Frontal and multi-frontal solvers: orderings, elimination trees, refinement trees

Maciej Paszynski

Department of Computer Science

AGH University of Science and Technology, Krakow, Poland

maciej.paszynski@agh.edu.pl

http://www.ki.agh.edu.pl/en/research-groups/a2s



EXEMPLARY SIMPLE 1D NUMERICAL PROBLEM

Find temperature distribution $R \ni x \mapsto u(x) \in R$ such that

$$\frac{d^2u}{dx^2} = 0 \text{ for } x \in [0,1] \qquad u(0) = 0 \qquad u(1) = 20$$

Finite difference disretization



 $h = \frac{1}{N}$ $u_i = u(x_i) = u\left(\frac{i}{N}\right)$ $[0,1] = \bigcup_{i=1}^N [x_{i-1}, x_i]$



TRIDIAGONAL MATRIX FOR EXEMPLARY 1D PROBLEM $u_0 = 0$ $\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = 0 \text{ for } i = 1, ..., N - 1$ $u_N = 20$ 1 0 ... 0 ... 0 0 $(u_i - 1) = 0$









Front matrix

Frontal matrix focuses on forward elimination of the first row





Front matrix

 2^{nd} row = 2^{nd} row - $1/h^2 * 1^{st}$ row





Front matrix

 2^{nd} row = 2^{nd} row - $1/h^2 * 1^{st}$ row





The first row has been eliminated

Frontral matrix focuses on the elimination of the second row





Front matrix

 $3^{rd} row = 3^{nd} row - [1/h^2] / [-2/h^2] * 2^{nd} row$



Front matrix

 $3^{rd} row = 3^{nd} row - [1/h^2] / [-2/h^2] * 2^{nd} row$

ELEMENT-WISE DECOMPOSITION





0 20

$\begin{bmatrix} 1 & 0 \\ 1/h^2 & -\frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_3^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_3^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_3^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_3^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_3^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_3^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ \frac{1}{h^2} & -\frac{1}{h^$

First all frontal matrices are constructed





First and second frontal matrices are sum up into new 3x3 frontal matrix Its first and second rows are fully assembled



 $\begin{bmatrix} 1 & 0 \\ 1/h^2 & -\frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2^{\mathrm{I}} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} = \begin{bmatrix} 0 \\ x_3^{\mathrm{I}} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_2^{\mathrm{II}} \\ x_3^{\mathrm{II}} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_3^{\mathrm{II}} \\ \frac{1}{h^2} & -\frac{1}{h^2$

First column is eliminated by using first row

 $2^{nd} row = 2^{nd} row - [1/h^2] * 1^{st} row$





 $\begin{bmatrix} 1 & 0 \\ 1/h^2 & -\frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_3^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ x_1^{II} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{II} \\ \frac{1}{h^2} & \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_$

 $2^{nd} row = 2^{nd} row - [1/h^2] * 1^{st} row$





 $\begin{bmatrix} 1 & 0 \\ 1/h^2 & -\frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ x_3^{\text{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ x_3^{\text{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ x_3^{\text{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ x_3^{\text{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ x_3^{\text{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ x_1^{\text{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ x_1^{\text{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ x_1^{\text{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ x_1^{\text{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ x_1^{\text{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ x_1^{\text{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ x_1^{\text{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ x_1^{\text{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ x_1^{\text{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ x_1^{\text{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ x_1^{\text{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ \frac{1}{h^2} & \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_1^{\text{I}} \\ \frac{1}{h^2} & \frac{1}{h^2}$

Third and fourth frontal matrices are sum up into new 3x3 frontal matrix Now only the second row is fully assembled





Change of the ordering







Why can I substract fully assembled 1st row from not fully assemled rows 2nd and 3rd ?



 $\begin{array}{c} 1 & 0 \\ 1/h^2 & -\frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{array} \left\{ \begin{array}{c} x_1 \\ x_2 \\ \frac{1}{h^2} \end{array} \right\} = \left\{ \begin{array}{c} 0 \\ 0 \end{array} \right\} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{array} \left\{ \begin{array}{c} x_2^{\text{II}} \\ x_3^{\text{II}} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{array} \right\} = \left\{ \begin{array}{c} 0 \\ 0 \end{array} \right\} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{bmatrix} \left\{ \begin{array}{c} x_3^{\text{II}} \\ x_4^{\text{II}} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{array} \right\} = \left\{ \begin{array}{c} 0 \\ 0 \end{array} \right\} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{array} \left\{ \begin{array}{c} x_3^{\text{II}} \\ x_5^{\text{II}} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{array} \right\} = \left\{ \begin{array}{c} 0 \\ 0 \end{array} \right\} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{array} \left\{ \begin{array}{c} x_4^{\text{II}} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{array} \right\} = \left\{ \begin{array}{c} 0 \\ 0 \end{array} \right\} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{array} \right\} = \left\{ \begin{array}{c} 0 \\ 0 \end{array} \right\} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{array} \right\} = \left\{ \begin{array}{c} 0 \\ 0 \end{array} \right\} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \\ \frac{1}{h^2} & -\frac{1}{h^2} \end{array} \right\}$



This is because substraction and addition are interchangable (now I am substructing from the 2nd not fully assembled row, and later I will add the remaining part)

Moreover the 1st row which is utilized for the substractions in other columns contains only zeros



 $\frac{1}{\frac{1}{h^2} - \frac{1}{h^2}} \begin{bmatrix} x_1 \\ x_2^{\mathrm{I}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_2^{\mathrm{II}} \\ x_3^{\mathrm{II}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_3^{\mathrm{II}} \\ x_3^{\mathrm{II}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_4^{\mathrm{II}} \\ x_5^{\mathrm{II}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_4^{\mathrm{II}} \\ x_5^{\mathrm{II}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_4^{\mathrm{II}} \\ x_5^{\mathrm{II}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_4^{\mathrm{II}} \\ x_5^{\mathrm{II}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_4^{\mathrm{II}} \\ x_5^{\mathrm{II}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_4^{\mathrm{II}} \\ x_5^{\mathrm{II}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_4^{\mathrm{II}} \\ x_5^{\mathrm{II}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_4^{\mathrm{II}} \\ x_5^{\mathrm{II}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_4^{\mathrm{II}} \\ x_5^{\mathrm{II}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_4^{\mathrm{II}} \\ x_5^{\mathrm{II}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_4^{\mathrm{II}} \\ x_5^{\mathrm{II}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_4^{\mathrm{II}} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_4^{\mathrm{II}} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h^2} & \frac{1}{h^2} \\ \frac{1}{h^2} - \frac{1}{h^2} \end{bmatrix} \begin{bmatrix} x_4^{\mathrm{II}} \\ \frac{1$





 $\begin{array}{c} 1 & 0 \\ 1 \\ h^{2} \\ h^$





Fifth and sixth frontal matrices are sum up into new 3x3 frontal matrix Now the second and third rows are fully assembled





Continue until root node





All frontal matrices are generated at the same time





Summing up and elimination are executed at the same time over different pairs of frontal matrices





Procesor 1 Procesor 2 Procesor 3 Procesor 4 Procesor 5 Procesor 6

Summing up and elimination are executed at the same time over different pairs of frontal matrices





The agorithm is recursively repeated until we reach the root of the tree The algorithm results in upper trianguler matrix stored in distributed manner Computational complexity = height of the tree = logN (where N = #unknowns-1)



Strong formulation

Find $u \in C^2(0, l)$ such that -(a(x)u'(x))'+b(x)u'(x)+c(x)u(x) = f(x) u(0) = 0 $a(l)u'(l) + \beta u(l) = \gamma$

Weak formulation

Find
$$u \in V$$
 such that

$$\int_{0}^{l} \{au'v'+bu'v+cuv\}dx + \beta u(l)v(l) = \int_{0}^{l} f v dx + \gamma v(l)$$

$$b(u,v) = l(v)$$

$$\forall v \in V = \{v \in H^{1}(0,l) : v(0) = 0\}$$

Finite element method disretization

$$u = \sum_{i=1}^{N} a_{i} e_{i} \qquad v = e_{j} \qquad \sum_{i=1}^{N} a_{i} b(e_{i}, e_{j}) = l(e_{j}) \qquad j = 1, \dots, N$$
$$b(e_{i}, e_{j}) = \int_{0}^{l} \{ae_{i} e_{j} + be_{i} e_{j} + ce_{i}e_{j}\} dx + \beta e_{i}(l)e_{j}(l) \qquad l(e_{j}) = \int_{0}^{l} f e_{j} dx + \gamma e_{j}(l)$$

Exemplary basis functions for [0,I] = [0,1], for two finite elements



$$u = \sum_{i=1}^{N} a_{i} e_{i} \quad v = e_{j} \qquad \begin{bmatrix} b(e_{1}, e_{1}) & b(e_{2}, e_{1}) & b(e_{3}, e_{1}) \\ b(e_{1}, e_{2}) & b(e_{2}, e_{2}) & b(e_{3}, e_{2}) \\ b(e_{1}, e_{3}) & b(e_{2}, e_{3}) & b(e_{3}, e_{3}) \end{bmatrix} \begin{bmatrix} a_{1} \\ a_{2} \\ a_{3} \end{bmatrix} = \begin{cases} l(e_{1}) \\ l(e_{2}) \\ l(e_{3}) \end{bmatrix}$$
$$b(e_{i}, e_{j}) = \int_{0}^{l} \{ae_{i} e_{j} + be_{i} e_{j} + ce_{i}e_{j}\} dx + \beta e_{i}(l)e_{j}(l) \qquad l(e_{j}) = \int_{0}^{l} f e_{j} dx + \gamma e_{j}(l)$$

Exemplary basis functions for [0,I] = [0,1], for two finite elements



$$u = \sum_{i=1}^{N} a_{i} e_{i} \quad v = e_{j} \qquad \begin{bmatrix} b(e_{1}, e_{1}) \quad b(e_{2}, e_{1}) \quad b(e_{3}, e_{1}) \\ b(e_{1}, e_{2}) \quad b(e_{2}, e_{2}) \quad b(e_{3}, e_{2}) \\ b(e_{1}, e_{3}) \quad b(e_{2}, e_{3}) \quad b(e_{3}, e_{3}) \end{bmatrix} \begin{bmatrix} a_{1} \\ a_{2} \\ a_{3} \end{bmatrix} = \begin{cases} l(e_{1}) \\ l(e_{2}) \\ l(e_{3}) \end{bmatrix}$$

$$b(e_{1}, e_{j}) = \int_{0}^{l} \{ae_{i}'e_{j}' + be_{i}'e_{j} + ce_{i}e_{j}\} dx + \beta e_{i}(l)e_{j}(l) \qquad l(e_{j}) = \int_{0}^{l} f e_{j} dx + \gamma e_{j}(l)$$
Exemplary basis functions for [0,I] = [0,1], for two finite elements
$$\int_{0}^{e_{2}} e_{2} = \chi_{1}^{K_{2}} + \chi_{2}^{K_{1}} \qquad e_{3} = \chi_{2}^{K_{2}} e_{3} = 1$$

$$b(e_{1}, e_{1}) = \int_{0}^{l} \{ae_{1}'e_{1}' + be_{1}'e_{1} + ce_{1}e_{1}\} dx + \beta e_{1}(l)e_{1}(l) = \int_{0}^{0.5} \{a\frac{d\chi_{1}^{K_{1}}}{dx} \frac{d\chi_{1}^{K_{1}}}{dx} + b\frac{d\chi_{1}^{K_{1}}}{dx} \chi_{1}^{K_{1}} + c(\chi_{1}^{K_{1}})^{2}\} dx$$

$$b(e_{2}, e_{2}) = \int_{0}^{l} \{ae_{2}'e_{2}' + be_{2}'e_{2} + ce_{2}e_{2}\} dx + \beta e_{2}(l)e_{2}(l) = 1$$

$$\int_{0}^{0.5} \{a\frac{d\chi_{2}^{K_{1}}}{dx} \frac{d\chi_{2}^{K_{1}}}{dx} + b\frac{d\chi_{2}^{K_{1}}}{dx} \chi_{1}^{K_{2}} + c(\chi_{1}^{K_{2}})^{2}\} dx + \beta e_{3}(l)e_{3}(l) = \int_{0.5}^{l} \{a\frac{d\chi_{1}^{K_{2}}}{dx} \frac{d\chi_{2}^{K_{2}}}{dx} + b\frac{d\chi_{2}^{K_{2}}}{dx} \chi_{2}^{K_{2}} + c(\chi_{2}^{K_{2}})^{2}\} dx + \beta e_{3}(l)e_{3}(l) = \int_{0.5}^{l} \{a\frac{d\chi_{2}^{K_{2}}}{dx} \frac{d\chi_{2}^{K_{2}}}{dx} + b\frac{d\chi_{2}^{K_{2}}}{dx} \chi_{2}^{K_{2}} + c(\chi_{2}^{K_{2}})^{2}\} dx + \beta e_{3}(l)e_{3}(l) = \int_{0.5}^{l} \{a\frac{d\chi_{2}^{K_{2}}}{dx} \frac{d\chi_{2}^{K_{2}}}{dx} + b\frac{d\chi_{2}^{K_{2}}}{dx} \chi_{2}^{K_{2}} + c(\chi_{2}^{K_{2}})^{2}\} dx + \beta e_{3}(l)e_{3}(l) = \int_{0.5}^{l} \{a\frac{d\chi_{2}^{K_{2}}}{dx} \frac{d\chi_{2}^{K_{2}}}{dx} + b\frac{d\chi_{2}^{K_{2}}}{dx} \chi_{2}^{K_{2}} + c(\chi_{2}^{K_{2}})^{2}\} dx + \beta e_{3}(l)e_{3}(l) = \int_{0.5}^{l} \{a\frac{d\chi_{2}^{K_{2}}}{dx} \frac{d\chi_{2}^{K_{2}}}{dx} + b\frac{d\chi_{2}^{K_{2}}}{dx} \chi_{2}^{K_{2}} + c(\chi_{2}^{K_{2}})^{2}\} dx + \beta e_{3}(l)e_{3}(l) = \int_{0.5}^{l} \{a\frac{d\chi_{2}^{K_{2}}}{dx} \frac{d\chi_{2}^{K_{2}}}{dx} \frac{d\chi_{2}^{K_{2}}}{dx} + b\frac{d\chi_{2}^{K_{2}}}{dx} \chi_{2}^{K_{2}} + c(\chi_{2}^{K_{2}})^{2}\} dx + \beta e_{3}(l)e_{3}(l) = \int_{0.5}^{l} \{a\frac{d\chi_{2}^{K_{2}}}{dx} \frac{d\chi_{2}^{K_{2}}}{dx} \frac{d\chi_{2}^{K_{2}}}{dx} \frac{d\chi_{2}^{K$$



Notice that when we switch from finite difference to finite elements, it only changes the local systems of equations at tree nodes

$$\begin{bmatrix} b(\chi_1^K, \chi_1^K) & b(\chi_2^K, \chi_1^K) \\ b(\chi_1^K, \chi_2^K) & b(\chi_2^K, \chi_2^K) \end{bmatrix} \begin{bmatrix} x_1^K \\ x_2^K \end{bmatrix} = \begin{bmatrix} l(\chi_1^K) \\ l(\chi_2^K) \end{bmatrix}$$



Global basis functions are composed with local shape functions, e.g.

$$e_2 = \chi_1^{K_2} + \chi_2^{K_1}$$

$$b(\chi_i^K, \chi_j^K) = \int_K \left\{ a\chi_i^K \chi_j^K + b\chi_i^K \chi_j^K + c\chi_i^K \chi_j^K \right\} dx + \beta \chi_i^K(l) \chi_i^K(l)$$
$$l(e_j) = \int_K f \chi_j^K dx + \gamma \chi_j^K(l)$$

Local system of equations generated over the element K

$$\begin{bmatrix} b(\chi_1^K, \chi_1^K) & b(\chi_2^K, \chi_1^K) \\ b(\chi_1^K, \chi_2^K) & b(\chi_2^K, \chi_2^K) \end{bmatrix} \begin{bmatrix} x_1^K \\ x_2^K \end{bmatrix} = \begin{bmatrix} l(\chi_1^K) \\ l(\chi_2^K) \end{bmatrix}$$



Notice that when we switch from finite difference to finite elements, it only changes the local systems of equations at tree nodes

2D hp FINITE ELEMENT METHOD

 $u = \sum_{i=1}^{15} u_{hp}^i e_{hp}^i$ We seek the solution *u* of some weak form of PDE as a linear combination of shape functions e_{hp}^{i} spread over finite element mesh e_{hp}^5 e_{hp}^3 e_{hp}^{1} 3 5 6 10 13 15 11 12 14 e_{hp}^2 e_{hp}^4 e_{hp}^9 e_{hp}^7

2D hp FINITE ELEMENT METHOD



FRONTAL SOLVER SOLUTION BASED ON LINEAR ORDER OF ELEMENTS



Generates frontal matrix for the first element, eliminates fully assembled degrees of freedom



FRONTAL SOLVER SOLUTION BASED ON LINEAR ORDER OF ELEMENTS



Generates frontal matrix for the second element, merges with the current frontal matrix eliminates fully assembled degrees of freedom



MULTI-FRONTAL SOLVER SOLUTION BASED ON THE ELIMINATION TREE







MULTI-FRONTAL SOLVER SOLUTION BASED ON THE ELIMINATION TREE







MULTI-FRONTAL SOLVER SOLUTION BASED ON THE ELIMINATION TREE



COMPARISON OF COSTS



Number of operations for partial forward elimination

$$\sum_{m=1}^{b} m^2 - \sum_{m=1}^{(b-a)} m^2 = \frac{a(6b^2 - 6ab + 6b + 2a^2 - 3a + 1)}{6}$$

Frontal solver

| Step | a | b | computational cost = $\frac{a(6b^2 - 6ab + 6b + 2a^2 - 3a + 1)}{6}$ |
|-------|---|---|---|
| 1 | 6 | 9 | 271 |
| 2 | 9 | 9 | 729 |
| Total | | | 1000 |

Multi-frontal solver

| Step | a | b | computational cost = $\frac{a(6b^2 - 6ab + 6b + 2a^2 - 3a + 1)}{6}$ | |
|-------|---|---|---|------|
| 1 | 6 | 9 | 271 | |
| 2 | 6 | 9 | 271 | |
| 3 | 3 | 3 | 27 | |
| Total | | | 569 | 2460 |

CONSTRUCTION OF THE ELIMINATION TREE BASED ON THE HISTORY OF MESH REFINEMENTS

For any initial mesh, the elimination tree can be created based on nested dissection algorithm.



CONSTRUCTION OF THE ELIMINATION TREE BASED ON THE HISTORY OF MESH REFINEMENTS

The elimination tree created for the initial mesh is updated when the mesh is refined (elimination tree is constructed dynamically, during mesh refinements)

CONSTRUCTION OF THE ELIMINATION TREE BASED ON THE HISTORY OF MESH REFINEMENTS

The elimination tree created for the initial mesh is updated when the mesh is refined (elimination tree is constructed dynamically, during mesh refinements)

1 2

| 3 | 4 | 5 | 6 |
|---|---|---|----|
| 7 | 8 | 9 | 10 |

| 3 | 4 | | | 5 | | | 6 |
|---------|----|----|-------|----|----|----|---|
| 7 11 12 | | 2 | 15 16 | | 16 | 10 | |
| | 13 | 19 | 20 | 23 | 24 | 18 | |
| | 15 | 21 | 22 | 25 | 26 | 10 | |

Local matrices for active elements – leaves of the elimination tree – are created

• Interior degrees of freedom are eliminated at every leaf

• Schur complement contributions are merged at parent level

 Fully assembled degrees of freedom are eliminated at parent nodes level (degrees of freedom related to common edges shared by both son elements can be eliminated now)

• Contributions to Schur complement are merged again at the next level

• Fully assembled degrees of freedom are eliminated

• Finally, Schur complement contributions are merged at the tree root node

• The common interface problem is solved at the tree root node (The size of the common interface problem corresponds to the size of crossection of the entire domain)

- The solution obtained at root node is utilized at son nodes.
- The backward substitution is executed

- The solution utilized at the second level nodes is utilizes at their sone nodes.
- The backward substitution is executed

- The solution obtained at the third level nodes is utilized at leaf nodes.
- The backward substitution is executed on the level of leaf nodes

PERFORMANCE OF THE 1st VERSION OF THE DISTRIBUTED MEMORY MULTI-FRONTAL PARALLEL SOLVER

1,482,570 degrees of freedom (68,826,475 non-zeros)

- Embeded into hp code
- + Outperforms MUMPS for large number of processors
- Slower than MUMPS for low number of processors

Profiling showed that the time consuming part for low number of processors was actually process of merging of matrices – performed on the level of unknowns, with moving of matrix entries.

Switch to the level of nodes, do not touch matrix entries -work with pointers

PAPERS

http://home.agh.edu.pl/~paszynsk/Publications.html

Maciej Paszyński, David Pardo, Carlos Torres-Verdin, Leszek Demkowicz, Victor Calo A PARALLEL DIRECT SOLVER FOR SELF-ADAPTIVE HP FINITE ELEMENT METHOD

Journal of Parallel and Distributed Computing, 70, 3 (2013) 270-281

Anna Paszynska, Maciej Paszynski, Konrad Jopek, Maciej Wozniak, Damian Goik, Piotr Gurgul, Hassan AbouEisha, Mikhail Moshkov, Victor Calo, Andrew Lenharth, Donald Nguyen, Keshav Pingali

QUASI-OPTIMAL ELIMINATION TREES FOR 2D GRIDS WITH SINGULARITIES

Scientiffic Programming, (2015) Article ID 303024, 1-18

Maciej Paszynski, David Pardo, Anna Paszynska, Leszek Demkowicz

OUT-OF-CORE MULTI-FRONTAL SOLVER FOR MULTI-PHYSICS HP ADAPTIVE PROBLEMS

Procedia Computer Science, 4 (2011) 1788-1797