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Implementation of FEM on HPC II – Solver types

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System of linear equations

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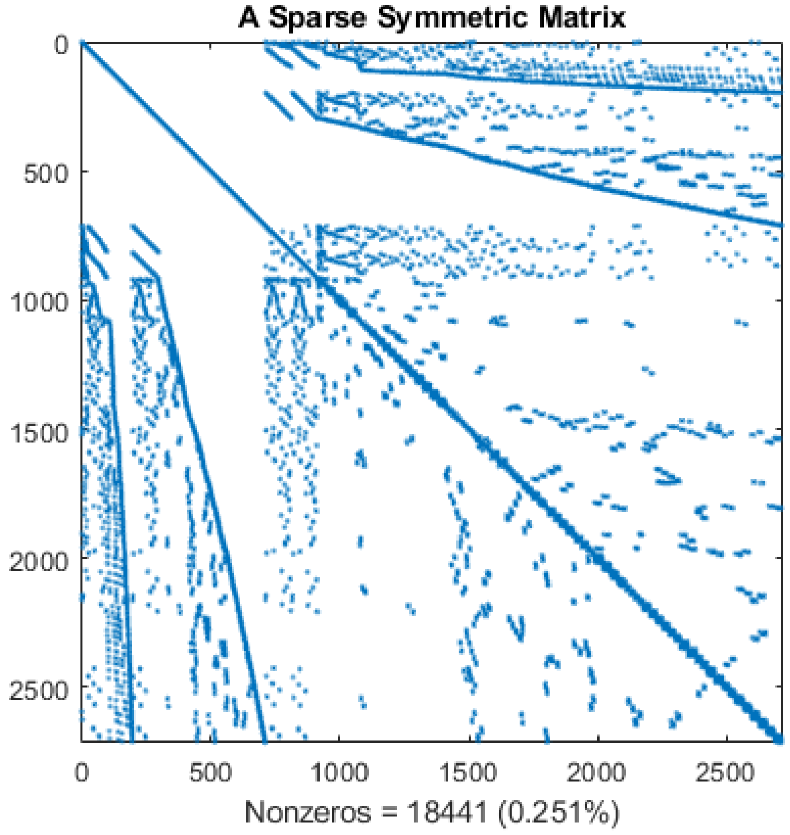
Different methods yield different systems of equations:

- Finite Difference Method (FDM) (large, sparse, unsymmetrical matrices)
- Finite Element Method (FEM) (large, sparse, generally unsymmetrical matrices)
- Finite Volume Method (FVM) (large, sparse, generally symmetric matrices)
- Boundary Element Method (BEM) (small systems, dense, unsymmetrical)



[1] https://au.mathworks.com/help/matlab/math/sparse-matrix-reordering.html

System of linear equations

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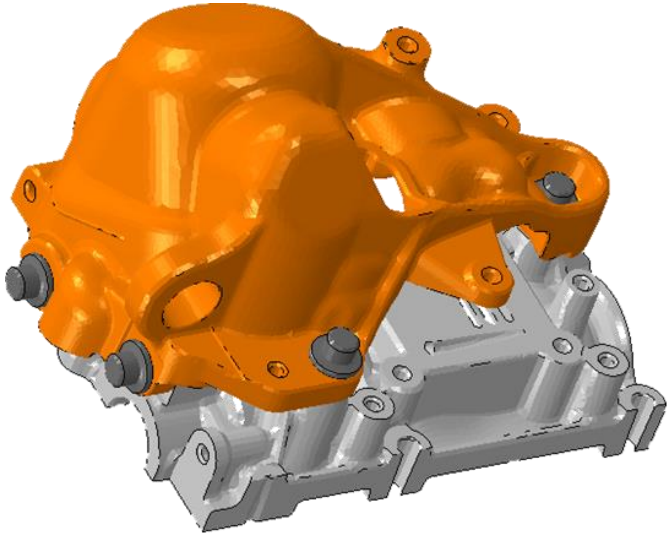
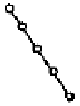
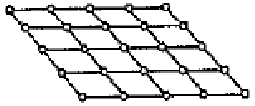
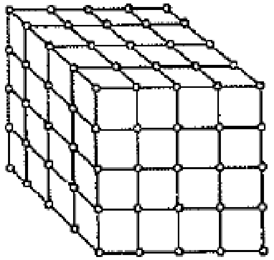
Different applications (meshes) result in different systems of equations:

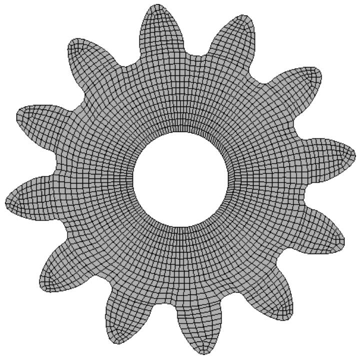
- Physical model is made from several parts or branches that are connected together (e.g. gears, spoked wheel)
- Space frames and other structures modelled with beams, trusses, and shells
- Blocky physical structures (solids, coupled structures in contact)
- 1D, 2D, 3D, degrees of freedom?
- Linear vs. nonlinear analysis?











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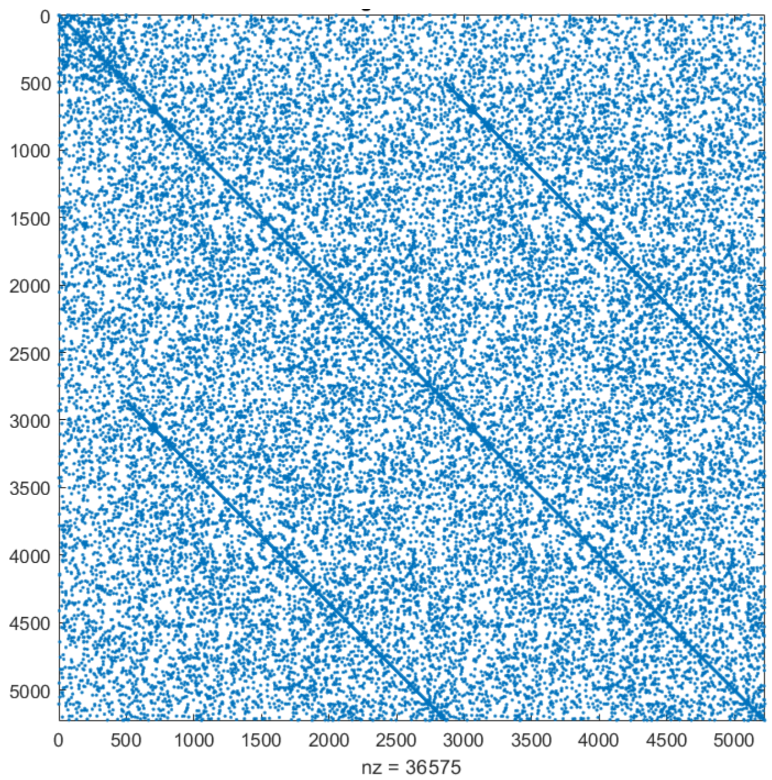
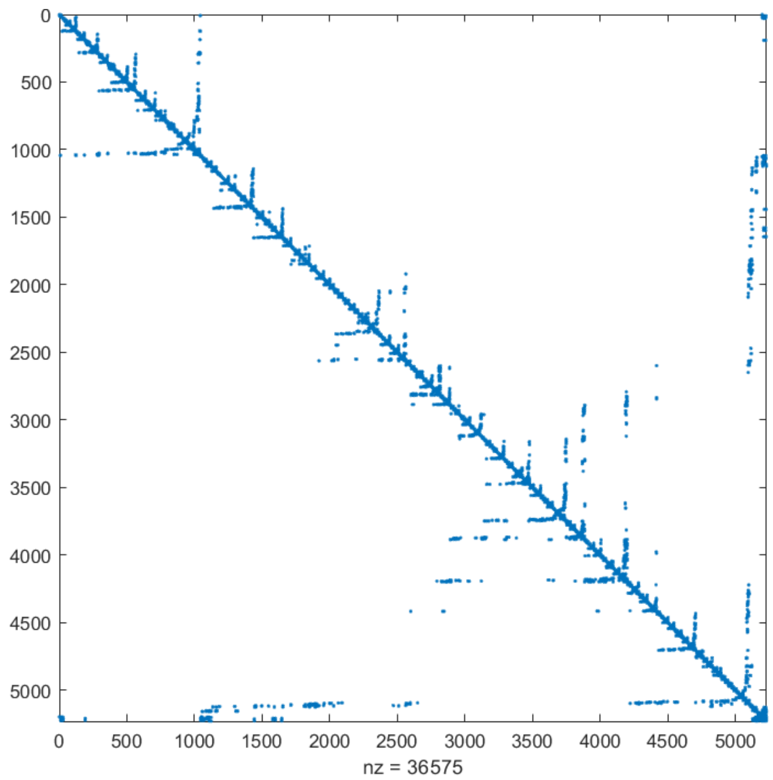
Sparse vs. dense matrices, bandwidth





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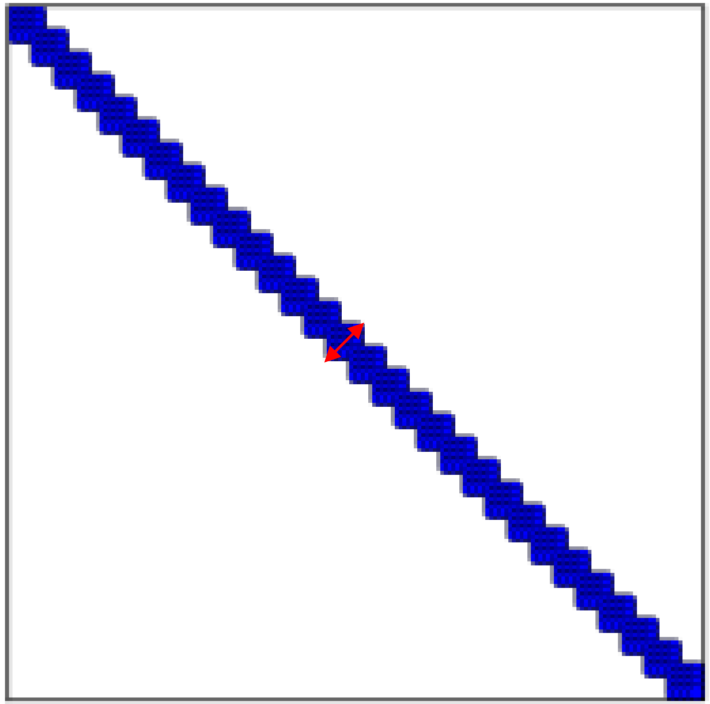
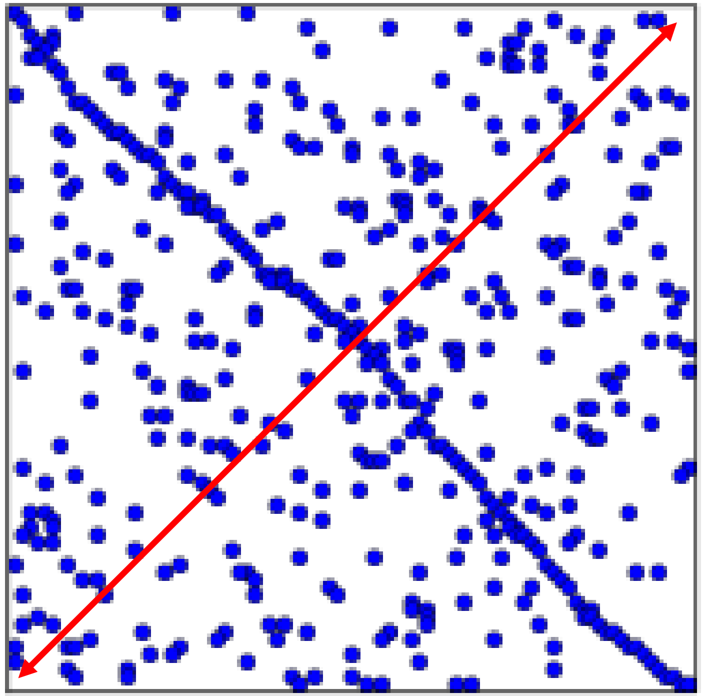
Influence of mesh numbering on bandwidth



Left-to-right numbering



Random numbering

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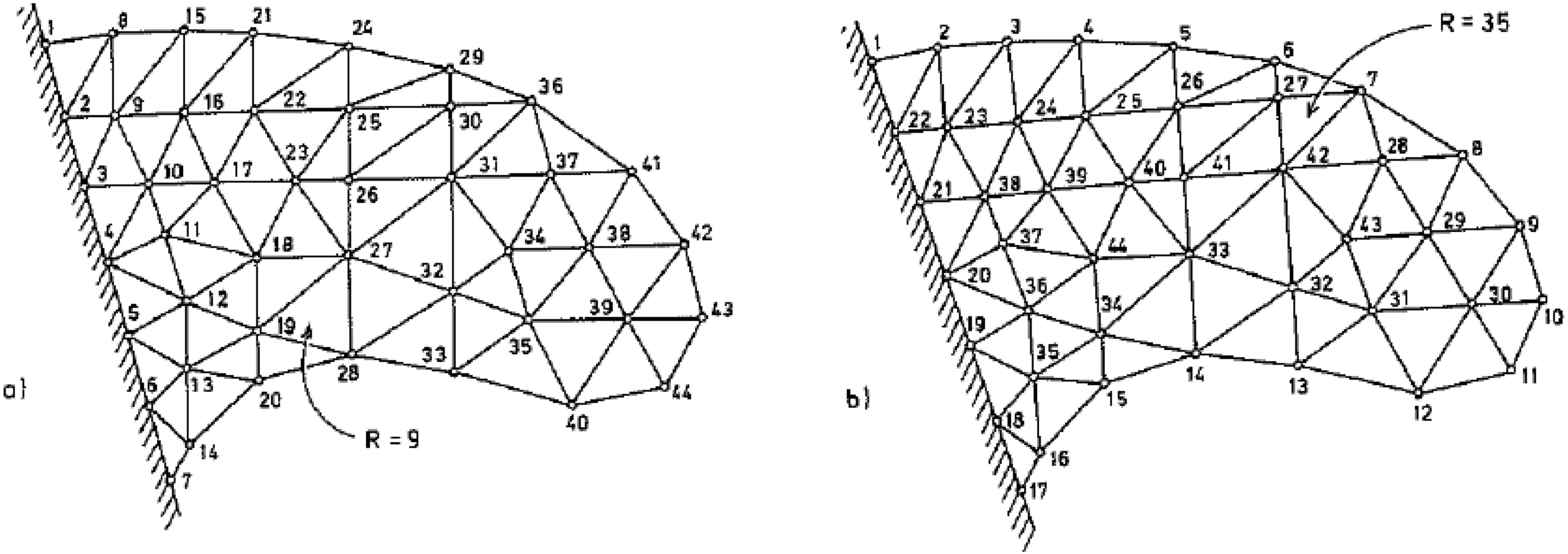
Influence of mesh numbering on bandwidth

$$B = (R+1)N_{DOF}$$



[2] N. S. Ottosen, H. Petersson : Introduction to the Finite Element Method

System of linear equations

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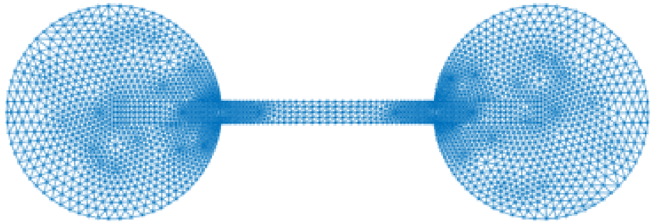
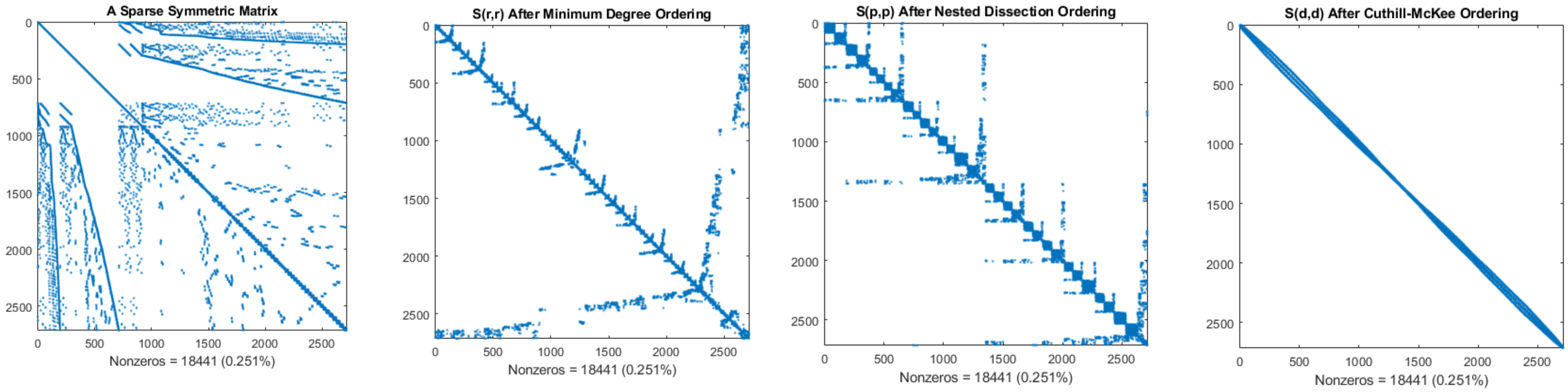
Reordering the rows and columns of a sparse matrix can influence the speed and storage requirements of a matrix operation



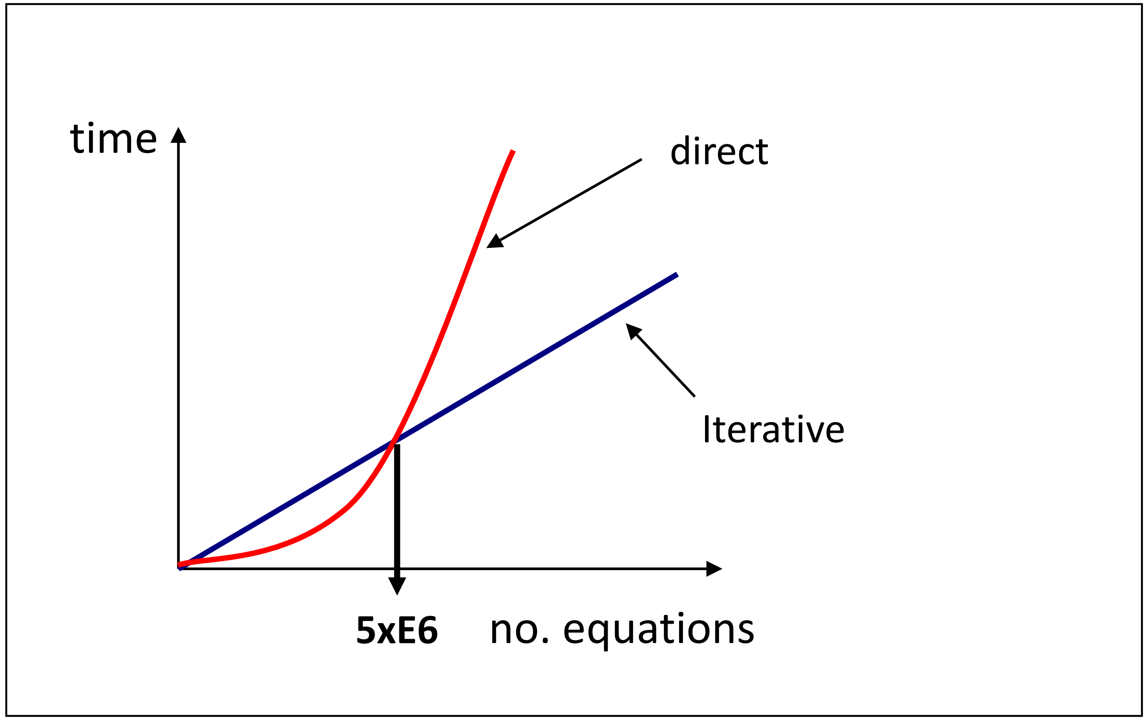


[1] https://au.mathworks.com/help/matlab/math/sparse-matrix-reordering.html

System of linear equations

Solution of a linear system of equations:

- Direct Solvers
  - Gauss elimination
  - Direct sparse solver (**MultiFront solver**)
  - LU decomposition
  - Cholesky method
  - **Domain Decomposition Method**
- Iterative Solvers
  - Gauss-Jacobi method
  - Gauss-Seidel method
  - **Krylov method**



System of linear equations

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Direct solvers:

- The direct linear equation solver finds the **exact solution to this system of linear equations** (up to machine precision).
- often represents the most time consuming part of the analysis (especially for large models) **— the storage of the equations occupies the largest part of the disk space during the calculations.**
- **Sparsity and bandwidth** have major impact on the **computational time**
- **physical model that is made from several parts or branches that are connected together;** a spoked wheel is a good example of a structure that has a sparse stiffness matrix

System of linear equations

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Iterative solvers:

- linear or nonlinear static, quasi-static, geostatic, pore fluid diffusion, heat transfer analysis ….
- **iterative -> a converged solution to a given system of linear equations cannot be guaranteed**
- when converges, **the accuracy of this solution depends on the relative tolerance** that is used
- **highly sensitive to the model geometry, favouring blocky type structures** (i.e., models that look more like a cube than a plate) **with a high degree of mesh connectivity and a relatively low degree of sparsity**
- The rate at which the approximate solution converges is directly related to the conditioning of the original system of equations. **A linear system that is well conditioned will converge faster than an ill-conditioned system.**

System of linear equations

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Deciding to use an iterative solver:

- Element type, contact and constraint equations, material and geometric nonlinearities and material properties
- Ill-conditioned models -> the iterative solver may converge very slowly or fail to converge. This may occur, for example, **if many elements have poor aspect ratios.**
- outperform the direct sparse solver only for **blocky models when number of DOF > 5 millions**
- **for some element types (i.e. cohesive) will likely lead to nonconvergence**
- **constraint equations** (multi-point constraints, surface-based tie constraints, kinematic couplings) solution cost grows linearly -> **recommended to keep such constraints to a minimum if possible, CONTACT -> special care must be taken due to large discontinuities**
- **material properties: large discontinuities in material behaviour (many orders of magnitude) will most likely converge slowly and possibly stagnate.**

System of linear equations

Gauss elimination:

$$computational\ cost = \alpha\ n\ B^2$$

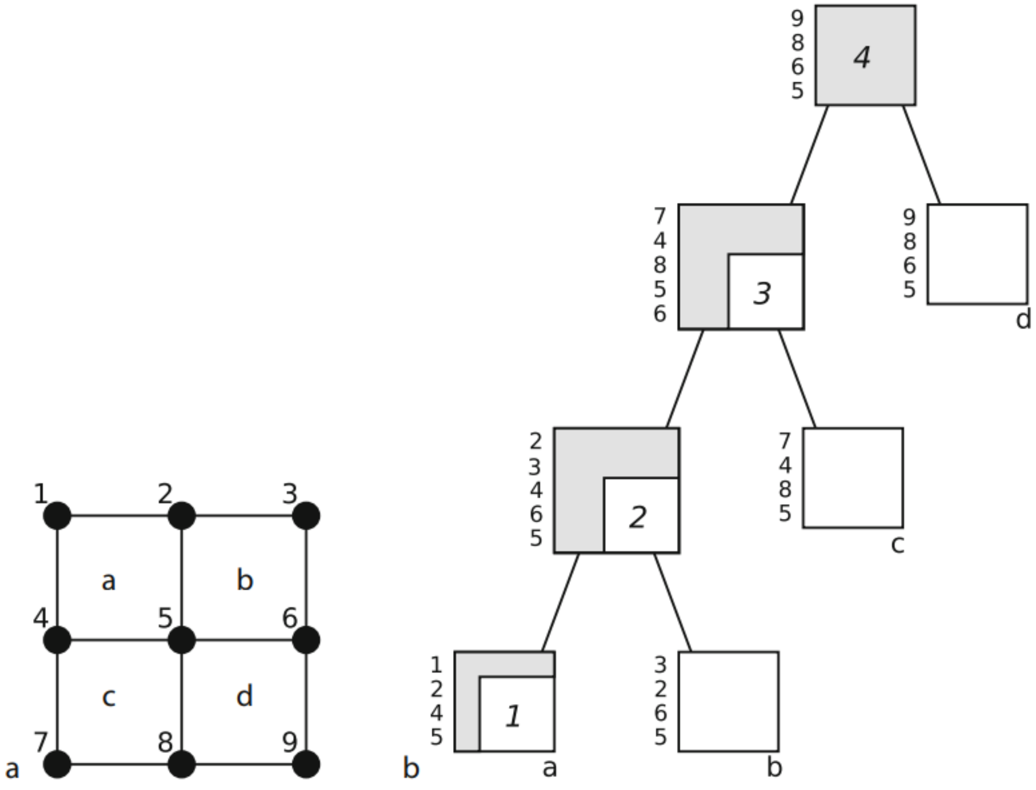
$$\begin{bmatrix} 2 & -2 & -2 & 0 \\ -2 & 4 & -2 & -2 \\ -2 & -2 & 12 & -2 \\ 0 & -2 & -2 & 22 \end{bmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ -5 \\ 7 \end{pmatrix} \qquad \begin{bmatrix} 2 & -2 & -2 & 0 \\ 0 & 2 & -4 & -2 \\ 0 & -4 & 10 & -2 \\ 0 & -2 & -2 & 22 \end{bmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ -4 \\ 7 \end{pmatrix}$$

$$\begin{bmatrix} 2 & -2 & -2 & 0 \\ 0 & 2 & -4 & -2 \\ 0 & 0 & 2 & -6 \\ 0 & 0 & -6 & 20 \end{bmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ -2 \\ 7 \end{pmatrix} \qquad \begin{bmatrix} 2 & -2 & -2 & 0 \\ 0 & 2 & -4 & -2 \\ 0 & 0 & 2 & -6 \\ 0 & 0 & 0 & 2 \end{bmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ -2 \\ 2 \end{pmatrix}$$

System of linear equations

direct sparse solver (MultiFront solver)

SPARSE symmetric matrices -> **assembly and static condensation process can be performed at the same time! -> Frontal Solver can reduce the computational time to solve the equations dramatically if the equation system has a sparse structure**



[3] https://link.springer.com/referenceworkentry/10.1007%2F978-0-387-09766-4_86

System of linear equations

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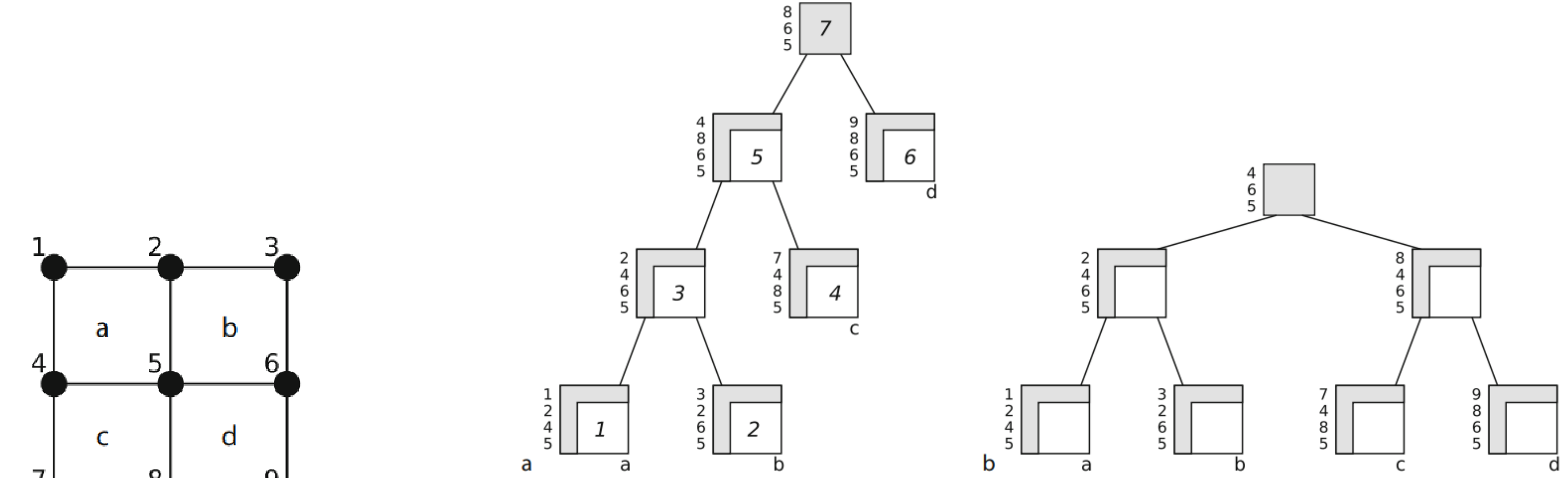
direct sparse solver (MultiFront solver):

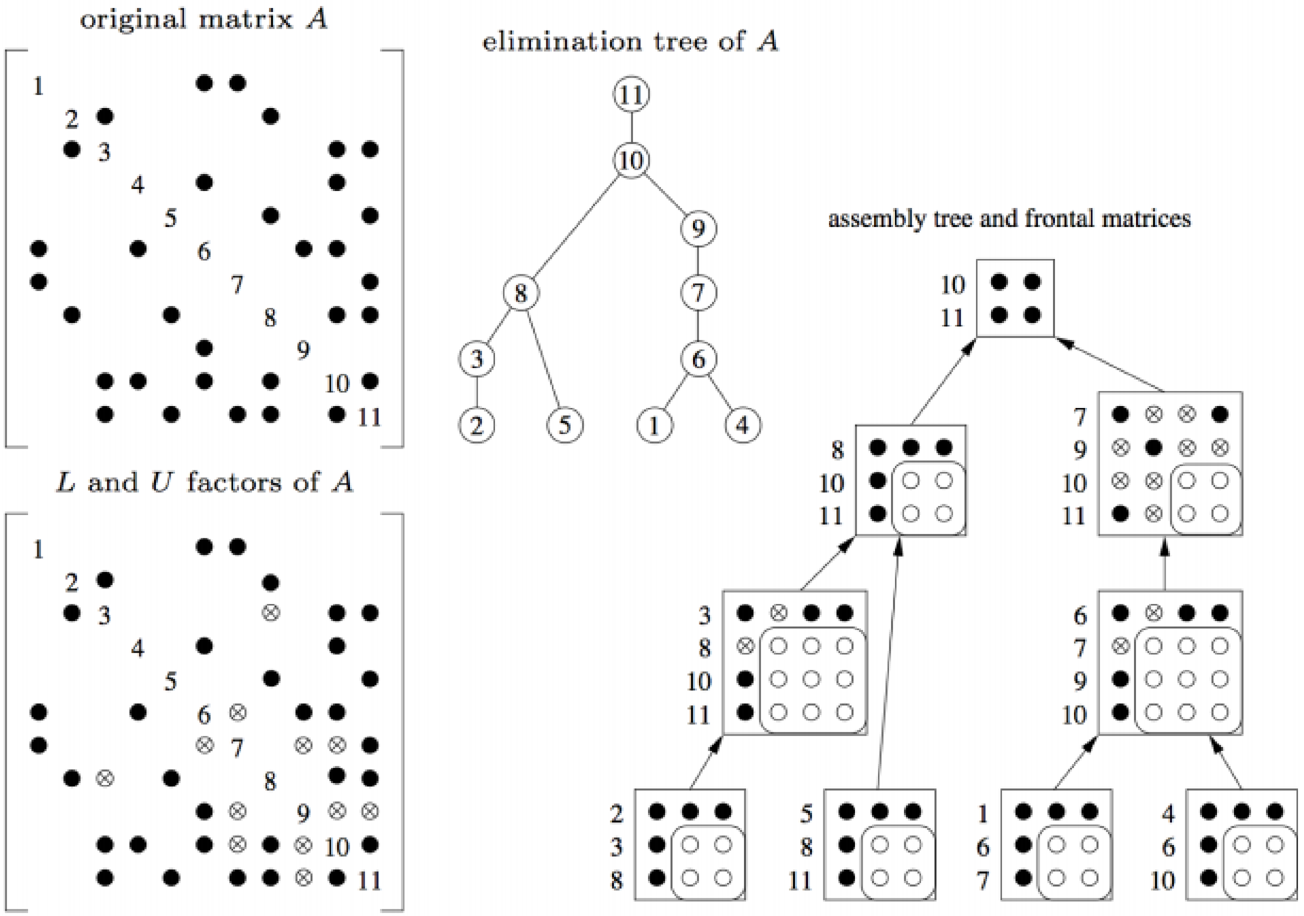


Multifrontal Method. Fig. 3 Finite-element problem and examples of associated assembly trees. Fully assembled variables are shown with a dark-shaded area within each frontal matrix

[3] https://link.springer.com/referenceworkentry/10.1007%2F978-0-387-09766-4_86

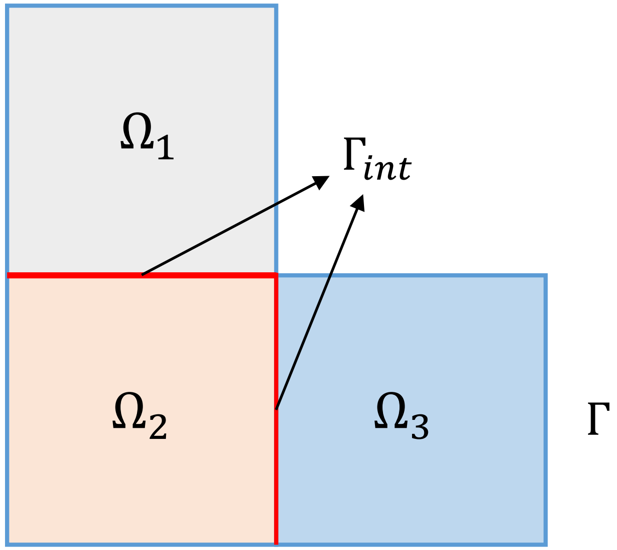
System of linear equations

direct sparse solver (MultiFront solver):



[3] https://link.springer.com/referenceworkentry/10.1007%2F978-0-387-09766-4_86

Domain Decomposition Method:



$x_1 \in \Omega_1$
$x_2 \in \Omega_2$
$x_3 \in \Omega_3$

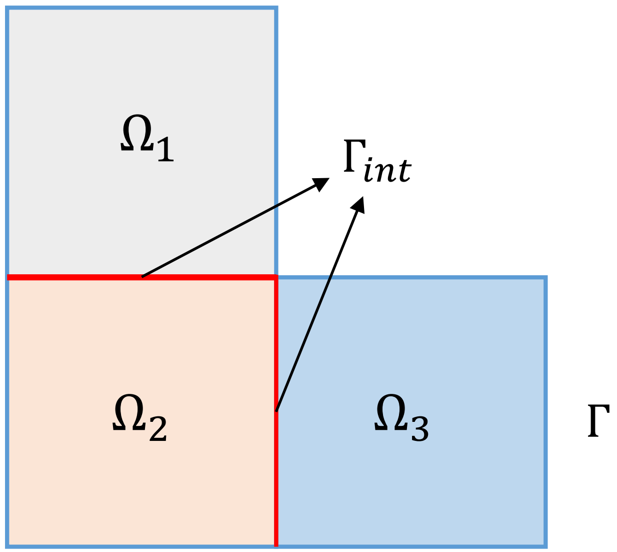
x_i - the solution of the domain internal points
y – the solution in the inter domain boundaries Γ_{int}.

The system of equations can be rewritten as:

$$\begin{bmatrix} \boldsymbol{B_1} & 0 & 0 & \boldsymbol{E_1} \\ 0 & \boldsymbol{B_2} & 0 & \boldsymbol{E_3} \\ 0 & 0 & \boldsymbol{B_3} & \boldsymbol{E_3} \\ \boldsymbol{F_1} & \boldsymbol{F_2} & \boldsymbol{F_3} & \boldsymbol{C} \end{bmatrix} \begin{pmatrix} \boldsymbol{x_1} \\ \boldsymbol{x_2} \\ \boldsymbol{x_3} \\ \boldsymbol{y} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f_1} \\ \boldsymbol{f_2} \\ \boldsymbol{f_3} \\ \boldsymbol{g} \end{pmatrix}$$

System of linear equations

Domain Decomposition Method:



$$\begin{bmatrix} B_1 & 0 & 0 & E_1 \\ 0 & B_2 & 0 & E_3 \\ 0 & 0 & B_3 & E_3 \\ F_1 & F_2 & F_3 & C \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ y \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ g \end{pmatrix} \Rightarrow$$

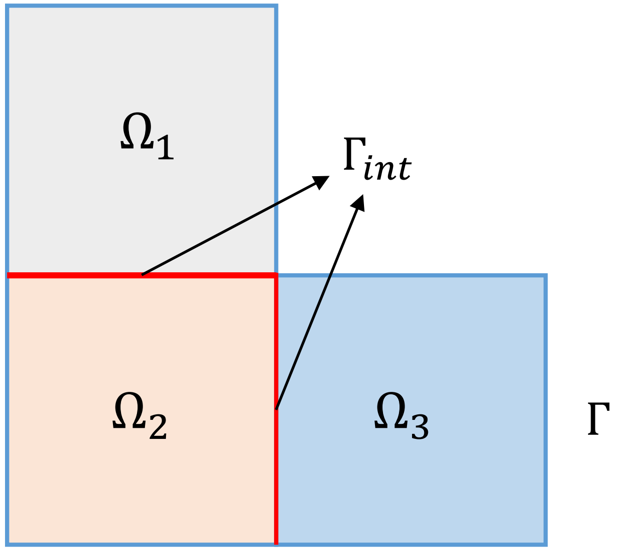
$$\begin{bmatrix} B & E \\ F & C \end{bmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix} \qquad B\,x + E\,y = f \Rightarrow x = B^{-1}(f - E\,y)$$

$$FB^{-1}(f - E\,y) + C\,y = g \Rightarrow \left(C - FB^{-1}E\right)y = g - FB^{-1}f$$

$$\Downarrow$$

$$S\ (Schur\ Component) \qquad \boxed{y = S^{-1}(g - FB^{-1}f)}$$

Domain Decomposition Method:



$$\begin{bmatrix} B_1 & 0 & 0 & E_1 \\ 0 & B_2 & 0 & E_3 \\ 0 & 0 & B_3 & E_3 \\ F_1 & F_2 & F_3 & C \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ y \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ g \end{pmatrix}$$

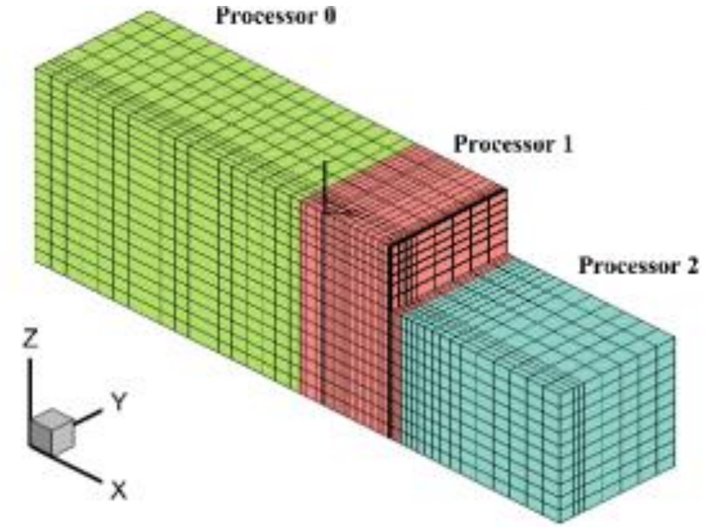
$$y = S^{-1}(g - FB^{-1}f)$$

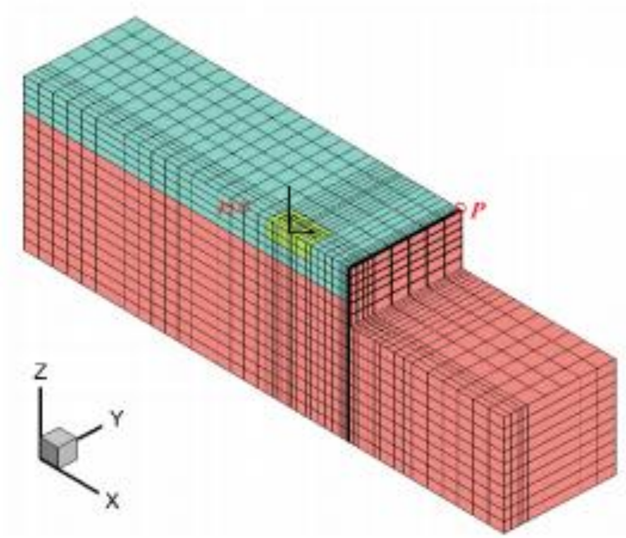
$$x_1 = B_1^{-1}(f_1 - E_1\, y)$$

$$x_2 = B_2^{-1}(f_2 - E_2\, y)$$

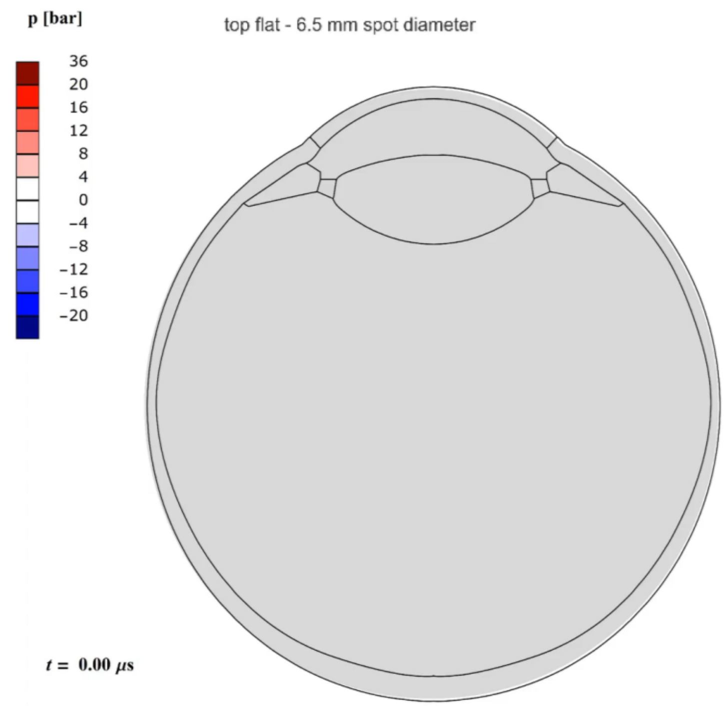
$$x_3 = B_3^{-1}(f_3 - E_3\, y)$$

Domain Decomposition Method:





Best practices – simulation of an laser-induced mechanical waves inside the human eye following laser medical procedures



Thank you for your attention!

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