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Implementation of Parallel Processing Inside the Finite Element Method

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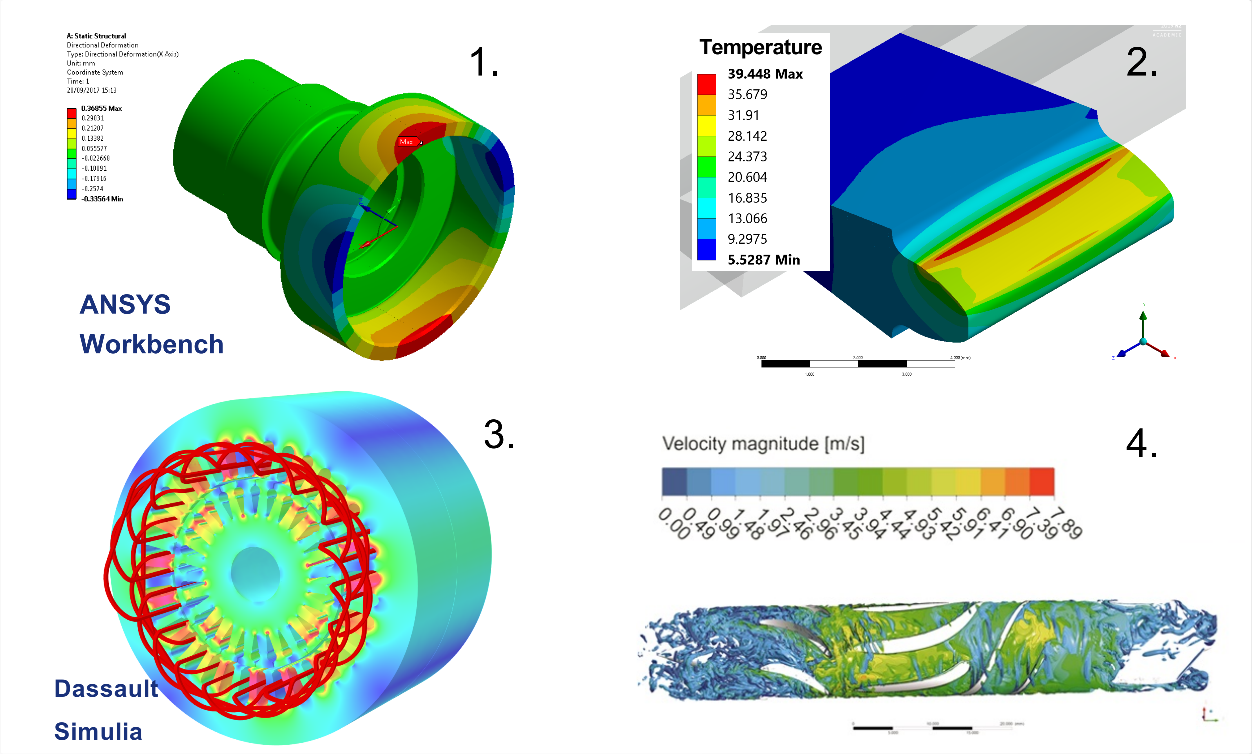
Parallel programming with MPI / OpenMP

EuroCC Competence Center Slovenia Training Course

Introduction to the Finite Element Method (FEM)

- Most widely used numerical method for solving physical problems described by partial differential equations (PDEs)
- First developed to solve structural analysis problems and civil and aeronautical engineering
- Used for problems related to:
  1. Structural mechanics
  2. Heat diffusion
  3. Electromagnetism
  4. Fluid mechanics
  5. Other



Introduction to the Finite Element Method (FEM)

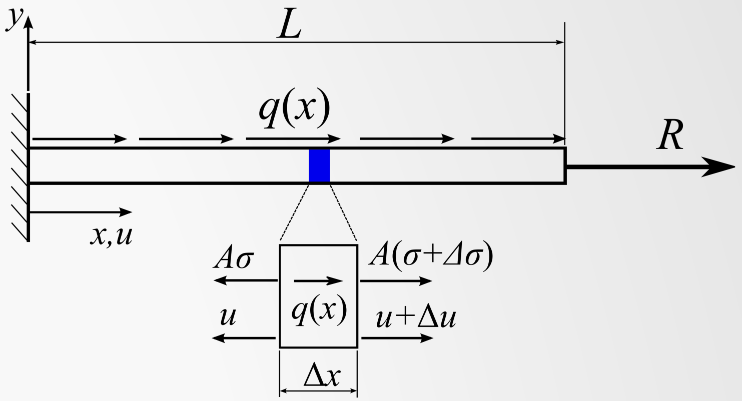
- FEM application to structural analysis problems – axially loaded bar

1. Strong form:

$$AE\frac{\mathrm{d}^2\mathbf{u}}{\mathrm{d}x^2} + \mathbf{q}(\mathbf{x}) = 0, \quad \text{where} \quad \mathbf{q}(\mathbf{x}) = a\mathbf{x}$$

BCs: 1. At $\mathbf{x} = 0$, $\mathbf{u}$

2. At $\mathbf{x} = L$, $\mathbf{f} = AE\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}x} = \mathbf{R}$



1. Weak form (virtual work principle):

   - Energy conservation principle:

$$\delta W_{\text{int}} = \delta W_{\text{ext}} + \delta W_{\text{body}} \quad \rightarrow \quad \text{Virtual work}$$

$$AE\int_0^L \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}x}\frac{\mathrm{d}(\delta\mathbf{u})}{\mathrm{d}x} = \int_0^L \mathbf{q}\delta\mathbf{u}\mathrm{d}x + \mathbf{R}\delta\mathbf{u}|_{x=L} \quad \rightarrow \quad \delta\mathbf{u} \; - \; \text{Virtual displacement}$$

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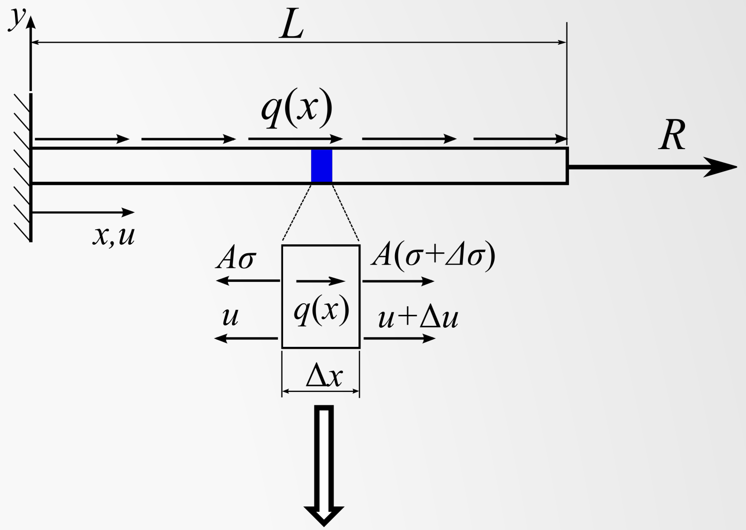
3. Galerkin method approximation

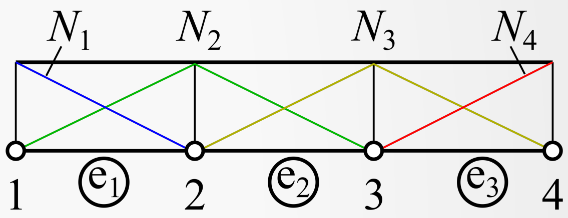
$$\underbrace{\int_0^L \frac{\mathrm{d}N_j}{\mathrm{d}x} AE \frac{\mathrm{d}N_i}{\mathrm{d}x} \mathrm{d}x}_{K_{ij}} \cdot u_i = \underbrace{\int_0^L N_j \mathbf{q} \mathrm{d}x + N_j \mathbf{R}|_{x=L}}_{f_j}$$

→ u_i - Approx. displacement vector

→ N_i - Shape functions



Finite element discretization:



4. System of equations to solve

$$\mathbf{Ku} = \mathbf{f}$$

→ $\mathbf{K}$ - Stiffness matrix

→ $\mathbf{u}$ - Displacement vector

→ $\mathbf{f}$ - External loads vector

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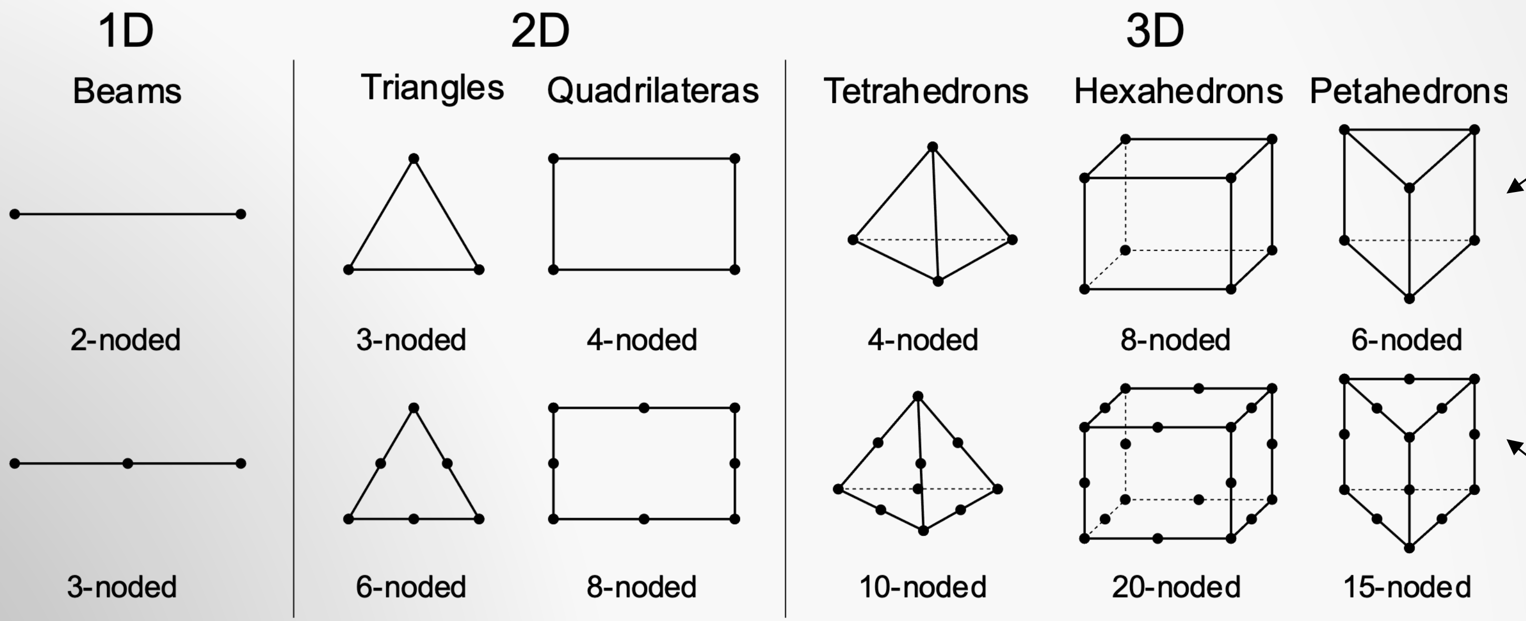
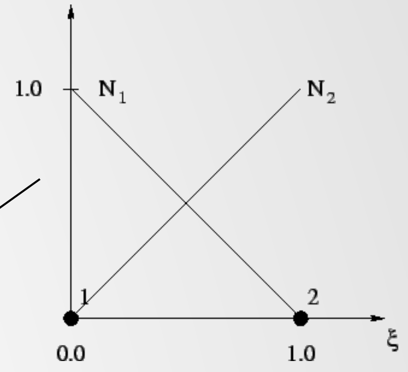
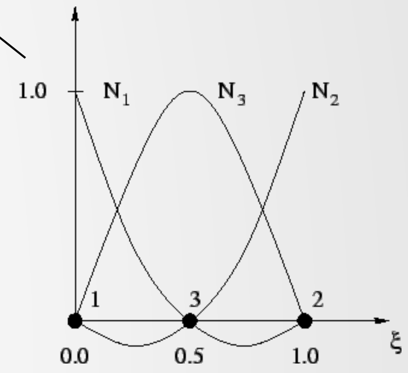
- Finite element (FE) types



Linear shape functions (SF):



Quadratic SF:



Introduction to the Finite Element Method (FEM)

- **Different problem types**

1. Thermal problems - heat equation:

$$\mathbf{S}\dot{\mathbf{T}} + \mathbf{HT} = \mathbf{q}$$

$\rightarrow$ $\mathbf{S}$ - Time dep. component matrix $\rightarrow$ $\mathbf{q}$ - Thermal load

$\rightarrow$ $\mathbf{H}$ - Conductivity component matrix $\rightarrow$ $\mathbf{T}$ - Temperature

- Numerical method for solving time dep. differential equation necessary

2. Electrostatic problems:

$$\mathbf{Ev} = \mathbf{b}$$

$\rightarrow$ $\mathbf{E}$ - Permittivity matrix $\rightarrow$ $\mathbf{v}$ - Electrostatic potential vector

$\rightarrow$ $\mathbf{b}$ - Volume charge + electric flux density vector

2. Time dependent/dynamical structural problems:

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{C}\dot{\mathbf{u}} + \mathbf{Ku} = \mathbf{f}$$

$\rightarrow$ $\mathbf{M}$ - Mass matrix

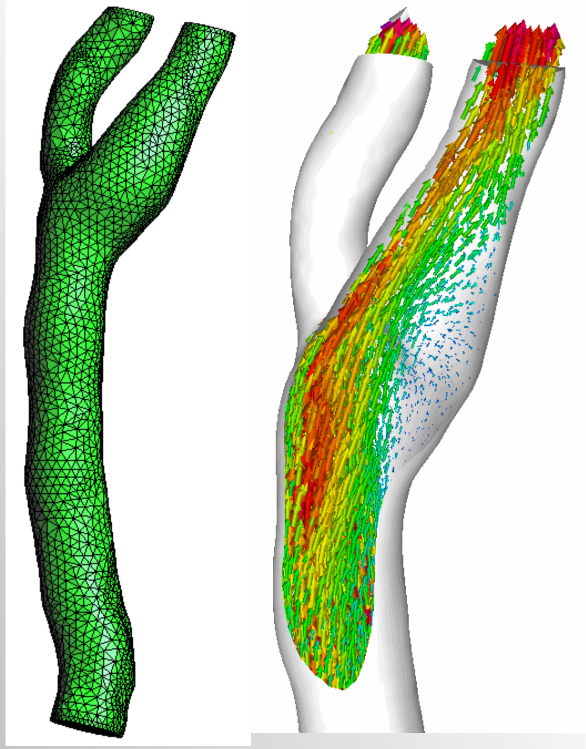
$\rightarrow$ $\mathbf{C}$ - Damping matrix

2. Nonlinear problems

- iterative solver methods like Newton-Raphson m. required

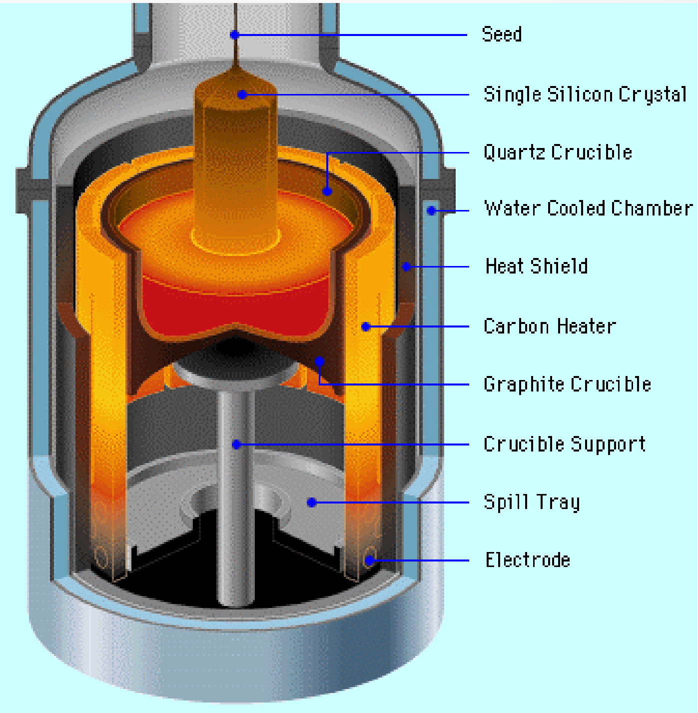
FEM for Multiphysics Problems

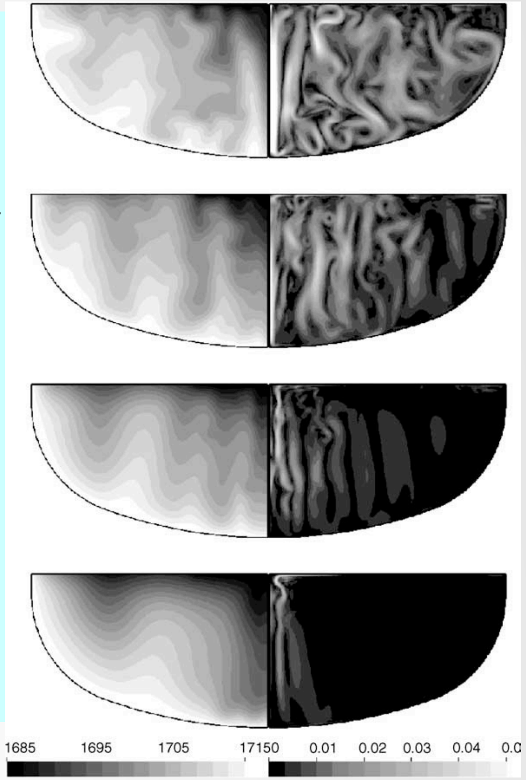
- Fluid structure interaction (FSI)



E. Järvinen, P. Råback, M. Lyly, J. Salonius. Medical Eng. & Physics, 30 (2008), 917-923

- Coupled field analyses





Temperature (K) Velocity (m/s)

V. Savolainen et al., J. Crystal Growth 243 (2002), 243-260.

Practical FEM Implementation

- The method is applicable using multiple software packages

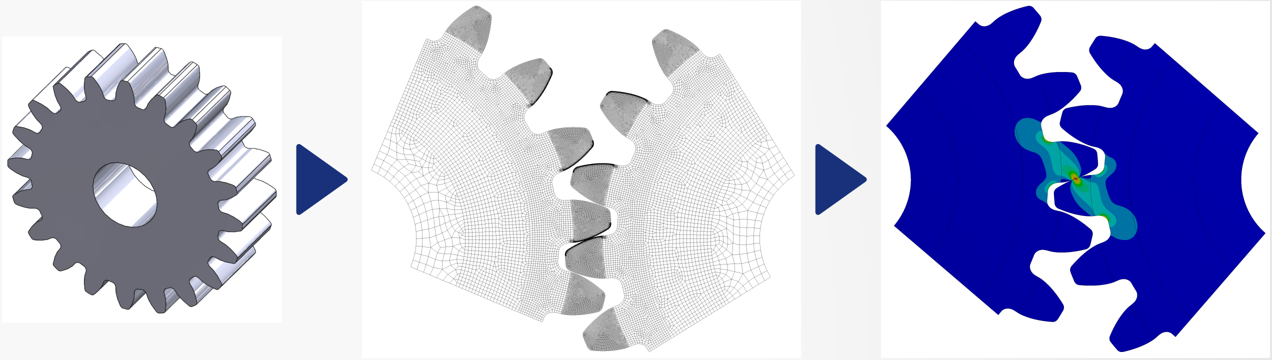
A. Open source:
  - Elmer FEM,
  - Code Aster,
  - CalculiX,
  - FreeFEM, etc.

B. Commercial:
  - ANSYS,
  - Abaqus,
  - Comsol Multiphysics,
  - Altair,
  - Nastran, etc.

Practical FEM Implementation

- ***Typical FEM analysis procedure***:

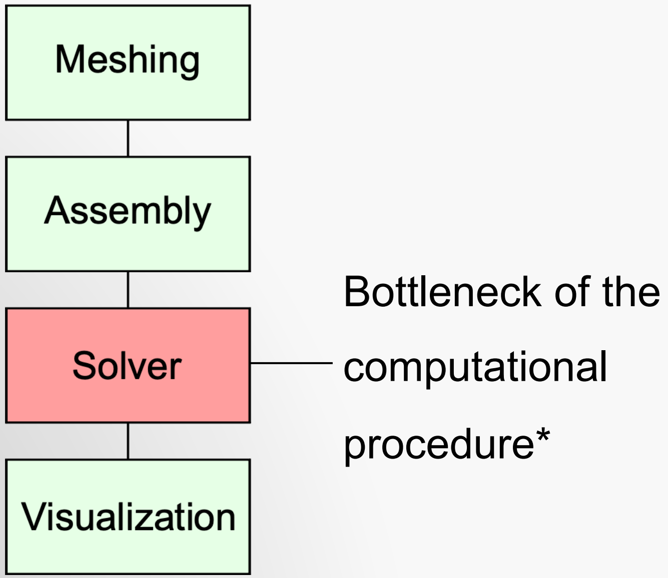
1. **Preliminary problem dissection:**
   - Analysis type: Static, thermal, modal…
   - Constitutive/physical model
   - Geometry: single body/multibody
   - Geom. space: 2D/3D
   - Element types: Line/surface/solid elements
   - Symmetry conditions, etc.
2. **Preprocessing:**
   - Import/create geometry
   - Mesh geometry
   - Material properties
   - Loads and boundary conditions (BCs)
3. **Solving the model**
4. **Postprocessing:**
   - Review results
   - Data analysis
   - Verify/validate solution



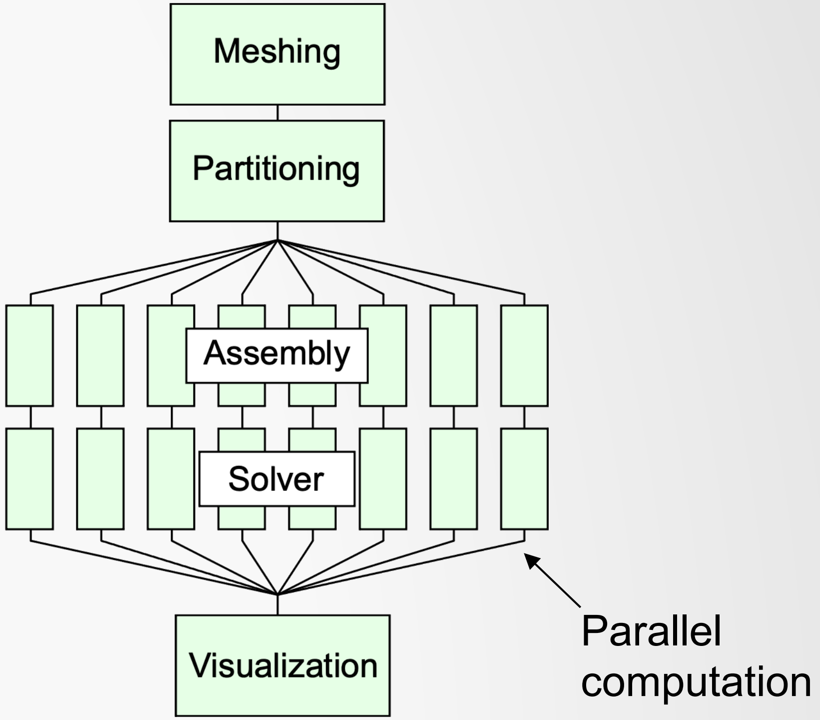
Parallelization of FEM problems

- Computational steps in typical FEM analysis:

1. Serial computation:



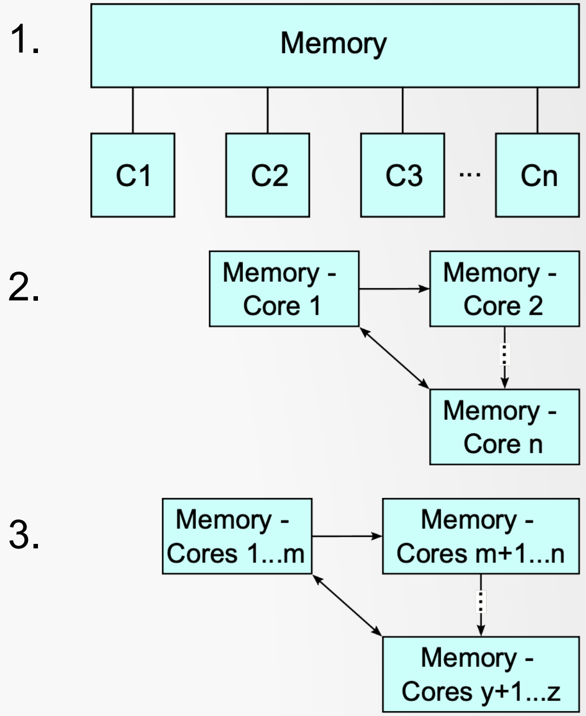
2. Parallelized computation



- * For large cases the other steps can also be highly time consuming – parallelization there also required

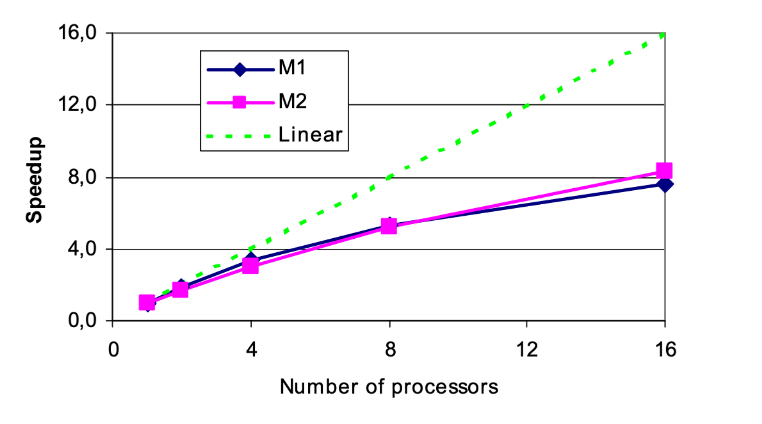
Parallelization of FEM problems

- Data dependency – does the computation of one task require data from other tasks to proceed?
  - FEM is inherently data dependent – reflection of the physical reality of the problem
    - Parallel computers:
      1. Shared memory – all cores access the whole memory
      2. Distributed memory:
         - Each core has its own memory unit
         - Communication protocol for memory access between different cores
      3. Typical HPC combines distributed and shared memory capabilities



Parallelization of FEM problems

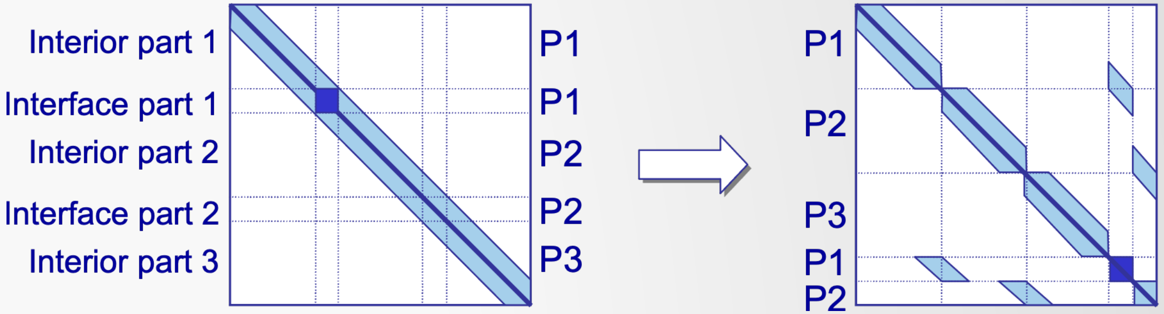
- Parallelization possible using OpenMP (shared memory processing), MPI (shared and/or distributed memory processing) or other libraries and protocols
- Scalability of parallelized FEM computations:
  - *Strong scaling* – how the solution time decreases with an increased number of processors for a fixed total problem size
    - Best case scenario: $N_p \cdot T$ = const.
  - *Weak scaling* – how the solution time varies with the number of processors for a fixed problem size per processor
    - Best case scenario: T = const.
  - Typically >10^4 FEs needed for suitable scaling



V. Rischmüller, M. Haas, S. Kurz, and W. M. Rucker, IEEE Trans. on Magnetics, Vol. 36, No. 4, July 2000

Parallel Processing Algorithms in FEM

- **Iterative methods:**
  - Parallelized Conjugate Gradient (CG) with
    - Incomplete Cholesky *preconditioner* (ICCG) – block (BICCG) or renumbering process (PICCG-RP) methods
    - Diagonal preconditioning (DPCG) method
  - BI-Conjugate Gradient Stabilized method (BICGSTAB)
  - Quasi-Minimal Residual (QMR) method
  - QCR, GMRes, TFQMR,…
- **Direct methods:**
  - Sparse LU decomposition solvers
  - Suitable for ill-conditioned cases (very stiff bodies, large displacements, etc.)
  - MUMPS parallel sparse solver

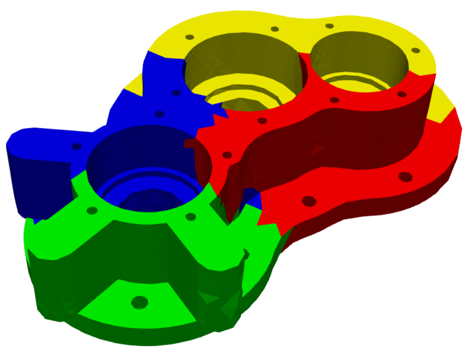


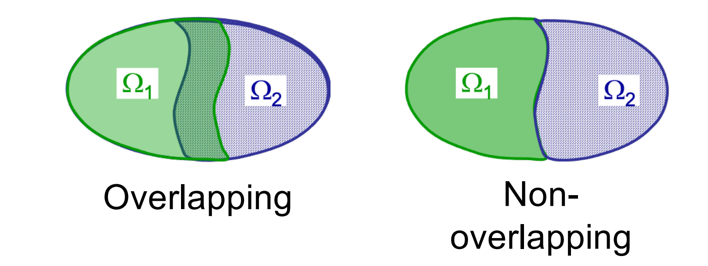
Example: PICCG-RP algorithm

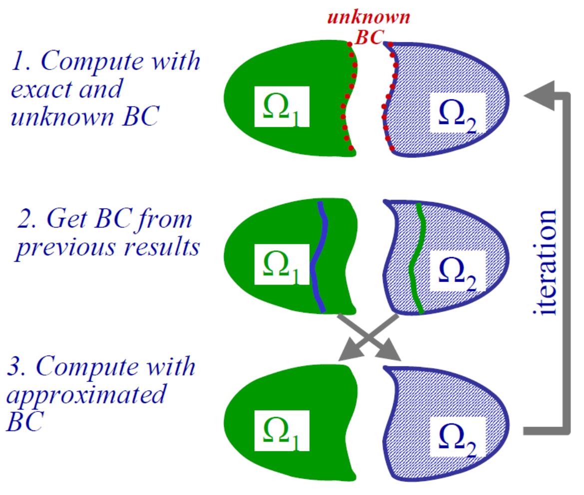
B. Butrylo, F. Musy, L.Nicolas, R.Perrussel, R. Scorretti, et al., *COMPEL: The Int. J. for Comp. and Math. in Elec. and Electronic Eng.*, Emerald, 2004, 23 (2), pp.531-546. ⟨10.1108/03321640410510721⟩. ⟨hal-00140344⟩

Parallel Processing Algorithms in FEM

- **Domain decomposition (I):**
  - Decomposition of the spatial domain into subdomains
  - Iterative algorithms preferred to direct solvers (better efficiency)
  - Overlapping or non-overlapping decomposition methods
  - *Overlapping decomposition method:*
    - Schwarz iterative methods
    - Approximation of BCs on interface
    - On each subdomain – iterative or direct solver can be used







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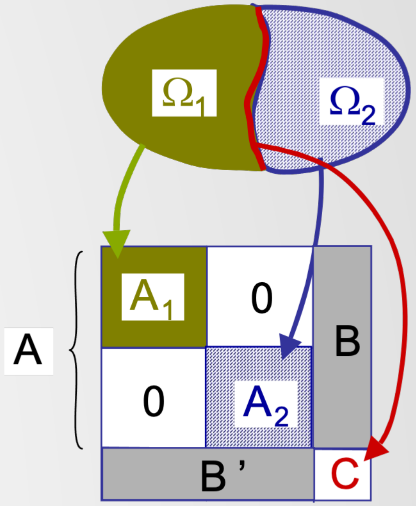
- **Domain decomposition (II):**
  - *Non-overlapping decomposition method:*
    - Schur complement system method

$$\begin{bmatrix} A & B \\ B' & C \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \Rightarrow \begin{cases} x = A^{-1}b_1 - A^{-1}By \\ (C - B'A^{-1}B)y = b_2 - B'A^{-1}b_1 \end{cases}$$

→ Base system
→ Schur comp. s.



Schur complement system method

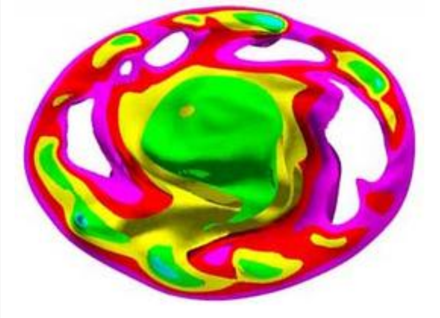
    - Continuity of BCs on subdomain interfaces can also be obtained using Lagrange multipliers:
      - Similar approach used in contact mechanics
      - FE Tearing and Interconnecting (FETI) method uses such approach

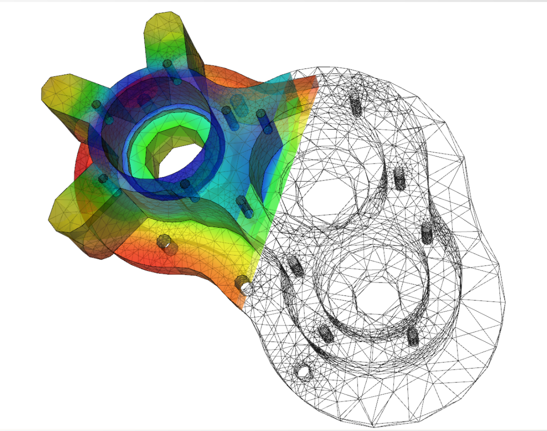
B. Butrylo, F. Musy, L.Nicolas, R.Perrussel, R. Scorretti, et al., *COMPEL: The Int. J. for Comp. and Math. in Elec. and Electronic Eng.*, Emerald, 2004, 23 (2), pp.531-546. ⟨10.1108/03321640410510721⟩. ⟨hal-00140344⟩

Elmer FEM

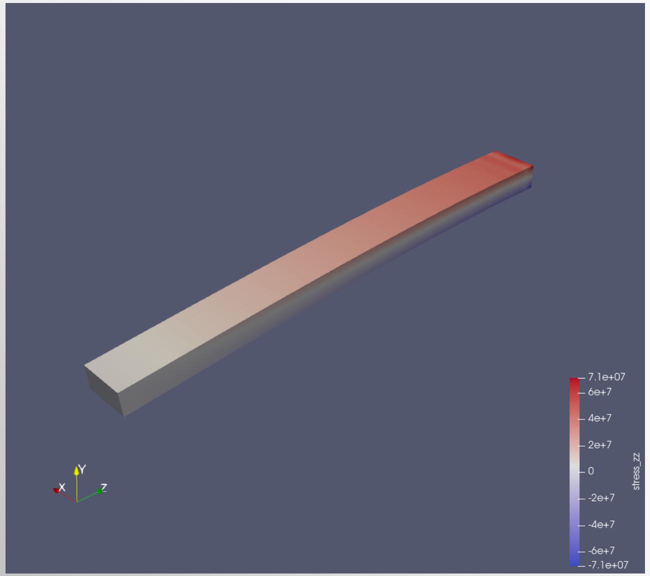
- **Open source multiphysics FEM software** – developed by CSC – IT Center of Science
- Physical models:
  - Solid mechanics
  - Fluid mechanics
  - Heat transfer
  - Acoustics
  - Electromagnetism, etc.
- Parallelization primarily based on MPI
- Suitable scalability has been shown using above 10^3 cores
- Preconditioners not always the same in parallel computations
  - Might deteriorate parallel performance

Elmer

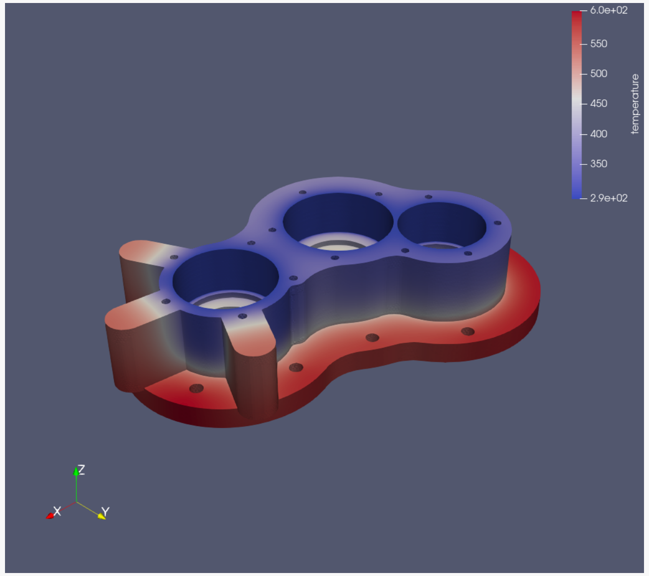




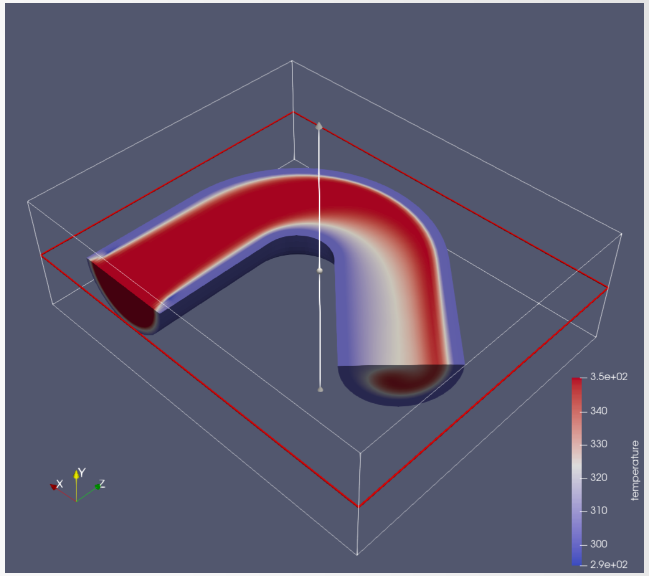
- Practical examples



Solid mechanics



Heat transfer



Coupled field-thermal flow

Thank you!

This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 951732. The JU receives support from the European Union’s Horizon 2020 research and innovation programme and Germany, Bulgaria, Austria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Greece, Hungary, Ireland, Italy, Lithuania, Latvia, Poland, Portugal, Romania, Slovenia, Spain, Sweden, United Kingdom, France, Netherlands, Belgium, Luxembourg, Slovakia, Norway, Switzerland, Turkey, Republic of North Macedonia, Iceland, Montenegro