);
y= SolveDD(f',eta,a,b,ga,gb);
for j=1:Imax-1
    % Dirichlet on (a,c)
    f1=f(1:Nc-1);
    u1=SolveDD((f1)',eta,a,c,ga,g(j));
    %extraction de u_1'(c) : second order
    up1= (-u1(end-1)+(1+eta*step^2/2)*u1(end))/step-step*f(Nc)/2;
     % Neumann on (c,b) with u_2'(c)=u_1'(c)
    f2=f(Nc:end);
    u2=SolveND((f2)',eta,c,b,up1,gb);
    g(j+1)=(1-t)*g(j)+t*u2(1);
    h=figure
    plot(x1,u1,'b',x2,u2,'m',x,y,'r',c,linspace(u1(end),u2(1),100),'k');
    legend('u_1','u_2','solution discrete')
    title({['Algorithme de Dirichlet-Neumann',' c=',num2str(c),'\theta=',
        num2str(t)];...
        ['Iteration number ',int2str(j)]})
        filename = ['figDNpos' int2str(Nc) 'relax' num2str(t) 'iter' int2str
            (j) '.eps']
        print(h,'-depsc',filename)

    pause%(1)
end
```

```
function u=algoSchur(f,eta,a,b,h,ga,gb,Nc)
% algoSchur solves the Laplace equation by the Schur method
%[g,u1,u2]=algoSchur(f,eta,a,b,step,ga,gb,Nc)
%solves the Laplace equation eta u -Delta u = f in (a,b)
% by the Schur method m on (a+Nc*h) and (Nc*h,c)
J=length(f);
e=ones(J,1);
A=spdiags([-e/h^2 (eta+2/h^2)*e -e/h^2],[-1 0 1],J,J);
% decomposition of A
A11=A(1:Nc-1,1:Nc-1);
A22=A(Nc+1:end,Nc+1:end);
A1g=A(1:Nc-1,Nc);
Ag1=A(Nc,1:Nc-1);
A2g=A(Nc+1:end,Nc);
Ag2=A(Nc,Nc+1:end);
Agg=A(Nc,Nc);
%decomposition of f
f1=f(1:Nc-1);
f2=f(Nc+1:end);
fg=f(Nc);
% Construction of the Schur problem
funS=@(x) Agg*x-Ag1*(A11\(A1g*x))-Ag2*(A22\(A2g*x));
fS=fg-Ag1*(A11\f1)-Ag2*(A22\f2);
ug=pcg(funS,fS)
%reconstruct u1 and u2
u1=A11\(f1-A1g*ug)
u2=A22\(f2-A2g*ug)
%reconstruct u
u=[ga; u1 ; ug ; u2 ; gb];
```

```
clear all;close all;
% Validation of the Dirichlet and Neumann codes
a=0;
b=1;
Step=(b-a)*0.1./10.^(0:2);
for j=1:length(Step)
    step=Step(j);
    x=(a:step:b);
    y=sin(pi*x);
    eta=1;
    f=(eta+pi^2)*y(2:end-1);
    ga=0;gb=0;
    sol=SolveDD(f',eta,a,b,ga,gb);
    X=a:step/100:b;
    Y=sin(pi*X);
    figure(1)
    plot(x,sol,'b',X,Y,'r');
    hold on

    e1d(j)=max(abs(sol-y'));
    f=(eta+pi^2)*y(1:end-1);
    ga=pi;
    sol1=SolveND(f',eta,a,b,ga,gb);
    plot(x,sol1,'b',X,Y,'r');

    e1n(j)=max(abs(sol1-y'));
    figure(2)
    plot(x,sol1-y');
    %       pause
end

figure(3)
loglog(Step,e1d,'m*-')
hold on
loglog(Step,e1n,'bo-')
hold on
loglog(Step,Step.^2,'r')
legend('Dirichlet','Neumann','slope 2')


% Algorithme de Dirichlet Neumann sur (a,c), (c,b)
clear all; close all;
a=0;
b=1;
J=9;
h=(b-a)/(J+1);
x=(a:h:b);
% eta=1;
% y=x.^3;
% f=-6*x(2:end-1)+eta*y(2:end-1);
% ga=0;gb=1;
eta=1;
y=sin(pi*x);
f=(eta+pi^2)*y(2:end-1);
ga=0;gb=0;
```

```
sol=SolveDD(f',eta,a,b,ga,gb);
% position de l interface
Nc=floor(length(x)/2);
Nc=2;
c=a+Nc*h;
% nombre d'iterations
Imax=10;
%parametre de relaxation
t=0.3;
% initialisation avec la valeur exacte
g1=y(Nc+1);
% ou initialisation avec 0
g1=0;
[g,u1,u2]=algoDN(f,eta,a,b,h,ga,gb,g1,Nc,Imax,t)
% algorithme
figure(99)
plot(g)
title('Interface value')
xlabel('Iteration number')

% Methode de Schur
u=algoSchur(f',eta,a,b,h,ga,gb,Nc);
%plot(x,y,'r',x,yd,'g',x,u,'b')
figure(55)
plot(x,sol,'g',x,u,'b')


%%
N=10;
chi=linspace(0,N,N*100)
Y=tanh(4*chi)./tanh(chi)+1;
plot(chi,Y,'b')
xlabel('\chi')
ylabel('\alpha')
title('Slope of the convergence factor')
```

# Bibliographie


[1] Suzanne.C Brenner and Ridgway Scott. *The mathematical theory of finite element methods.* Springer-Verlag, 1994.

[2] William L. Briggs and Van Emden Henson. A multigrid tutorial. www.llnl.gov/CASC/people/henson/mgtut/ps/mgtut.pdf.

[3] Charles F Loan Gene H Golub. *Matrix computations.* Johns Hopkins University Press, 1996.

[4] Wolfgang Hackbusch. *Multigrid methods and applications.* Springer-Verlag, 1985.

[5] Hans Petter Langtangen and Aslak Tveitog. What is multigrid ? folk.uio.no/infima/doc/mg-underscore-nmfpd.pdf.

[6] Pierre-Arnaud Raviart and Jean-Marie Thomas. *Introduction à l'analyse numérique des équations aux dérivées partielles.* Masson, 1988.

[7] P. Wesseling. *An introduction to multigrid methods.* Wiley -Interscience, 1992.