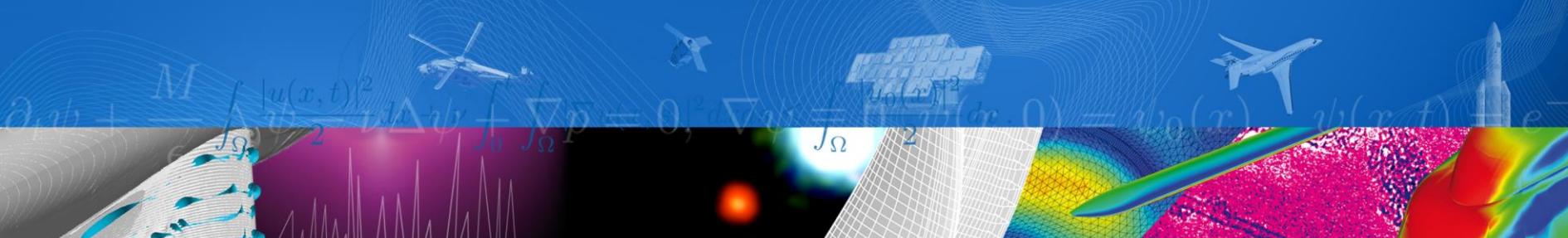


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Dirichlet to Neumann, Schur complement, Robin, interconnecting and coupling

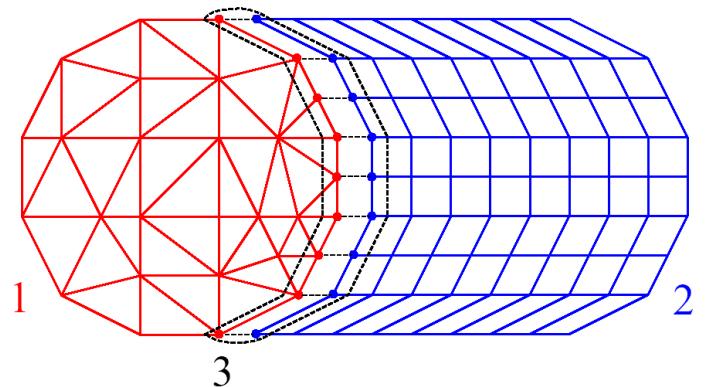
François-Xavier Roux
High Performance Computing Unit



Domain decomposition methods, algebraic approach

- Global system of equations

$$\begin{pmatrix} K_{11} & 0 & K_{13} \\ 0 & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$



- Local systems of equations

$$\begin{pmatrix} K_{11} & K_{13} \\ K_{31} & K_{33}^{(1)} \end{pmatrix}, \quad \begin{pmatrix} x_1 \\ x_3^{(1)} \end{pmatrix}, \quad \begin{pmatrix} b_1 \\ b_3^{(1)} \end{pmatrix}$$

$$\begin{pmatrix} K_{22} & K_{23} \\ K_{32} & K_{33}^{(2)} \end{pmatrix}, \quad \begin{pmatrix} x_2 \\ x_3^{(2)} \end{pmatrix}, \quad \begin{pmatrix} b_2 \\ b_3^{(2)} \end{pmatrix}$$

$$K_{33}^{(1)} + K_{33}^{(2)} = K_{33}$$

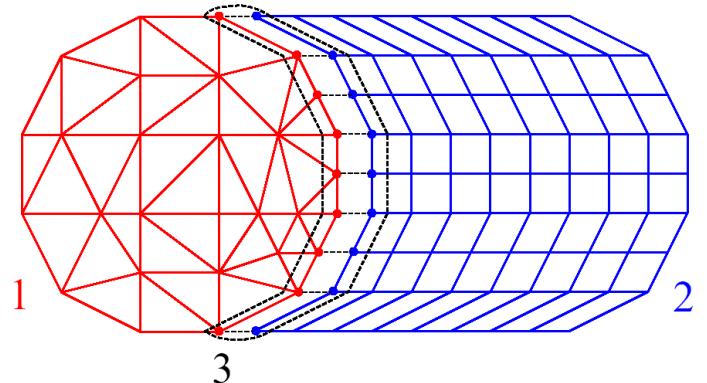
$$b_3^{(1)} + b_3^{(2)} = b_3$$

Local equations, interface interconnecting conditions

- Local inner equations

$$K_{11} x_1 + K_{13} x_3^{(1)} = b_1$$

$$K_{22} x_2 + K_{23} x_3^{(2)} = b_2$$



- Admissibility condition at interface

$$x_3^{(1)} = x_3^{(2)} \quad (= x_3)$$

- Equilibrium condition at interface

$$K_{31} x_1 + K_{32} x_2 + K_{33} x_3 = b_3$$

$$K_{31} x_1 + K_{33}^{(1)} x_3^{(1)} + K_{32} x_2 + K_{33}^{(2)} x_3^{(2)} = b_3^{(1)} + b_3^{(2)}$$

Dirichlet to Neumann and Schur complement

- Local problems with Dirichlet boundary conditions

$$K_{11} x_1 = b_1 - K_{13} x_3^{(1)}$$

$$K_{22} x_2 = b_2 - K_{23} x_3^{(2)}$$

- Local contributions to interface residual

$$\begin{pmatrix} K_{11} & K_{13} \\ K_{31} & K_{33}^{(1)} \end{pmatrix} \begin{pmatrix} x_1 \\ x_3^{(1)} \end{pmatrix} - \begin{pmatrix} b_1 \\ b_3^{(1)} \end{pmatrix} = \begin{pmatrix} 0 \\ (K_{33}^{(1)} - K_{31} K_{11}^{-1} K_{13}) x_3^{(1)} - (b_3^{(1)} - K_{31} K_{11}^{-1} b_1) \end{pmatrix}$$

$$\begin{pmatrix} K_{22} & K_{23} \\ K_{32} & K_{33}^{(2)} \end{pmatrix} \begin{pmatrix} x_2 \\ x_3^{(2)} \end{pmatrix} - \begin{pmatrix} b_2 \\ b_3^{(2)} \end{pmatrix} = \begin{pmatrix} 0 \\ (K_{33}^{(2)} - K_{32} K_{22}^{-1} K_{23}) x_3^{(2)} - (b_3^{(2)} - K_{32} K_{22}^{-1} b_2) \end{pmatrix}$$

- Local problems with Neumann boundary conditions

$$\begin{pmatrix} K_{11} & K_{13} \\ K_{31} & K_{33}^{(1)} \end{pmatrix} \begin{pmatrix} x_1 \\ x_3^{(1)} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_3^{(1)} + \lambda_1 \end{pmatrix}$$

$$\begin{pmatrix} K_{22} & K_{23} \\ K_{32} & K_{33}^{(2)} \end{pmatrix} \begin{pmatrix} x_2 \\ x_3^{(2)} \end{pmatrix} = \begin{pmatrix} b_2 \\ b_3^{(2)} + \lambda_2 \end{pmatrix}$$

Dirichlet to Neumann and Schur complement

- Solution of local problems with Dirichlet boundary conditions

$$K_{11} x_1 = b_1 - K_{13} x_3^{(1)}$$

$$K_{22} x_2 = b_2 - K_{23} x_3^{(2)}$$

- Solution of local problems with Neumann boundary conditions

$$\begin{pmatrix} K_{11} & K_{13} \\ K_{31} & K_{33}^{(1)} \end{pmatrix} \begin{pmatrix} x_1 \\ x_3^{(1)} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_3^{(1)} + \lambda_1 \end{pmatrix}$$

$$\begin{pmatrix} K_{22} & K_{23} \\ K_{32} & K_{33}^{(2)} \end{pmatrix} \begin{pmatrix} x_2 \\ x_3^{(2)} \end{pmatrix} = \begin{pmatrix} b_2 \\ b_3^{(2)} + \lambda_2 \end{pmatrix}$$

- Schur complement = discrete Dirichlet to Neumann mapping

$$\lambda_1 = S_1 x_3^{(1)} - c_3^{(1)}$$

$$\lambda_2 = S_2 x_3^{(2)} - c_3^{(2)}$$

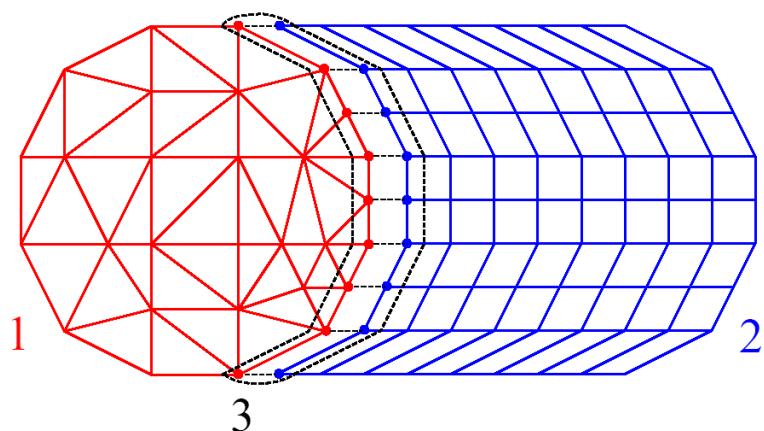
- Interface matching conditions

$$\left. \begin{array}{l} x_3^{(1)} = x_3^{(2)} \\ \lambda_1 + \lambda_2 = 0 \end{array} \right\} \Rightarrow (S_1 + S_2) x_3 = c_3$$

FETI-2LM: Robin interface interconnecting conditions

- Global system of equations

$$\begin{pmatrix} K_{11} & 0 & K_{13} \\ 0 & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$



- Local systems of equations with Robin boundary conditions

$$\begin{pmatrix} K_{11} & K_{13} \\ K_{31} & K_{33}^{(1)} + k_1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_3^{(1)} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_3^{(1)} + \lambda_1 \end{pmatrix}$$

$$\begin{pmatrix} K_{22} & K_{23} \\ K_{32} & K_{33}^{(2)} + k_2 \end{pmatrix} \begin{pmatrix} x_2 \\ x_3^{(2)} \end{pmatrix} = \begin{pmatrix} b_2 \\ b_3^{(2)} + \lambda_2 \end{pmatrix}$$

- Interface interconnecting conditions

$$\begin{cases} x_3^{(1)} = x_3^{(2)} \\ k_1 x_3^{(1)} + k_2 x_3^{(2)} = \lambda_1 + \lambda_2 \end{cases} \Leftrightarrow$$

$$\begin{cases} \lambda_1 + \lambda_2 - (k_1 + k_2) x_3^{(2)} = 0 \\ \lambda_1 + \lambda_2 - (k_2 + k_1) x_3^{(1)} = 0 \end{cases}$$

Condensed interface problem

- Solution of local systems of equations with Robin boundary conditions

$$(k_1 + K_{33}^{(1)} - K_{31} K_{11}^{-1} K_{13}) x_3^{(1)} = \lambda_1 + b_3^{(1)} - K_{31} K_{11}^{-1} b_1$$

$$(k_2 + K_{33}^{(2)} - K_{32} K_{22}^{-1} K_{23}) x_3^{(2)} = \lambda_2 + b_3^{(2)} - K_{32} K_{22}^{-1} b_2$$

- Substitution in interface interconnecting conditions : matrix of condensed interface problem

$$\begin{pmatrix} I & I - (k_1 + k_2)(k_2 + K_{33}^{(2)} - K_{32} K_{22}^{-1} K_{23})^{-1} \\ I - (k_2 + k_1)(k_1 + K_{33}^{(1)} - K_{31} K_{11}^{-1} K_{13})^{-1} & I \end{pmatrix}$$

Optimal interconnecting conditions

- Optimal Robin boundary conditions

$$k_1 = K_{33}^{(2)} - K_{32} K_{22}^{-1} K_{23}$$

$$k_2 = K_{33}^{(1)} - K_{31} K_{11}^{-1} K_{13}$$

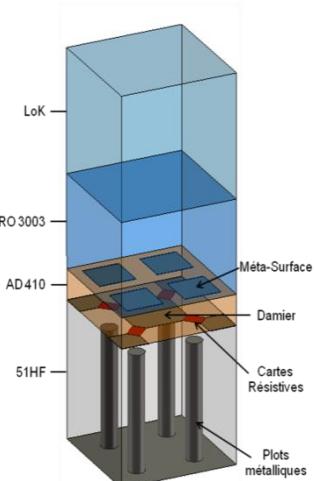
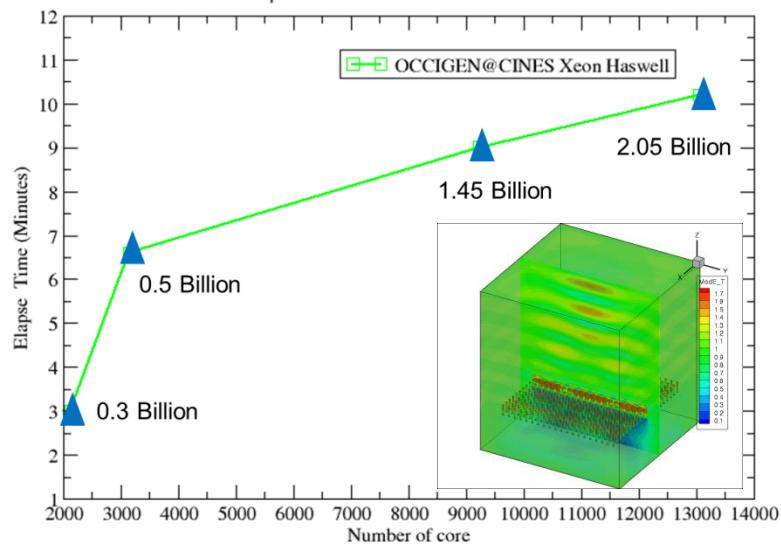
- Optimal Robin boundary conditions = Schur complement of outer domain
- Relationship with partial block LU factorization : local elimination of local equations in global system

$$\begin{pmatrix} K_{11} & K_{13} \\ K_{31} & K_{33}^{(1)} + K_{33}^{(2)} - K_{32} K_{22}^{-1} K_{23} \end{pmatrix} \begin{pmatrix} x_1 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_3^{(1)} + b_3^{(2)} - K_{32} K_{22}^{-1} b_2 \end{pmatrix}$$

Application to electromagnetism

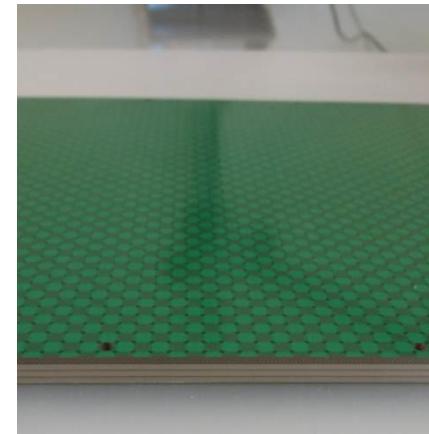
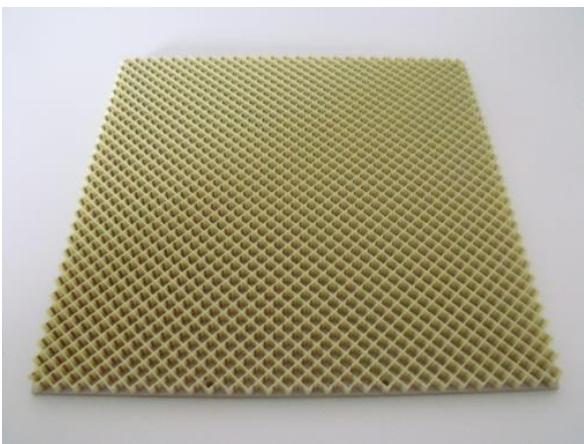
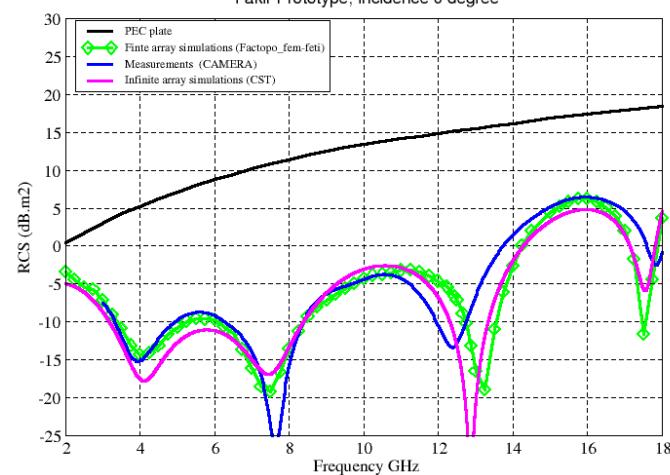
Curve of scalability code Factopo_fem-feti

Computer OCCIGEN@CINES Xeon Haswell

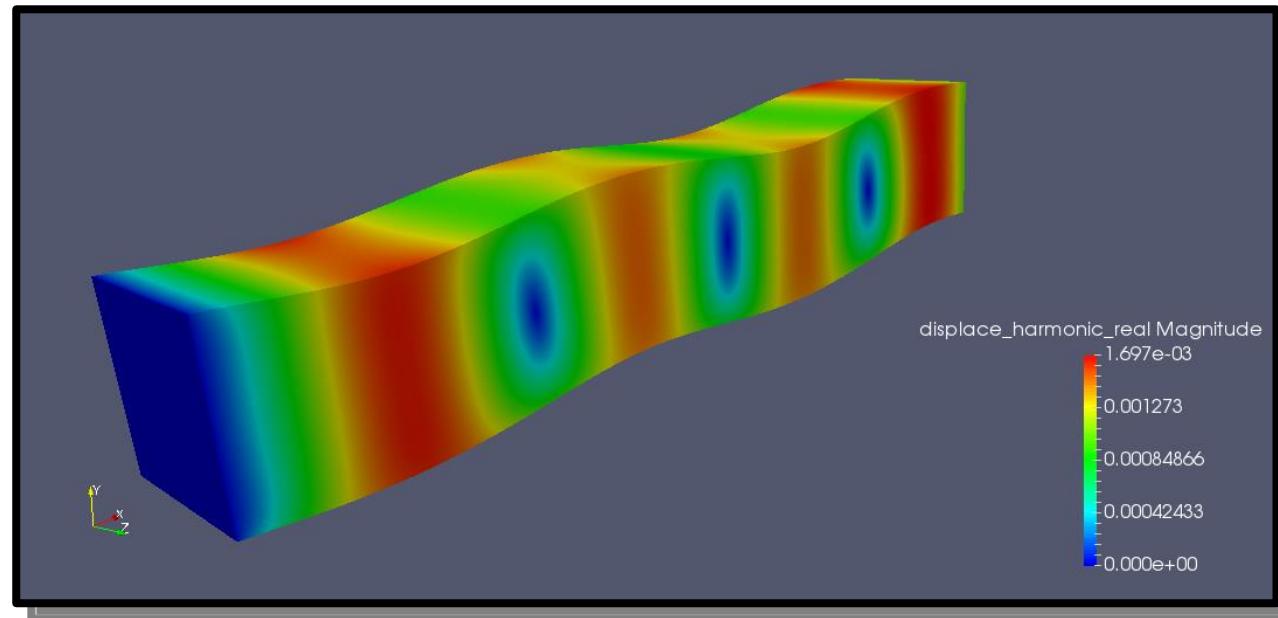


Finite periodisation 28x28; 198x198 cm²

Fakir Prototype; Incidence 0 degree



Application to time harmonic elasticity



Application to time harmonic elasticity

Uniform decomposition

var.	1.	2.	3.
#DOF	211,071	1,403,391	4,441,311
#subdom	48	48	48
#materials	1	1	1

3 steps(freq.)

1. fr.

#iter	83	128	153
time [s]	6.1	114	643.9

2. fr.

#iter	80	123	149
time [s]	5.8	111.9	628.0

3. fr.

#iter	80	140	163
time [s]	5.8	125.9	685.4

Alternate strategy for coupling : “Dirichlet–Neumann” method

- Solution of local problems with Dirichlet boundary conditions on one side and Neumann on the other side

$$x_3^{(1)p+\frac{1}{2}} = x_3^{(2)p}$$

$$\lambda_1^{p+\frac{1}{2}} = S_1 x_3^{(1)p+\frac{1}{2}} - c_3^{(1)}$$

$$\lambda_2^{p+\frac{1}{2}} = -\lambda_1^{p+\frac{1}{2}}$$

$$S_2 x_3^{(2)p+1} = \lambda_2^{p+\frac{1}{2}} + c_3^{(2)}$$

- Iteration of Dirichlet-Neumann method

$$S_2 x_3^{(2)p+1} = -S_1 x_3^{(2)p} + c_3^{(1)} + c_3^{(2)}$$

- Equation at convergence

$$(S_1 + S_2) x_3 = c_3 = c_3^{(1)} + c_3^{(2)}$$

- Iteration of Dirichlet-Neumann method : error reduction operator

$$S_2(x_3^{(2)p+1} - x_3) = -S_1(x_3^{(2)p} - x_3) \Leftrightarrow (x_3^{(2)p+1} - x_3) = -S_2^{-1}S_1(x_3^{(2)p} - x_3)$$

Must choose the right side

“Dirichlet-Robin” method

- Solution of local problems with Dirichlet boundary conditions on one side and Robin on the other side

$$x_3^{(1)p+\frac{1}{2}} = x_3^{(2)p}$$

$$\lambda_1^{p+\frac{1}{2}} = S_1 x_3^{(1)p+\frac{1}{2}} - c_3^{(1)}$$

$$\lambda_2^{p+\frac{1}{2}} = -\lambda_1^{p+\frac{1}{2}} + k_2 x_3^{(1)p+\frac{1}{2}}$$

$$(S_2 + k_2) x_3^{(2)p+1} = \lambda_2^{p+\frac{1}{2}} + c_3^{(2)}$$

- Iteration of Dirichlet-Robin method
- Equation at convergence

$$(S_2 + k_2) x_3^{(2)p+1} = -(S_1 - k_2) x_3^{(2)p} + c_3^{(1)} + c_3^{(2)}$$

$$(S_1 + S_2) x_3 = c_3 = c_3^{(1)} + c_3^{(2)}$$

- Iteration of Dirichlet-Robin method : error reduction operator

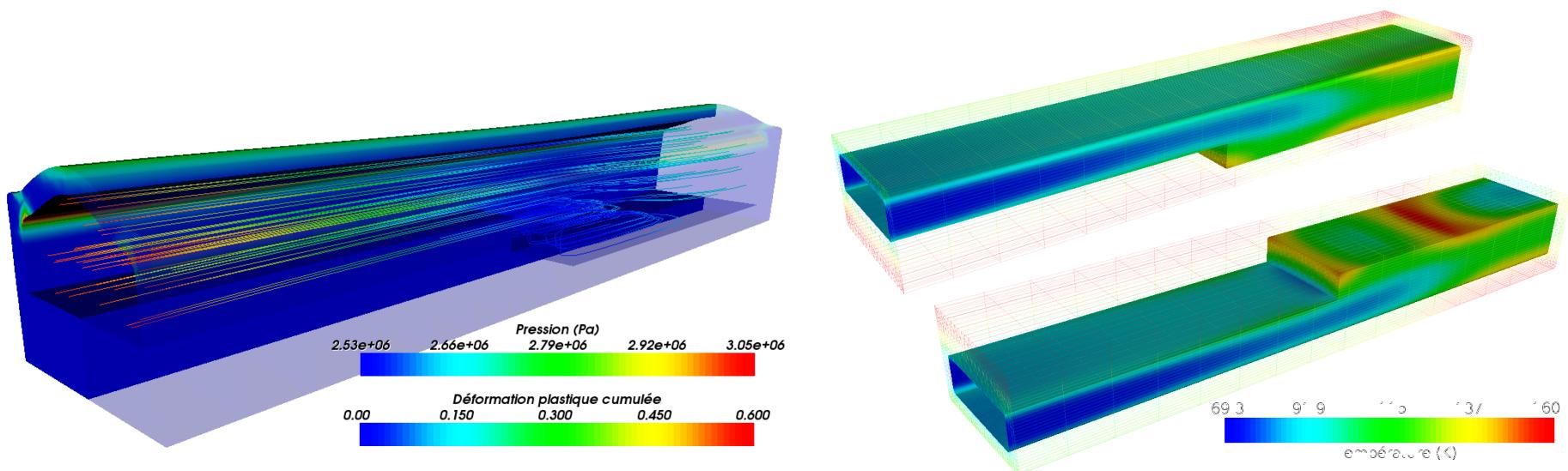
$$(S_2 + k_2) (x_3^{(2)p+1} - x_3) = -(S_1 - k_2) (x_3^{(2)p} - x_3)$$

$$(x_3^{(2)p+1} - x_3) = -(S_2 + k_2)^{-1} (S_1 - k_2)^{-1} (x_3^{(2)p} - x_3)$$

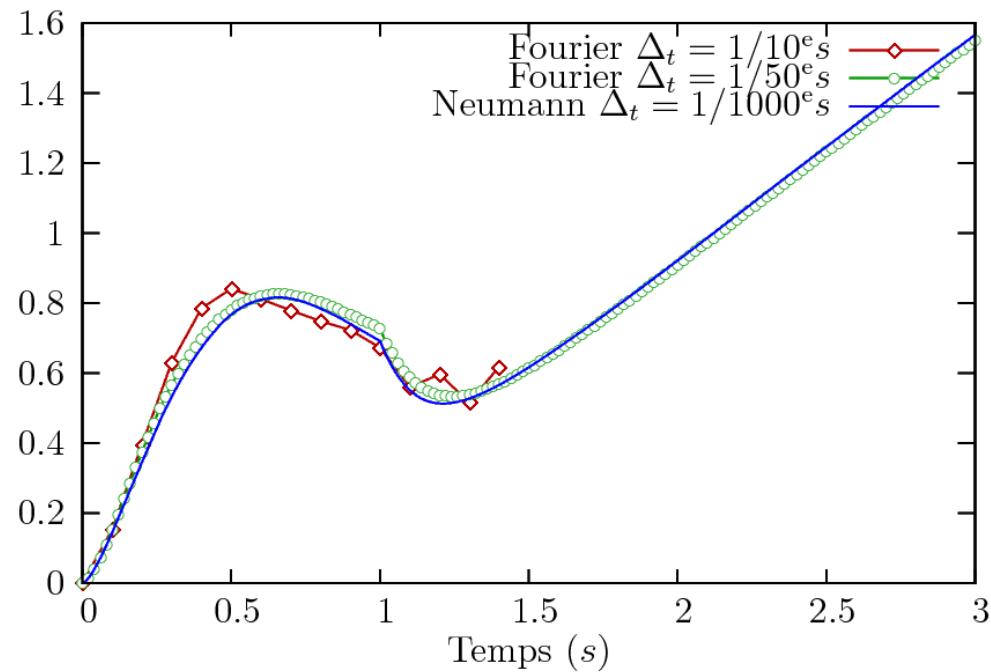
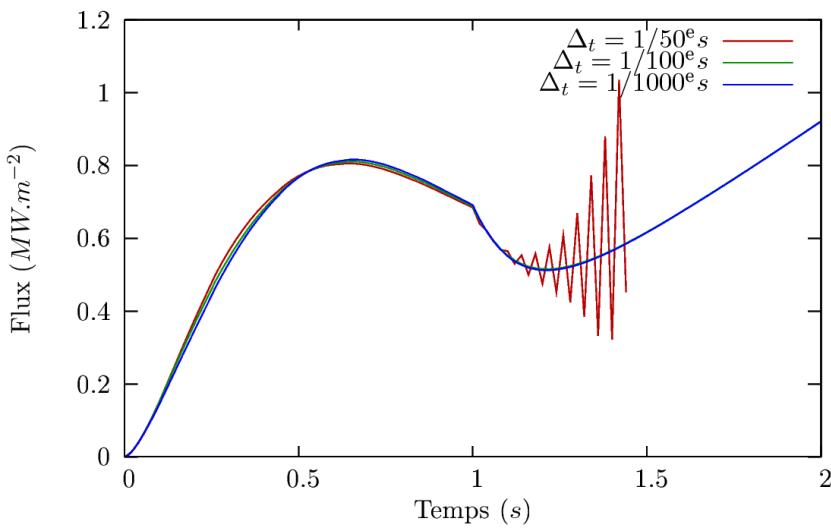
- Optimal Robin condition : $k_2 = S_1$

Application to fluid-structure thermal coupling

- Staggered time scheme
- Prediction phase + correction
- Prediction is better with the right Robin boundary conditions



Application to fluid-structure thermal coupling

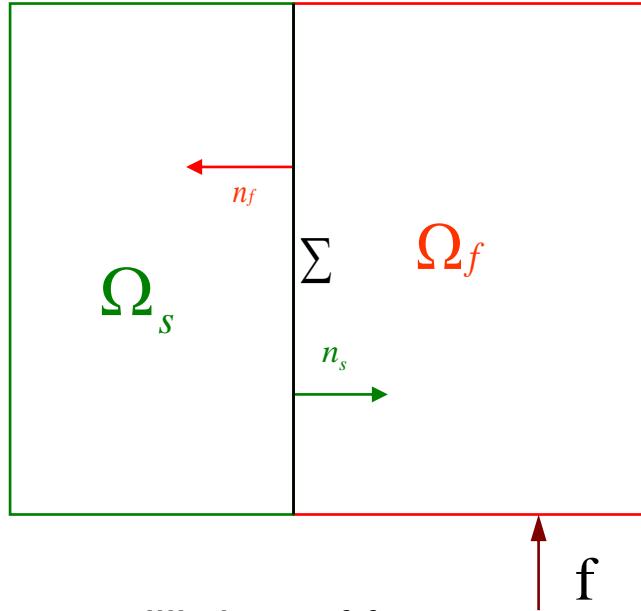


Coupled structure-fluid model in vibro-acoustics

- Helmholtz equation for pressure in fluid, time harmonic elasticity equations for motion in structure

$$\begin{cases} -\Delta p - k^2 p = f \text{ in } \Omega_f \\ + \text{C.L. on } \partial \Omega_f - \Sigma \end{cases}$$

$$\begin{cases} -\nabla \cdot \sigma - \rho_s \omega^2 u = F \text{ in } \Omega_s \\ + \text{C.L. on } \partial \Omega_s - \Sigma \end{cases}$$



- Interconnecting conditions : equality of motions, equilibrium of forces

$$\frac{\partial p}{\partial n_f} = \omega^2 \rho_f u \cdot n_f \text{ on } \Sigma$$

$$\sigma \cdot n_s = -p n_s \text{ on } \Sigma$$

Discretization

- Discrete coupled system of equations

$$\begin{pmatrix} \mathbf{Z}_f & \mathbf{C}_{fs} \\ \mathbf{C}_{sf} & \mathbf{Z}_s \end{pmatrix} \begin{pmatrix} p \\ u \end{pmatrix} = \begin{pmatrix} \mathbf{b}_f \\ \mathbf{b}_s \end{pmatrix}$$

$$(\mathbf{C}_{fs} \mathbf{u}, p) = -\omega^2 \rho_f \int_{\Sigma} \mathbf{u} \cdot \mathbf{n}_f p \, d\sigma$$

$$(\mathbf{C}_{sf} p, \mathbf{u}) = \int_{\Sigma} p \mathbf{n}_s \cdot \mathbf{u} \, d\sigma$$

- Symmetrization of system via simple change of variables
- Complex symmetric matrix : non Hermitian
- Heterogeneous system : ill conditioned
- Preconditioning via solution of local problems

Block preconditioning

- General coupled system

$$\begin{pmatrix} Z_1 & C_{12} \\ C_{21} & Z_2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

- Block Jacobi preconditioner
- Only local
- No coupling

$$M = \begin{pmatrix} Z_1^{-1} & 0 \\ 0 & Z_2^{-1} \end{pmatrix}$$

- Block Gauss Seidel preconditioner
- One way coupling
- Must choose the right side

$$M = \begin{pmatrix} Z_1 & C_{12} \\ 0 & Z_2 \end{pmatrix}^{-1} = \begin{pmatrix} Z_1^{-1} & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} I & -C_{12} \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & Z_2^{-1} \end{pmatrix}$$

Preconditioning via approximate block factorization

$$\begin{pmatrix} Z_1 & C_{12} \\ C_{21} & Z_2 \end{pmatrix} = \begin{pmatrix} Z_1 & 0 \\ C_{21} & I \end{pmatrix} \begin{pmatrix} I & Z_1^{-1}C_{12} \\ 0 & Z_2 - C_{21}Z_1^{-1}C_{12} \end{pmatrix}$$

- Approximation of Schur complement

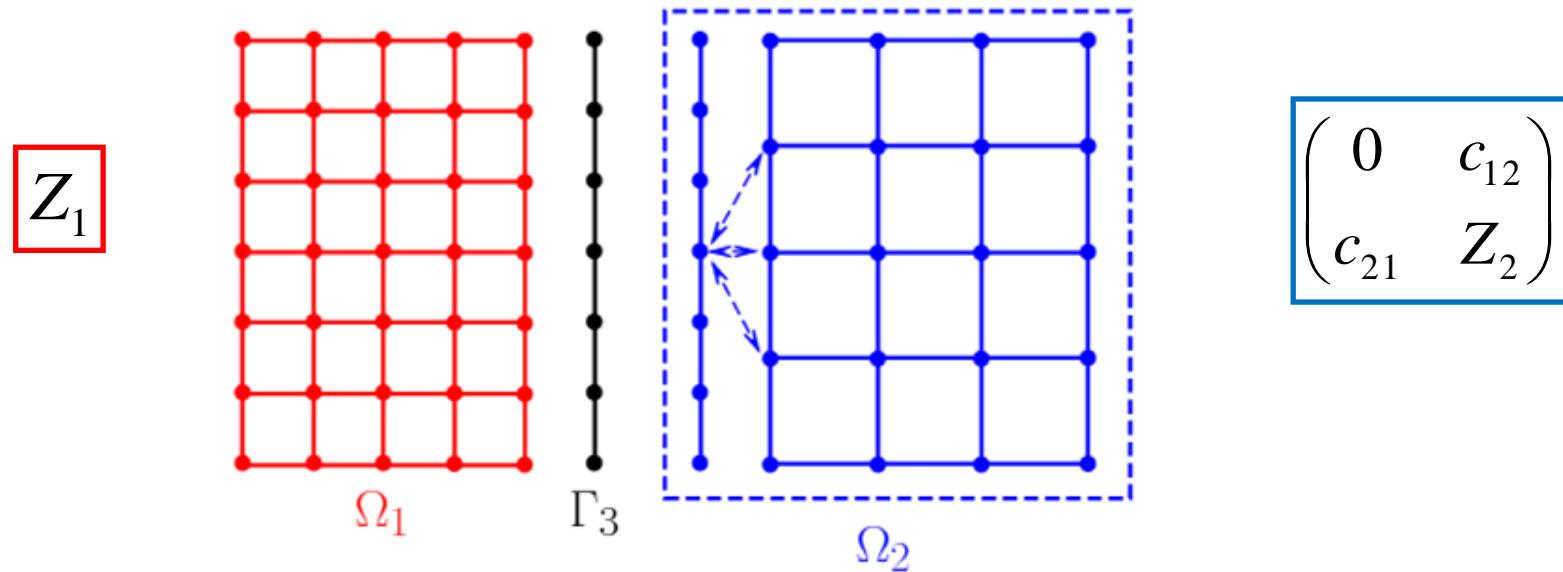
$$Z_2 - C_{21}Z_1^{-1}C_{12}$$
$$C_{12} = \begin{pmatrix} 0 \\ c_{12} \end{pmatrix}, C_{21} = (0 \ c_{21})$$

$$C_{21}Z_1^{-1}C_{12} = \begin{pmatrix} 0 & 0 \\ 0 & c_{21}S_1^{-1}c_{12} \end{pmatrix}$$

- Sparse approximation of Dirichlet to Neumann or Neumann to Dirichlet of domain 1
- Generalized Robin boundary conditions in domain 2

FETI-2LM for coupled problem

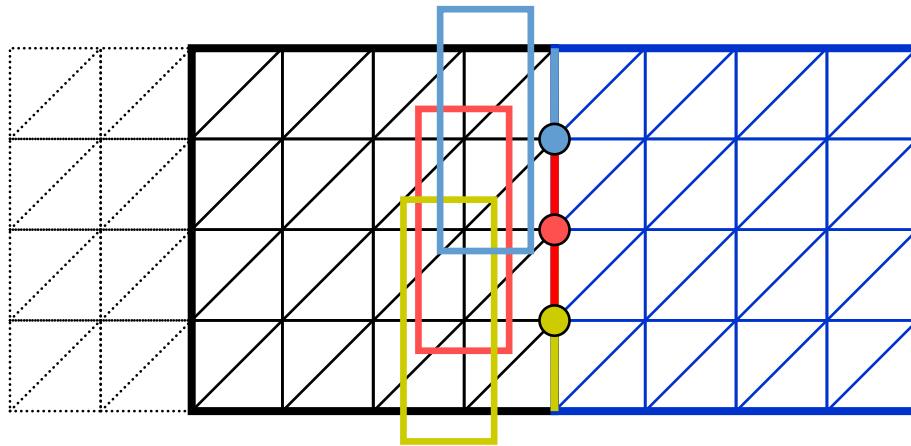
- Coupling terms on one side : standard interface



- With FETI-2LM approximate Schur complement of matrix of domain 1 makes matrix of domain 2 invertible
- Dirichlet to Neumann or Neumann to Dirichlet approximations

Algebraic approach for approximate Schur complement

- Assembling of Schur complements computed on small patches



- Black-box implementation
- Works well for elliptic problems
- Not good for wave equations

Test for model problem

- Fluid cavity with elastic membrane

Freq (Hz)	$\begin{pmatrix} Z_1^{-1} & 0 \\ 0 & Z_2^{-1} \end{pmatrix} \begin{pmatrix} Z_1 & C_{12} \\ 0 & Z_2 \end{pmatrix}_{\text{fluid}}^{-1}$	$\begin{pmatrix} Z_1 & C_{12} \\ 0 & Z_2 \end{pmatrix}_{\text{struct}}^{-1}$	approx block LU fluid	approx block LU struct	FETI-2LM fluid	FETI-2LM struct
20	16	8	11	13	9	16
110	28	13	16	64 12 19	31	76
200	41	15	23	80 17 12	38	154

- Algebraic approximation of Schur complements not so good
- Using sparse approximation of Dirichlet to Neumann or Neumann to Dirichlet will certainly bring a great improvement

Conclusion

- Deriving Robin boundary conditions from Dirichlet to Neumann or Neumann to Dirichlet operators of outer domain is the general methodology for designing fast and robust iterative coupling or interconnecting methods
- Domain decomposition approach : Krylov space method for condensed interface problem