



Solving the linear system

Numerical Flow Simulation

École polytechnique fédérale de Lausanne

Edouard Boujo Fall 2022

Linear system

 After discretization (and linearization if needed), the conservation equation(s) yield a linear system to be solved:

$$\mathbf{A}\phi = \mathbf{b}$$

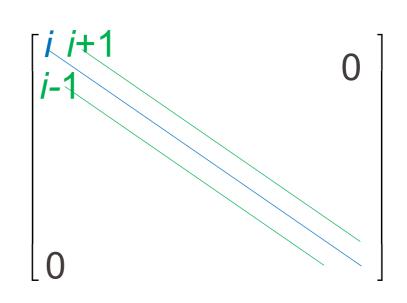
 $\mathbf{A}: n \times n \text{ matrix}$ $\phi, \mathbf{b}: n \times 1 \text{ vectors}$ $a_{i,j} \neq 0 \text{ if } \phi_i \text{ depends on } \phi_j$

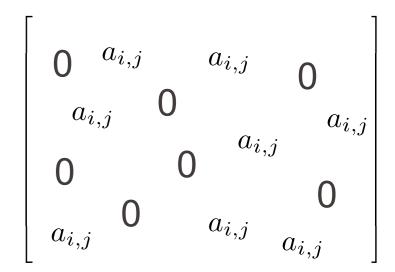
- The size *n* depends on:
 - the mesh: number of control volumes
 - the physical dimension: 1D/2D/3D
 - the equations: single vs. coupled (1 unknown vs. several unknowns)

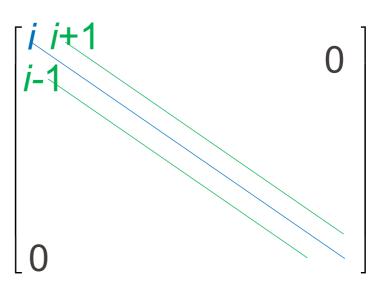
Linear system

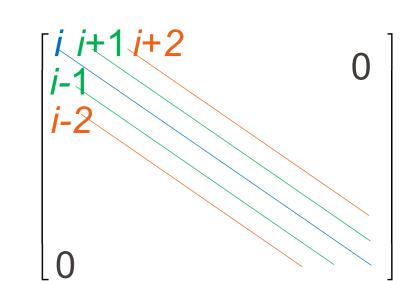
- The structure of the matrix **A** depends on:
 - The mesh: structured vs. unstructured
 - The equations that are solved (the order of the derivatives)
 - The discretization method: different schemes involve a different number of neighbors (e.g. UD vs. CD vs. QUICK, see week 2)
 - The physical dimension: 1D vs. 2D vs. 3D

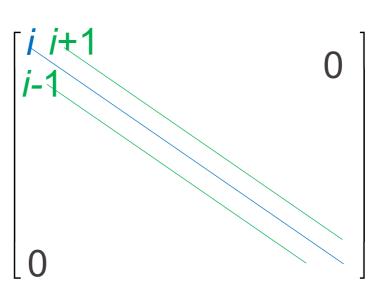
Solution methods depend on this structure.

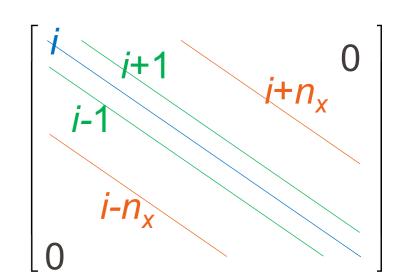












Direct vs. iterative methods

- Direct methods:
 - Build a series of equivalent exact systems
 - Compute the solution in a finite number of operations
 - Overall complexity generally $O(n^3)$
- Iterative methods:
 - Build a series of approximate solutions
 - May converge after an infinite number of steps
 - Complexity at each step generally $O(n^2)$
 - \rightarrow useful if practical number of steps is < n

$$\mathbf{A}\boldsymbol{\phi} = \mathbf{b} \begin{cases} a_{1,1}\phi_1 + a_{1,2}\phi_2 + \dots + a_{1,n}\phi_n = b_1 \\ a_{2,1}\phi_1 + a_{2,2}\phi_2 + \dots + a_{2,n}\phi_n = b_2 \\ \vdots \\ a_{n,1}\phi_1 + a_{n,2}\phi_2 + \dots + a_{n,n}\phi_n = b_n \end{cases}$$

- Naively:
 - Use eq. 1 to express ϕ_1 as function of $\phi_2 \dots \phi_n$
 - Substitute in other eqs. (2... n)
 - Repeat with $\phi_2, \phi_3 \dots$ until ϕ_n is known explicitly
 - Substitute back into eq. n-1 to get ϕ_{n-1} , eq. n-2 to get ϕ_{n-2} ,... eq. 1 to get ϕ_1
- Systematically: find suitable linear combinations of rows to eliminate variables successively
 - Step 1: "forward elimination" to make the system triangular
 - Step 2: "backward substitution" to solve the triangular system

$$\mathbf{A}\boldsymbol{\phi} = \mathbf{b} \begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{n,1} & a_{n,2} & a_{n,3} & \cdots & a_{n,n} \end{bmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

- Step 1: "forward elimination"
 - 1. Replace each row i>1 of A by $(row i) \frac{a_{i,1}}{a_{1,1}}(row 1)$
 - i.e. define new coefficients and rhs: $a_{i,j}^{(1)} = a_{i,j} \frac{a_{i,1}}{a_{1,1}} a_{1,j}$ $b_i^{(1)} = b_i \frac{a_{i,1}}{a_{1,1}} b_1$

$$\begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\ 0 & a_{2,2} - \frac{a_{2,1}}{a_{1,1}} a_{1,2} & a_{2,3} - \frac{a_{2,1}}{a_{1,1}} a_{1,3} & \cdots & a_{2,n} - \frac{a_{2,1}}{a_{1,1}} a_{1,n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & a_{n,2} - \frac{a_{n,1}}{a_{1,1}} a_{1,2} & a_{n,3} - \frac{a_{n,1}}{a_{1,1}} a_{1,3} & \cdots & a_{n,n} - \frac{a_{n,1}}{a_{1,1}} a_{1,n} \end{bmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 - \frac{a_{n,1}}{a_{1,1}} b_1 \\ \vdots \\ b_n - \frac{a_{2,1}}{a_{1,1}} b_1 \end{pmatrix}$$

$$\mathbf{A}^{(1)}\boldsymbol{\phi} = \mathbf{b}^{(1)}$$

$$\mathbf{A}^{(1)}\boldsymbol{\phi} = \mathbf{b}^{(1)} \begin{bmatrix} a_{1,1}^{(1)} & a_{1,2}^{(1)} & \cdots & a_{1,n}^{(1)} \\ 0 & a_{2,2}^{(1)} & \cdots & a_{2,n}^{(1)} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & a_{n,2}^{(1)} & \cdots & a_{n,n}^{(1)} \end{bmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_n \end{pmatrix} = \begin{pmatrix} b_1^{(2)} \\ b_2^{(2)} \\ \vdots \\ b_n^{(2)} \end{pmatrix}$$

- Step 1: "forward elimination"
- 2. Replace each row i > 2 of $\mathbf{A}^{(1)}$ by $(\text{row } i) \frac{a_{i,2}^{(1)}}{a_{2,2}^{(1)}}(\text{row } 2)$ i.e. define new coefficients and rhs: $a_{i,j}^{(2)} = a_{i,j}^{(1)} \frac{a_{i,2}^{(1)}}{a_{2,2}^{(1)}}a_{2,j}^{(1)}$ $b_i^{(2)} = b_i^{(1)} \frac{a_{i,2}^{(1)}}{a_{2,2}^{(1)}}b_2^{(1)}$

$$a_{i,j}^{(2)} = a_{i,j}^{(1)} - \frac{a_{i,2}^{(1)}}{a_{2,2}^{(1)}} a_{2,j}^{(1)}$$

$$b_i^{(2)} = b_i^{(1)} - \frac{a_{i,2}^{(1)}}{a_{2,2}^{(1)}} b_2^{(1)}$$

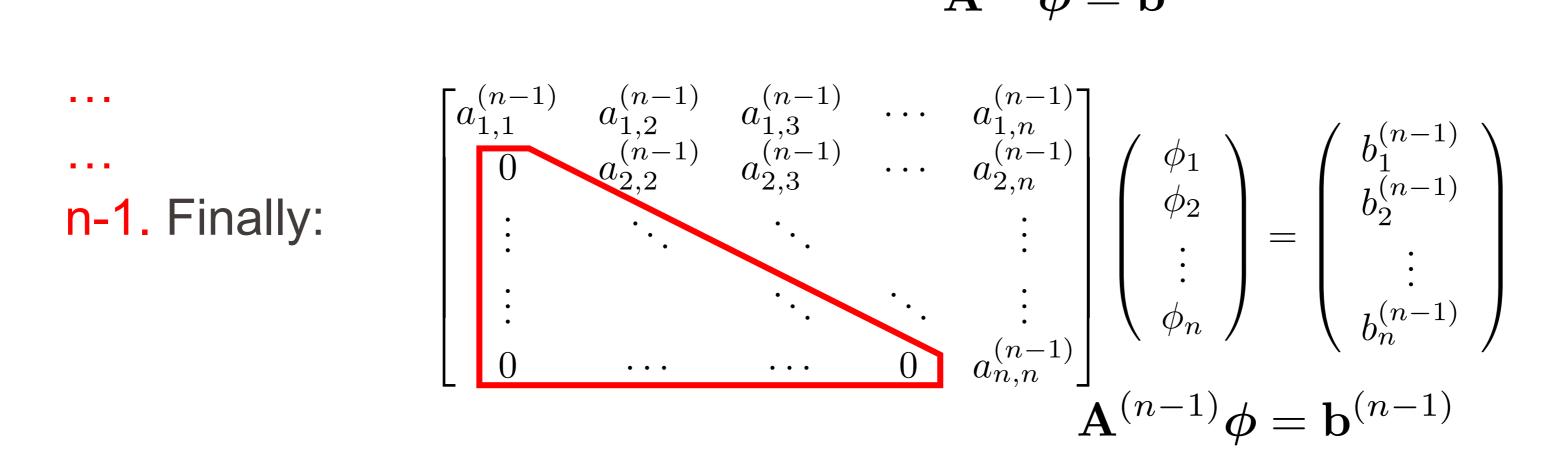
$$\begin{bmatrix} a_{1,1}^{(2)} & a_{1,2}^{(2)} & a_{1,3}^{(2)} & \cdots & a_{1,n}^{(2)} \\ 0 & a_{2,2}^{(2)} & a_{2,3}^{(2)} & \cdots & a_{2,n}^{(2)} \\ \vdots & 0 & \vdots & \vdots & \vdots \\ 0 & \vdots & \vdots & \vdots & \vdots \\ 0 & a_{n,3}^{(2)} & \cdots & a_{n,n}^{(2)} \end{bmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_n \end{pmatrix} = \begin{pmatrix} b_1^{(2)} \\ b_2^{(2)} \\ \vdots \\ b_n^{(2)} \end{pmatrix}$$

$$\mathbf{A}^{(2)}\boldsymbol{\phi} = \mathbf{b}^{(2)}$$

$$\mathbf{A}^{(k-1)}\boldsymbol{\phi} = \mathbf{b}^{(k-1)}$$

Step 1: "forward elimination"

k. Replace each row
$$i > k$$
 of $\mathbf{A}^{(k-1)}$ by $(\operatorname{row} i) - \frac{a_{i,k}^{(k-1)}}{a_{k,k}^{(k-1)}}(\operatorname{row} k)$ i.e. define: $a_{i,j}^{(k)} = a_{i,j}^{(k-1)} - \frac{a_{i,k}^{(k-1)}}{a_{k,k}^{(k-1)}} a_{k,j}^{(k-1)}$ $b_i^{(k)} = b_i^{(k-1)} - \frac{a_{i,k}^{(k-1)}}{a_{k,k}^{(k-1)}} b_k^{(k-1)}$ $\mathbf{A}^{(k)} \phi = \mathbf{b}^{(k)}$

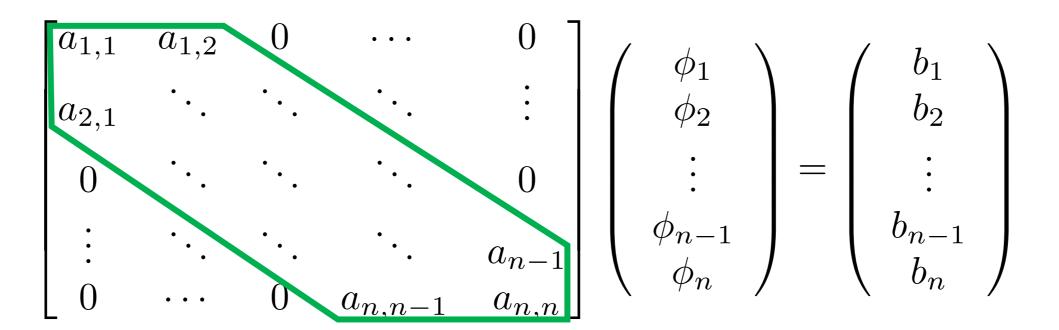


$$\mathbf{A}^{(n-1)}\boldsymbol{\phi} = \mathbf{b}^{(n-1)} \quad \begin{bmatrix} a_{1,1}^{(n-1)} & a_{1,2}^{(n-1)} & a_{1,3}^{(n-1)} & \cdots & a_{1,n}^{(n-1)} \\ 0 & a_{2,2}^{(n-1)} & a_{2,3}^{(n-1)} & \cdots & a_{2,n}^{(n-1)} \\ \vdots & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & 0 & a_{n,n}^{(n-1)} \end{bmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_n \end{pmatrix} = \begin{pmatrix} b_1^{(n-1)} \\ b_2^{(n-1)} \\ \vdots \\ b_n^{(n-1)} \end{pmatrix}$$

- Step 2: "backward substitution" to solve the triangular system
 - Row n: $\phi_n = \frac{b_n}{a_{m,n}}$ (omit superscript (n-1))
 - Row *n*-1: $\phi_{n-1} = \frac{b_{n-1} a_{n-1,n}\phi_n}{a_{n-1,n-1}}$
 - Row i: $\phi_i = \frac{1}{a_{i,i}} \left(b_i \sum_{k=i+1}^n a_{i,k} \phi_k \right)$
- Complexity $O(n^3)$ → not practical for large systems.

Direct methods: TDMA algorithm

- "TriDiagonal Matrix Algorithm" (also called Thomas algorithm)
- Particular case of Gaussian elimination for tridiagonal systems (suitable for 1D problems)



• Complexity O(n)

Direct methods: TDMA algorithm

$$\begin{bmatrix} a_{1,1} & a_{1,2} & 0 & \cdots & 0 \\ a_{2,1} & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & a_{n-1} \\ 0 & \cdots & 0 & a_{n,n-1} & a_{n,n} \end{bmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_{n-1} \\ \phi_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_{n-1} \\ b_n \end{pmatrix}$$

- Step 1: forward elimination

• Express
$$\phi_1$$
 as fct of ϕ_2 : $\phi_1 = \frac{b_1 - a_{1,2}\phi_2}{a_{1,1}} = P_1\phi_2 + Q_1$

• Express ϕ_2 as fct of ϕ_3 :

$$a_{2,2}\phi_2 = b_2 - a_{2,1}\phi_1 - a_{2,3}\phi_3$$

$$a_{2,2}\phi_2 = b_2 - a_{2,1}\phi_1 - a_{2,3}\phi_3$$

$$p_2 = \frac{b_2 - a_{2,1}Q_1 - a_{2,3}\phi_3}{a_{2,2} + a_{2,1}P_1}$$

$$p_3 = \frac{-a_{2,3}}{a_{2,2} + a_{2,1}P_1}$$

$$Q_4 = \frac{b_2 - a_{2,1}Q_1 - a_{2,3}\phi_3}{a_{2,2} + a_{2,1}P_1}$$

- Express ϕ_i :
- Obtain finally:

 $\phi_i = P_i \phi_{i+1} + Q_i$

$$\phi_n = Q_n = \frac{b_n - a_{n,n-1}Q_{n-1}}{a_{n,n} + a_{n,n-1}P_{n-1}}$$

$$P_1 = -\frac{a_{1,2}}{a_{1,1}}$$

$$Q_1 = \frac{b_1}{a_{1,1}}$$

$$P_2 = \frac{-a_{2,3}}{a_{2,2} + a_{2,1}P_1}$$

$$Q_2 = \frac{b_2 - a_{2,1}Q_1}{a_{2,2} + a_{2,1}P_1}$$

$$P_{i} = \frac{-a_{i,i+1}}{a_{i,i} + a_{i,i-1}P_{i-1}}$$

$$Q_{i} = \frac{b_{i} - a_{i,i-1}Q_{i-1}}{a_{i,i} + a_{i,i-1}P_{i-1}}$$

Direct methods: TDMA algorithm

$$\begin{bmatrix} a_{1,1} & a_{1,2} & 0 & \cdots & 0 \\ a_{2,1} & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & a_{n-1} \\ 0 & \cdots & 0 & a_{n,n-1} & a_{n,n} \end{bmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_{n-1} \\ \phi_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_{n-1} \\ b_n \end{pmatrix}$$

• Step 2: backward substitution $\phi_n = Q_n$

$$\phi_n = Q_n$$

$$\phi_{n-1} = P_{n-1}\phi_n + Q_{n-1}$$

$$\cdots$$

$$\phi_i = P_i\phi_{i+1} + Q_i$$

$$\cdots$$

$$\phi_1 = P_1\phi_2 + Q_1$$

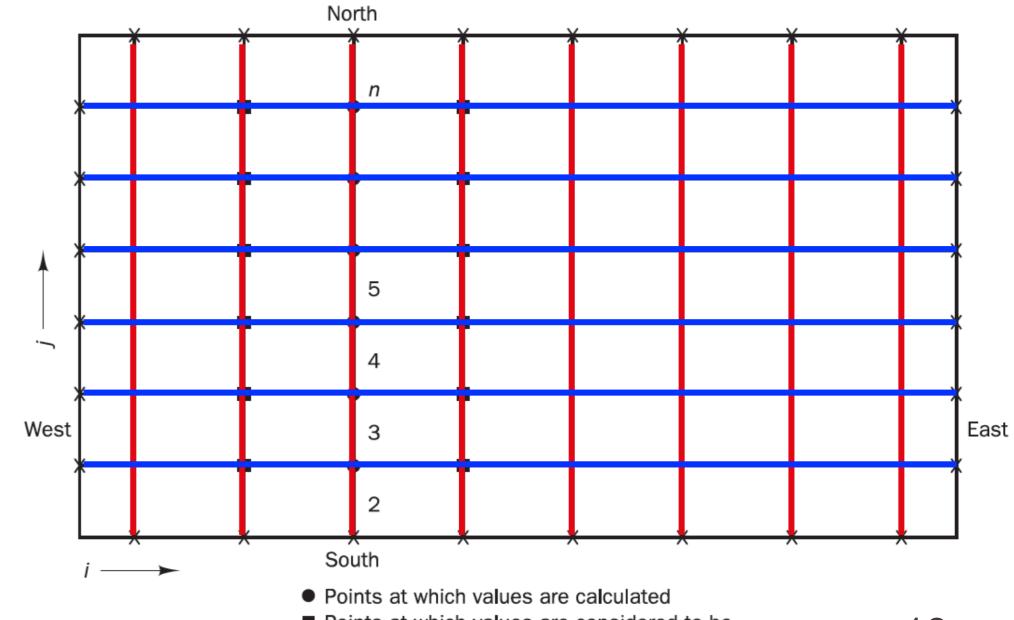
- Algorithm:
 - Compute P_1 , Q_1 , then P_2 , Q_2 , etc.
 - Set $\phi_n = Q_n$
 - Compute ϕ_{n-1} , then ϕ_{n-2} , etc.

TDMA extended to 2D/3D problems

- TDMA can be applied iteratively to 2D/3D structured meshes
- First applied in 1D along one line, e.g. in the North-South direction:

rewrite
$$a_P\phi_P=a_W\phi_W+a_E\phi_E+a_S\phi_S+a_N\phi_N+b$$
 as $a_P\phi_P=a_S\phi_S+a_N\phi_N+(b+a_W\phi_W^*+a_E\phi_E^*)$ with guess values for W, E

- Repeat for all N-S lines, sweeping the domain from W to E.
- Repeat for all W-E lines, sweeping the domain from S to N.
- Iterate, alternating the line/sweep directions to improve the propagation of boundary conditions within the domain.



Points at which values are considered to be temporarily known

X Known boundary values

Iterative methods

- Build a series of approximate solutions $\phi^{(k)}$ to the actual system $\mathbf{A}\phi = \mathbf{b}$
- Error vector: $e^{(k)} = \phi \phi^{(k)}$ (but generally the true solution is unknown)
- Residual vector: $\mathbf{r}^{(k)} = \mathbf{A} \boldsymbol{\phi}^{(k)} \mathbf{b}$ (useful: can actually be computed)
- Convergence: $\lim_{k\to\infty} ||\mathbf{e}^{(k)}|| = \mathbf{0}$ $\lim_{k\to\infty} ||\mathbf{r}^{(k)}|| = 0$
- Convergence can be assessed with different criteria: $||\phi^{(k)} \phi^{(k-1)}|| \quad \text{or} \quad \frac{||\phi^{(k)} \phi^{(k-1)}||}{||\phi^{(k-1)}||} < \text{tol}$

 - Absolute residual: $||\mathbf{r}^{(k)}|| < \text{tol}$
 - Normalized residual (most common): $\frac{||\mathbf{r}^{(k)}||}{||\mathrm{diag}(\mathbf{A})\boldsymbol{\phi}^{(k)}||} \quad \text{or} \quad \frac{||\mathbf{r}^{(k)}||}{||\mathbf{r}^{(k_0)}||} < \mathrm{tol}$ $2 \le k_0 \lesssim 10$

Typically use
$$L^1$$
 norm $||\mathbf{x}|| = \sum_{i=1}^n |x_i|$ or $||\mathbf{x}|| = \frac{1}{n} \sum_{i=1}^n |x_i|$

Point-iterative methods

• At each iteration, solve each equation i for ϕ_i , using guess values ϕ_j^* for the other unknows:

Jacobi method: guess value taken from previous iteration.

$$\phi_i^{(k)} = \frac{1}{a_{i,i}} \left(b_i - \sum_{j \neq i} a_{i,j} \phi_j^{(k-1)} \right)$$

Point-iterative methods

 Gauss-Seidel method: guess value taken from previous or current iteration, using the most recently updated one.

$$\phi_i^{(k)} = \frac{1}{a_{i,i}} \left(b_i - \sum_{j < i} a_{i,j} \phi_j^{(k)} - \sum_{j > i} a_{i,j} \phi_j^{(k-1)} \right)$$

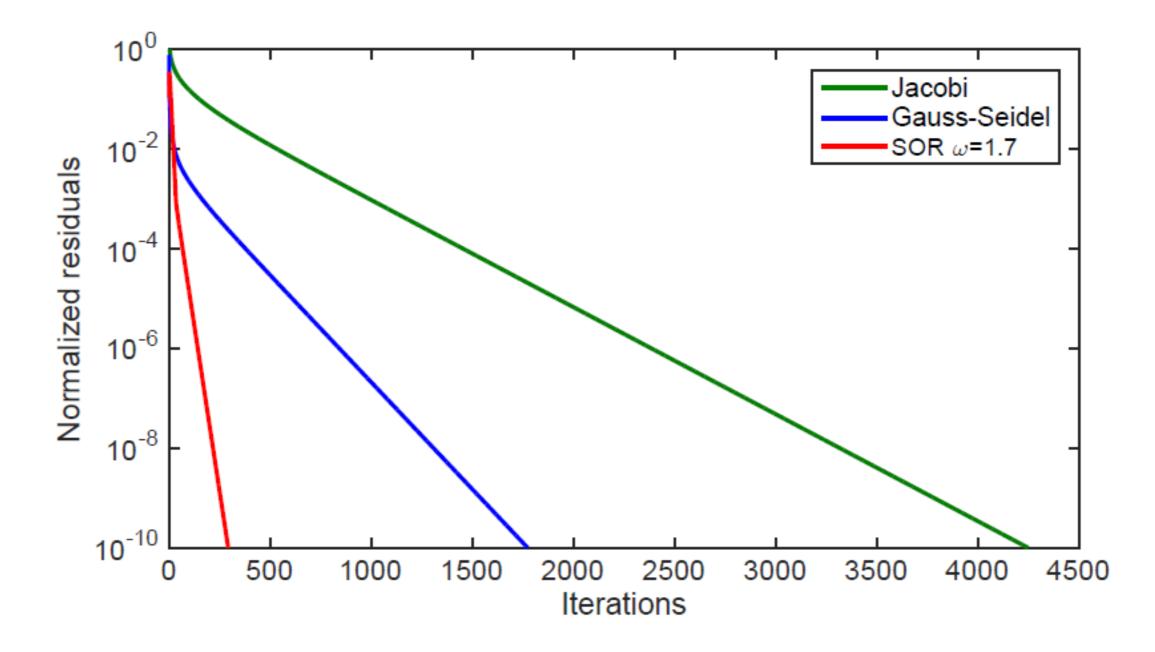
- Both Jacobi and GS require $O(n^2)$ iterations. GS often faster than Jacobi.
- Successive Over-Relaxation (SOR) method:

$$\phi_i^{(k)} = (1 - \omega)\phi_i^{(k-1)} + \frac{\omega}{a_{i,i}} \left(b_i - \sum_{j < i} a_{i,j} \phi_j^{(k)} - \sum_{j > i} a_{i,j} \phi_j^{(k-1)} \right) \qquad 0 < \omega < 2$$

- $\omega > 1$: can speed up convergence
- $\omega < 1$: can stabilize the iterative procedure if needed
- Optimal value of ω is case-dependent.

Point-iterative methods

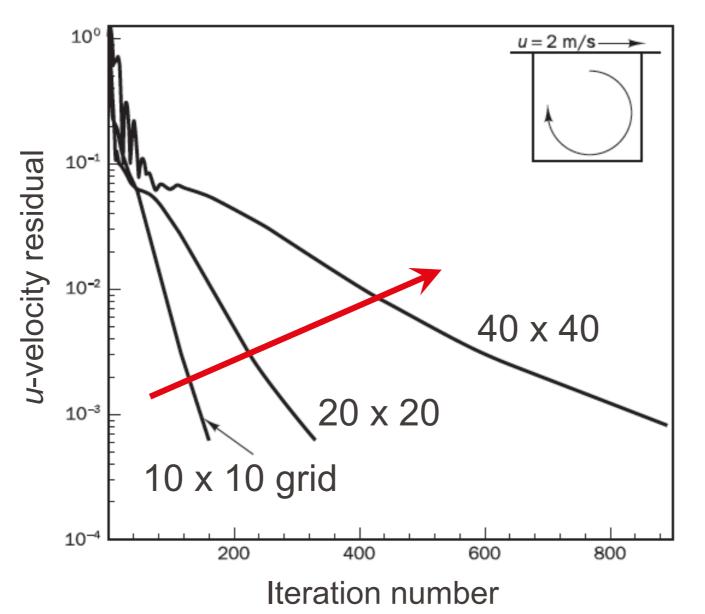
Example: 1D steady diffusion, Dirichlet BCs, *n*=33 (see week 2)



Still need hundreds of iterations, for a small number of unknows...
Can we do even faster?

Two observations about iterative methods:

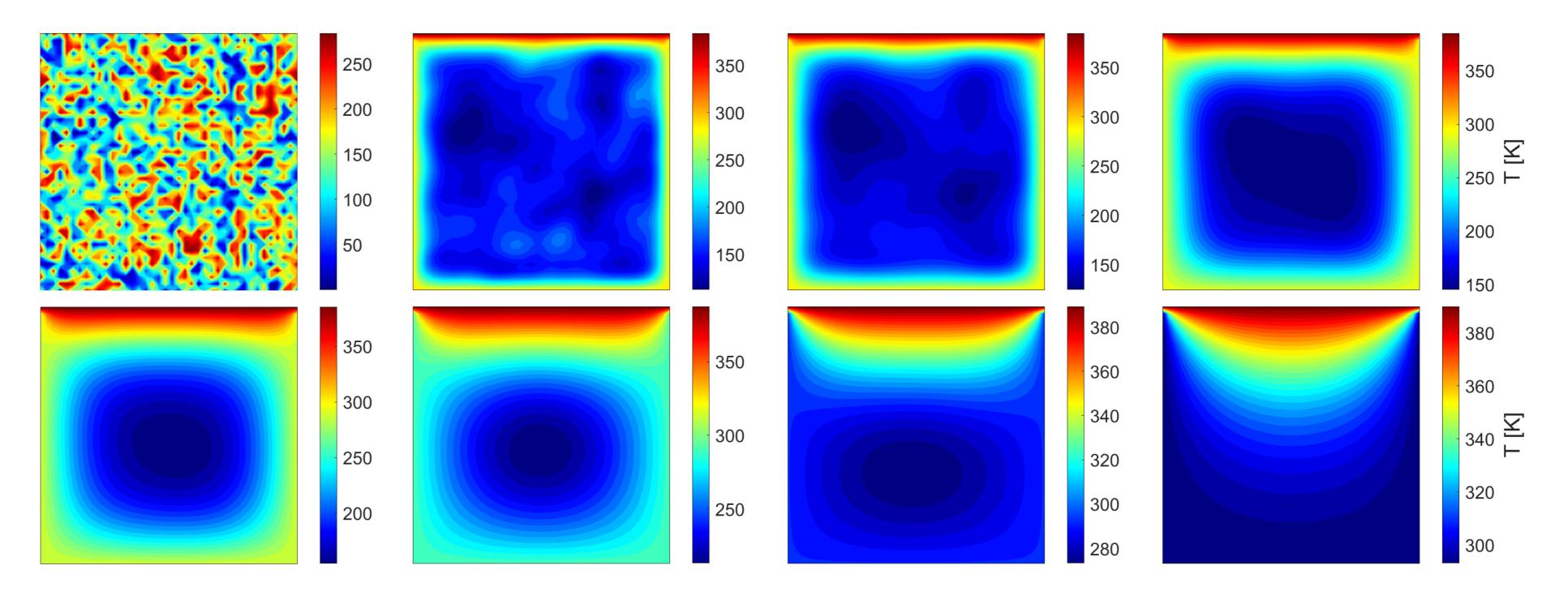
1. Finer mesh: more accurate solution (smaller final error), but slower convergence (more iterations needed to decrease the residuals, and each iteration is more expensive).



Example: flow in a lid-driven cavity

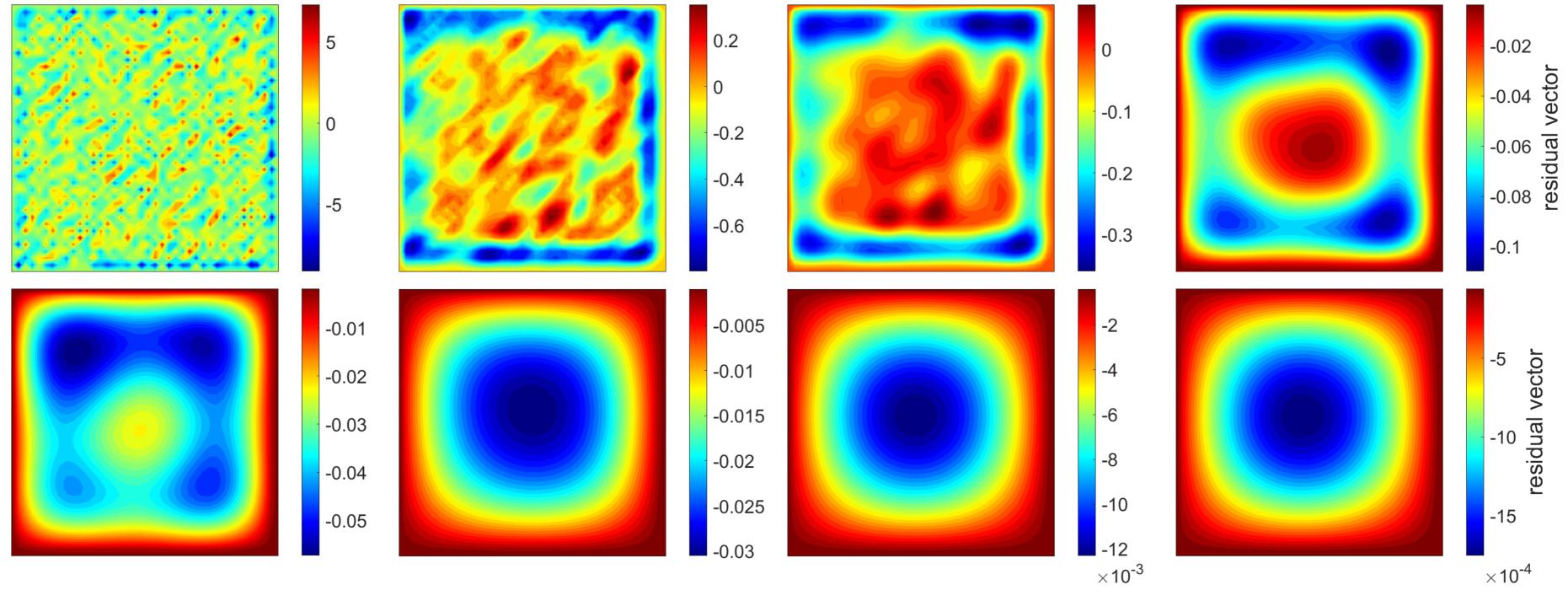
Two observations about iterative methods:

2. Consider this example (2D steady diffusion; see week 2). What do we observe?



Two observations about iterative methods:

2. Consider this example (2D steady diffusion; see week 2). What do we observe?

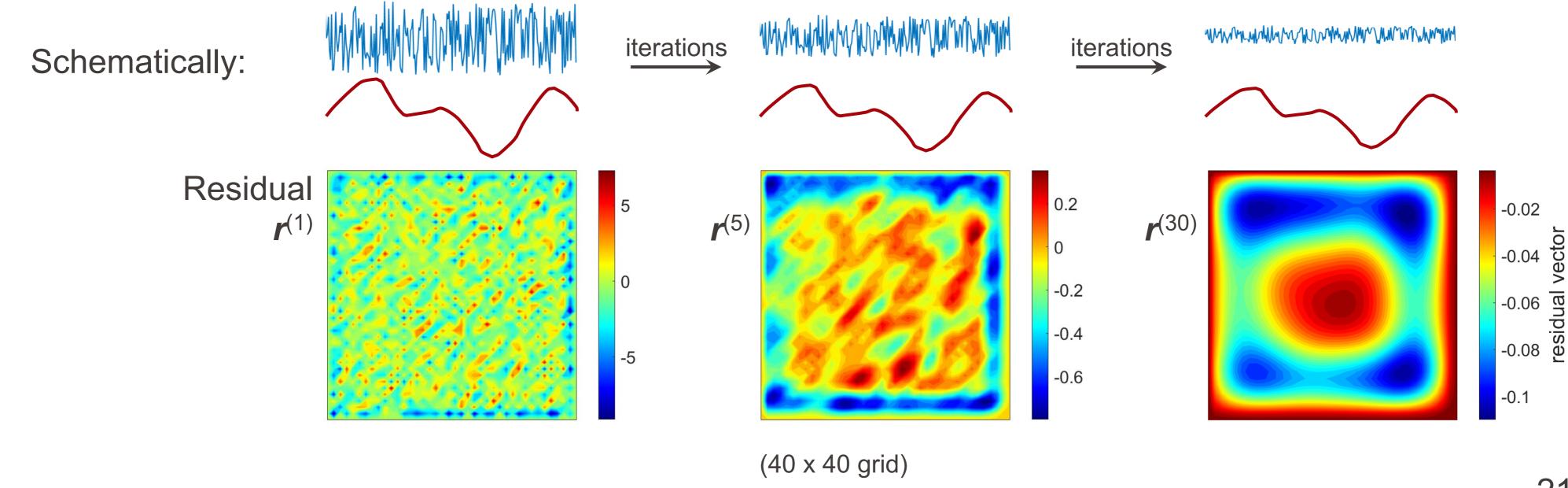


Residual vector $r^{(k)} = AT^{(k)} - b$

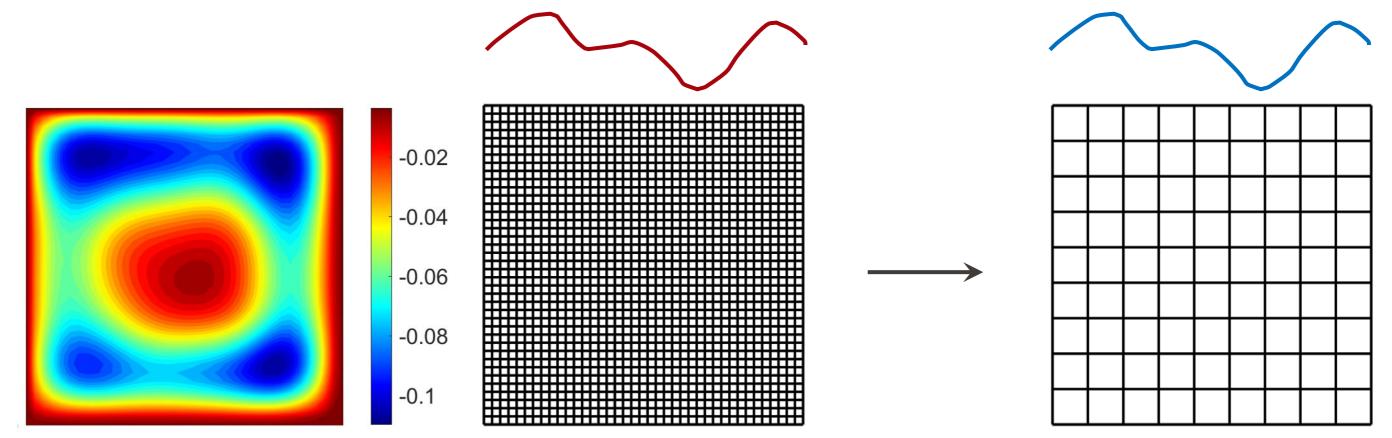
(40 x 40 grid, iterations *k*=1, 5, 10, 30, 60, 150, 300, 600)

Two observations about iterative methods:

2. These methods only have a local effect: they quickly reduce the short-wavelength components of the error (wavelengths comparable to the mesh size), but they act slowly on long wavelengths.



• If we change to a **coarser** grid, the long-wavelength error becomes a "short" wavelength (comparable to the mesh size). "Smooth becomes rough".

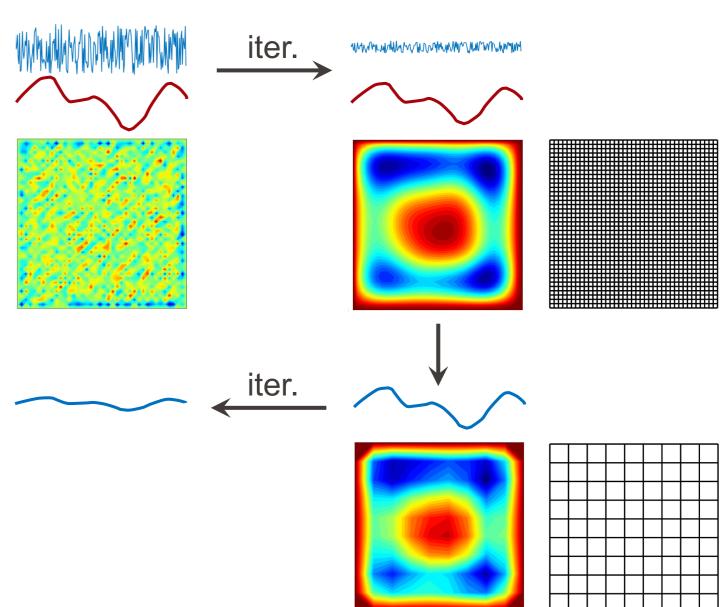


 Now, on this coarser grid, the short-wavelength error can be reduced very quickly.

• Multigrid idea: combine iterations on meshes of different sizes. Schematically:

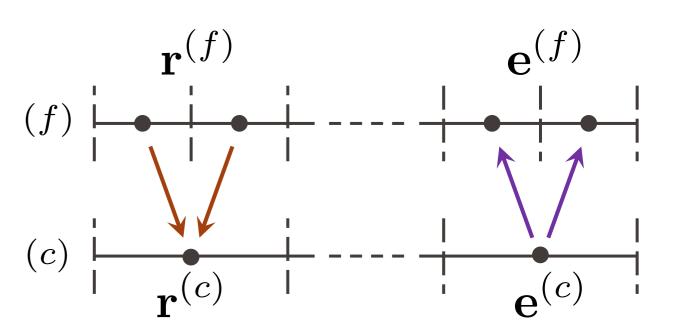
Initial solution on original fine mesh
 → quickly reduce short-wavelength error.

 Propagate on coarse mesh → quickly reduce the original long-wavelength error (which is now a short wavelength).



Come back to original fine mesh → improve final accuracy.

System to be solved (on fine mesh): $\mathbf{A}^{(f)}\phi = \mathbf{b}$



- Initial fine-mesh iterations:
 - A few steps only (e.g. GS) \rightarrow approximate solution $\phi^{(f)}$
 - Compute the residual from $\mathbf{A}^{(f)}\phi^{(f)} = \mathbf{b} \mathbf{r}^{(f)}$
 - Note that the error $e^{(f)} = \phi \phi^{(f)}$ satisfies $A^{(f)}e^{(f)} = r^{(f)}$
- Restriction + coarse-mesh iterations:
 - Transfer the residual to the coarser mesh (interpolation): ${f r}^{(c)}$
 - Solve for the error, which satisfies $\mathbf{A}^{(c)}\mathbf{e}^{(c)}=\mathbf{r}^{(c)}$
- Prolongation:
 - Transfer back the error to the finer mesh (interpolation): $\mathbf{e}^{(f)}$
- Update $\phi_{new}^{(f)} = \phi^{(f)} + \mathbf{e}^{(f)}$; perform a few fine-mesh iterations $\mathbf{A}^{(f)}\phi = \mathbf{b}$
- Repeat the whole process until convergence.

Examples of restriction/prolongation operators on uniform 1D meshes:

5-CV and 9-CV meshes

$$R^{(0)} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & 0 & 0 & 0 & 1 \end{pmatrix}$$

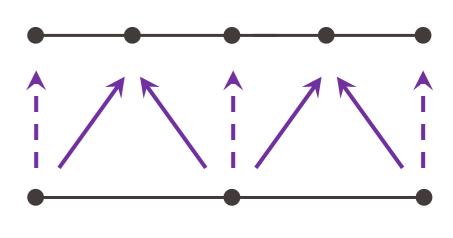
$$R^{(1)} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$T^{(1)} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

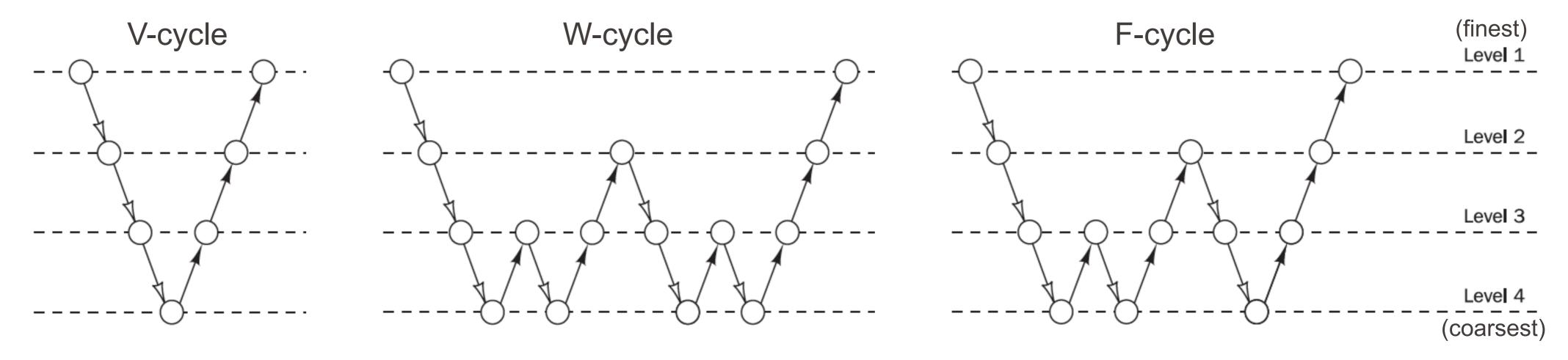
3-CV and 5-CV meshes

$$R^{(1)} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$T^{(2)} = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 1 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & 1 \end{pmatrix}$$

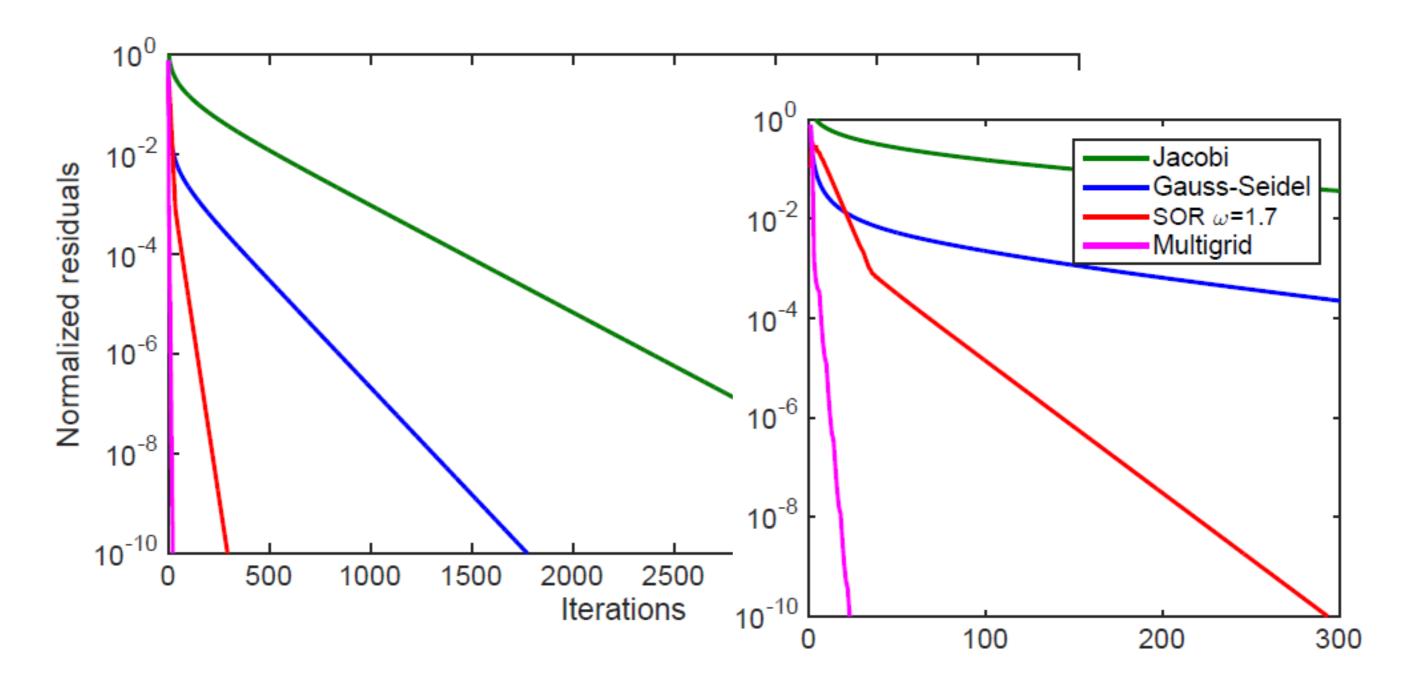


- Can use more than 2 meshes:
 - At each level *i*, solve for the error of the equation solved at level *i*-1.
 - Use only a few iterations, except on the coarsest mesh (full solution).
- Can use different types of cycles:



Coarse-grid iterations are comparatively very cheap.

Example: 1D steady diffusion, Dirichlet BCs, *n*=33 (see week 2)



 Multigrid methods require much less fine-mesh iterations than singlegrid iterative methods. Widely used in CFD, including in Fluent.

In Fluent:

