Méthodes Itératives

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Cours 1, 10/03/2025 Méthodes Multigrilles

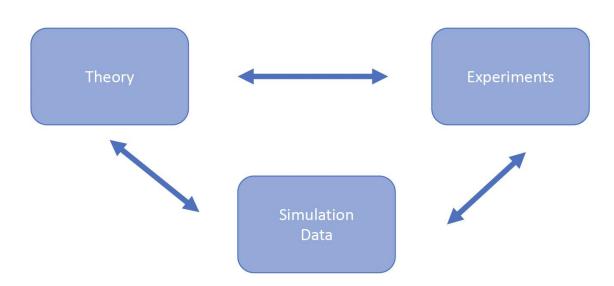
Organisation

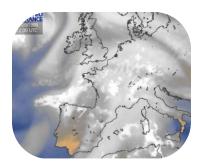
- 4 séances de Cours « Méthodes Multigrilles »
 - 10/03/25 10h
 - 11/03/25 10h
 - 14/03/25 14h
 - 18/03/25 18h
- 2 TP qui vont mettre en pratique la méthode multigrilles
 - 24/03/25 14h
 - 24/03/25 16h

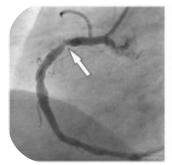
Numerical simulation

Third pillar for the development of scientific discoveries at the same level as theory and experiments.







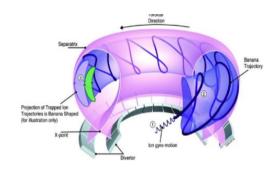






Many problems come down to **solving** a

- Linear system of type Ax = b
- An eigenvalue problem of type $Ax = \lambda b$



What kind of solvers exists?

Direct methods

- Accurate to machine precision
- High computational cost
- Efficient, parallel sparse direct solvers exist

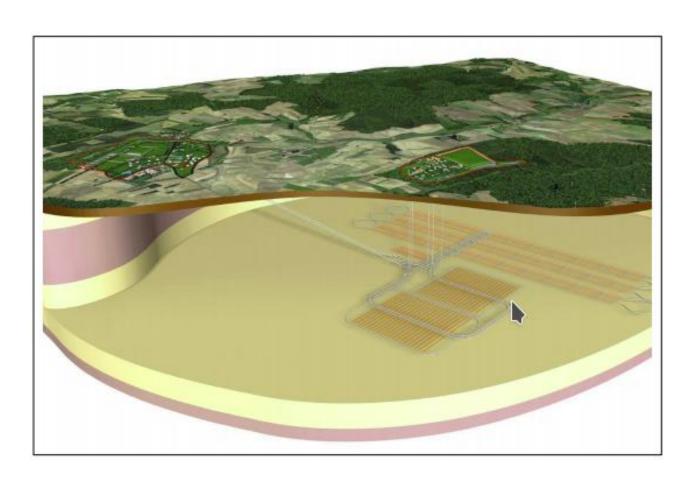
Iterative methods

- Classical relaxation schemes
- Krylov methods
- Preconditioning
- Multigrid methods
- Accurate to a predefined precision
- (Generally) lower computational cost





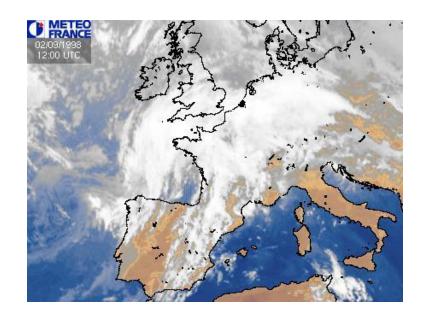
Examples – Discretization of PDE

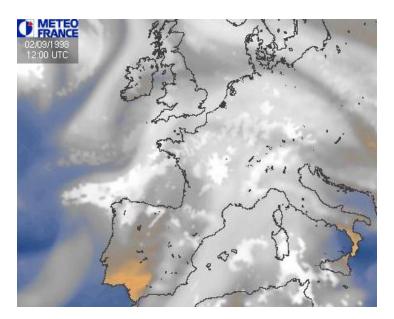


- Gallery crossing model
- 3D thermo-hydro-mechanics modelling (Biot's consolidation problem)
- Discretization of PDE leads to non-symmetric systems with about 100 million unknowns.
- We need fast iterative solvers!

Examples – Weather forecasting

• Time constraints: The weather forecast has to be done for 'soonish'





What will we look at

Solving linear systems of the form

$$Ax = b$$

- Matrix A shall be sparse (and large)
- Solve this problem iteratively (e.g. stationary methods, Krylov methods, multigrid)
- Do this in an inexpensive and fast way.

Large scale problems – mind experiment

• Let us take a matrix of size $N \times N$.

Let us suppose that we have three algorithms with different computational complexities

• Algorithm 1: $10^6 N$ operations

• Algorithm 2: $10^3 N^2$ operations

• Algorithm 3: N^3 operations

- Suppose that the problem size N is chosen, such that Algorithm 1 requires 1 second to compute the result.
- How long do the others need?

Speed of algorithms

N	Algorithm 1 10 ⁶ N operations	Algorithm 2 $10^3 N^2$ operations	Algorithm 1 N ³ operations	Computer Speed (ops/sec)
1	1 sec	0.001 sec	0.000001 sec	1M (~10 ⁶) (1980's)
10 ³	1 sec	1 sec	1 sec	1G (~10 ⁹) (1990's)
10 ⁶	1 sec	17 min	12 days	1T (~10 ¹²) (2000's)
10 ⁹	1 sec	12 days	31710 years	1P (~10 ¹⁵) (2010's)

Stronger computers



Greater advantage (necessity) of efficient algorithms!

Message

- Computational complexity is important!
- For very large problems, an algorithm with optimal complexity (i.e., the work grows only linearly with problem size) wins dramatically against an algorithm whose complexity is quadratic.
- Not seen, but: Also the energy consumption will become a bottleneck.

Classic schemes

Classical iterative methods - basic theory

• Let $A \in \mathbb{R}^{n \times n}$ be a non-singular matrix and $\mathbf{f} \in \mathbb{R}^n$.

Problem: Find $\mathbf{u} \in \mathbb{R}^n$, such that

$$A\mathbf{u} = \mathbf{f} \tag{1}$$

• Decompose the matrix into a non-singular matrix M and a matrix N as

$$A = M - N$$

• Equation (1) can then be written as

$$M\mathbf{u} = N\mathbf{u} + \mathbf{f}$$

or

$$\mathbf{u} = \underbrace{M^{-1}N}_{:=S} \mathbf{u} + M^{-1} \mathbf{f}$$

Classical iterative schemes – fixed point iterations

Let $oldsymbol{u}^0$ be an initial guess. Then a fixed point iteration can be applied to the equation

$$\mathbf{u}^{(m+1)} = S\mathbf{u}^{(m)} + M^{-1}\mathbf{f}$$

For u being a solution, u must be a fixed point.

This basic iterative approach might also be damped.

$$\mathbf{u}^* = S\mathbf{u}^{(m)} + M^{-1}\mathbf{f}$$
$$\mathbf{u}^{(m+1)} = \omega\mathbf{u}^* + (1 - \omega)\mathbf{u}^{(m)}$$

Then we get

$$\mathbf{u}^{(m+1)} = (\omega S + (1 - \omega)\mathbf{I})\mathbf{u}^{(m)} + \omega M^{-1}\mathbf{f}$$

The error and residual equation

• Let $\boldsymbol{u}^{(m)}$ be the approximation at step m. The error is defined by

$$\mathbf{e}^{(m)} = \mathbf{u} - \mathbf{u}^{(m)}$$

The residual at step m is defined by

$$\mathbf{r}^{(m)} = \mathbf{f} - A\mathbf{u}^{(m)}$$

• For both the weighted and the non-weighted iterative schemes above, the residual equation has the form

$$A\mathbf{e}^{(m)} = \mathbf{r}^{(m)}$$

• In some methods (e.g. multigrid), this residual equation is used to update the new $u^{(m+1)}$ by computing an approximation $\tilde{e}^{(m)}$ and then the new iterate

$$\boldsymbol{u}^{(m+1)} = \boldsymbol{u}^{(m)} + \tilde{\boldsymbol{e}}^{(m)}.$$

The error equation

• Let ${m u}$ be the solution of Au=f and ${m u}^{(m)}$ an approximation. We have

$$\mathbf{u}^{(1)} = S\mathbf{u}^{(0)} + M^{-1}\mathbf{f}$$

• The solution $oldsymbol{u}$ is a fixed point

$$\mathbf{u} = S\mathbf{u} + M^{-1}\mathbf{f}$$

Substraction of the initial error

$$\mathbf{e}^{(1)} = S\mathbf{u} - S\mathbf{u}^{(0)} = S\mathbf{e}^{(0)}$$

Repeating this argument, we have

$$\mathbf{e}^{(m)} = S\mathbf{u} - S\mathbf{u}^{(m-1)} = S\mathbf{e}^{(m-1)}$$

Recursively, we then get

$$\mathbf{e}^{(m)} = S^m \mathbf{e}^{(0)}$$

Convergence

From the previous equation follows

$$\|\mathbf{e}^{(m)}\| \le \|S^m\| \|\mathbf{e}^{(0)}\|$$

The iteration is called convergent, if

$$\lim_{m \to \infty} ||S^m|| = 0$$

 $\parallel S \parallel$ is called contraction number of the fixed point iteration.

Theorem

Let $\rho(S) = \max(\lambda(S))$ be the spectral radius of S. The iteration associated with the matrix S converges for **all** initial guesses, **if and only if**

$$\rho(S) < 1.$$

Convergence – Error reduction

• Suppose the matrix is symmetric positive definite (spd). We have

$$\frac{\|\mathbf{e}^{(m)}\|}{\|\mathbf{e}^{(0)}\|} \le \|S^m\| \approx \rho(S^m) = \rho(S)^m \approx 10^{-1}$$

How many iterations do we need to guarantee the reduction of the error by a factor of 10?

$$m \ge -\frac{1}{\log_{10}|\rho(S)|}$$

• Convergence factor

$$\rho(S)$$

Loosely speaking: The worst factor for the Reduction of the error in each step.

• Convergence rate

$$-\log_{10}|\rho(S)|$$
 \longrightarrow

The convergence becomes the faster, the higher the convergence rate.

Jacobi method

• Correct x_i^{old} by x_i^{new} such that the *i-th* equation of Ax = f is correct.

• Then the Jacobi method is given by

$$x_i^{(m+1)} := \frac{1}{a_{ii}} \left(b_i - \sum_{i \neq j} a_{ij} x_j^{(m)} \right), \qquad i = 1, .., n$$

$$a_{11} \cdot x_1 + \dots + a_{1n} \cdot x_n = b_1$$
 $a_{21} \cdot x_1 + \dots + a_{2n} \cdot x_n = b_2$
 \vdots
 $a_{n1} \cdot x_1 + \dots + a_{nn} \cdot x_n = b_n$

Jacobi Method

• Let D be the diagonal part and -L and -U the strictly lower and upper triangular parts of A, thus

$$A = D - L - U$$

Jacobi Method

• Calculate the relaxations simultaneously for all i = 1, ..., n. In matrix notation

$$\mathbf{x}^{(m+1)} = D^{-1}(L+U)\mathbf{x}^{(m)} + D^{-1}\mathbf{f}$$

Define $S_J := D^{-1}(L+U)$

Weighted Jacobi Method

• Let $\omega \in \mathbb{R}$ be a weighting factor. Then

$$\mathbf{x}^{(m+1)} = \left[(1 - \omega)\mathbf{I} + \omega S_J \right] \mathbf{x}^{(m)} + \omega D^{-1} \mathbf{r}^{(m)}$$

Define $S_{\omega} := (1 - \omega)I + \omega S_J$

Gauss-Seidel Method

The Gauss-Seidel method is given by

$$x_k^{(m+1)} := \frac{1}{a_{kk}} \left(b_k - \sum_{i=1}^{k-1} a_{ki} x_i^{(m+1)} - \sum_{i=k+1}^n a_{ki} x_i^{(m)} \right)$$

$$a_{11} \cdot x_1 + \dots + a_{1n} \cdot x_n = b_1$$
 $a_{21} \cdot x_1 + \dots + a_{2n} \cdot x_n = b_2$
 \vdots
 $a_{n1} \cdot x_1 + \dots + a_{nn} \cdot x_n = b_n$

- Components of the new approximation are used as soon as they are computed
- Gauss-Seidel method is sequential: To compute a new entry, we first need to compute all previous entries.

Relaxation schemes

Gauss-Seidel method

• Calculate an entry x_k of the new iteration and use it in the computation of x_i , i = k + 1, ..., n.

$$\mathbf{x}^{(m+1)} = (\mathbf{D} - \mathbf{L})^{-1} \mathbf{U} \mathbf{x}^{(m)} + (\mathbf{D} - \mathbf{L})^{-1} \mathbf{f}$$

Define $S_{GS} := (D - L)^{-1}U$

SOR method

$$\mathbf{x}^{(m+1)} = (\mathbf{D} - \omega \mathbf{L})^{-1} (\omega \mathbf{U} - (\omega - 1)\mathbf{D}) \mathbf{x}^{(m)} + (\frac{1}{\omega} \mathbf{D} - \mathbf{L})^{-1} \mathbf{f}$$

• If $\omega = 1$, then the Gauss-Seidel method is recovered.

Define $S_{CS\omega} := (D - \omega L)^{-1} (-\omega U + (\omega - 1)D)$

Properties

Weighted Jacobi

- For $A \in \mathbb{R}^{n \times n}$, weighted Jacobi converges for all initial \mathbf{x}^0 , if $\omega \in (0, 2/(\lambda_{\max} (D^{-1}A))$.
- The rate of convergence depends on ω .
- The convergence does not depend on the numbering of the unknowns.
- Entries can be computed all at once.

$$a_{11} \cdot x_1 + \cdots + a_{1n} \cdot x_n = b_1$$
 $a_{21} \cdot x_1 + \cdots + a_{2n} \cdot x_n = b_2$
 \vdots
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SOR

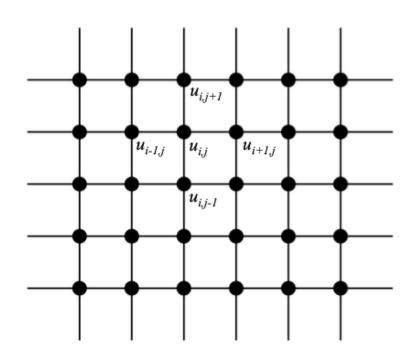
- For $A \in \mathbb{R}^{n \times n}$, SOR converges for all initial x^0 , if $\omega \in (0, 2)$.
- The rate of convergence depends on ω .
- The convergence depends on the numbering of the unknowns.
- We could also first solve for x_{nn} instead of x_{11}
- We could also alternate between ascending and descending order (symmetric Gauss-Seidel)

Example: 2D Poisson equation

$$-\Delta u = f,$$
 in $\Omega = [0, \pi] \times [0, \pi]$
 $u = u_0,$ on $\Gamma = \partial \Omega$

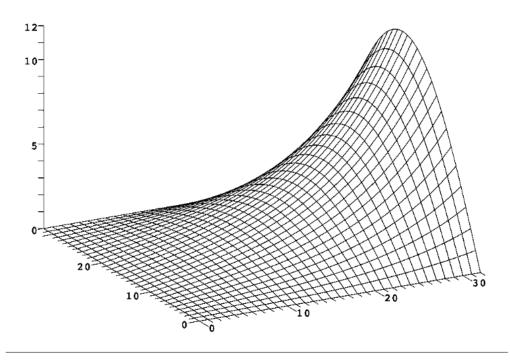
- Discretize Ω into a regular grid with N intervals in x and y
- We discretize using a 5-point stencil

$$\Delta u_{ij} \approx \frac{1}{h^2} (u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{ij}), \quad \text{for } i, j = 1, ..., n$$



- Boundary values are given.
- Imagine: Temperature at each node = average of neighboring temperatures.

Choice of an exact solution



We choose

$$u = \sinh(x)\sin(y)$$

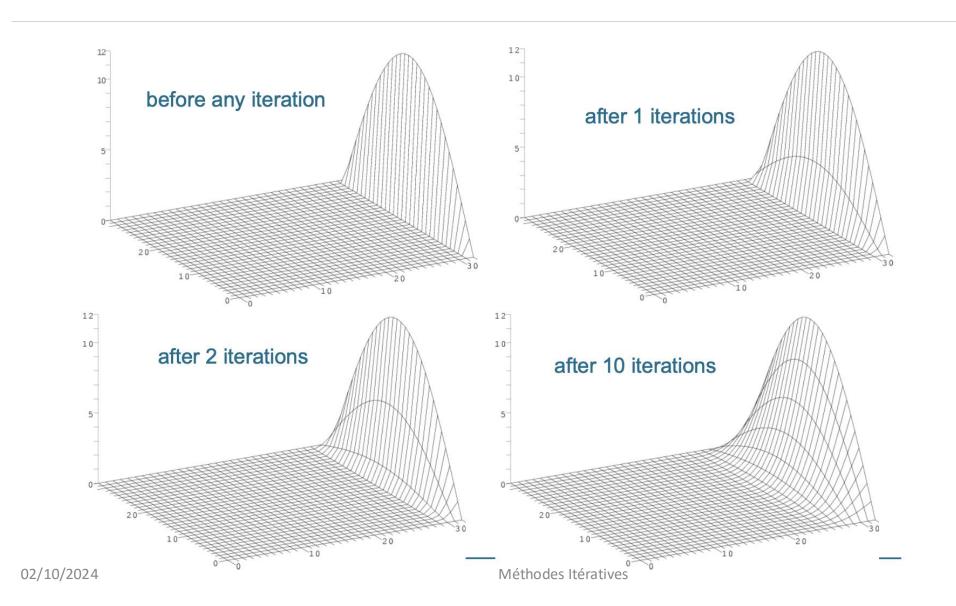
and obtain the right-hand side

$$f = 0$$

- We can thus compute the error at each node.
- We discretize the domain $\Omega = [0,\pi] \times [0,\pi]$ into a mesh with n intervals, so the matrix is of size $N=n^2$ and $h=\frac{\pi}{n}$.

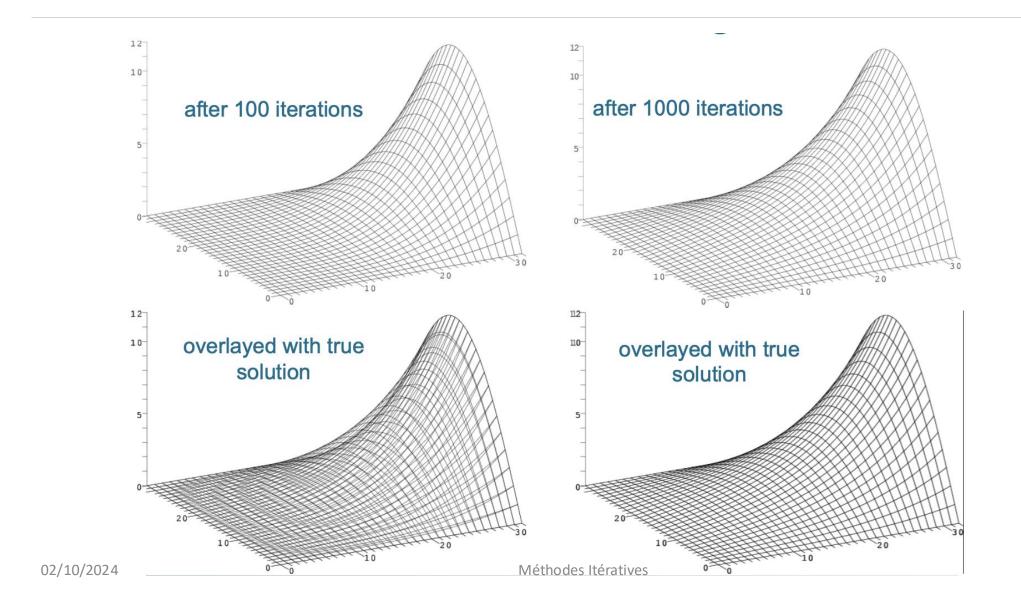
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Visualization of Gauss-Seidel iterations

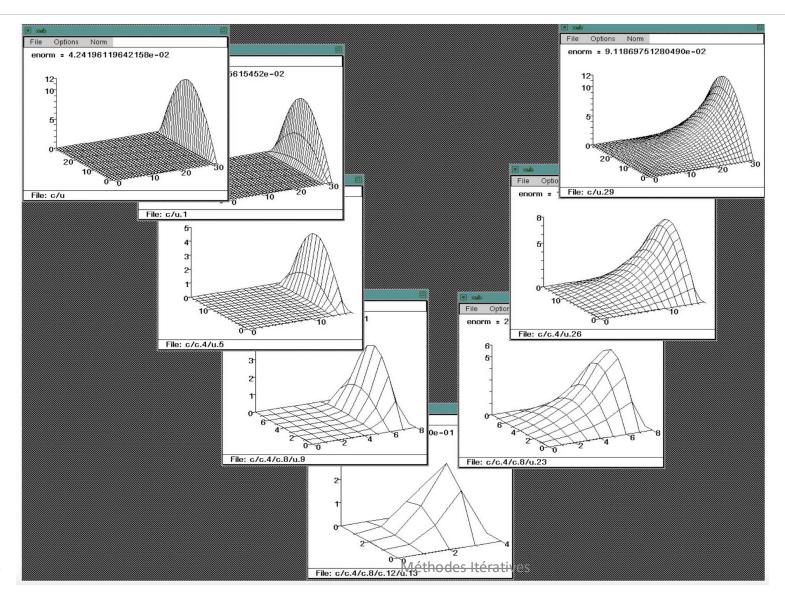


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Visualization of Gauss-Seidel iterations



Multigrid



Trying out algorithms

• Let us now apply some algorithms to the 2D Poisson problem.

level	h	d.o.f.	SSOR		PCG		MG		FGMRES+MG		UMFPACK	
			ite	$_{ m time}$	ite	time	ite	$_{ m time}$	ite	time	ite	time
1	1/4	25	49	0	3	0	11	0	6	0	1	0
2	1/8	81	164	0	9	0	13	0	8	0	1	0
3	1/16	289	543	0	31	0	13	0	8	0	1	0
4	1/32	1089	2065	0.07	66	0.01	14	0.03	8	0.01	1	0.01
5	1/64	4225	7998	0.92	132	0.02	14	0.11	8	0.03	1	0.03
6	1/128	16641	31054	14.61	263	0.16	13	0.35	8	0.21	1	0.12
7	1/256	66049	> 100000		524	1.79	13	1.55	8	1.06	1	0.75
8	1/512	263169			1038	16.55	12	6.09	8	3.90	1	5.40
9	1/1024	1050625			1986	127.76	12	27.46	7	18.32	1	46.46
10	1/2048	4198401			3944	1041.68	12	111.03	7	68.38		
fac	tor ≈	4	4	16	2	8	1	4	1	4	1	

Multigrid

- Framework: common concepts, different methods
- Efficient: usually O(N) or $O(N \log N)$ operations
- The importance of efficient methods becomes greater, as computers grow stronger!
- Iterative: Most nontrivial problems in our field cannot be solved directly
- Many variables: the larger the number of variables, the greater the gain of efficient methods

A framework of efficient iterative methods for solving problems with many variables and many scales.

This lecture is based on:

- A Multigrid Tutorial W.L. Briggs, V.E. Henson, S.F. McCormick
- Why Multigrid Methods Are So Efficient Irad Yavneh, Computing in Science and Engineering, 8(6):12 22
- Multigrid Methods, the basics Luke Olson, Copper Mountain Multigrid Conference tutorial, 2021
- Multi-Grid Methods and Applications W. Hackbusch

Some nice illustrations in jupyter notebooks:

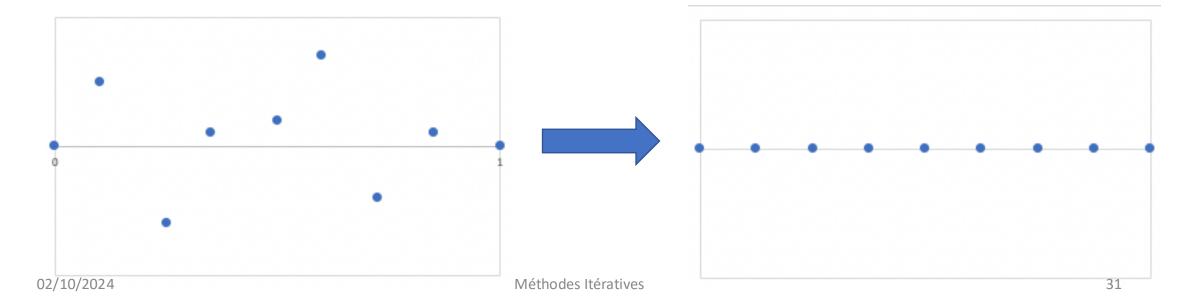
https://github.com/lukeolson/imperial-multigrid/tree/master/lecture-1-mg-basics

A multiscale approach

Following Irad Yaneh (Why Multigrid Methods Are So Efficient)

Imagine:

- A football coach wants to line up his players in equal distances on the goal line.
- Player 0 and player N shall stand on the left and right goal post.
- The remaining players stand in between them. He now moves them according to some rule.



1. possibility: Global processing

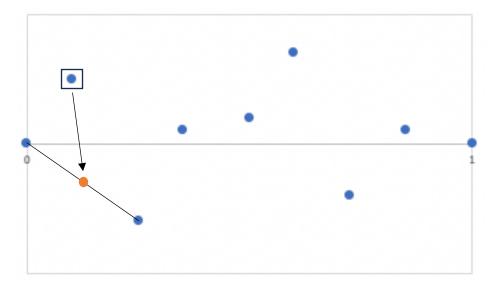
- The coach numbers its players from *O* to *N*.
- He tells player j to move to the goal line connecting player 0 to player N and then at a distance $j \frac{L}{N}$ from player 0.
- This solves the problem directly.

But

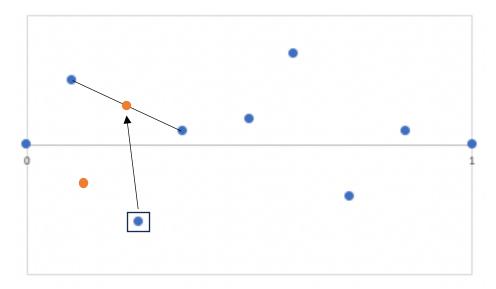
- Each player has to recognize the extreme players to find the 'goal line'.
- He has to do some 'fancy' arithmetic $\binom{L}{N}$, and has to move j times of this.

Let us see how we could achieve the same goal with some local processing.

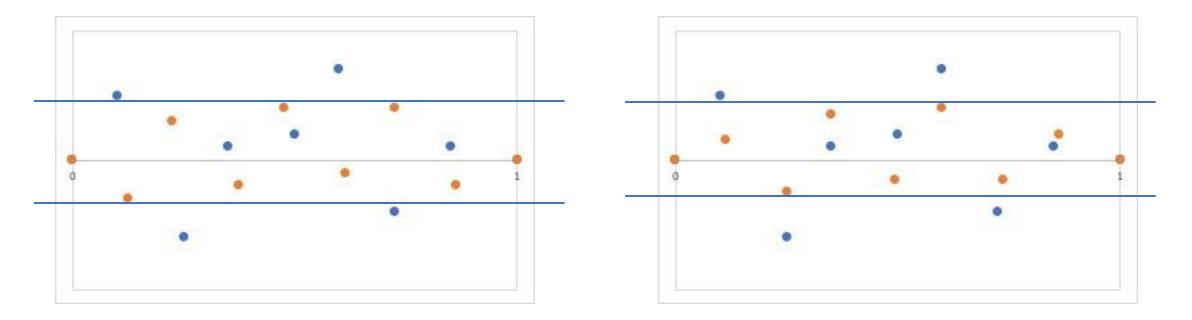
- We now require that each player detects the two players next to him and moves to the midpoint of the straight line connecting them.
- This is done at the whistle blow of the coach.
- Blue: initial position, Orange: new position



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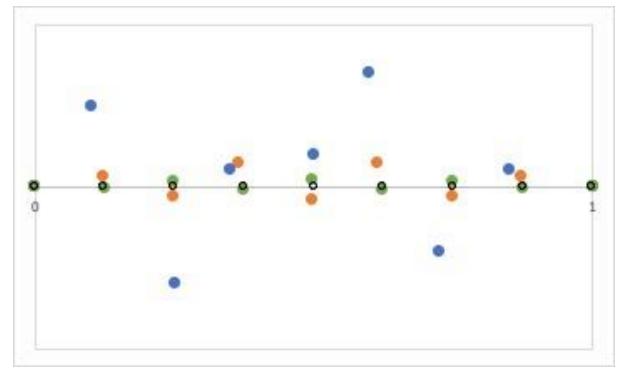


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- Blue: initial position, black: final position
- orange: after 15 iterations, green: after 30 iterations, black: after 64 iterations ($err \approx 5 \cdot 10^{-3}$)



Local movements – as formula

- Let us look at the distance of each player to the goal line. We have 9 players (N=8), with 7 players moving.
- At each whistle blow, the following update is done

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_7 \end{pmatrix}^{(m+1)} = \frac{1}{2} \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 1 & 0 & 1 & \ddots & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 & 1 \\ 0 & \dots & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_7 \end{pmatrix}^{(m)}$$

• This is nothing else than the Jacobi method for the 1D Poisson problem with mesh size 1. We derive this later on.

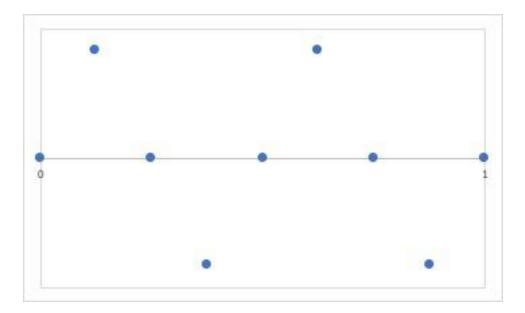
Some slow convergence

- Blue: initial position,
- Orange: new position after the whistle blow



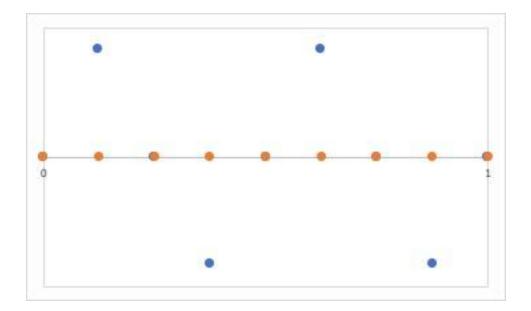
Fast convergence

- Blue: initial position,
- Orange: new position after the whistle blow



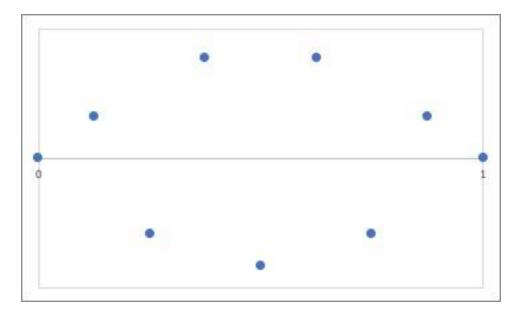
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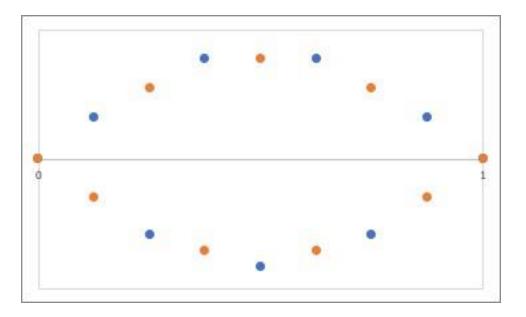
Slow convergence

- Blue: initial position,
- Orange: position after one whistle blow
- Green: position after two whistle blows



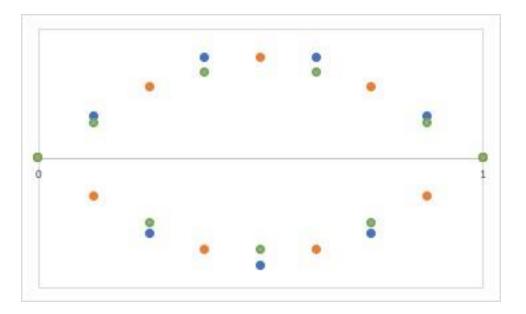
Slow convergence

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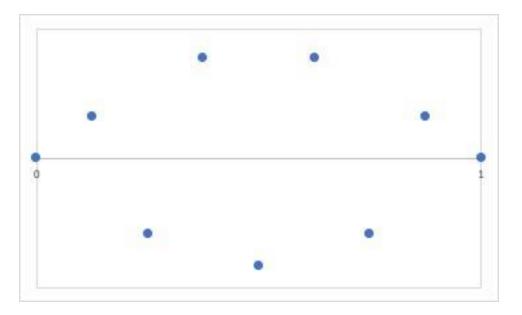
Slow convergence

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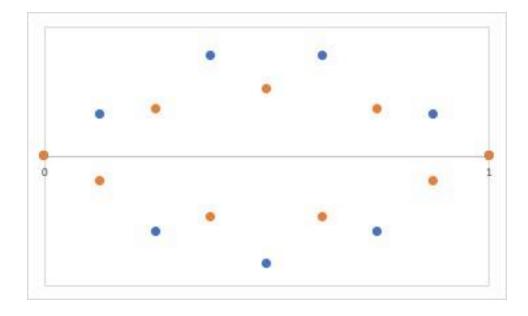
Slow convergence - improvement through damping

- Blue: initial position,
- Orange: position after one whistle blow
- Green: position after two whistle blows



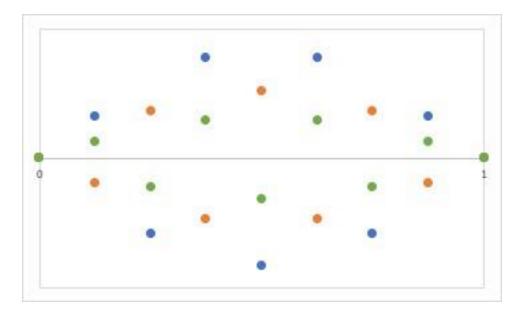
Slow convergence - improvement through damping

- Blue: initial position,
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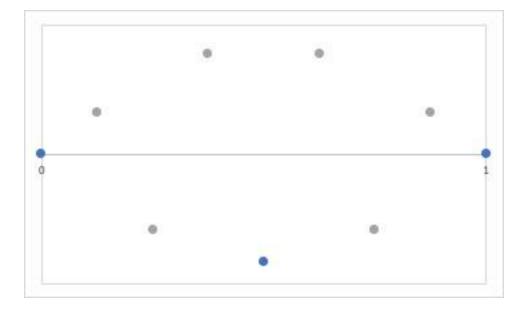


Slow convergence - improvement through damping

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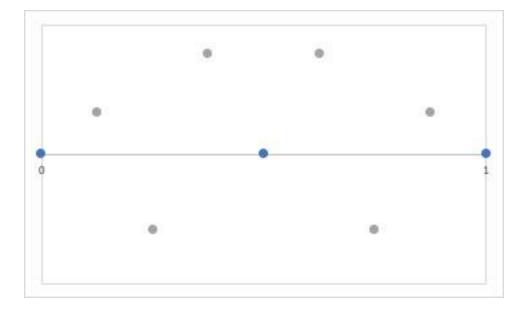


- Employ the local processing with simple arithmetic.
- Do this on different scales.



Large scale

- Employ the local processing with simple arithmetic.
- Do this on different scales.



Large scale

- Employ the local processing with simple arithmetic.
- Do this on different scales.



Intermediate scale

- Employ the local processing with simple arithmetic.
- Do this on different scales.



Intermediate scale

- Employ the local processing with simple arithmetic.
- Do this on different scales.



Small scale

- Employ the local processing with simple arithmetic.
- Do this on different scales.



Small scale

How much do we save?

- The local movements (Jacobi method) require about N^2 iterations and $N^2 \cdot N = N^3$ operations to improve the accuracy by an order of magnitude
- The multiscale approach solves the problem in about $log_2(N)$ iterations (whistle blows) and only about N operations.
- Example: For *N*=1000 we require about
 - Multiscale: 10 iterations and 1000 operations
 - Jacobi: 1 000 000 iterations and 1 000 000 000 operations

Geometric Multigrid methods

Elements of multigrid

Relaxation schemes and smoothing properties

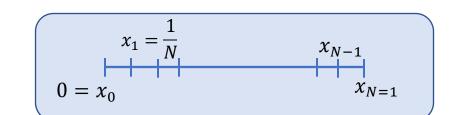
Model problem: 1D Poisson equation

• The 1D Poisson equation:

$$-u'' = f$$
$$u(0) = u(1) = 0$$

Grid points

 $h = \frac{1}{N}, \quad x_i = ih, \quad i = 0, ..., N$



Finite difference scheme

$$u_i'' \approx \frac{-u_{i-1} + 2u_i - u_{i+1}}{h^2} = f_i, \quad i = 1, .., N-1$$

$$u_0 = u_N = 0$$

• We obtain a linear system
$$A\mathbf{u} = \frac{1}{h^2} \left(\begin{array}{cccc} 2 & -1 & 0 & \dots & 0 \\ -1 & 2 & -1 & \ddots & \vdots \\ 0 & -1 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 2 & -1 \\ 0 & \dots & \mathsf{MéthOdes} & \mathsf{HéIntives} & 2 \end{array} \right) \left(\begin{array}{c} u_1 \\ u_2 \\ \vdots \\ u_{N-1} \end{array} \right) = \left(\begin{array}{c} f_1 \\ f_2 \\ \vdots \\ f_{N-1} \end{array} \right)$$

Application to our example: Jacobi method

• Remember the discretization at point i (this gives one matrix row):

$$-u_{i-1} + 2u_i - u_{i+1} = h^2 f_i$$

• Solving for u_i :

$$u_i = \frac{1}{2}(u_{i-1} + u_{i+1} + h^2 f_i)$$

We can write this iteratively as

$$u_i^{(m+1)} = \frac{1}{2} (u_{i-1}^{(m)} + u_{i+1}^{(m)} + h^2 f_i)$$

This can be expressed in matrix form as

$$\mathbf{u}^{(m+1)} = D^{-1}(L+U)\mathbf{u}^{(m)} + D^{-1}h^{2}\mathbf{f}$$

$$= \underbrace{(I-D^{-1}A)}_{:=R} \mathbf{u}^{(m)} + D^{-1}h^{2}\mathbf{f}$$

$$:= R$$
Méthodos Itérativos

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

$$R = \frac{1}{2} \begin{pmatrix} 0 & 1 & & \\ 1 & 0 & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & 0 \end{pmatrix}$$

Weighted Jacobi method

To increase convergence properties, we next look at the weighted Jacobi method.

We compute

$$u_i^* = \frac{1}{2}(u_{i-1} + u_{i+1} + h^2 f_i)$$

This is now only an intermediate step, and we define the new weighted iterate by

$$u_i^{(m+1)} = (1-\omega)u_i^{(m)} + \omega u_i^*, \qquad i \le j \le N-1$$

In matrix notation, we can express it by

$$\mathbf{u}^{(m+1)} = [(1 - \omega)\mathbf{I} + \omega S_J] \mathbf{u}^{(m)} + \omega D^{-1} \mathbf{f}^{(m)}$$
$$= (1 - \omega D^{-1}) A \mathbf{u}^m + \omega D^{-1} \mathbf{f}$$

Define R_{ω} : = $(I - \omega D^{-1}A)$

Eigenvectors and Eigenvalues

• The matrix is spd and sparse (not more than 3 non-zero entries per row and column).

• It has the eigenvalues $(\lambda_k \mathbf{w}_k = A\mathbf{w}_k)$

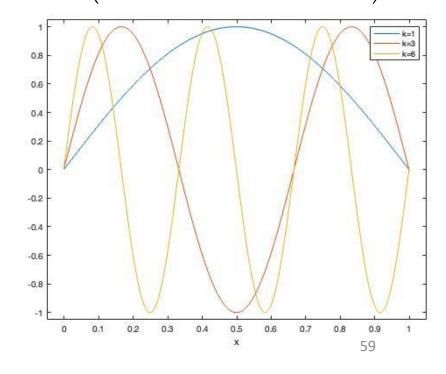
$$\lambda_k = \frac{4}{h^2} \sin^2 \left(\frac{k\pi}{2N} \right)$$

And the eigenvectors

$$(w_k)_j = \sin\left(\frac{jk\pi}{N}\right)$$

- This denotes the *j*-th component of the *k*-th eigenvector.
- The eigenvectors are Fourier modes.

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Definition

Modes in the upper half of the spectrum, i.e.

$$\frac{N}{2} \le k < N - 1$$

are called high-frequency or oscillatory modes.

Modes in the lower half of the spectrum, i.e.

$$1 \le k < \frac{N}{2}$$

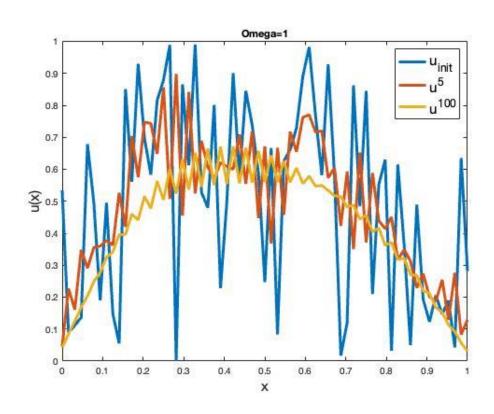
are called low-frequency or smooth modes.

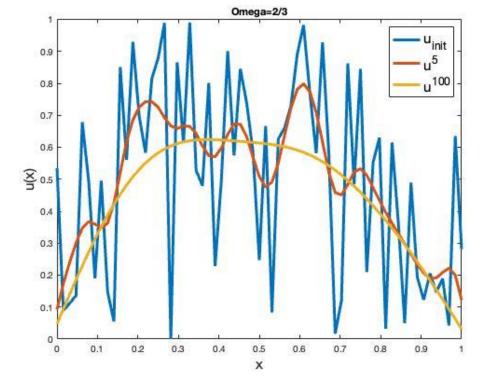
Note that the classification of smooth or oscillatory wave number depends on the total number N of grid points. A fixed wave number k might thus be smooth on one, but oscillatory on another grid.

Smoothing with Jacobi and weighted Jacobi

• Let f = 0 (thus solution u = 0). Then random initial guess \rightarrow random error

Méthodes Itératives





Jacobi $R = I - D^{-1}A$

Weighted Jacobi $R_{\omega} = I - \frac{2}{3}D^{-1}A$

Weighted Jacobi

- Let us use the four modes: k = 1, 3, 6, 48, as initial guess.
- Then smooth modes will dampen less quickly than higher ones.

