Scientific Computing

Lecture 7

Delft University of Technology

Vandana Dwarka and Kees Vuik

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Today

- Chapter 5:
  - Jacobi method
  - Gauss-Seidel (GS) method
  - Convergence
  - Block Jacobi/GS method
  - damped Jacobi/SOR

Recap: Basic Iterative Methods

Notation: u^k is the k-th iteration.

- Error: $e^k = u - u^k$
- Residual: $r^k = f - Au^k$
- Residual equation: $Ae^k = Au - Au^k = f - Au^k = r^k$

Splitting method: $A = M - N$.
$Au = f \Rightarrow Mu^{k+1} = f + Nu^k$
$u^{k+1} = M^{-1}f + M^{-1}Nu^k$

Substituting $N = M - A$ we get:

$$\begin{aligned} u^{k+1} &= M^{-1}f + M^{-1}(M - A)u^k \\ &= u^k + M^{-1}(f - Au^k) \\ &= u^k + M^{-1}(r^k) \end{aligned}$$

Recap: Convergence

Does this iterative scheme converge? I.e. $u^{k+1} \to u$ as k goes to infinity?

$$u^{k+1} = u^k + M^{-1}\left(f - Au^k\right)$$

$$u - u^{k+1} = u - u^k - M^{-1}\left(Au - Au^k\right)$$

$$e^{k+1} = e^k - M^{-1}Ae^k \Rightarrow e^{k+1} = \left(I - M^{-1}A\right)e^k$$

We define the iteration matrix $B = I - M^{-1}A$ such that:

$$e^{k+1} = B^k e^0$$

For convergence: $\lim_{k\to\infty}\left\|B^k\right\|_2 = 0$, which using theorem 2.7.2 is equivalent to:

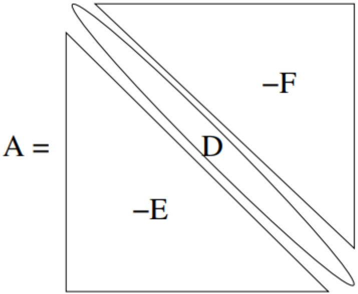
$$\lim_{k\to\infty}\left\|B^k\right\|_2 = 0 \Leftrightarrow \rho(B) < 1$$

§ 5.3: Prototypes

Different notation:

$$A = D - E - F \in \mathbb{R}^{n \times n}$$

where $D, -E$ and $-F$ denote the diagonal, the strictly lower and the strictly upper triangular part of A.



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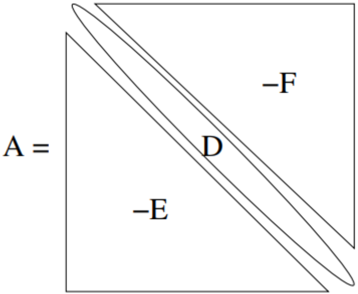

Using this, we can write:

$$\hat{E} = D^{-1}E \text{ and } \hat{F} = D^{-1}F.$$

§ 5.3.1: Jacobi

Example with 1D Poisson (BC eliminated)

$A \in \mathbb{R}^{3\times 3}$ with

$$A = \frac{1}{h^2}\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}, \quad f = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad u = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}$$

such that $Au = f$

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This is equivalent to:

$$\begin{aligned} 2u_1 - u_2 &= 1 \\ -u_1 + 2u_2 - u_3 &= 1 \\ -u_2 + 2u_3 &= 1 \end{aligned}$$

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But also to:

$$\begin{aligned} 2u_1 &= 1 + u_2 \\ 2u_2 &= 1 + u_1 + u_3 \\ 2u_3 &= 1 + u_2 \end{aligned}$$

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In an iterative scheme we can update using previous information!

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Using iteration k:

$$\begin{aligned} 2{u_1}^{k+1} &= 1 + {u_2}^k \\ 2{u_2}^{k+1} &= 1 + {u_1}^k + {u_3}^k \\ 2{u_3}^{k+1} &= 1 + {u_2}^k \end{aligned}$$

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Splitting notation:
$Mu^{k+1} = f + Nu^k$, with

$$M = \frac{1}{h^2}\begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}, N = \frac{1}{h^2}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

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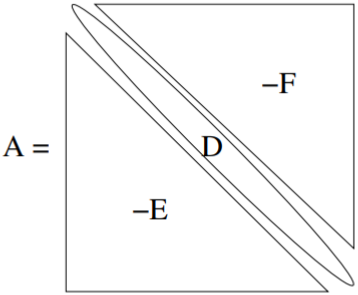

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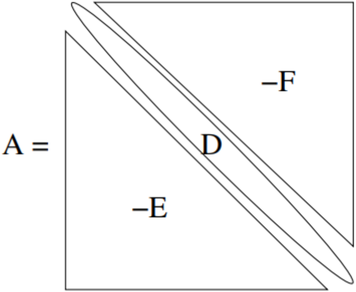

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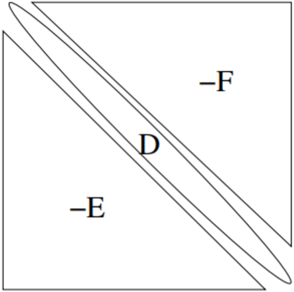
$A =$ 

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Jacobi:

$$2\mathbf{u_1}^{\mathbf{k+1}} = 1 + {u_2}^k$$
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Gauss-Seidel:

$$\begin{aligned} 2{u_1}^{k+1} &= 1 + {u_2}^k \\ -\mathbf{u_1}^{\mathbf{k+1}} + 2{u_2}^{k+1} &= 1 + {u_3}^k \\ -\mathbf{u_2}^{\mathbf{k+1}} + 2{u_3}^{k+1} &= 1 \end{aligned}$$

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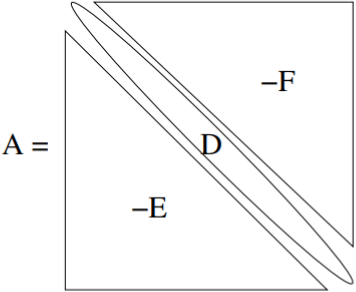

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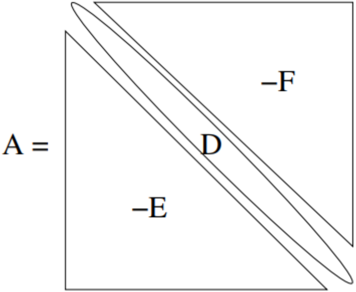

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§ 5.3.1: Jacobi and GS

Jacobi:

$$u^{k+1} = D^{-1}\left[(E+F)u^k + f\right]$$

Component wise update:

$$u_i^{k+1} = \left[f_i - \sum_{j=1, j\neq i}^{n} a_{ij} u_j^k\right] / a_{ii}$$

GS:

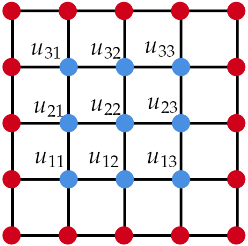
$$u^{k+1} = \hat{E}u^{k+1} + \hat{F}u^k + D^{-1}f$$

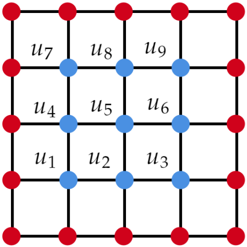
Component wise update:

$$u_i^{k+1} = \left[f_i - \sum_{j=1}^{i-1} a_{ij} u_j^{k+1} - \sum_{j=i+1}^{n} a_{ij} u_j^k\right] / a_{ii}$$

§ 5.3.1: Faster Convergence (Block methods)

Recall: x-line lexicographic ordering (2D)





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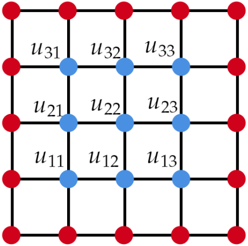
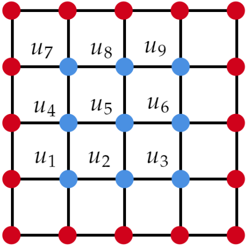
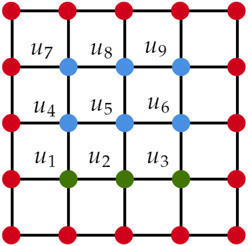




Update in blocks or 'aggregates' of *u* to accelerate convergence!

§ 5.3.1: Faster Convergence (Block methods)



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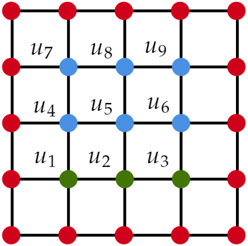

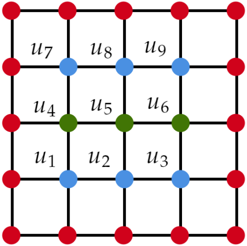

$$\hat{U}_1 = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} \qquad \hat{U}_2 = \begin{pmatrix} u_4 \\ u_5 \\ u_6 \end{pmatrix}$$

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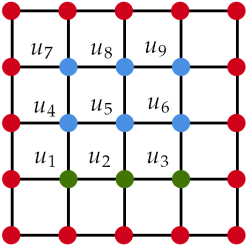

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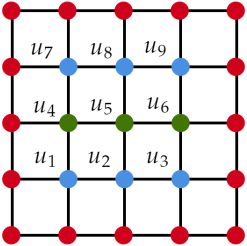
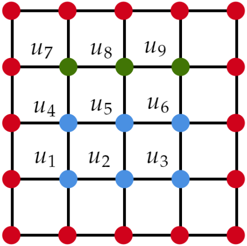


$$\hat{U}_2 = \begin{pmatrix} u_4 \\ u_5 \\ u_6 \end{pmatrix}$$



$$\hat{U}_3 = \begin{pmatrix} u_7 \\ u_8 \\ u_9 \end{pmatrix}$$

§ 5.3.1: Faster Convergence (Block methods)

Then $Au = f$ can be written as:

$$\left(\begin{array}{ccc} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{array}\right) \begin{pmatrix} \hat{U}_1 \\ \hat{U}_2 \\ \hat{U}_3 \end{pmatrix} = \begin{pmatrix} \hat{F}_1 \\ \hat{F}_2 \\ \hat{F}_3 \end{pmatrix}.$$

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For the 2D poisson problem with elim. (lecture 3, slide 7), we get:

$$A_{11} = A_{22} = A_{33} = \frac{1}{h^2} \begin{pmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{pmatrix},$$

$$A_{12} = A_{21} = A_{23} = A_{32} = \frac{1}{h^2} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$A_{13} = A_{31} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

§ 5.3.1: Faster Convergence (Block-Jacobi)

Block-Jacobi: $M = [A_{11}, A_{22}, A_{33}]$ (block-diagonal of A).

At iteration k:

$$
\begin{aligned}
A_{11}\hat{U}_1^{k+1} &= \hat{F}_1 - A_{12}\hat{U}_2^k \\
A_{22}\hat{U}_2^{k+1} &= \hat{F}_2 - A_{21}\hat{U}_1^k - A_{23}\hat{U}_3^k \\
A_{33}\hat{U}_3^{k+1} &= \hat{F}_3 - A_{32}\hat{U}_2^k
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§ 5.3.1: Faster Convergence (Block-Jacobi)

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A_{33}\hat{U}_3^{k+1} &= \hat{F}_3 - A_{32}\hat{U}_2^k
\end{aligned}
$$

Block wise update:

$$
\hat{U}_i^{k+1} = A_{i,i}^{-1}\left[F_i - \sum_{j=1, j\neq i}^{q} A_{i,j}\hat{U}_j^k\right] \quad \forall i = 1, \ldots, q
$$

§ 5.3.1: Error Propagation

For the iteration matrices $B_{JAC} = I - {M_{JAC}}^{-1}A$ and $B_{GS} = I - {M_{GS}}^{-1}A$, we get[1]

$$
\begin{aligned}
B_{JAC} &= I - D^{-1}(D - E - F) \\
&= I - I + D^{-1}E + D^{-1}F \\
&= \hat{E} + \hat{F},
\end{aligned}
$$

$$
\begin{aligned}
B_{GS} &= I - (D - E)^{-1}(D - E - F) \\
&= I - I + (D - E)^{-1}F \\
&= (D - E)^{-1}DD^{-1}F \\
&= (I - E)^{-1}\hat{F}
\end{aligned}
$$

[1] Note: $A = D - E - F$

§ 5.4.1: Convergence (General)

Theorem 5.4.1

$\rho(B) = \rho\left(I - M^{-1}A\right) < 1 \Leftrightarrow \left\{\mathbf{u}^k\right\}_{k=1}^{\infty}$ converges.

§ 5.4.1: Convergence (General)

Theorem 5.4.1

$\rho(B) = \rho\left(I - M^{-1}A\right) < 1 \Leftrightarrow \left\{\mathbf{u}^k\right\}_{k=1}^{\infty}$ converges.

Recall: iteration matrix $B = I - M^{-1}A$ defines error propagation:

$$e^{k+1} = B^k e^0$$

For convergence: $\lim_{k\to\infty} \left\|B^k\right\|_2 = 0$, which using theorem 2.7.2 is equivalent to:

$$\lim_{k\to\infty} \left\|B^k\right\|_2 = 0 \Leftrightarrow \rho(B) < 1$$

§ 5.4.4: Convergence (Jacobi)

Diagonal Dominance

Theorem 5.4.2

Theorem 5.4.2 Assume $A \in \mathbb{R}^{n \times n}$ to be strongly row diagonally dominant. Then the Jacobi and GaussSeidel method applied to A converge, i.e.,

$$\sum_{j=1, j \neq i}^{n} |a_{ij}| < |a_{ii}| \quad \forall i = 1, \ldots, n \Rightarrow \|B_{GS}\|_\infty \leq \|B_{JAC}\|_\infty < 1$$

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$\|B_{JAC}\|_\infty = \|\hat{E} + \hat{F}\|_\infty = \max_{1\leq i\leq n} \sum_{j=1,j\neq i}^{n} \frac{|a_{ij}|}{|a_{ii}|} < 1$ [row sum criterion]

§ 5.4.4: Convergence (GS)

Lemma 5.3.1 (Elementwise bound on the Gauss-Seidel)

Assume $A \in \mathbb{R}^{n \times n}$ and assume B_{GS} to be the Gauss-Seidel iteration matrix defined by (5.19). Then

$$|B_{GS}| \leq (I - |\hat{E}|)^{-1} |\hat{F}|$$

§ 5.3.2: Richardson and damped Jacobi

- Richardson: $M_{RICH} = I$ or $M = \tau I$
- Damped Jacobi: $M_{JAC(\omega)} = \frac{1}{\omega} D$

One can show equivalence of the methods with $\tau = \omega^{-1}$ applied to $D^{-1}Au = D^{-1}f$

§ 5.3.3: Successive overrelaxation (SOR)

- SOR: $M_{SOR} = \frac{1}{\omega} D - E$

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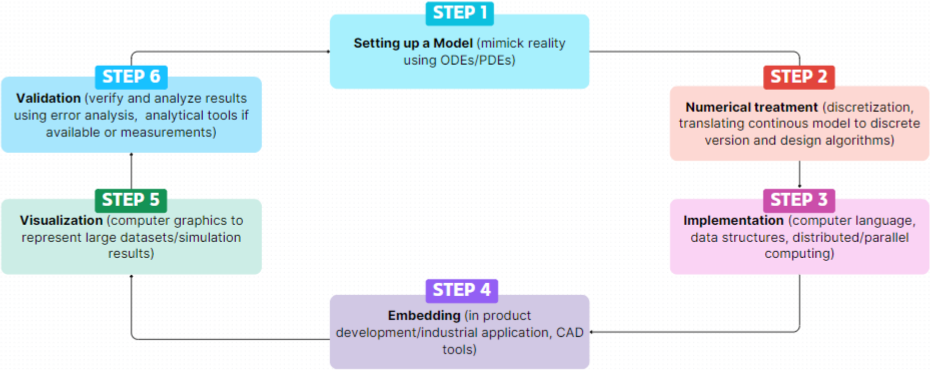
- SOR: $M_{SOR} = \frac{1}{\omega} D - E$

Note that this is GS with damping!

Summary (Part I of this course)



- Lecture 1-3 (step 1,2): elliptic problems, from PDE to $Au = f$ (discretization) and properties of the continuous/discrete problem

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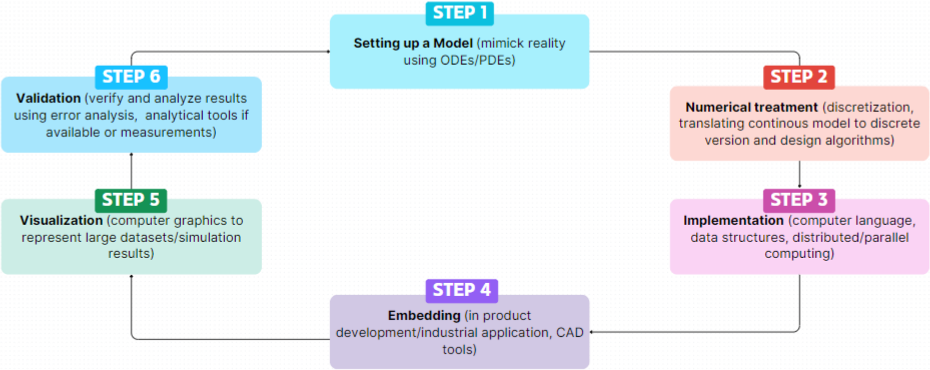

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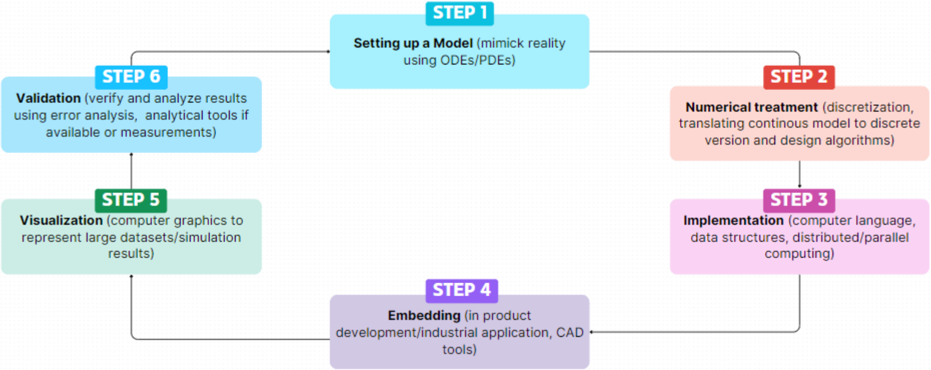

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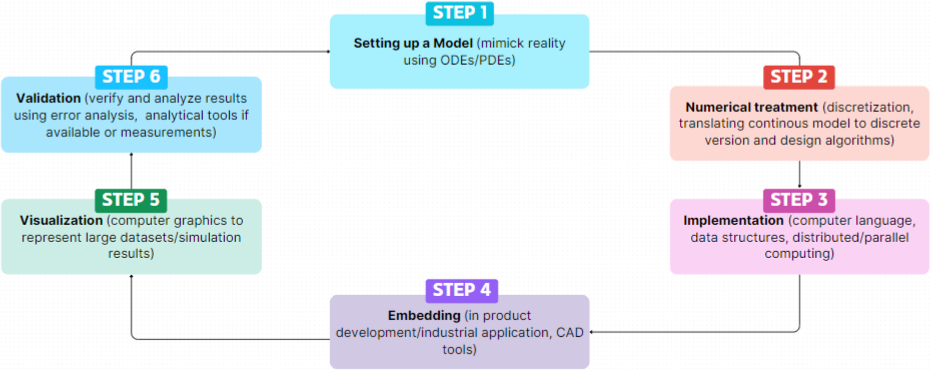

- Lecture 1-3 (step 1,2): elliptic problems, from PDE to $Au = f$ (discretization) and properties of the continuous/discrete problem
- Lecture 4 (step 6): metrics to perform validation steps (rounding errors, floating points, conditioning)
- Lecture 5-7 (step 2): design of algorithms to solve $Au = f$
  - Direct solvers (LU decomposition)
  - Basic iterative solvers (Jacobi, GS, Richardson)

Part II of this course

- Multigrid
- Krylov methods
- Power methods

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MSc. projects in our group ▸ (graduation)

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MSc. projects in our group (graduation)

- Machine learning, computational finance, discretization methods and iterative solvers.
- Projects with me: computational and sustainable finance, plasma fusion simulation, electromagnetics simulation