Mathematical modelling in science and engineering

Lecture 3
Finite element solution procedures

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Finite element formulation for stationary heat transfer problems

- For differential formulation of the form (with zero Dirichlet BC only, for simplicity):

$$-\nabla \cdot (k(T,\boldsymbol{x})\nabla T) = s$$

- The following weak statement can be derived:

Find approximate function $T^h \in V_T^h$, such that the following statement:

$$\int_\Omega k(T^h,\boldsymbol{x})T^h_{,i}w^h_{,i}d\Omega = \int_\Omega sw^h d\Omega$$

holds for every test function $w^h \in V_w^h$.

- For material properties being the function of $\boldsymbol{x}$ only, the problem is (quasi-)linear
- For material properties being the function of T as well, the problem has material non-linearity

Finite element formulation for stationary heat transfer problems

- Adding Neumann and Robin boundary conditions:

$$-k(T^h,\boldsymbol{x})\frac{dT}{d\boldsymbol{n}} = -k(T^h,\boldsymbol{x})T_{,i}n_i = -q_N \qquad \text{on} \qquad \Gamma_N$$

$$-k(T^h,\boldsymbol{x})\frac{dT}{d\boldsymbol{n}} = -k(T^h,\boldsymbol{x})T_{,i}n_i = c(T^h,\boldsymbol{x})(T-T_{ext}) \qquad \text{on} \qquad \Gamma_R$$

- Lead to the formulation with additional terms:

Find approximate function $T^h \in V_T^h$, such that the following statement:

$$\int_\Omega k(T^h,\boldsymbol{x})T^h_{,i}w^h_{,i}d\Omega = \int_\Omega sw^h d\Omega + \int_{\Gamma_N} q_N w^h d\Gamma - \int_{\Gamma_R} c(T-T_{ext})w^h d\Gamma$$

holds for every test function $w^h \in V_w^h$

Finite element formulation for stationary heat transfer problems

- The final formulation for linear stationary heat transfer problems:

Find approximate function $T^h \in V_T^h$, such that the following statement:

$$\int_\Omega kT^h_{,i} w^h_{,i} d\Omega + \int_{\Gamma_R} cTw^h d\Gamma = \int_\Omega sw^h d\Omega + \int_{\Gamma_N} q_N w^h d\Gamma + \int_{\Gamma_R} cT_{ext} w^h d\Gamma$$

holds for every test function $w^h \in V_w^h$

- ... leads to the following formulae for the entries of the global stiffness matrix and the global load vector

$$\mathrm{A}_{ML} = \int_\Omega k \frac{d\psi_M}{dx_i} \frac{d\psi_L}{dx_i} d\Omega + \int_{\Gamma_R} c\psi_M \psi_L d\Gamma$$

$$\mathrm{b}_M = \int_\Omega s\psi_M d\Omega + \int_{\Gamma_N} q_N \psi_M d\Gamma + \int_{\Gamma_R} cT_{ext} \psi_M d\Gamma$$

Finite element systems of linear equations

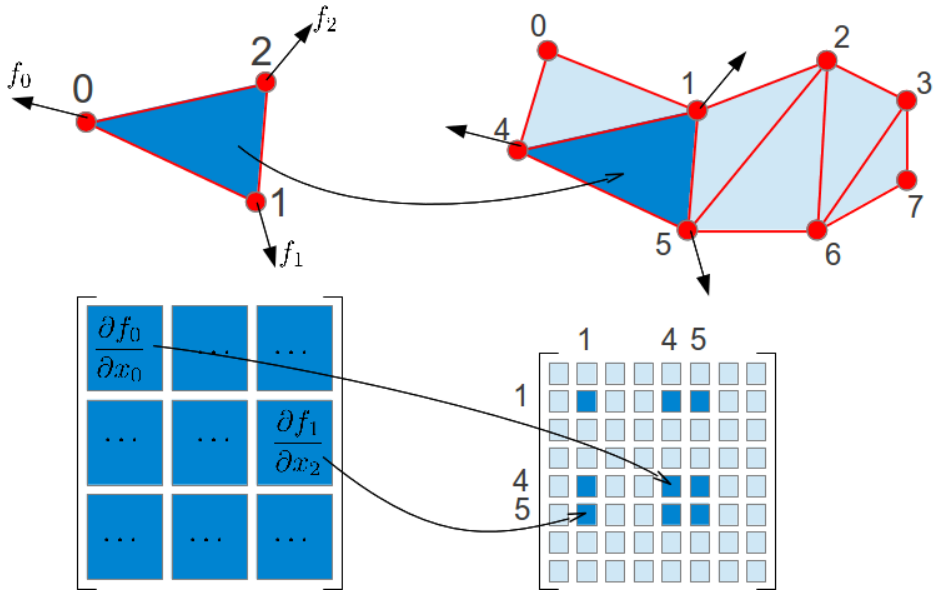
- Standard discretizations for linear stationary problems require the solution of a system of linear equations

$$\sum_{L=1}^{N} \mathrm{A}_{ML}\mathrm{U}_L^h = \mathrm{b}_M \qquad M = 1, 2, ..., N \qquad \equiv \qquad \mathbf{A}\mathbf{U}^h = \mathbf{b}$$

  - for non-stationary problems and implicit time integration a system of linear equations is solved at every time step
  - for non-linear problems a system of linear equations is solved for every iteration of the solution method
- The procedures for solving a linear system include
  - the creation of the system of linear equations that includes the integration of the terms from the weak statement for suitable pairs of basis functions
    - the integrals are calculated separately for each element, forming local, element system matrices and right hand side vectors
    - the local matrices and vectors are than assembled into the global system matrix and the global right hand side vector
  - the solution of the system, that takes into account its special form

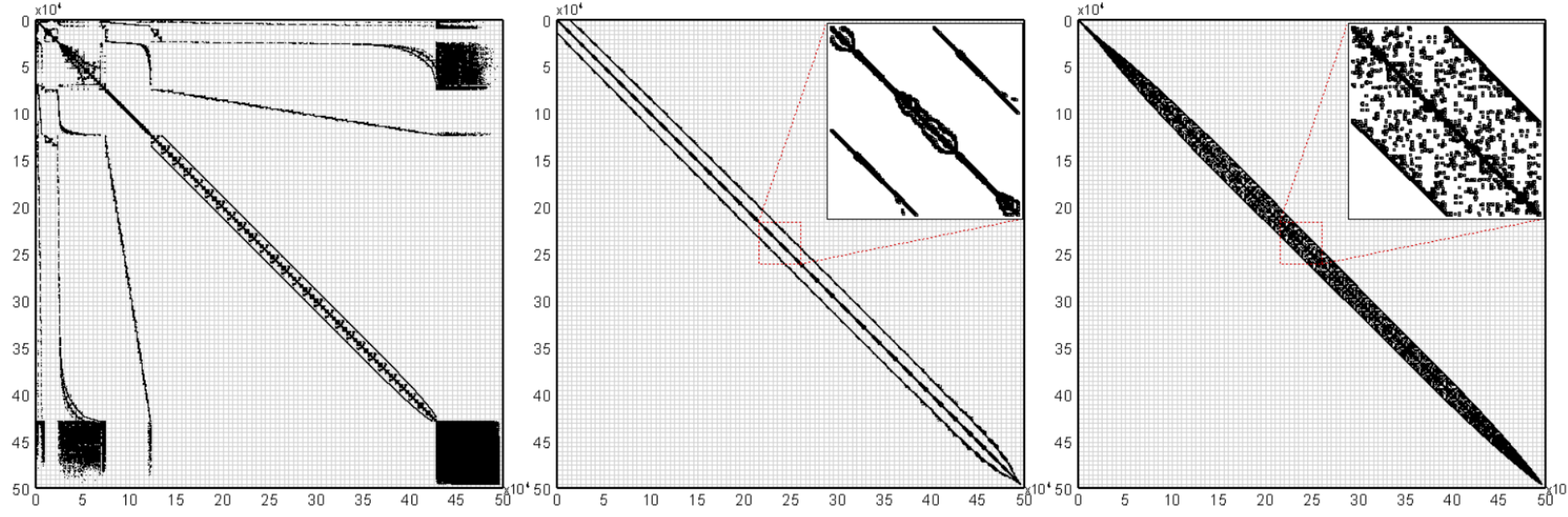
Finite element systems of linear equations

- The assembly of global finite element systems of linear equations
  - local element matrices computed using numerical integration
  - numerical integration usually using Gaussian quadratures **defined for the reference elements** (transformation to the reference elements required for the application of The Change of Variables Theorem)
  - local numbering of degrees of freedom for integration
  - the assembly to the global system using the mapping of the local numbers to the global numbers - for element's nodes



Finite element systems of linear equations

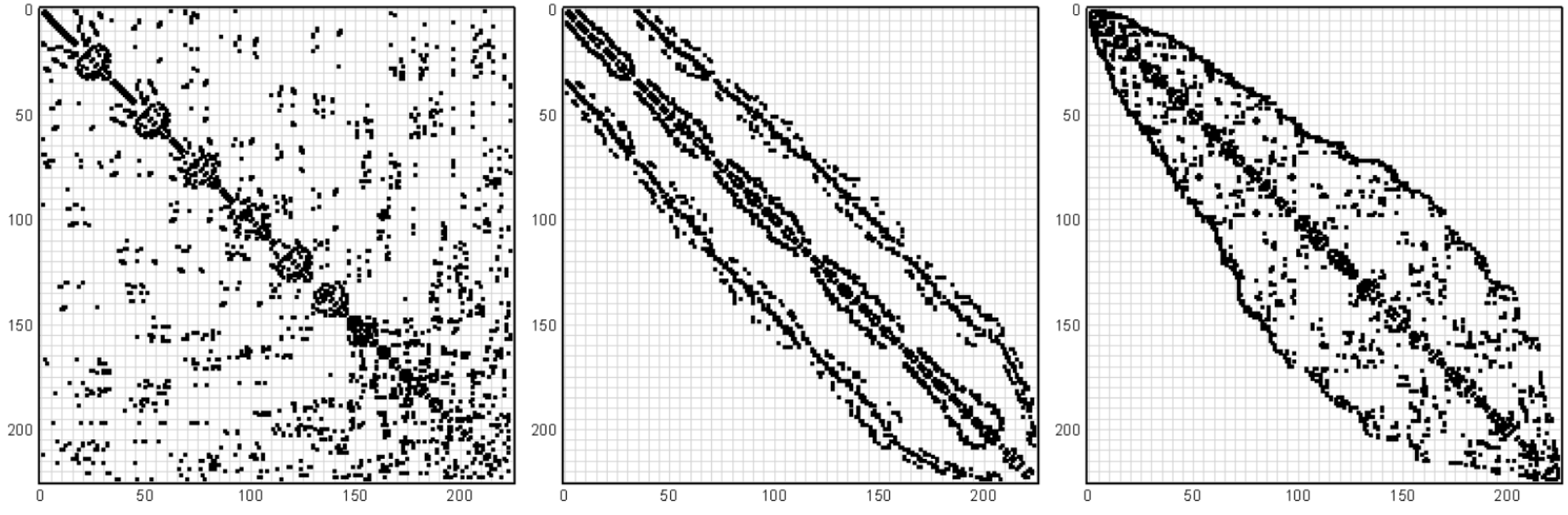
- The solved equations are
  - usually large (up to billions of unknowns)
  - sparse (for large systems more than 99.99% entries in the system matrix are zero)
  - often ill conditioned – with large condition number and slow convergence of iterative methods



Finite element systems of linear equations

Practical solutions for solving FEM systems of linear equations

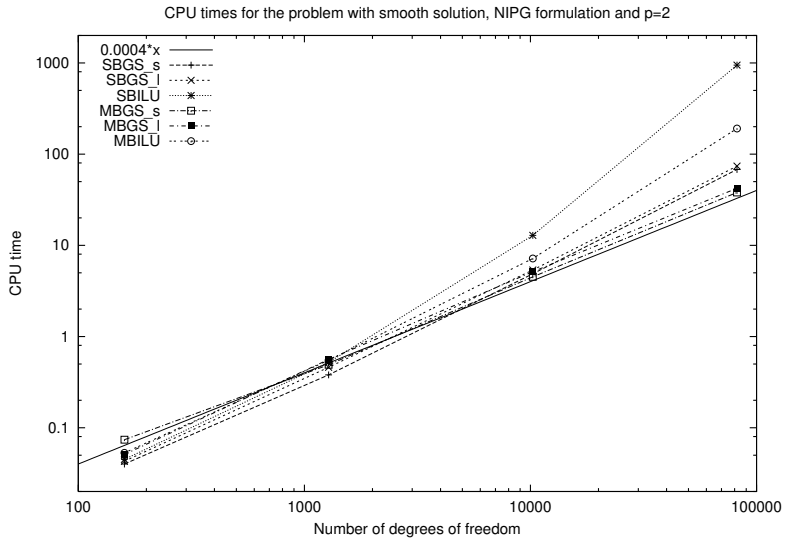
- Direct methods for solving large sparse systems of linear equations
  - the variants of Gaussian elimination
  - the problem of fill-in
    - renumbering
    - frontal methods

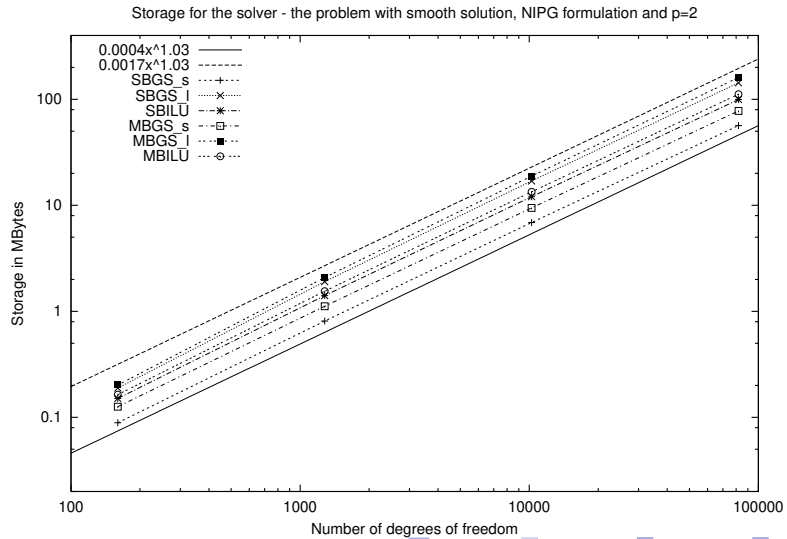


Finite element systems of linear equations

Practical solutions for solving FEM systems of linear equations

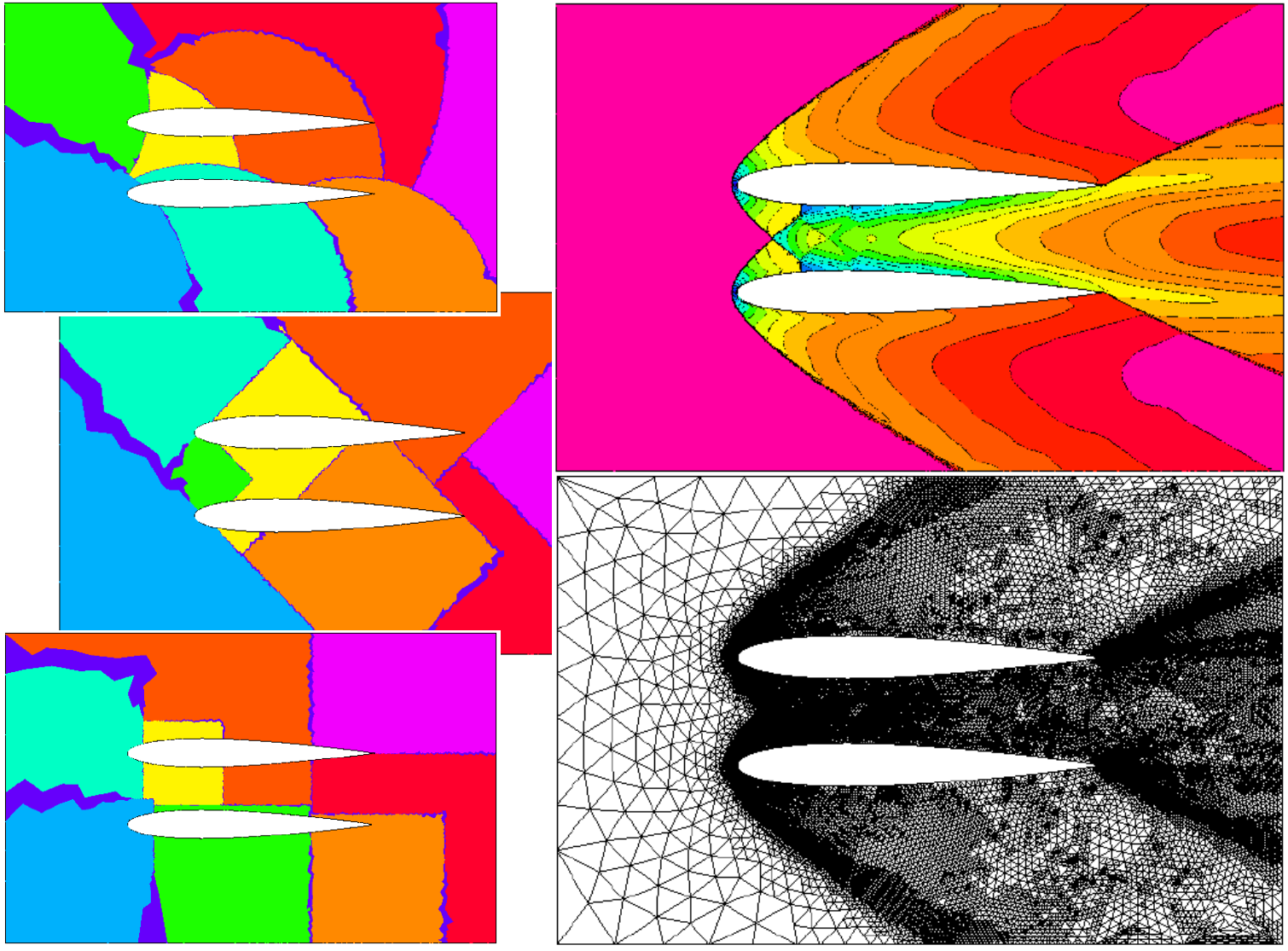
- Iterative methods for solving large sparse systems of linear equations
  - slow convergence of standard iterative methods
  - simple preconditioners: Jacobi (diagonal scaling), Gauss-Seidel, incomplete LU factorization
  - complex preconditioners: multigrid, special preconditioners for specific problems
  - the best iterative solvers can have linear complexity, both in terms of solution time and storage requirements





Finite element solution procedures

Parallel solution based on domain decomposition



Non-linear problem solution

- Finite element space discretization of non-linear problems leads to the set of non-linear algebraic equations for the vector of degrees of freedom $\mathbf{U}^h$, that can be shortly written as:

$$\mathbf{A}(\mathbf{U}^h)\mathbf{U}^h = \mathbf{b}$$

- The general methods for solving multidimensional systems of the form

$$\mathbf{F}(\mathbf{U}) = 0$$

usually refer to the Newton's iterative method, that finds the subsequent approximations

$$\mathbf{U}_{k+1} = \mathbf{U}_k + \boldsymbol{\Delta}\mathbf{U}_k$$

where $\boldsymbol{\Delta}\mathbf{U}_k$ is the solution to the equation

$$\mathbf{J}(\mathbf{U}_k) \cdot \boldsymbol{\Delta}\mathbf{U}_k = -\mathbf{F}(\mathbf{U}_k)$$

with the Jacobian matrix $\mathbf{J}$ representing the gradient of the function $\mathbf{F}$

$$\mathbf{J} = \partial\mathbf{F}/\partial\mathbf{U}$$

Non-linear problem solution

- Applying the Newton's method to the system:

$$\mathbf{A}(\mathbf{U}^h)\mathbf{U}^h = \mathbf{b}$$

leads to the equation

$$\left(\frac{\partial \mathbf{A}}{\partial \mathbf{U}^h}(\mathbf{U}_k^h)\mathbf{U}_k^h + \mathbf{A}(\mathbf{U}_k^h)\right) \cdot \boldsymbol{\Delta}\mathbf{U}_k^h = -\mathbf{A}(\mathbf{U}_k^h)\mathbf{U}_k^h + \mathbf{b}$$

- When the derivative $\frac{\partial \mathbf{A}}{\partial \mathbf{U}^h}$ is assumed to vanish, the system reduces to the form

$$\mathbf{A}(\mathbf{U}_k^h) \cdot \mathbf{U}_{k+1}^h = \mathbf{b}$$

that can be interpreted as using fixed point (Picard's) iterations

$$\mathbf{U}_{k+1}^h = \mathbf{A}(\mathbf{U}_k^h)^{-1} \cdot \mathbf{b}$$

for the original nonlinear problem

Non-linear problem solution

- In general (for 1D case) Picard's (fixed point) iterations are defined as subsequent computations

$$x_{k+1} = g(x_k)$$

that after convergence lead to the satisfaction of the nonlinear problem

$$x = g(x)$$

- Newton's method iterations for the problem $f(x) = 0$:

$$x_{k+1} = x(k) - f'(x_k)^{-1} \cdot f(x_k) \quad [= g(x_k)]$$

can be interpreted as a special case of fixed point iterations