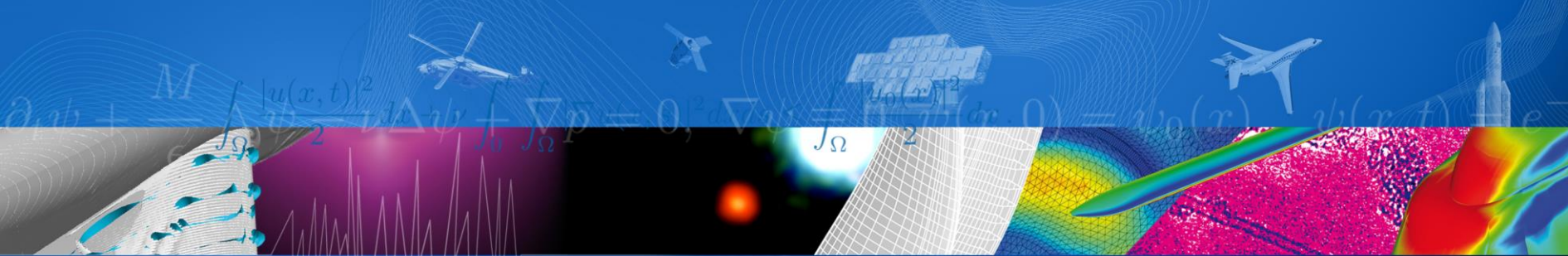


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Efficient iterative solvers : FETI methods with multiple search directions

François-Xavier Roux



Parallel architectures

Direct sparse solvers

Non overlapping domain decomposition methods

FETI-2LM

Multi-RHS antenna array

FETI-1LM

S-FETI : multiple search directions

Parallel architecture

Direct sparse solvers

Domain decomposition context

Computer architecture

Networked compute nodes, more and more nodes and cores per node

Each node is a hierarchical memory SMP with possibly parallel accelerator (many-core, GPU)

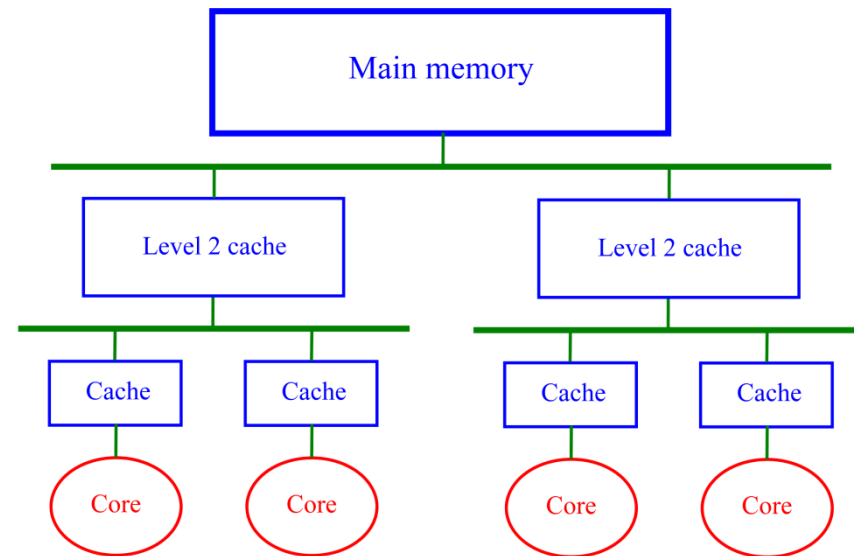
Space and time locality of data required for performance

Need of multi-level parallel methods :

direct solvers , BLAS (shared memory),

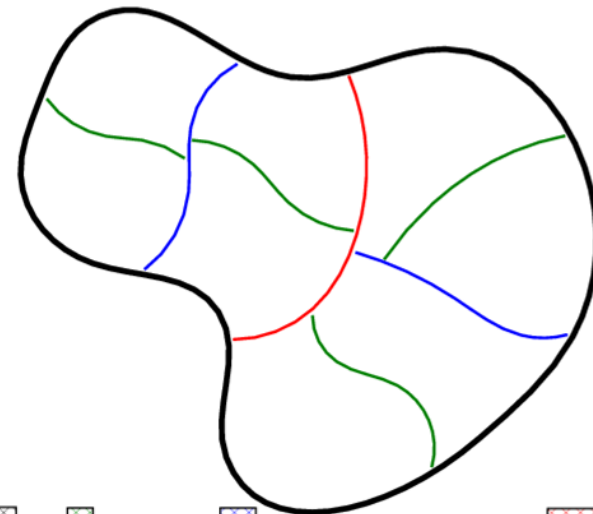
domain decomposition methods (MPI) ,

+ parallel in time (or quasi-static non linear iterations → PANLIM project)



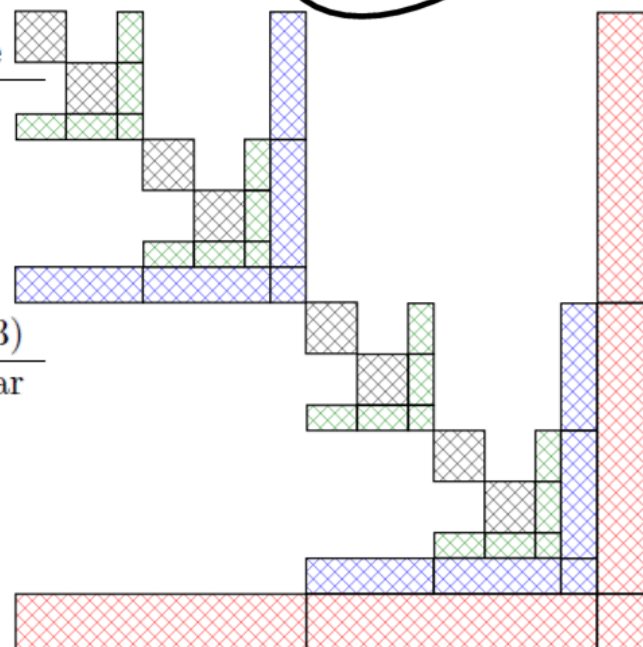
Sparse direct solver on SMP compute node

Sparse direct solver based on nested bisection
 P-threads multi-threading management
 Splitting of blocks in small sub-blocks
 Atsushi Suzuki, research granted by Total at LJLL



# cores	Dissection		Pardiso	
	CPU time	elapsed time	CPU	esapsed time
1	74.84	72.824	85.04	82.941
2	74.81	38.162	87.79	43.627
4	77.32	20.454	92.66	23.141
6	79.96	15.200	104.38	17.391
8	83.56	12.008	118.25	14.786
12	94.08 ($\times 1.26$)	9.873 ($/7.38$)	165.99 ($\times 1.95$)	13.993 ($/5.93$)

elstct1, $N = 206,763$, nonsingular



Efficiency of parallel forward-backward substitution

Actual performance limited by global memory access

Parallelization of forward-backward substitution for a single RHS gives very limited performance (speed-up < 2)

With multiple RHS, higher arithmetic complexity with same memory access requirement (better data locality)

	1RHS @ 1core	12 RHS @ 12core	efficiency
Dissection	0.6194 sec.	0.5135 sec	120.6%
Pardiso	0.7054 sec.	1.2642 sec	55.8%



With more than one subdomain per compute node, memory bandwidth available for each MPI process is even smaller

Performance of each single RHS forward-backward substitution is even lower



Efficiency of parallel Gram Schmidt orthogonalization

Test on a cluster of 12-core Westmere Xeon nodes with Gigabit Ethernet connection

Up to 8 compute nodes, maximum 6 cores per MPI process

Dimension of vectors = 50000

Number of new/old vectors = 20/80 , 20/4x20

#threads/MPI process	#MPI process	Modif GS	Simultaneous GS	Modif block GS
1	1	2	9.9	9.2
1	12	0.5	7.5	6.5
6	1	4.7	45	35
6	2	3.2	41	31
6	16	0.8	28	18

Krylov space methods with domain decomposition

Optimal decomposition for 3D regular grid

Number of DOF = dN^3

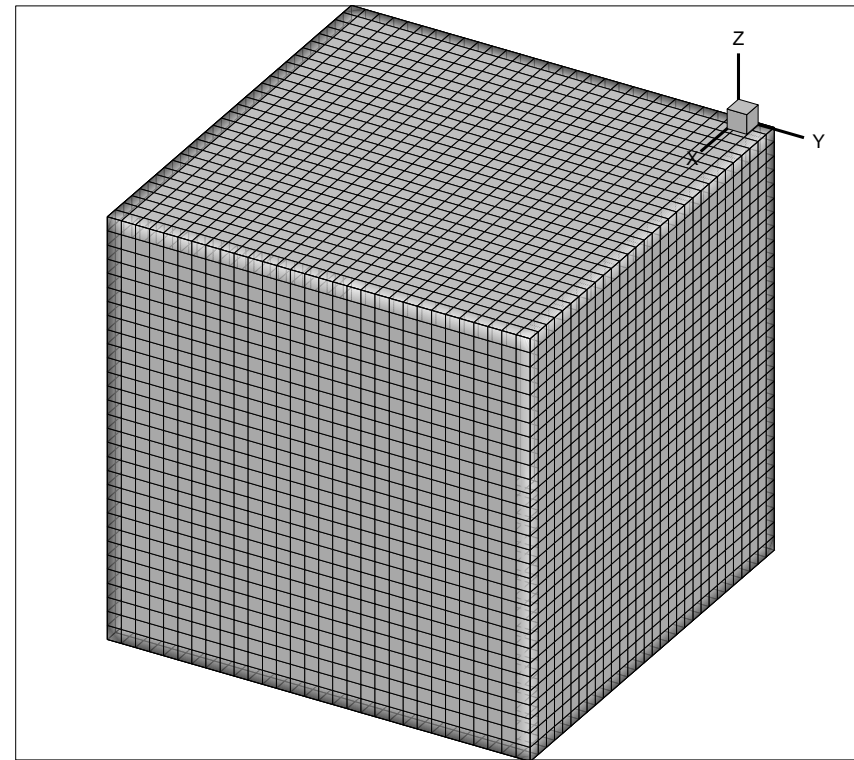
Number of interface DOF = $6dN^2$ → complexity of a dot product

Fill in with sparse direct solver = $O(d^2N^4)$
→ complexity of a forward-backward substitution

Order of magnitude of $N = 100$

Storage and orthogonalization of many search directions affordable

Use Krylov methods with full orthogonalization



Non overlapping domain decomposition method

Schur complement method

Schur complement = discrete Dirichlet to Neumann mapping

Boundary value problem, inner and boundary degrees of freedom

Block structure
$$\begin{pmatrix} K_{ii} & K_{ib} \\ K_{bi} & K_{bb} \end{pmatrix}, \begin{pmatrix} x_i \\ x_b \end{pmatrix}, \begin{pmatrix} b_i \\ b_b \end{pmatrix}$$

Solution of Dirichlet problem

$$\begin{cases} K_{ii}x_i + K_{ib}x_b = b_i \\ x_b = x_b \end{cases} \Rightarrow K_{ii}x_i = b_i - K_{ib}x_b \Rightarrow x_i = -K_{ii}^{-1}K_{ib}x_b + K_{ii}^{-1}b_i$$

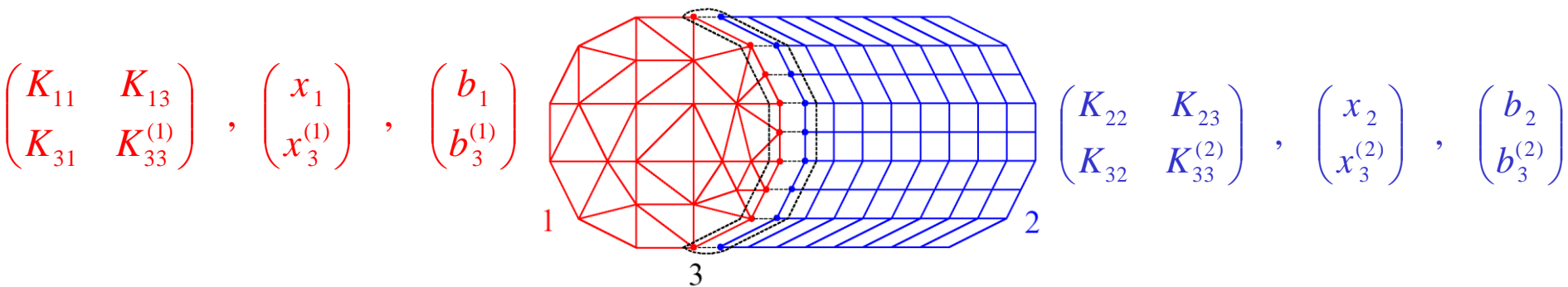
Neumann problem with same solution

$$\begin{aligned} K_{bi}x_i + K_{bb}x_b &= K_{bb}x_b - K_{bi}K_{ii}^{-1}K_{ib}x_b + K_{bi}K_{ii}^{-1}b_i \\ \Rightarrow \begin{pmatrix} K_{ii} & K_{ib} \\ K_{bi} & K_{bb} \end{pmatrix} \begin{pmatrix} x_i \\ x_b \end{pmatrix} &= \begin{pmatrix} b_i \\ (K_{bb} - K_{bi}K_{ii}^{-1}K_{ib})x_b + b_b - K_{bi}K_{ii}^{-1}b_i \end{pmatrix} \end{aligned}$$

Non overlapping domain decomposition

Element based splitting of the global problem

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



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

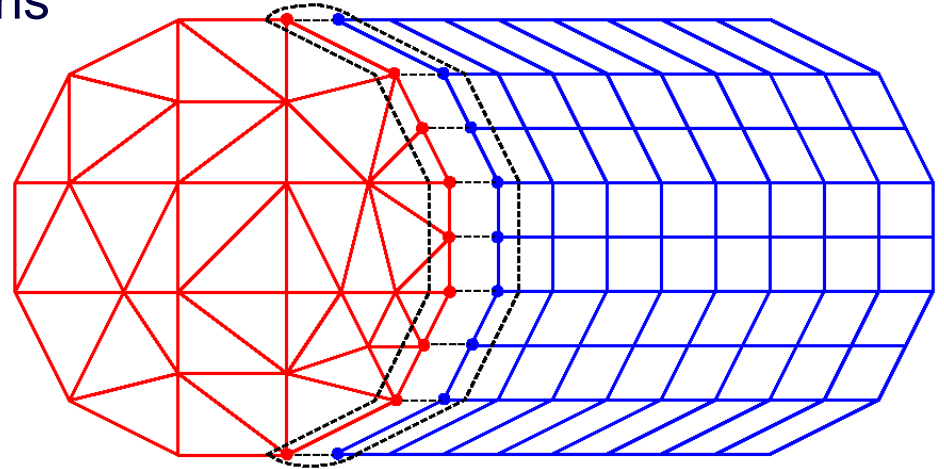
$$b_3^{(1)} + b_3^{(2)} = b_3$$

Local equations, interface matching conditions

Local equations inside subdomains

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

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



Admissibility condition on the interface = continuity condition

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

Equilibrium condition on interface

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

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

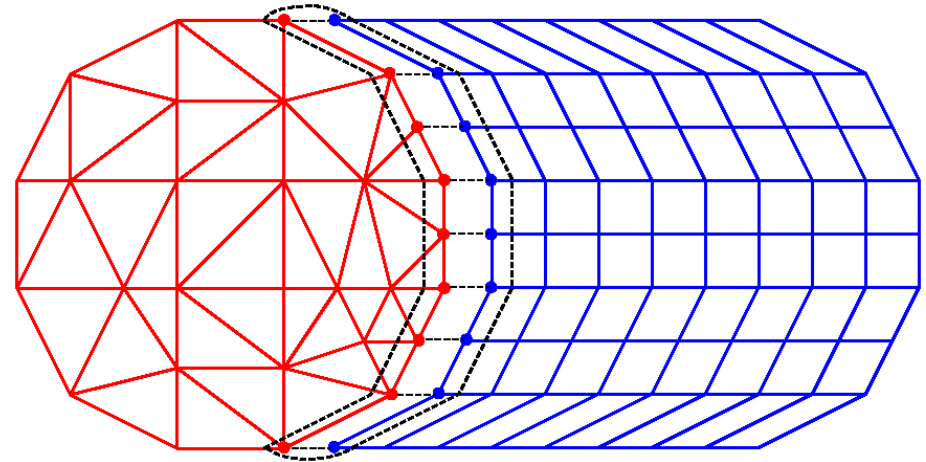
Local condensation : Schur complement method

Interface unknown : $x_3 = x_3^{(1)} = x_3^{(2)}$

Solution of internal equations in subdomains

$$K_{11} x_1 = b_1 - K_{13} x_3$$

$$K_{22} x_2 = b_2 - K_{23} x_3$$



Equilibrium condition on interface => definition of residual

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

$$\left(K_{33} - K_{31} K_{11}^{-1} K_{13} - K_{32} K_{22}^{-1} K_{23} \right) x_3 - \left(b_3 - K_{31} K_{11}^{-1} b_1 - K_{32} K_{22}^{-1} b_2 \right)$$

Implementation

Solution of local system via a direct method (Gauss, Cholesky)

$$K_{11} x_1 = b_1 - K_{13} x_3$$

$$K_{22} x_2 = b_2 - K_{23} x_3$$

Local contribution to interface residual

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

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

Global interface residual obtained by assembling local contributions

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

Robin interface conditions

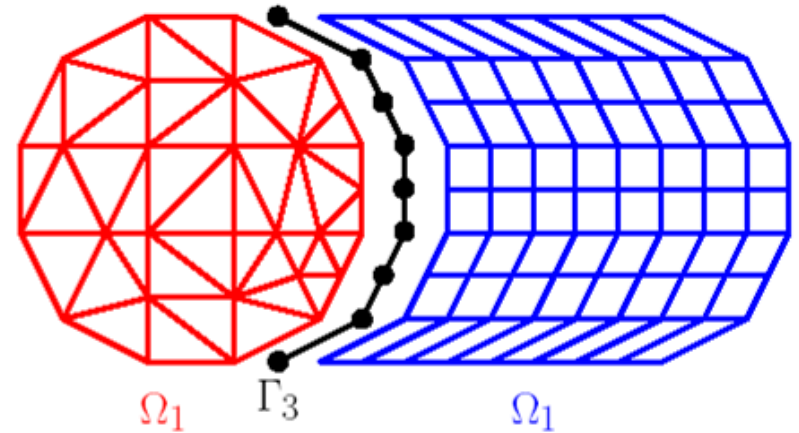
FETI-2LM method

Application to Maxwell equations

Robin conditions on interfaces

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 system of equations

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

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

Interface matching conditions

$$\begin{cases} x_3^{(1)} = x_3^{(2)} \\ K_{31}x_1 + K_{32}x_2 + K_{33}^{(1)}x_3^{(1)} + K_{33}^{(2)}x_3^{(2)} = b_3 \\ \Leftrightarrow \lambda_1 + \lambda_2 - k_1x_3^{(1)} - k_2x_3^{(2)} = 0 \end{cases}$$

FETI-2LM : homogenized interface matching conditions

Interface matching conditions are mixed

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

Combine the equations to find two homogeneous conditions

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

Definition of condensed interface problem

Condensed interface problem for FETI-2LM

Local elimination of inner unknowns

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

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

Matrix of condensed interface problem

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

Optimal interface conditions

Optimal interface conditions

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

Optimal conditions = condensation on interface of remaining structure
= discrete Dirichlet to Neumann operator of outer domain

Interpretation via local condensation in global system of equations

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

Main features of the method

Well posed local problems, even with irregular mesh splitting with correct Robin conditions

Convergence in $p - 1$ iterations in case of one-way splitting into p subdomains



optimal cv

Issue : computation of exact optimal operator impossible (Schur complement)

Approximation of discrete Dirichlet to Neumann mapping required

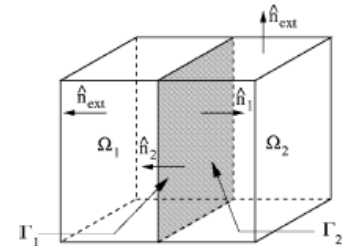
For wave equations approximate “transparent” boundary conditions

FETI-2LM applied to Maxwell

$$\Omega = \Omega_1 \cup \Omega_2 \dots \cup \Omega_N$$

Domain partition

$$\left\{ \begin{array}{l} \nabla \times \left(\frac{1}{\vec{\mu}_r} \nabla \times \vec{E}_i \right) - k_0^2 \vec{\epsilon}_r \vec{E}_i = k_0^2 (\epsilon_{r,i} - \mu_{r,i}^{-1}) \vec{E}_{incident} \quad \text{in} \quad \Omega_i \subset R^3 \\ \vec{n}_i \times \left(\frac{1}{\vec{\mu}_{r,i}} \nabla \times \vec{E}_i \right) + jk_0 \vec{n}_i \times (\vec{n}_i \times \vec{E}_i) = \vec{\Lambda}_j^i \quad \text{on} \quad \Gamma_i \quad (\text{Robin}) \\ \vec{n} \times (\nabla \times \vec{E}_i) + jk_0 \vec{n} \times (\vec{n} \times \vec{E}_i) = 0 \quad \text{on} \quad \Gamma_{ext} = \partial\Omega_i \setminus \Gamma_i \end{array} \right.$$



Robin

Additional variables on the interface (2 LM method)

Lagrange multipliers with approximate transparent Robin condition (approximate outer Dirichlet-Neumann)

$$\vec{n}_i \times (\mu_{r,i}^{-1} \nabla \times \vec{E}_j^i) + jk_0 \vec{n}_i \times (\vec{n}_i \times \vec{E}_j^i) = \vec{\Lambda}_j^i$$

Electric and Magnetic field Continuity

$$\vec{n}_j \times (\mu_{r,j}^{-1} \nabla \times \vec{E}_i^j) + jk_0 \vec{n}_j \times (\vec{n}_j \times \vec{E}_i^j) = \vec{\Lambda}_i^j$$

$$\vec{n}_i \times (\vec{n}_i \times \vec{E}_j^i) = \vec{n}_j \times (\vec{n}_j \times \vec{E}_i^j) \quad (1)$$



$$\vec{n}_i \times (\mu_{r,i}^{-1} \nabla \times \vec{E}_j^i) = -\vec{n}_j \times (\mu_{r,j}^{-1} \nabla \times \vec{E}_i^j) \quad (2)$$

$$\Lambda_j^i + \Lambda_i^j - 2jk_0 \vec{n}_i \times (\vec{n}_i \times \vec{E}_j^i) = 0$$

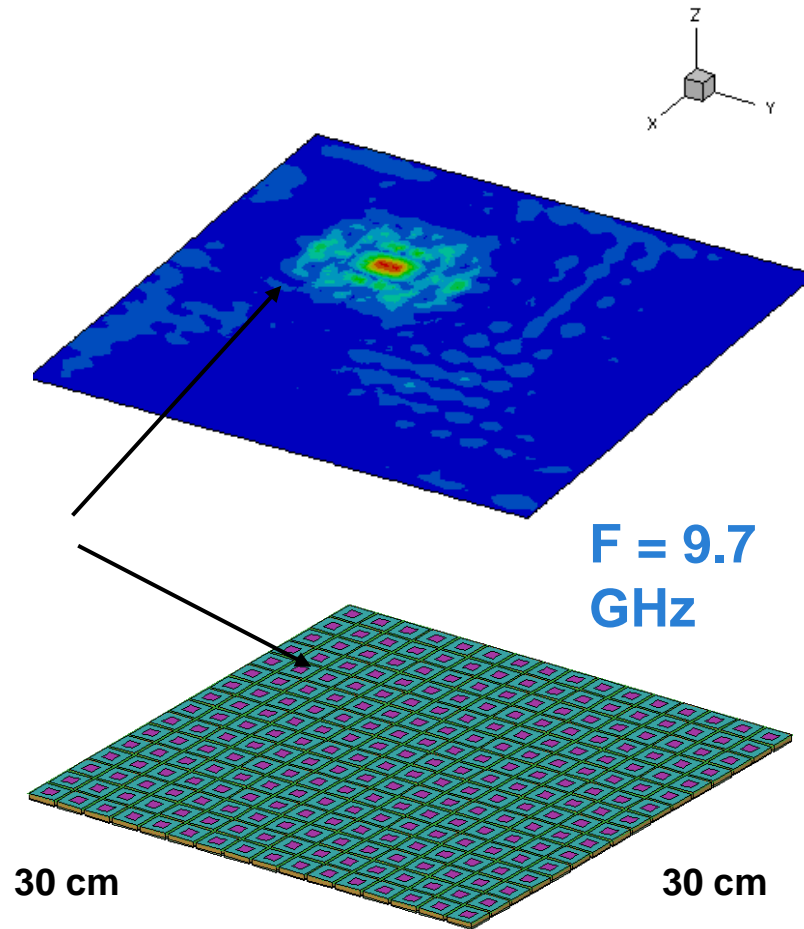
$$\Lambda_j^i + \Lambda_i^j - 2jk_0 \vec{n}_j \times (\vec{n}_j \times \vec{E}_i^j) = 0$$

Antenna arrays

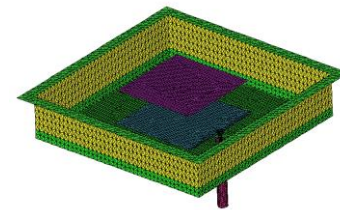
Reuse of search directions with ORTHODIR or ORTHOMIN

Block method

Antenna arrays



2D device, attached to the fuselage of the plane
Complex treatment to orient the radar beam
Larger arrays for higher intensity



Fine local mesh to take into account the heterogeneous structure of each element

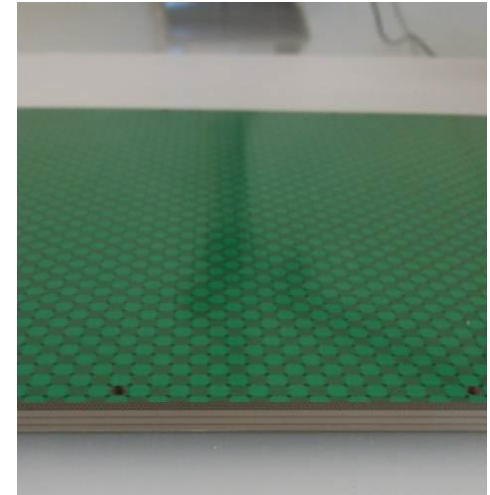
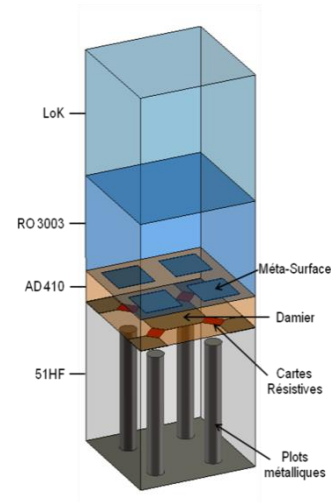
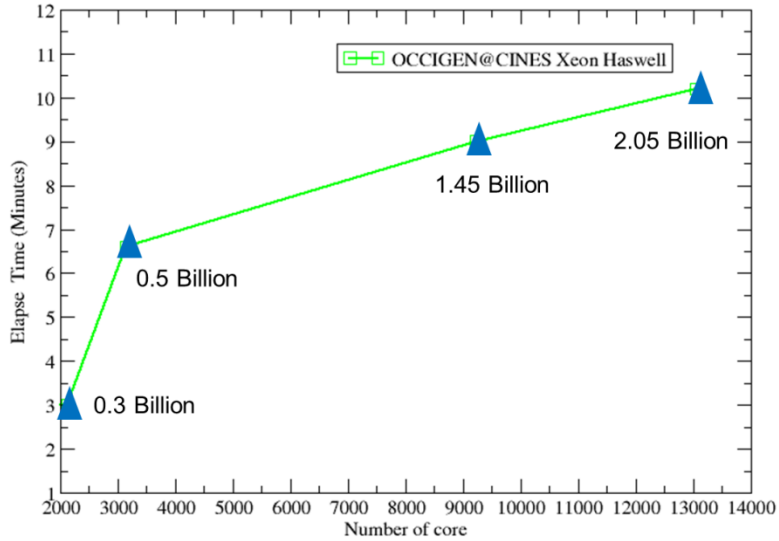


Solution for multiple incident waves or for various emitting modes : many RHS

Antenna simulations : nearly weak scalability

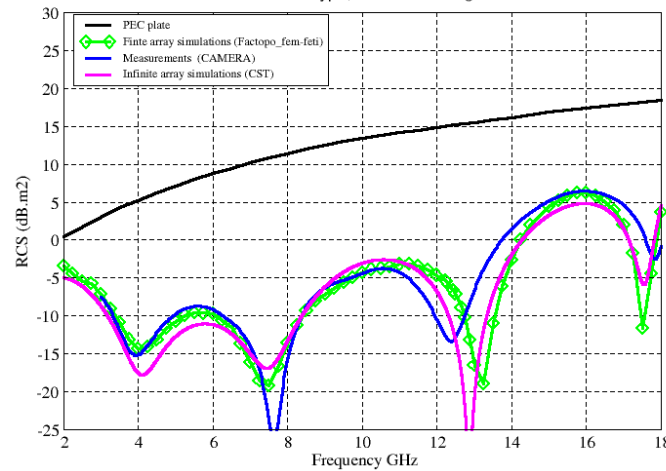
Curve of scalability code Factopo_fem-feti

Computer OCCIGEN@CINES Xeon Haswell



Finite periodisation 28x28; 198x198 cm²

Fakir Prototype; Incidence 0 degree



Krylov method with full orthogonalization : ORTHODIR

ORTHODIR : build a F^*F -orthogonal basis of Krylov space

$$\left\{ \begin{array}{l} g_0 = F\lambda_0 - d \\ v_0 = g_0 \\ Fv_0 \\ d_0 = \|Fv_0\|^2 \end{array} \right. \left\{ \begin{array}{l} \lambda_p = \lambda_{p-1} + \rho_{p-1}v_{p-1} \\ g_p = g_{p-1} + \rho_{p-1}Fv_{p-1} \\ (Fv_{p-1})^* g_p = 0 \Leftrightarrow d_{p-1}\rho_{p-1} = -(Fv_{p-1})^* g_{p-1} \\ \qquad \qquad \qquad - (Fv_{p-1})^* g_0 \end{array} \right. \left\{ \begin{array}{l} v_p = Fv_{p-1} + \sum_{i=0}^{p-1} \gamma_{ip} v_i \\ Fv_p = FFv_{p-1} + \sum_0^{p-1} \gamma_{ip} Fv_i \\ \gamma_{ip} = -(Fv_i)^* FFv_{p-1} \\ d_p = \|Fv_p\|^2 \end{array} \right.$$

ORTHODIR : block formulation (Fv_{p-1} replaced by g_{p-1} : ORTHOMIN)

$$V^p = [v_0 v_1 \cdots v_{p-1}], \quad (FV^p)^*(FV^p) = D_p, \quad D_p P_p = -(FV^p)^* g_0$$

$$\left\{ \begin{array}{l} \lambda_p = \lambda_0 + V^p P_p \\ g_p = g_0 + FV^p P_p \end{array} \right.$$

Continued ORTHODIR with multiple RHS

V^p and $F V^p$ are given , $(F V^p)^* (F V^p) = D_p$

Optimal starting λ_0^{opt}

$$\begin{cases} \lambda_0^{opt} = \lambda_0 + V^p P_p \\ g_0^{opt} = g_0 + F V^p P_p \end{cases} \quad - (F V^p)^* g_0^{opt} = 0 \Leftrightarrow D_p P_p = - (F V^p)^* g_0$$

Start new iterations with new search directions F^*F -orthogonal to V^p

F^*F -projected ORTHODIR

In practice same as if continuing ORTHODIR from iteration p

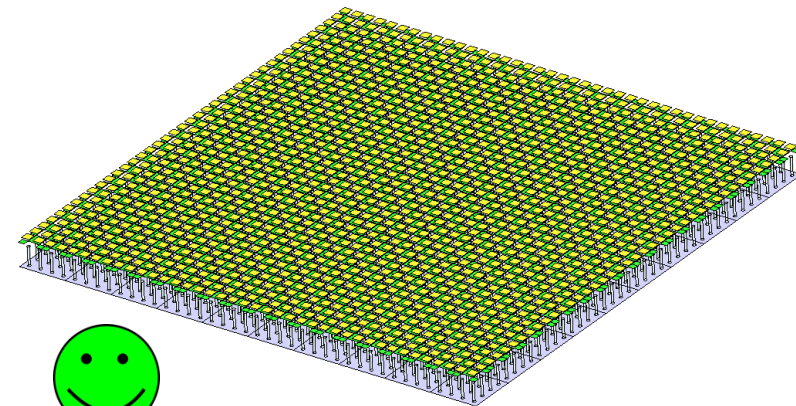
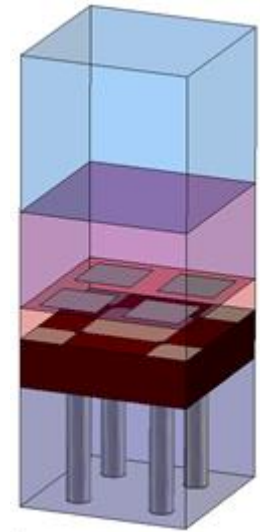
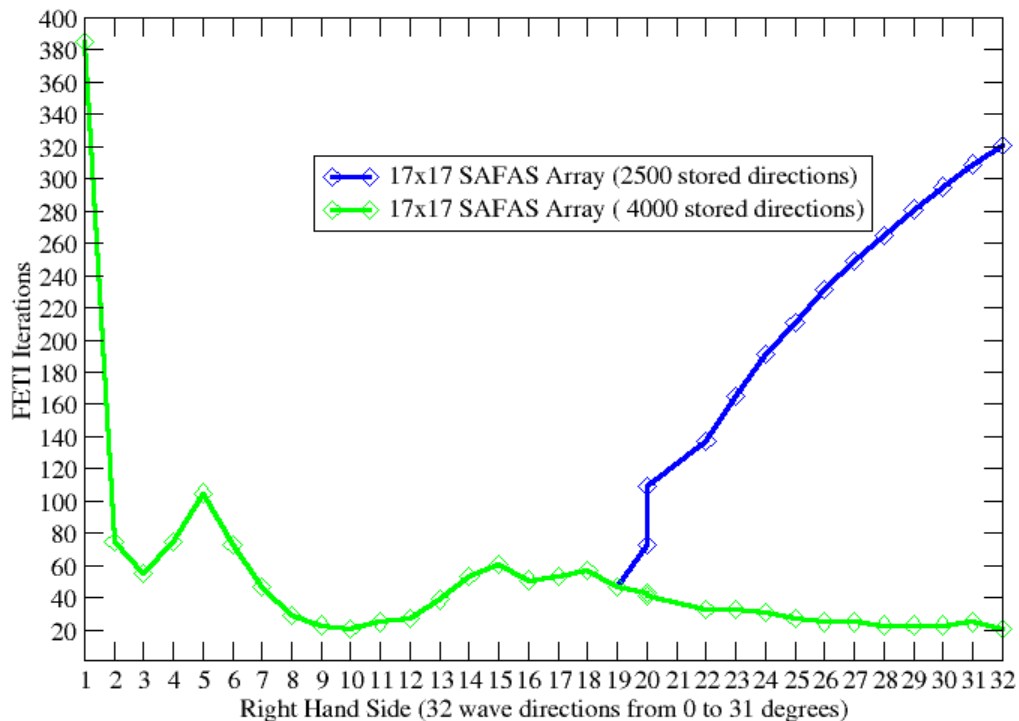
Accumulation of search directions with successive RHS

Dependency upon number of stored directions

17x17 array

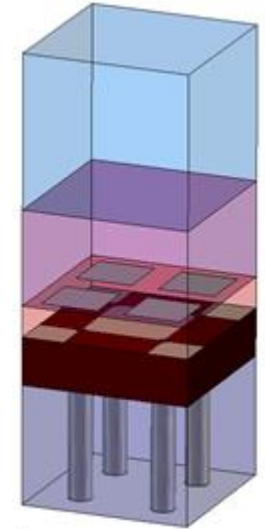
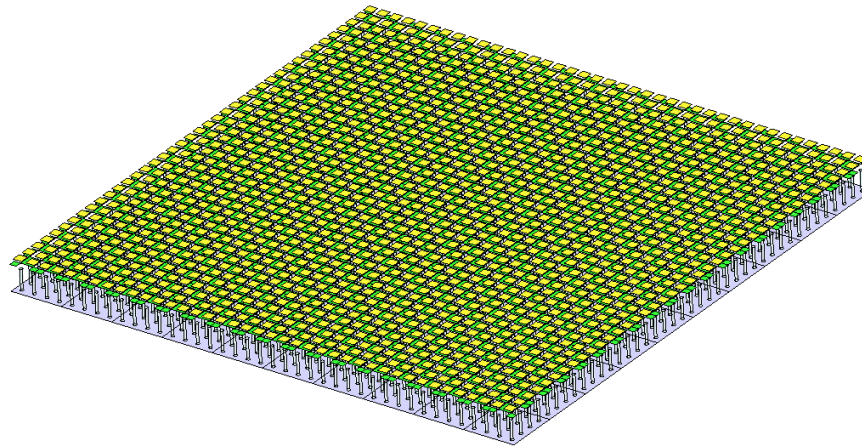
289 subdomains, 50 Million unknowns

31 RHS, incident waves with various angles

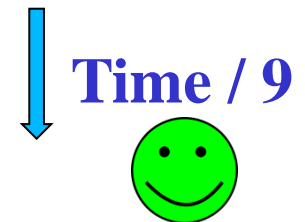


Application of multi-RHS techniques

17x17 array, 289 subdomains,
1 core per subdomain,
50M unknowns,
31 RHS,
16 RHS per block



	Elapsed time
Successive ORTHODIR	29.7
Continued ORTHODIR	3.3



Block ORTHODIR algorithm

Block ORTHODIR initialization

$$\begin{cases} \mathbf{g}_0^k = F\lambda_0^k - d^k \\ \mathbf{v}_0^k = \mathbf{g}_0^k \end{cases}, k = 1, n_{block}$$

$$\begin{cases} \Lambda^0 = [\lambda_0^1 \lambda_0^2 \dots \lambda_0^{n_{block}}] \\ \mathbf{G}^0 = [\mathbf{g}_0^1 \mathbf{g}_0^2 \dots \mathbf{g}_0^{n_{block}}] \\ \mathbf{V}^0 = [\mathbf{v}_0^1 \mathbf{v}_0^2 \dots \mathbf{v}_0^{n_{block}}] \\ \mathbf{D}_0 = (F\mathbf{V}^0)^* (F\mathbf{V}^0) = \mathbf{L}_0 \mathbf{L}_0^* \end{cases}$$

Block ORTHODIR iteration

$$\begin{cases} \Lambda^p = \Lambda^{p-1} + \mathbf{V}^{p-1} \mathbf{P}_{p-1} \\ \mathbf{G}^p = \mathbf{G}^{p-1} + F\mathbf{V}^{p-1} \mathbf{P}_{p-1} \\ (F\mathbf{V}^{p-1})^* \mathbf{G}^p = \mathbf{0} \Leftrightarrow \mathbf{D}_{p-1} \mathbf{P}_{p-1} = -(F\mathbf{V}^{p-1})^* \mathbf{G}^p \end{cases}$$

$$\begin{cases} \mathbf{V}^p = F\mathbf{V}^{p-1} + \sum_{i=0}^{p-1} \mathbf{V}^i \Gamma_{ip} \\ F\mathbf{V}^p = FF\mathbf{V}^{p-1} + \sum_{i=0}^{p-1} F\mathbf{V}^i \Gamma_{ip} \\ \mathbf{D}_i \Gamma_{ip} = -(F\mathbf{V}^i)^* FF\mathbf{V}^{p-1} \\ \mathbf{D}_p = (F\mathbf{V}^p)^* (F\mathbf{V}^p) = \mathbf{L}_p \mathbf{L}_p^* \end{cases}$$

Rank revealing Cholesky factorization

Use all directions for all RHS

Block ORTHODIR implementation

Optimal solution for each RHS using all search directions computed for all RHS

Rank revealing LL^* factorization of D_p , automatic detection of dependencies between search directions, reduction of number of search directions

Same property as continued ORTHODIR in term of decrease of global number of directions to be computed

n_{block} simultaneous forward-backward substitutions at each iteration, good parallel efficiency on multi-core nodes

Simultaneous computation of dot products, BLAS3, good parallel efficiency on multi-core nodes, global reduction for a block of scalars at once, reduced MPI overhead



Continued block ORTHODIR straightforward

Application of multi-RHS techniques

17x17 array, 289 subdomains,
1 core per subdomain,
50M unknowns,
31 RHS,
16 RHS per block

	Elapsed time
Successive ORTHODIR	29.7
Continued ORTHODIR	3.3
Block ORTHODIR	0.8




Improved local performance with multi-threading

32x1 array, 32 subdomains,
12 cores per subdomain,
57M unknowns,
32 RHS,
16 RHS per block

	Elapsed time
Successive ORTHODIR	21.8
Continued ORTHODIR	12.1
Block ORTHODIR	0.63



Time / 1.8

Time / 34.6

Limited improvement with continued ORTHODIR in this case, due to right-hand-sides

Neumann interface conditions

FETI method

Coarse grid projection

Neumann local problems

Local systems of equations

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

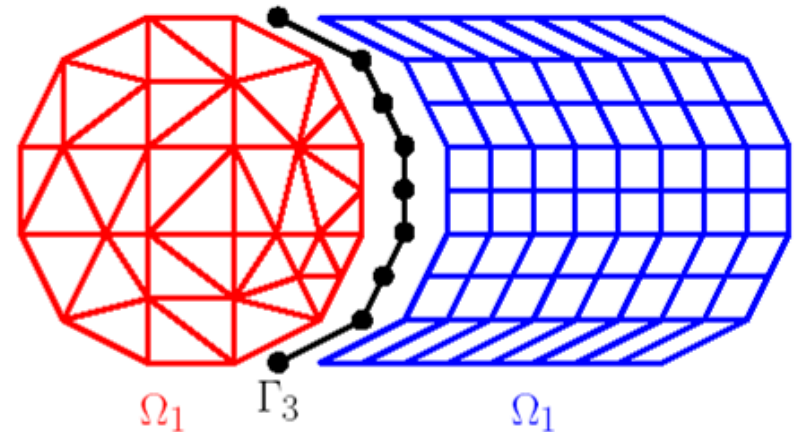
$$\begin{pmatrix} K_{22} & K_{23} \\ K_{32} & K_{33}^{(2)} \end{pmatrix} \begin{pmatrix} x_2 \\ x_3^{(2)} \end{pmatrix} = \begin{pmatrix} b_2 \\ b_3^{(2)} + \lambda_2 \end{pmatrix}$$

Interface continuity condition

$$x_3^{(1)} - x_3^{(2)} = 0$$

Interface equilibrium condition

$$\lambda_1 + \lambda_2 = 0$$



Interface unknown : $\lambda = \lambda_1 = -\lambda_2$

Local problems :

$$\begin{pmatrix} K_{11} & K_{13} \\ K_{31} & K_{33}^{(1)} \end{pmatrix} \begin{pmatrix} x_1 \\ x_3^{(1)} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_3^{(1)} + \lambda \end{pmatrix} \quad \begin{pmatrix} K_{22} & K_{23} \\ K_{32} & K_{33}^{(2)} \end{pmatrix} \begin{pmatrix} x_2 \\ x_3^{(2)} \end{pmatrix} = \begin{pmatrix} b_2 \\ b_3^{(2)} - \lambda \end{pmatrix}$$

Interface residual : $x_3^{(1)} - x_3^{(2)}$

Use CG to converge to the solution of the implicit condensed interface problem

Condensed interface problem for FETI

Local systems of equations

$$\begin{pmatrix} K_{11} & K_{13} \\ K_{31} & K_{33}^{(1)} \end{pmatrix} \begin{pmatrix} x_1 \\ x_3^{(1)} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_3^{(1)} + \lambda \end{pmatrix} \quad \begin{pmatrix} K_{22} & K_{23} \\ K_{32} & K_{33}^{(2)} \end{pmatrix} \begin{pmatrix} x_2 \\ x_3^{(2)} \end{pmatrix} = \begin{pmatrix} b_2 \\ b_3^{(2)} - \lambda \end{pmatrix}$$

Condensation on interface

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

$$S^{(1)} x_3^{(1)} = c_3^{(1)} + \lambda$$

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

$$S^{(2)} x_3^{(2)} = c_3^{(2)} - \lambda$$

Condensed interface problem

$$x_3^{(1)} - x_3^{(2)} = 0 \Leftrightarrow (S^{(1)-1} + S^{(2)-1}) \lambda = -S^{(1)-1} c_3^{(1)} + S^{(2)-1} c_3^{(2)}$$

Optimal local preconditioner

FETI condensed interface operator

$$F = \left(S^{(1)-1} + S^{(2)-1} \right)$$

Optimal local preconditioner (convergence independent of mesh size)

$$\tilde{F}^{-1} = \left(\frac{1}{2} S^{(1)} \frac{1}{2} + \frac{1}{2} S^{(2)} \frac{1}{2} \right)$$

Computation of preconditioned gradient

$$K_{11} v_1 = -K_{13} \frac{1}{2} g \quad \begin{pmatrix} K_{11} & K_{13} \\ K_{31} & K_{33}^{(1)} \end{pmatrix} \begin{pmatrix} v_1 \\ \frac{1}{2} g \end{pmatrix} = \begin{pmatrix} 0 \\ \left(K_{33}^{(1)} - K_{31} K_{11}^{-1} K_{13} \right) \frac{1}{2} g \end{pmatrix}$$

$$K_{22} v_2 = -K_{23} \frac{1}{2} g \quad \begin{pmatrix} K_{22} & K_{23} \\ K_{32} & K_{33}^{(2)} \end{pmatrix} \begin{pmatrix} v_2 \\ \frac{1}{2} g \end{pmatrix} = \begin{pmatrix} 0 \\ \left(K_{33}^{(2)} - K_{32} K_{22}^{-1} K_{23} \right) \frac{1}{2} g \end{pmatrix}$$

Solution of Dirichlet problem in each subdomain

Ill posed local Neumann problem

Local null modes

$$\begin{cases} \mathbf{x}_3^{(1)} = \mathbf{S}^{(1)+} (\mathbf{c}_3^{(1)} + \lambda) + \mathbf{N}^{(1)} \alpha^{(1)} \\ \mathbf{N}^{(1)t} (\mathbf{c}_3^{(1)} + \lambda) = 0 \end{cases} \quad \begin{cases} \mathbf{x}_3^{(2)} = \mathbf{S}^{(2)+} (\mathbf{c}_3^{(2)} - \lambda) + \mathbf{N}^{(2)} \alpha^{(2)} \\ \mathbf{N}^{(2)t} (\mathbf{c}_3^{(2)} - \lambda) = 0 \end{cases}$$

Mixed condensed interface problem

$$\begin{pmatrix} \mathbf{S}^{(1)+} + \mathbf{S}^{(2)+} & \mathbf{N}^{(1)} & -\mathbf{N}^{(2)} \\ \mathbf{N}^{(1)t} & \mathbf{0} & \mathbf{0} \\ -\mathbf{N}^{(2)t} & \mathbf{0} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \lambda \\ \alpha^{(1)} \\ \alpha^{(2)} \end{pmatrix} = \begin{pmatrix} -\mathbf{S}^{(1)+} \mathbf{c}_3^{(1)} + \mathbf{S}^{(2)+} \mathbf{c}_3^{(2)} \\ \mathbf{N}^{(1)t} \mathbf{c}_3^{(1)} \\ -\mathbf{N}^{(2)t} \mathbf{c}_3^{(2)} \end{pmatrix}$$

FETI null modes projection

Mixed condensed interface problem

$$\begin{pmatrix} F & G \\ G^t & 0 \end{pmatrix} \begin{pmatrix} \lambda \\ \alpha \end{pmatrix} = \begin{pmatrix} d \\ c \end{pmatrix}$$

Solution via projection

$$g = F\lambda - d$$

$$Pg = g + G\alpha$$

Orthogonal projection in $\text{Ker}(G^t)$

$$G^t Pg = 0 \Rightarrow G^t G\alpha = -G^t g$$

$$P = I - G(G^t G)^{-1} G^t$$

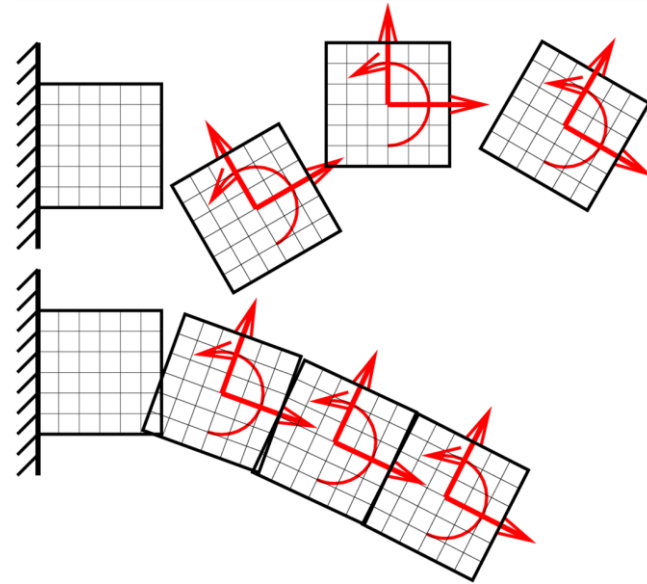
Coupling of local null modes

$$G^t G = \begin{pmatrix} N^{(1)t} N^{(1)} & -N^{(1)t} N^{(2)} \\ -N^{(2)t} N^{(1)} & N^{(2)t} N^{(2)} \end{pmatrix}$$

Coarse grid preconditioner effect of FETI projection

Projection for rigid body motion (linear elasticity context)

- ⇒ computation of local rigid body motions which minimize interface jump
- ⇒ solution of a global problem whose unknowns are rigid body motions



Global coarse grid preconditioner

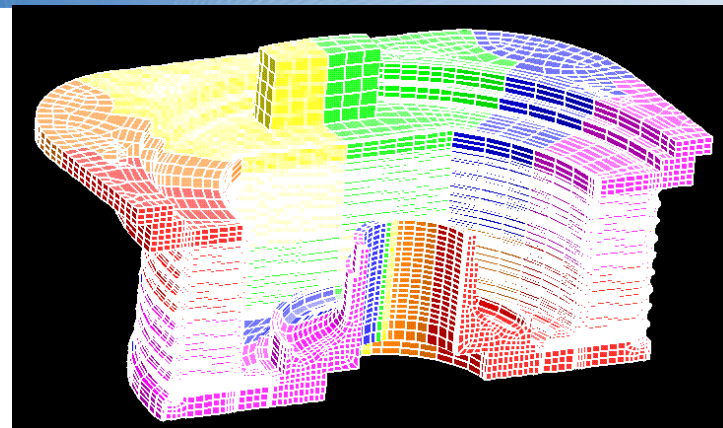
- ⇒ convergence independent upon number of subdomains

Heterogeneous problems, weighted Dirichlet preconditioner

S-FETI method

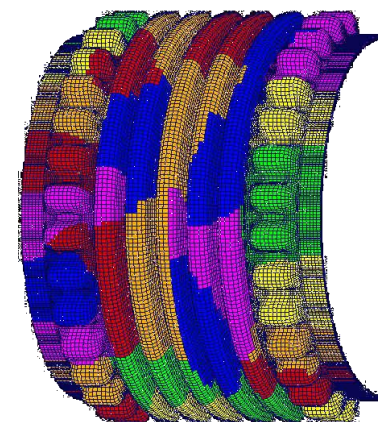
Heterogeneous materials, heterogeneous finite element models

Geometrical heterogeneity created by automatic mesh splitting



Weighted preconditioner

$$\tilde{F}^{-1} = \left(d_1 S^{(1)} d_1 + d_2 S^{(2)} d_2 \right) , \quad d_1 + d_1 = 1$$



Mechanical interpretation of weighting

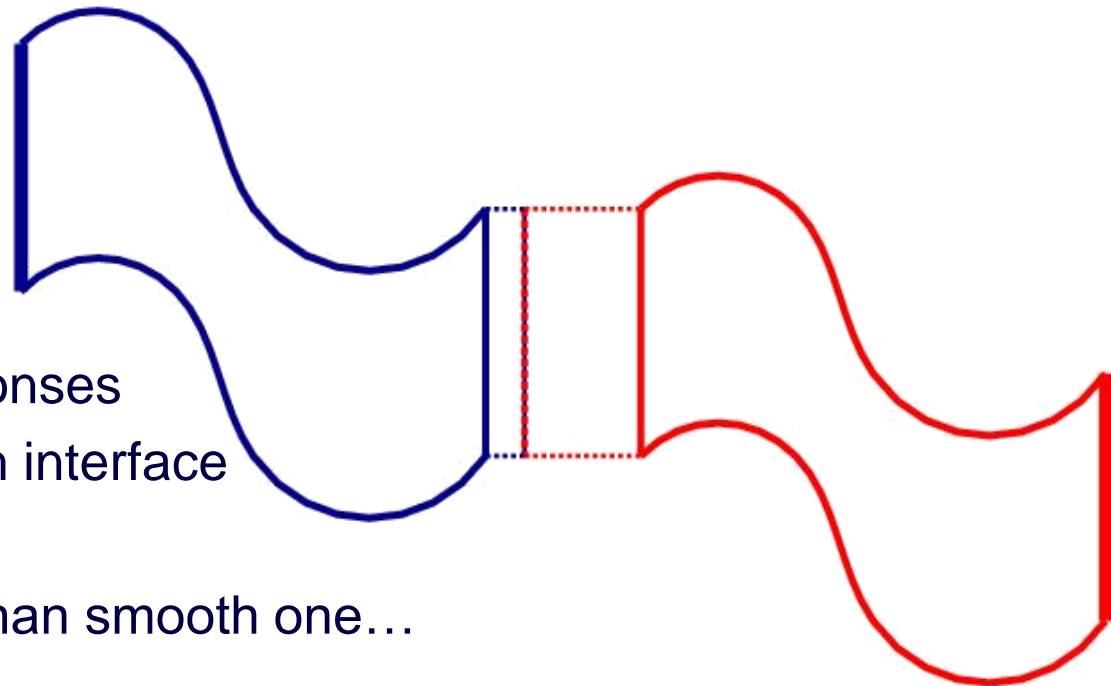
The interface gradient is the jump of displacements

Find the interaction force which will make the gap to vanish

Impose each subdomain interface to move a fraction of the gap, compute the local force to impose (Dirichlet to Neumann)

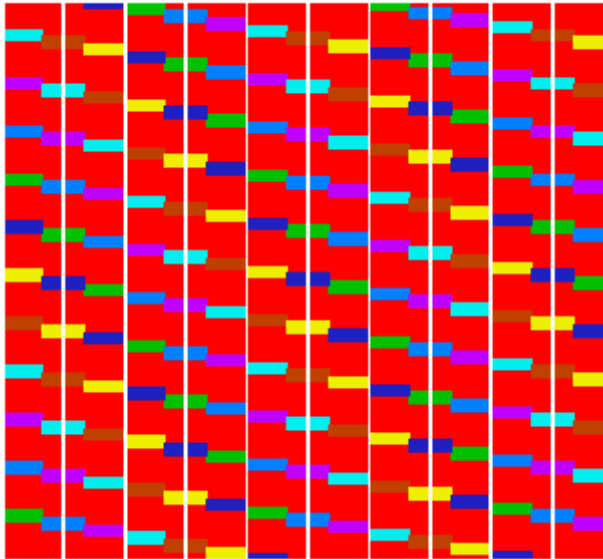
Take an average of the responses from both subdomain on each interface

Stiff subdomain moves less than smooth one...



Heterogeneity across and/or along the interface

Hard to derive correct weighting factor when heterogeneity is not only across the interface but also along the interface



Model problem

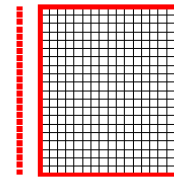
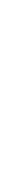
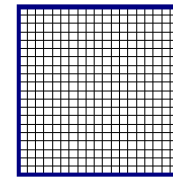
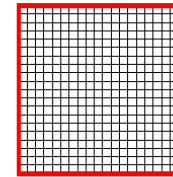
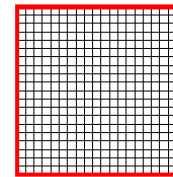
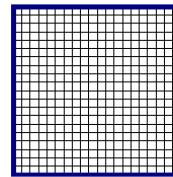
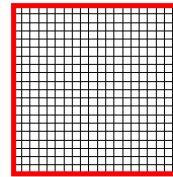
Polymer matrix smooth,
nearly incompressible

Heterogeneous fibers with
varying E from 10 to 10^6

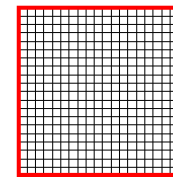
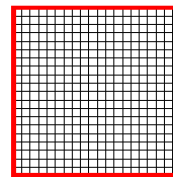
Badly shaped subdomain creates anisotropy

S-FETI method, Nicole Spillane, Daniel Rixen

FETI, one preconditioned gradient on all interfaces obtained by adding two contributions on each interface



S-FETI, keep both contributions as two independent candidate directions, split interface per interface



Total number of candidate directions = 2 x total number of interfaces

“Coarse space” : dimension depends only on number of subdomains, only a few “modes” of the coarse space are non zero in one subdomain

Block CG algorithm with full reconjugation

Block CG iteration

$$\begin{cases} \lambda_p = \lambda_{p-1} + W^{p-1} P_{p-1} \\ g_p = g_{p-1} + FW^{p-1} P_{p-1} \\ W^{p-1t} g_p = 0 \Leftrightarrow (W^{p-1t} FW^{p-1}) P_{p-1} = -W^{p-1t} g_{p-1} \end{cases}$$

Computation of multiple search directions

$$g_p = F\lambda_p - d$$

$$Pg_p$$

Local Dirichlet solve \rightarrow coarse space C^p

Rank revealing Cholesky

$$\begin{cases} W^p = PC^p + \sum_0^{p-1} W^i \Gamma_{ip} \\ \Gamma_{ip} = -(FW^i)^t PC^p \\ FW^p = FPC^p + \sum_0^{p-1} FW^i \Gamma_{ip} \\ W^{pt} FW^p = L_p L_p^t \end{cases}$$

Computing cost for the coarse space

Computation of projected coarse space and product by FETI operator

$$PC^p = C^p + GA_p$$

$$G^t PC^p = 0 \Rightarrow (G^t G)A_p = -G^t C^p$$

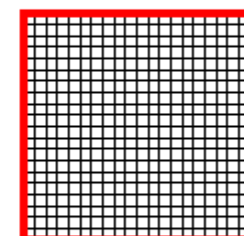
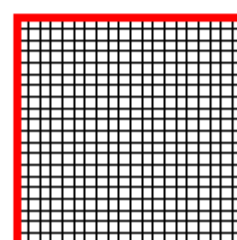
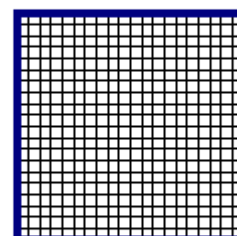
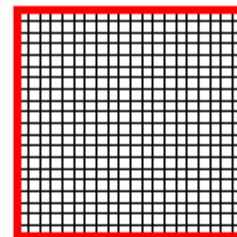
$$FPC^p = FC^p + FGA_p$$

Number of coarse modes with non zero trace in a subdomain:

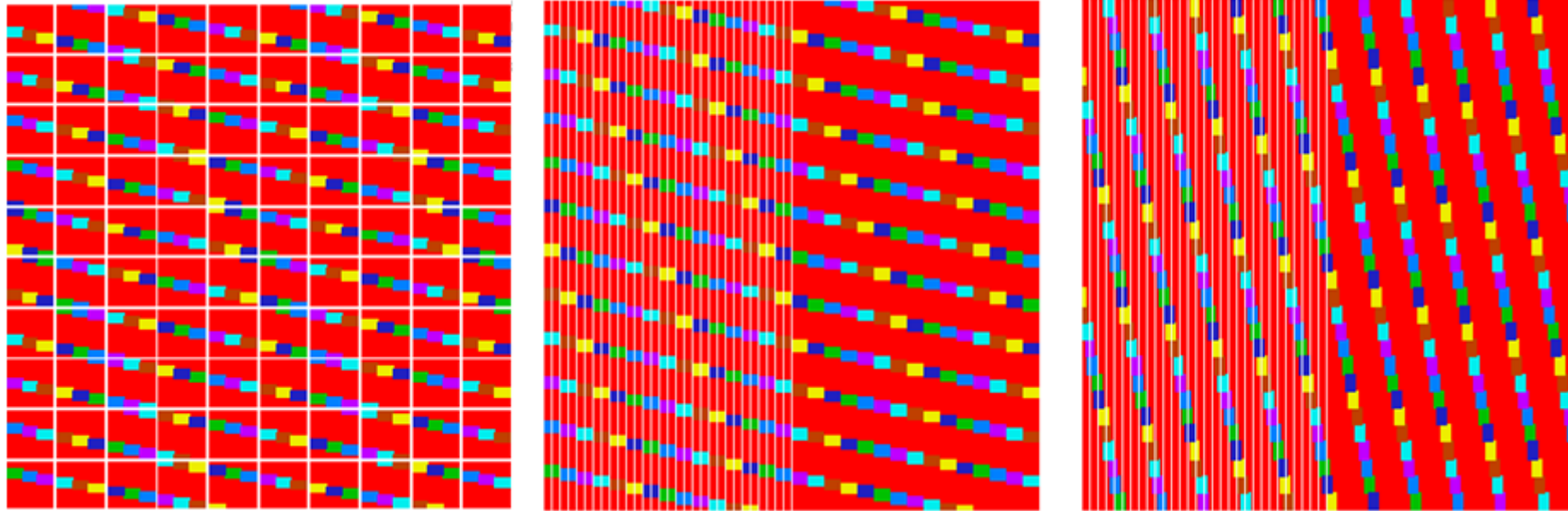
2 x number of interfaces = number of local Neumann solution

$G^t C^p$ sparse : small number of non zero coarse and rigid body modes in each subdomain

FG coarse, computed at initialization



Test case



Number of subdomains = 100

Poisson ratio of polymer matrix = 0.45 or 0.4999

180 000 degrees of freedom per subdomain

4 cores per subdomain, 50 8-core compute nodes

Performance tests

Splitting	Poisson	Solver	#iterations	#search directions	Max #local solutions	Elapsed time
Checker	0.4999	FETI	233	233	466	991
		S-FETI	46	4600	414	320
Slices X	0.4999	FETI	> 800	> 800	> 1600	> 7300
		S-FETI	152	15200	760	4653
Slices Y	0.4999	FETI	> 800	> 800	> 1600	> 7300
		S-FETI	144	14400	720	4455
Slices X	0.45	FETI	> 800	> 800	> 1600	> 7300
		S-FETI	48	4800	240	493
Slices Y	0.45	FETI	409	409	818	1979
		S-FETI	36	3600	180	363

Conclusion

Multiple search directions approach good for both numerical and parallel performances

S-FETI more robust than FETI for very ill-conditioned problems

For 3D, large number of degrees of freedom on interface, memory requirement and reconjugation time may become prohibitive, need for selective and/or sparse approach