An introduction to the FEM accuracy

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Outline

1. An introduction to the FEM accuracy
   - Convergence of FEM
   - Error estimate

2. An introduction to the solution of sparse systems of equations
   - Methods of sparse matrix storing
   - Parallel solution of equation systems

Convergence of FEM:

- FEM is based on the dicretization of the original continuous domain by a set of elements - generally it is a discretization of the weak form $\Rightarrow$ the result is the approximated solution
- The accuracy of the approximated solution depends on
  - type of finite elements
  - size of elements
  - weak form
  - for time-dependent problems, on the time distretization type and the algorithm of solution
- FEM in strongly influenced by the finite element mesh construction (basis functions)

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Convergence of FEM:

- The convergence theory is elaborated very well in problems of mechanics (linear statics) - findings are exploited in transport problems (stationary $\rightarrow$ non-stationary)
- Convergence (Cauchy principle): we say that the sequence of real numbers a_n converge in the limit to a, if for an arbitrary $\epsilon > 0$, we can find n_0 so that for each $n \geq n_0$, it is $|a - a_n| \leq \epsilon$. So we write:

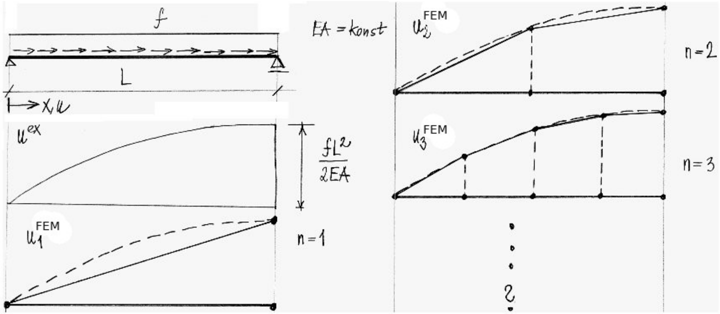
$$\lim_{n \to \infty} a_n = a$$

- The previous definition says we are able to approximate the limit a by a sequence a_n with an arbitrary accuracy $\epsilon > 0$
- In FEM, we approximate the weak solution u^{ex} by a FE solution u_n^{FEM} with a given accuracy:

$$u_n^{\text{FEM}}(x) \rightarrow u^{\text{ex}}$$

Convergence of FEM:

- FEM deals with the convergence of functions
- Example: bar element



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Convergence of FEM:

- We can define an *energy norm* of the function u as

$$\|u(x)\| = \int_L E(x)A(x)\left(\frac{\mathrm{d}u}{\mathrm{d}x}\right)^2 \mathrm{d}x,$$

which has a physical meaning of the structure energy with a given displacement u

- We verify if it is valid:

$$\|u_n^{\mathrm{FEM}}(x)\| \to \|u^{\mathrm{ex}}(x)\|$$

- In FEM, we parametrize solutions by the element size h instead of the number of elements n
- In the ideal case, it has to be satisfied:

$$\lim_{h \to 0} \|u_h^{\mathrm{FEM}}(x)\| \to \|u^{\mathrm{ex}}(x)\|$$

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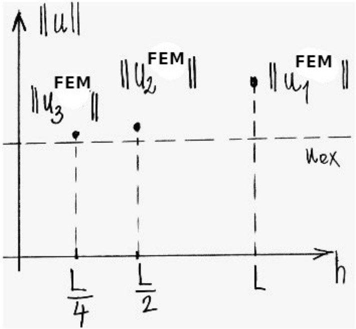
Convergence of FEM:



- For the given accuracy, $\epsilon > 0$, we can find such element size h, so that:

$$\|u_h^{\text{FEM}}(x) - u^{\text{ex}}(x)\| < \epsilon.$$

We are able approximate weak solution with an arbitrary accuracy in *energy norm*.

Convergence of FEM:

Basis functions have to satisfy following conditions:

- Smoothness requirement: functions have derivatives of one degree higher than derivatives appearing in the weak form
- Continuity requirement: functions have to be continuous within the element and on the boundary
- Completeness requirement: e. g., in elasticity:
  - the displacement field and its derivative can take constant values so that the finite elements can represent rigid body motion and constant strain states exactly
- Finite element with approximation functions satisfying continuity and completeness is called "*conforming*" → *monotonous convergence*
- If the completeness is satisfied but the continuity is not, the finite element is *non-conforming*
- For non-conforming elements, the analysis of the condition completeness is difficult. The PATCH TEST can be then used for the solution control

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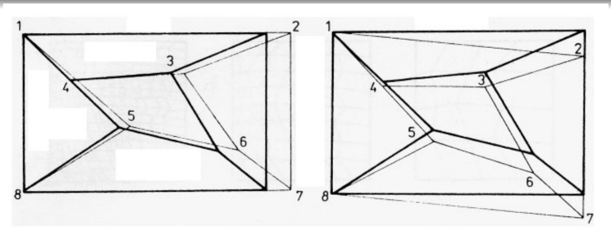
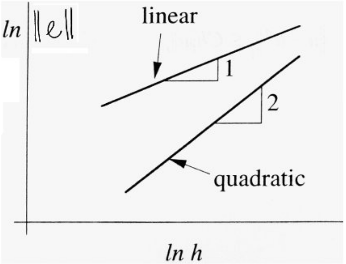


Adaptive techniques in FEM:

- Adaptive techniques in FEM deal with the mesh refinement and the increasing of the approximation function polynomial degree, and the speed of convergence
- The speed of convergence can be affected by
  - mesh refinement $h \rightarrow 0 = h$ convergence
  - increasing of the approximation function polynomial degree $= p$ convergence
  - combination of both effects $= hp$ convergence
- From the computational point of view, it is beneficial to perform the mesh refinement or the increasing of the approximation function polynomial degree, where the approximated solution doesn't approximate the exact solution as precise as possible $\rightarrow$ adaptive FEM,
  - e .g., areas of hight stresses concentration, extreme temperature gradients, etc.

Error estimate:



- For adaptive methods, it is necessary to know the error of the approximated solution

$$e(x) = u^{\mathrm{FEM}}(x) - u^{\mathrm{ex}}(x) \tag{1}$$

respectively

$$\|e(x)\| = \|u^{\mathrm{FEM}}(x) - u^{\mathrm{ex}}(x)\| \tag{2}$$

- To describe the behavior of the problem we define the variation of the *relative energy norm error* as

$$\eta = \frac{\|e\|}{\|u\|} \tag{3}$$

Error estimate:

- The exact solution u^{ex} is not generally known. We have to work with an error estimate ${}^{0}\|e\|$ or relative error estimate ${}^{0}\eta$
- The efficiency index:

$$\vartheta = \frac{{}^{0}\|e\|}{\|e\|}.$$

- For asymptotic effective error estimate methods, it holds:

$$\lim_{h\to 0} \vartheta = 1$$

- Error estimate methods:
  - ZZ method (introduced by Zienkiewiczem a Zhuem) - suitable for h adaptive method

O. C. Zienkiewicz and J. Z. Zhu, A simple error estimator and adaptive procedure for practical engeneering analysis, International Journal for Numerical Methods in Engineering 24 (1987), 337-357.

ZZ method:

- Suitable for h adaptive method
- Simple for the computation - based on known nodal displacements $\boldsymbol{r}$
- Approximated displacements u^{FEM} by linear basis functions:

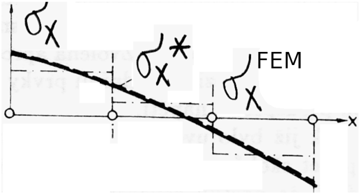
$$\boldsymbol{u}^{\text{FEM}}(\boldsymbol{x}) \approx \boldsymbol{N}(\boldsymbol{x})\boldsymbol{r}$$

- Stresses $\boldsymbol{\sigma}^{\text{FEM}}$ and strains $\boldsymbol{\varepsilon}^{\text{FEM}}$ are piecewise constant:

$$\boldsymbol{\varepsilon}^{\text{FEM}}(\boldsymbol{x}) \approx \boldsymbol{B}(\boldsymbol{x})\boldsymbol{r}$$

- Consider stresses $\boldsymbol{\sigma}^{\star}$ is closed to exact solution $\boldsymbol{\sigma}^{\text{ex}}$

$$\boldsymbol{\sigma}^{\star}(\boldsymbol{x}) = \boldsymbol{N}(\boldsymbol{x})\boldsymbol{r}_{\sigma}$$



Error estimate:

- Coefficients in the vector $\boldsymbol{r}_\sigma$ are determined for the minimal error between approximated $\boldsymbol{\sigma}^{\mathrm{FEM}}$ and recovered stresses $\boldsymbol{\sigma}^\star$ with help of least square method:

$$\int_\Omega \left(\boldsymbol{\sigma}^\star(\boldsymbol{x}) - \boldsymbol{\sigma}^{\mathrm{FEM}}(\boldsymbol{x})\right)^{\mathrm{T}} \left(\boldsymbol{\sigma}^\star(\boldsymbol{x}) - \boldsymbol{\sigma}^{\mathrm{FEM}}(\boldsymbol{x})\right) \mathrm{d}x$$

- Then

$$\begin{aligned} \frac{\partial}{\partial \boldsymbol{r}_\sigma} \int_\Omega \left(\boldsymbol{N}(\boldsymbol{x})\boldsymbol{r}_\sigma - \boldsymbol{B}(\boldsymbol{x})\boldsymbol{r}\right)^{\mathrm{T}} \left(\boldsymbol{N}(\boldsymbol{x})\boldsymbol{r}_\sigma - \boldsymbol{B}(\boldsymbol{x})\boldsymbol{r}\right) \mathrm{d}x &= 0 \\ \int_\Omega \boldsymbol{N}^{\mathrm{T}}(\boldsymbol{x}) \left(\boldsymbol{N}(\boldsymbol{x})\boldsymbol{r}_\sigma - \boldsymbol{B}(\boldsymbol{x})\boldsymbol{r}\right) \mathrm{d}x &= 0 \end{aligned}$$

- Nodal values of recovered stresses are calculated from this system of equations:

$$\left(\int_\Omega \boldsymbol{N}^{\mathrm{T}}(\boldsymbol{x})\boldsymbol{N}(\boldsymbol{x})\mathrm{d}x\right) \boldsymbol{r}_\sigma = \left(\int_\Omega \boldsymbol{N}^{\mathrm{T}}(\boldsymbol{x})\boldsymbol{B}(\boldsymbol{x})\mathrm{d}x\right) \boldsymbol{r}$$

$$\boldsymbol{A}\boldsymbol{r}_\sigma = \boldsymbol{b}$$

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Error estimate:

- The error estimate is based on the following difference:

$$\boldsymbol{\sigma}^{\star}(\boldsymbol{x}) - \boldsymbol{\sigma}^{\mathrm{FEM}}(\boldsymbol{x})$$

- For 1D problem, we obtain:

$$^{0}\|e\| = \int_{l} \frac{A(\boldsymbol{x})}{E(\boldsymbol{x})} \left(\boldsymbol{\sigma}^{\star}(\boldsymbol{x}) - \boldsymbol{\sigma}^{\mathrm{FEM}}(\boldsymbol{x})\right)^{2} \mathrm{d}x$$

- In case of general problem (2D and 3D), the energy norm is expressed by:

$$\|u\| = \int_{\Omega} \boldsymbol{\varepsilon}^{\mathrm{T}}(\boldsymbol{x})\boldsymbol{D}(\boldsymbol{x})\boldsymbol{\varepsilon}(\boldsymbol{x})\mathrm{d}\boldsymbol{x} = \int_{\Omega} \boldsymbol{\sigma}^{\mathrm{T}}(\boldsymbol{x})\boldsymbol{D}^{-1}(\boldsymbol{x})\boldsymbol{\sigma}(\boldsymbol{x})\mathrm{d}\boldsymbol{x}$$

- The energy norm error:

$$\|e\| = \int_{\Omega} \left(\boldsymbol{\sigma}^{\star}(\boldsymbol{x}) - \boldsymbol{\sigma}^{\mathrm{FEM}}(\boldsymbol{x})\right)^{\mathrm{T}} \boldsymbol{D}^{-1}(\boldsymbol{x}) \left(\boldsymbol{\sigma}^{\star}(\boldsymbol{x}) - \boldsymbol{\sigma}^{\mathrm{FEM}}(\boldsymbol{x})\right) \mathrm{d}\boldsymbol{x}$$

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Error estimate:

- Let's remind the definition of energy norm:

$$\|u\| = \int_l E(x)A(x)\left(\frac{\mathrm{d}u}{\mathrm{d}x}\right)^2 \mathrm{d}x = \int_l \varepsilon_x(x)E(x)A(x)\varepsilon_x(x)\mathrm{d}x = \frac{A(x)}{E(x)}\boldsymbol{\sigma}_x^2(x)$$

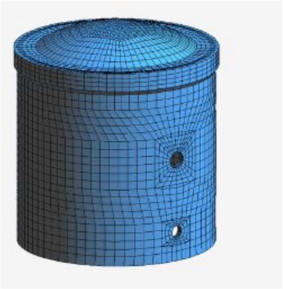
An introduction to the FEM accuracy

An introduction to the solution of sparse systems of linear algebraic equations

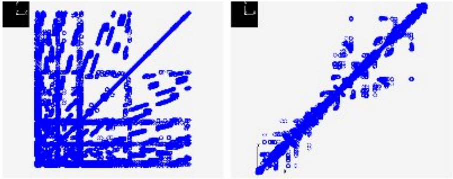
- Solution of the system:

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b},$$

where the number of equation is huge (10^6) and the matrix $\boldsymbol{A}$ is sparse



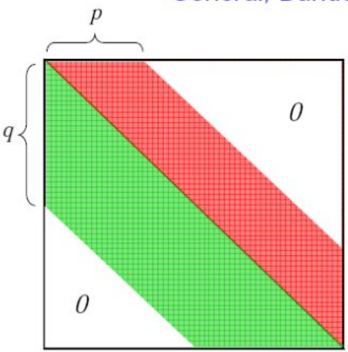
Containment of Temelin NP:
- **Number of elements** 14970
- **Number of nodes** 11764
- **Number of equations** 43875
- **Profile** 676,00,240; **after renumbering** 5,866,165



Methods of sparse matrix storing:

- Banded matrix

General, Banded Coefficient Matrix



$$\left.\begin{array}{l} j > i + p \\ i > j + q \end{array}\right\} a_{ij} = 0$$

p super-diagonals
q sub-diagonals
$w = p+q+1$ bandwidth

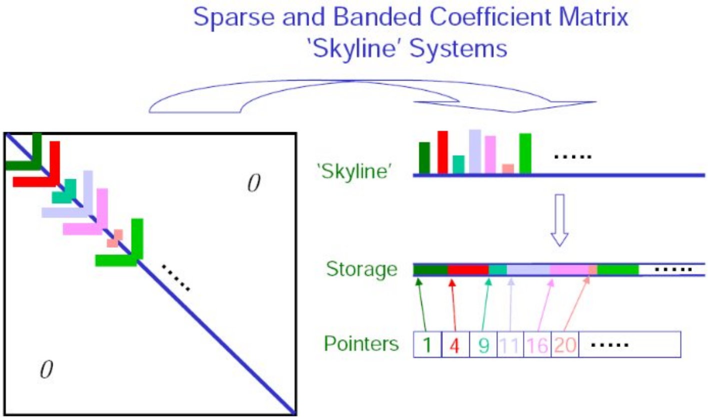
Banded Symmetric Matrix

$$a_{ij} = a_{ji}\,, \quad |i-j| \leq b$$
$$a_{ij} = a_{ji} = 0\,, \quad |i-j| > b$$

b is half-bandwidth

Methods of sparse matrix storing:

- Skyline



- Coordinate scheme for storing sparse matrices - suitable for iterative solvers

Direct solvers:

- Maind idea: factorization of the matrix in to multiplication of two matrices, which are invertible (and triangular) with possible permutation for the stability reaching
- Example: LU decomposition $\boldsymbol{A} = \boldsymbol{L}\boldsymbol{U}$, where $\boldsymbol{L}$ a $\boldsymbol{U}$ are the lower and upper triangular matrices, respectively. If we have the decomposition, then:

$$\boldsymbol{A}\boldsymbol{x} = (\boldsymbol{L}\boldsymbol{U})\boldsymbol{x} = \boldsymbol{L}(\boldsymbol{U}\boldsymbol{x}) = \boldsymbol{b},$$
$$\boldsymbol{L}\boldsymbol{y} = \boldsymbol{b}, \quad \boldsymbol{U}\boldsymbol{x} = \boldsymbol{y}$$

- The main benefit of the matrix decomposition is the simple solution of both problem by backward and forward substitution

Direct solvers:

- Advantages:
  - known number of operations
  - ability of the large systems solution (2D a 3D problems)
  - speed and robustness
- Disadvantages:
  - assembly of the whole matrix - it can be complicated

Iterative solvers:

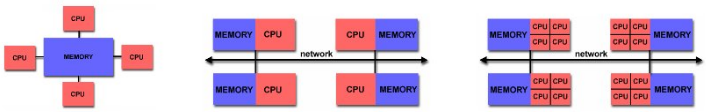
- Two main iterative algorithms: relaxation (Jacobi, Gauss-Seidel) a project (Krylovov method: CG, GMRES)
- Idea: generation of a sequence of approximation solutions $x_0, x_1, \ldots x_n$ so than lim$x_n \rightarrow x^*$, where x^* is the exact solution
- In comparison with the direct solvers, the solution can be end ahead of time with help of a suitable criterion
- Advantages:
  - the explicit matrix assembly is not needed
  - low memory requirements
  - effective for very sparse systems, mainly for 3D problems
- Disadvantages:
  - huge number of iterations
  - effective preconditioning is often needed

Hybrid methods:

- Multigrid methods

Parallel solution of equation systems:

- The size of solved problem is limited on one computer by the CPU speed and the size of memory $\rightarrow$ parallel and distributed computations in modern clusters and computers
- Architecture:
  - shared memory
  - distributed memory
  - hybrid systems

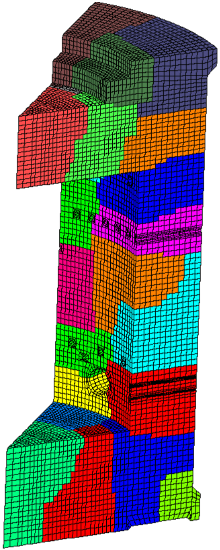


- Computing models:
  - threads - shared memory (POSIX, OpenMP)
  - Message passing interface - distributed systems (MPI)
  - parallel data model - shared memory (F90, HPF)

Domain decomposition:

- Idea: the decomposition of solved problem into sub-problems, that can be solved on individual clusters and the mutual correspondence enforces mutual communication
- In FEM, the domain decomposition method is used = the decomposition of a domain into several sub-domains. A parallel solver is needed for the effective processing
- Requirements: constant work distribution (equal number of elements and nodes), minimal boundary between subdomains (communication)
- Solution methods:
  1. Primary domain decomposition method - Schur complement method
  2. Dual decomposition method - FETI method (Finite Element Tearing and Interconnecting method)
- Load balancing - distributed work among clusters (static, dynamic), is inevitable for the effective computation

Example of domain decomposition:



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