

Adaptive Coarse Spaces and Multiple Search Directions: Tools for Robust Domain Decomposition Algorithms

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FÍSICAS Y MATEMÁTICAS
UNIVERSIDAD DE CHILE



Acknowledgements

Collaborators

- ▶ Pierre Gosselet (CNRS, ENS Cachan)
- ▶ Frédéric Nataf (CNRS, Université Pierre et Marie Curie)
- ▶ Daniel J. Rixen (University of Munich)
- ▶ François-Xavier Roux (ONERA, Université Pierre et Marie Curie)

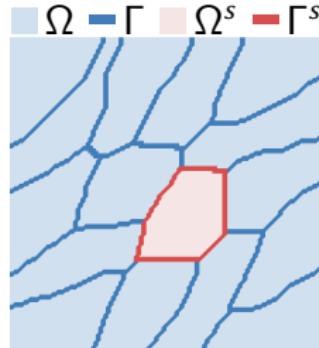
Funding

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Balancing Domain Decomposition (BDD): $\mathbf{K}\mathbf{u}_* = \mathbf{f}$ (\mathbf{K} spd)

BDD reduces the problem to the interface Γ :



$$\mathbf{A}\mathbf{u}_{*,\Gamma} = \mathbf{b}, \text{ where } \begin{aligned} \mathbf{A} &:= \mathbf{K}_{\Gamma\Gamma} - \mathbf{K}_{\Gamma I} \mathbf{K}_{II}^{-1} \mathbf{K}_{I\Gamma}, \\ \mathbf{b} &:= \mathbf{f}_{\Gamma} - \mathbf{K}_{\Gamma I} \mathbf{K}_{II}^{-1} \mathbf{f}_I. \end{aligned}$$

The operator \mathbf{A} is a sum of local contributions:

$$\mathbf{A} = \sum_{s=1}^N \mathbf{R}^{s\top} \mathbf{S}^s \mathbf{R}^s, \quad \mathbf{S}^s := \mathbf{K}_{\Gamma_s \Gamma_s}^s - \mathbf{K}_{\Gamma_s I_s}^s (\mathbf{K}_{I_s I_s}^s)^{-1} \mathbf{K}_{I_s \Gamma_s}^s,$$

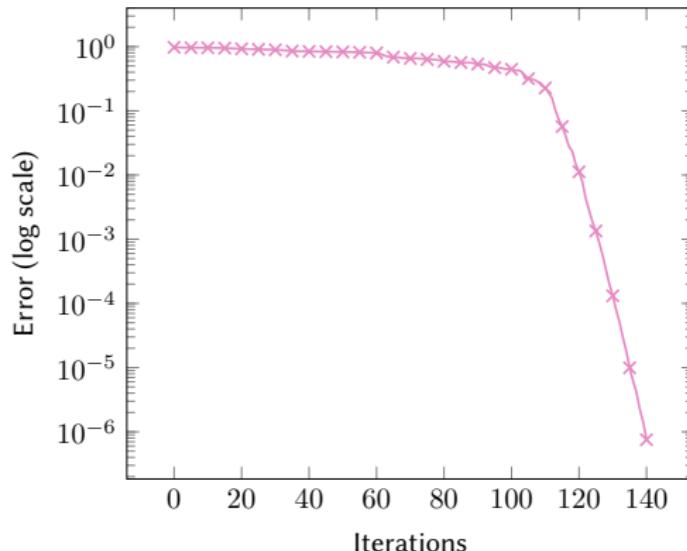
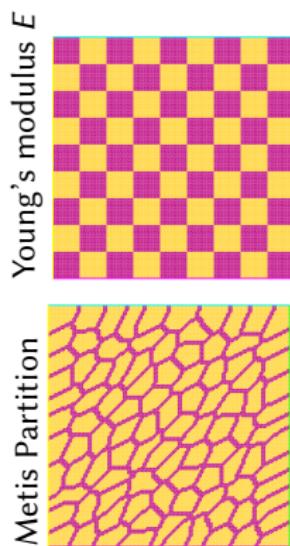
The preconditioner \mathbf{H} also:

$$\mathbf{H} := \sum_{s=1}^N \mathbf{R}^{s\top} \mathbf{D}^s \mathbf{S}^{s\dagger} \mathbf{D}^s \mathbf{R}^s, \text{ with } \sum_{s=1}^N \mathbf{R}^{s\top} \mathbf{D}^s \mathbf{R}^s = \mathbf{I}.$$

The coarse space is $\text{range}(\mathbf{U}) := \sum_{s=1}^N \mathbf{R}^{s\top} \mathbf{D}^s \text{Ker}(\mathbf{S}^s)$.

Illustration of the Problem: Heterogeneous Elasticity

$N = 81$ subdomains, $\nu = 0.4$, $E_1 = 10^7$ and $E_2 = 10^{12}$

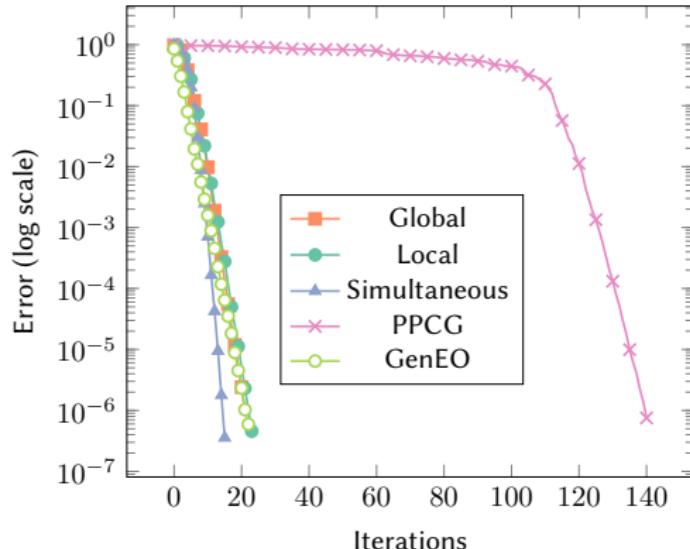
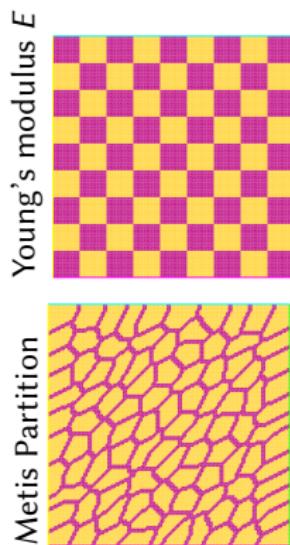


Problem: We want to design new DD methods with three objectives:

- **Reliability:** robustness and scalability.
- **Efficiency:** adapt automatically to difficulty.
- **Simplicity:** non invasive implementation.

Illustration of the Problem: Heterogeneous Elasticity

$N = 81$ subdomains, $\nu = 0.4$, $E_1 = 10^7$ and $E_2 = 10^{12}$



Problem: We want to design new DD methods with three objectives:

- **Reliability:** robustness and scalability.
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Contents

Adaptive Coarse Spaces (GenEO)

Multi Preconditioned CG (Simultaneous BDD)

Adaptive Multi Preconditioned CG

Projected PCG [Nicolaides, 1987 – Dostál, 1988]

for $\mathbf{A}\mathbf{x}_* = \mathbf{b}$ preconditioned by \mathbf{H} and projection $\boldsymbol{\Pi}$

- ▶ Assume that $\mathbf{A}, \mathbf{H} \in \mathbb{R}^{n \times n}$ are spd and $\mathbf{U} \in \mathbb{R}^{n \times n_0}$ is full rank,
- ▶ Define $\boldsymbol{\Pi} := \mathbf{I} - \mathbf{U}(\mathbf{U}^\top \mathbf{A} \mathbf{U})^{-1} \mathbf{U}^\top \mathbf{A}$.

```

1  $\mathbf{x}_0 = \mathbf{U}(\mathbf{U}^\top \mathbf{A} \mathbf{U})^{-1} \mathbf{U}^\top \mathbf{b};$            ← Initial Guess
2  $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0;$            ← Initial residual
3  $\mathbf{z}_0 = \mathbf{H}\mathbf{r}_0;$ 
4  $\mathbf{p}_0 = \boldsymbol{\Pi}\mathbf{z}_0;$            ← Initial search direction
5 for  $i = 0, 1, \dots$ , convergence do
6    $\mathbf{q}_i = \mathbf{A}\mathbf{p}_i;$ 
7    $\alpha_i = (\mathbf{q}_i^\top \mathbf{p}_i)^{-1}(\mathbf{p}_i^\top \mathbf{r}_i);$ 
8    $\mathbf{x}_{i+1} = \mathbf{x}_i + \alpha_i \mathbf{p}_i;$            ← Update approximate solution
9    $\mathbf{r}_{i+1} = \mathbf{r}_i - \alpha_i \mathbf{q}_i;$            ← Update residual
10   $\mathbf{z}_{i+1} = \mathbf{H}\mathbf{r}_{i+1};$            ← Precondition
11   $\beta_i = (\mathbf{q}_i^\top \mathbf{p}_i)^{-1}(\mathbf{q}_i^\top \mathbf{z}_{i+1});$ 
12   $\mathbf{p}_{i+1} = \boldsymbol{\Pi}\mathbf{z}_{i+1} - \beta_i \mathbf{p}_i;$            ← Project and orthogonalize
13 end
14 Return  $\mathbf{x}_{i+1};$ 

```

Convergence

[Kaniel, 66 – Meinardus, 63]

$$\frac{\|\mathbf{x}_* - \mathbf{x}_i\|_{\mathbf{A}}}{\|\mathbf{x}_* - \mathbf{x}_0\|_{\mathbf{A}}} \leq 2 \left[\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right]^i$$

- ▶ $\kappa = \frac{\lambda_{\max}}{\lambda_{\min}}$,
- ▶ λ_{\max} and λ_{\min} : extreme eigenvalues of $\mathbf{H}\mathbf{A}\boldsymbol{\Pi}$ excluding 0.

→ GenEO is a choice of range(\mathbf{U}) that guarantees fast convergence.

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Multigrid

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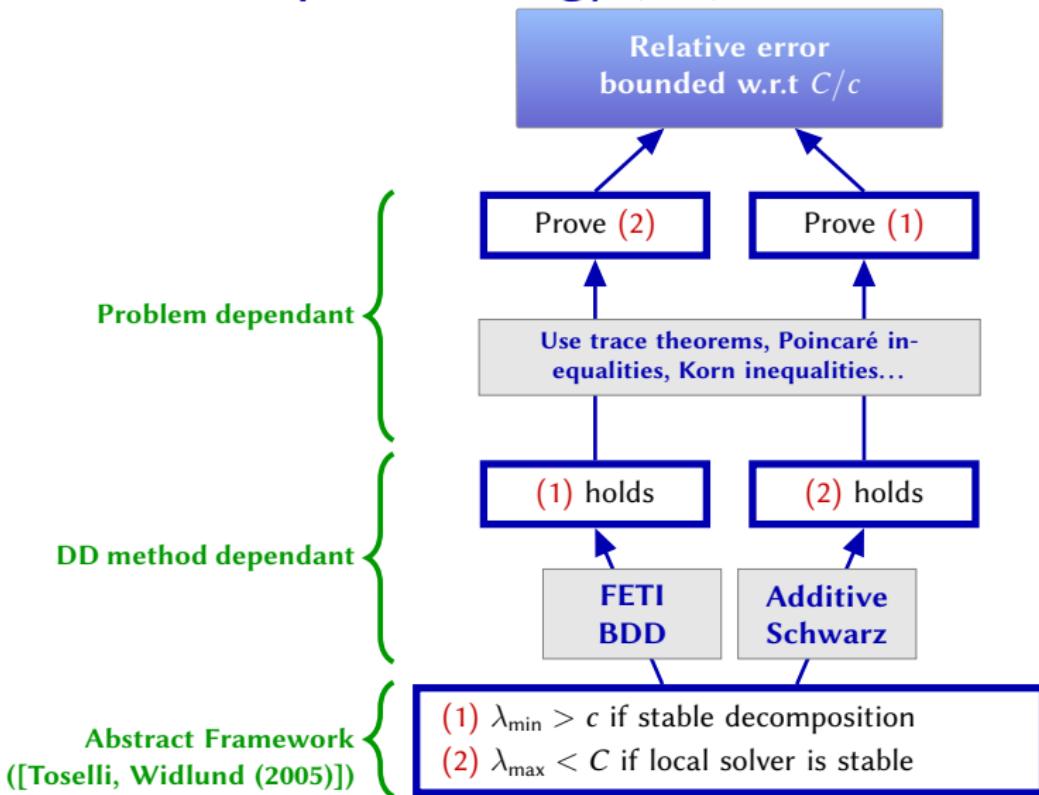
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And many other talks at this conference:

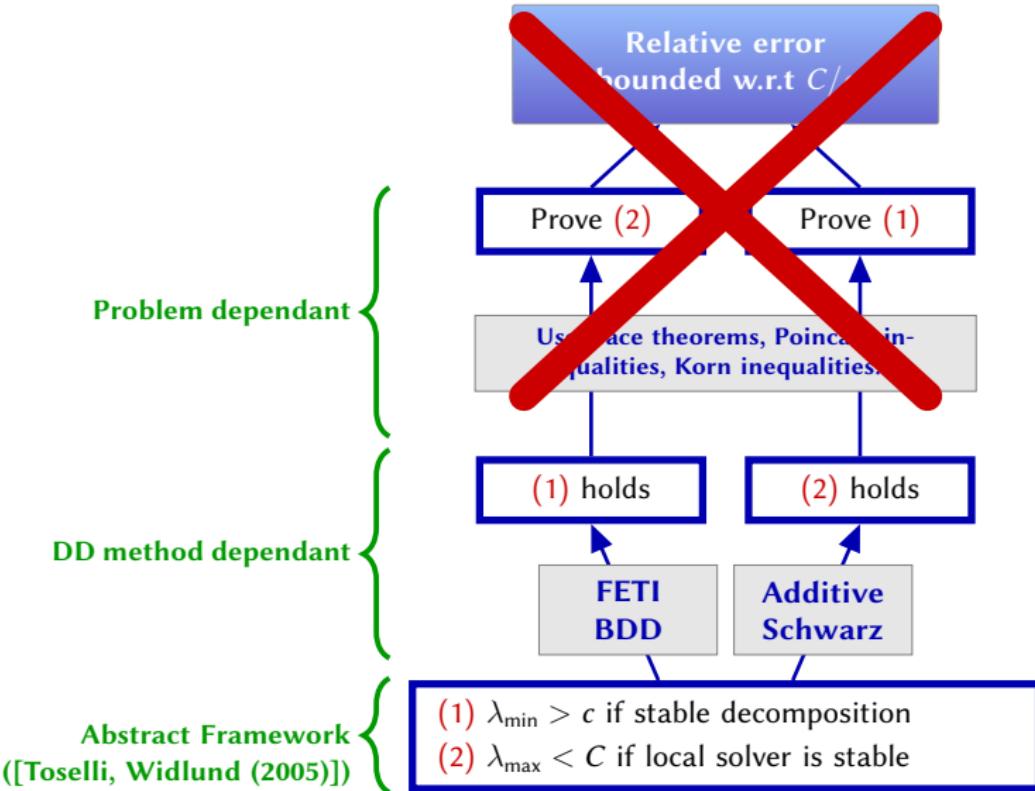
- ▶ Minisymposium on monday: Olof B. Widlund, Clark R. Dohrmann (with Clemens Pechstein),
- ▶ Pierre Jolivet (HPDDM <https://github.com/hpddm>),
- ▶ Frédéric Nataf's plenary talk tomorrow !
- ▶ Session on friday morning (CT 7) !

Adaptive Coarse Space: Strategy (1/5)



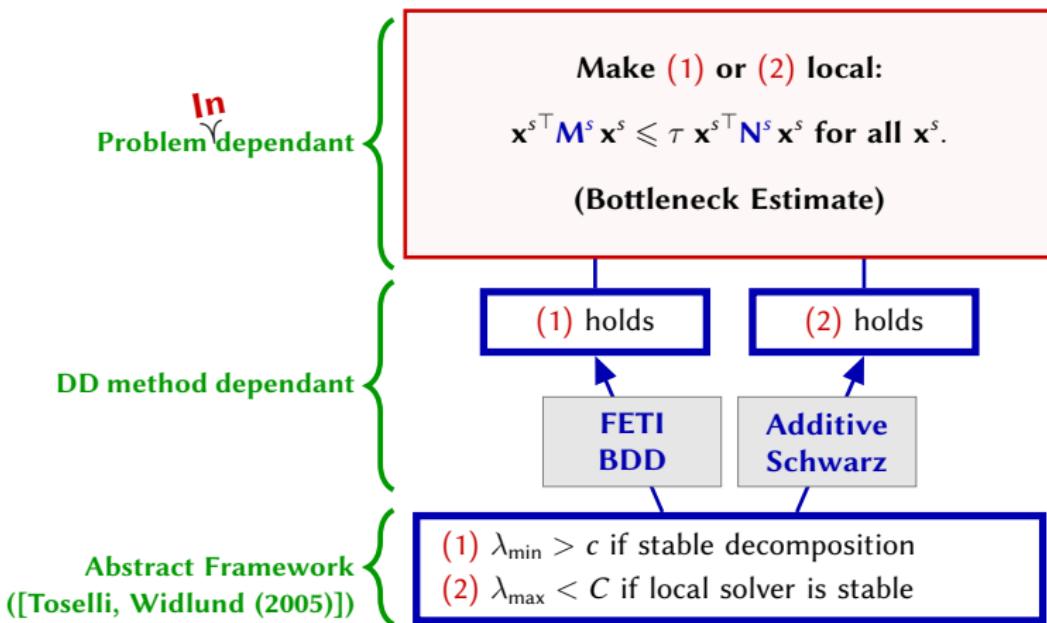
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Adaptive Coarse Space: Strategy (2/5)



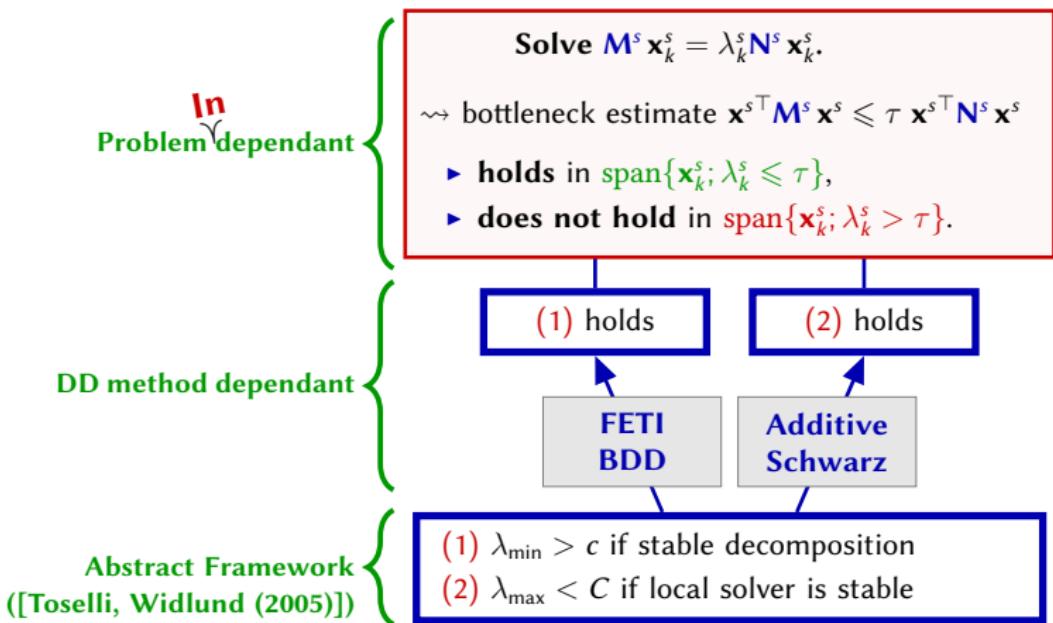
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Adaptive Coarse Space: Strategy (3/5)



[N. S., D. J. Rixen, 2013] [N. S., V. Dolean, P. Hauret, F. Nataf, C. Pechstein, and R. Scheichl, 2014]

Adaptive Coarse Space: Strategy (4/5)



[N. S., D. J. Rixen, 2013] [N. S., V. Dolean, P. Hauret, F. Nataf, C. Pechstein, and R. Scheichl, 2014]

Adaptive Coarse Space: Strategy (5/5)

Π : A-orthogonal projection onto the space where the bottleneck estimate holds

$\mathbf{A}\mathbf{x}_* = \mathbf{b}$ is equivalent to :

$$\underbrace{(\mathbf{I} - \Pi)^\top \mathbf{A} \mathbf{x}_*}_{\text{Direct Solver}} = \underbrace{(\mathbf{I} - \Pi)^\top \mathbf{b}}_{\text{DD method}}$$

and

$$\underbrace{\Pi^\top \mathbf{A} \mathbf{x}_*}_{\text{DD method}} = \Pi^\top \mathbf{b}.$$

Relative error bounded w.r.t τ and number of neighbours \mathcal{N}

$$\text{Solve } \mathbf{M}^s \mathbf{x}_k^s = \lambda_k^s \mathbf{N}^s \mathbf{x}_k^s.$$

$$\rightsquigarrow \text{bottleneck estimate } \mathbf{x}^s \top \mathbf{M}^s \mathbf{x}^s \leqslant \tau \mathbf{x}^s \top \mathbf{N}^s \mathbf{x}^s$$

- ▶ holds in $\text{span}\{\mathbf{x}_k^s; \lambda_k^s \leqslant \tau\}$,
- ▶ does not hold in $\text{span}\{\mathbf{x}_k^s; \lambda_k^s > \tau\}$.

DD method dependant

(1) holds

(2) holds

FETI
BDD

Additive
Schwarz

Abstract Framework
([Toselli, Widlund (2005)])

- (1) $\lambda_{\min} > c$ if stable decomposition
- (2) $\lambda_{\max} < C$ if local solver is stable

[N. S., D. J. Rixen, 2013] [N. S., V. Dolean, P. Hauret, F. Nataf, C. Pechstein, and R. Scheichl, 2014]

GenEO Coarse Space for BDD

- ▶ $\lambda_{\min} \geqslant 1$.
- ▶ the bottleneck estimate for λ_{\max} is

$$\mathbf{x}^s{}^\top \mathbf{R}^s \mathbf{A} \mathbf{R}^{s\top} \mathbf{x}^s \leqslant (1/\tau) \mathbf{x}^s{}^\top \mathbf{D}^{s-1} \mathbf{S} \mathbf{D}^{s-1} \mathbf{x}^s.$$

So we solve in each subdomain :

$$\mathbf{D}^{s-1} \mathbf{S}^s \mathbf{D}^{s-1} \mathbf{x}_k^s = \lambda_k^s \mathbf{R}^s \mathbf{A} \mathbf{R}^{s\top} \mathbf{x}_k^s,$$

and define the coarse space as

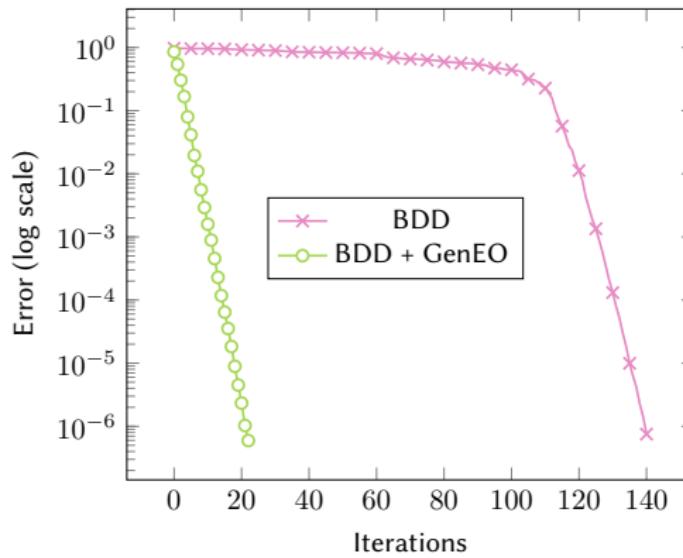
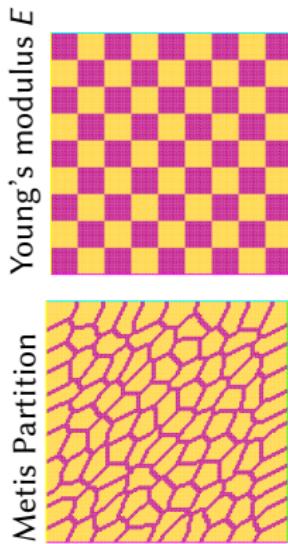
$$\text{range}(\mathbf{U}) = \text{span}\{\mathbf{R}^{s\top} \mathbf{x}_k^s; s = 1, \dots, N \text{ and } \lambda_k^s \leqslant \tau\}.$$

The effective condition number is bounded by :

$$\kappa(\mathbf{H} \mathbf{A} \boldsymbol{\Pi}) \leqslant \frac{\mathcal{N}}{\tau}; \quad \mathcal{N}: \text{number of neighbours of a subdomain.}$$

Numerical Illustration: Heterogeneous Elasticity

$N = 81$ subdomains, $\nu = 0.4$, $E_1 = 10^7$ and $E_2 = 10^{12}$, $\tau = 0.1$



Size of the coarse space: $n_0 = 349$ including 212 rigid body modes.

Conclusion for GenEO and introduction for MPCG

- ▶ Convergence guaranteed in few iterations,
- ▶ This is achieved with **local** contributions to the coarse space.

→ **Only drawback could be the cost of the eigensolves.**

 Instead of precomputing a coarse space, take advantage of the local components already being computed:

$$\mathbf{H} := \sum_{s=1}^N \underbrace{\mathbf{R}^{s\top} \mathbf{D}^s \mathbf{S}^{s\dagger} \mathbf{D}^s \mathbf{R}^s}_{:=\mathbf{H}^s}.$$

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Multi Preconditioned CG for $\mathbf{A}\mathbf{x}_* = \mathbf{b}$ prec. by $\{\mathbf{H}^s\}_{s=1,\dots,N}$ and $\boldsymbol{\Pi}$

► $\mathbf{A}, \mathbf{H} \in \mathbb{R}^{n \times n}$ spd ► $\mathbf{U} \in \mathbb{R}^{n \times n_0}$ full rank, ► $\mathbf{H} = \sum_{s=1}^N \mathbf{H}^s$, where \mathbf{H}^s spsd.

MPCG

Remark

- 1 $\mathbf{x}_0 = \mathbf{U}(\mathbf{U}^\top \mathbf{A} \mathbf{U})^{-1} \mathbf{U}^\top \mathbf{b}; \quad \leftarrow \text{Initial Guess}$
 $\mathbf{r}_i, \mathbf{x}_i \in \mathbb{R}^n$
- 2 $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0;$
 $\mathbf{Z}_i, \mathbf{P}_i, \mathbf{Q}_i \in \mathbb{R}^{n \times N}$
- 3 $\mathbf{Z}_0 = [\mathbf{H}^1 \mathbf{r}_0 | \dots | \mathbf{H}^N \mathbf{r}_{i+1}];$
 $\beta_{i,j} \in \mathbb{R}^{N \times N}$
- 4 $\mathbf{P}_0 = \boldsymbol{\Pi} \mathbf{Z}_0; \quad \leftarrow \text{Initial search directions}$
 $\alpha_i \in \mathbb{R}^N$
- 5 **for** $i = 0, 1, \dots$, convergence **do**

- 6 $\mathbf{Q}_i = \mathbf{A}\mathbf{P}_i;$
 $\mathbf{P}_i^\top \mathbf{A}\mathbf{P}_j = 0 \quad (i \neq j).$
- 7 $\alpha_i = (\mathbf{Q}_i^\top \mathbf{P}_i)^\dagger (\mathbf{P}_i^\top \mathbf{r}_i);$
 $\mathbf{r}_i^\top \mathbf{P}_j = 0 \quad (j < i).$
- 8 $\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{P}_i \alpha_i; \quad \leftarrow \text{Update approximate solution}$
 $\mathbf{P}_i^\top \mathbf{A}\mathbf{P}_i = 1.$
- 9 $\mathbf{r}_{i+1} = \mathbf{r}_i - \mathbf{Q}_i \alpha_i; \quad \leftarrow \text{Update residual}$
 $\mathbf{Q}_i^\top \mathbf{Q}_i = 1.$
- 10 $\mathbf{Z}_{i+1} = [\mathbf{H}^1 \mathbf{r}_{i+1} | \dots | \mathbf{H}^N \mathbf{r}_{i+1}]; \quad \leftarrow \text{Multi Precondition}$
 $\mathbf{Q}_i^\top \mathbf{H}^s = 0 \quad (s > i).$
- 11 $\beta_{i,j} = (\mathbf{Q}_j^\top \mathbf{P}_i)^\dagger (\mathbf{Q}_j^\top \mathbf{Z}_{i+1}), \quad j = 0, \dots, i;$
 $\mathbf{P}_i^\top \mathbf{Q}_j = 0 \quad (j > i).$
- 12 $\mathbf{P}_{i+1} = \boldsymbol{\Pi} \mathbf{Z}_{i+1} - \sum_{j=0}^i \mathbf{P}_j \beta_{i,j}; \quad \leftarrow \text{Project and orthog.}$
 $\mathbf{P}_{i+1}^\top \mathbf{A}\mathbf{P}_i = 0.$
- 13 **end**
- 14 Return $\mathbf{x}_{i+1};$

Properties

1. $\mathbf{P}_i^\top \mathbf{A}\mathbf{P}_j = 0 \quad (i \neq j).$
2. $\mathbf{r}_i^\top \mathbf{P}_j = 0 \quad (j < i).$
3. **no** short recurrence.
4. $\|\mathbf{x}_* - \mathbf{x}_{i+1}\|_{\mathbf{A}} = \min\{\|\mathbf{x}_* - \mathbf{x}\|_{\mathbf{A}}; \mathbf{x} \in \mathbf{x}_i + \text{range}(\mathbf{P}_i)\}.$

Multi Preconditioned CG for $\mathbf{A}\mathbf{x}_* = \mathbf{b}$ prec. by $\{\mathbf{H}^s\}_{s=1,\dots,N}$ and $\boldsymbol{\Pi}$

► $\mathbf{A}, \mathbf{H} \in \mathbb{R}^{n \times n}$ spd ► $\mathbf{U} \in \mathbb{R}^{n \times n_0}$ full rank, ► $\mathbf{H} = \sum_{s=1}^N \mathbf{H}^s$, where \mathbf{H}^s spsd.

MPCG

```

1  $\mathbf{x}_0 = \mathbf{U}(\mathbf{U}^\top \mathbf{A} \mathbf{U})^{-1} \mathbf{U}^\top \mathbf{b};$            ← Initial Guess
2  $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0;$ 
3  $\mathbf{Z}_0 = [\mathbf{H}^1 \mathbf{r}_0 | \dots | \mathbf{H}^N \mathbf{r}_{i+1}];$ 
4  $\mathbf{P}_0 = \boldsymbol{\Pi} \mathbf{Z}_0;$            ← Initial search directions
5 for  $i = 0, 1, \dots$ , convergence do
6    $\mathbf{Q}_i = \mathbf{A}\mathbf{P}_i;$ 
7    $\boldsymbol{\alpha}_i = (\mathbf{Q}_i^\top \mathbf{P}_i)^\dagger (\mathbf{P}_i^\top \mathbf{r}_i);$ 
8    $\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{P}_i \boldsymbol{\alpha}_i;$      ← Update approximate solution
9    $\mathbf{r}_{i+1} = \mathbf{r}_i - \mathbf{Q}_i \boldsymbol{\alpha}_i;$        ← Update residual
10   $\mathbf{Z}_{i+1} = [\mathbf{H}^1 \mathbf{r}_{i+1} | \dots | \mathbf{H}^N \mathbf{r}_{i+1}];$  ← Multi Precondition
11   $\boldsymbol{\beta}_{i,j} = (\mathbf{Q}_j^\top \mathbf{P}_j)^\dagger (\mathbf{Q}_j^\top \mathbf{Z}_{i+1}), \quad j = 0, \dots, i;$ 
12   $\mathbf{P}_{i+1} = \boldsymbol{\Pi} \mathbf{Z}_{i+1} - \sum_{j=0}^i \mathbf{P}_j \boldsymbol{\beta}_{i,j};$  ← Project and orthog.
13 end
14 Return  $\mathbf{x}_{i+1};$ 

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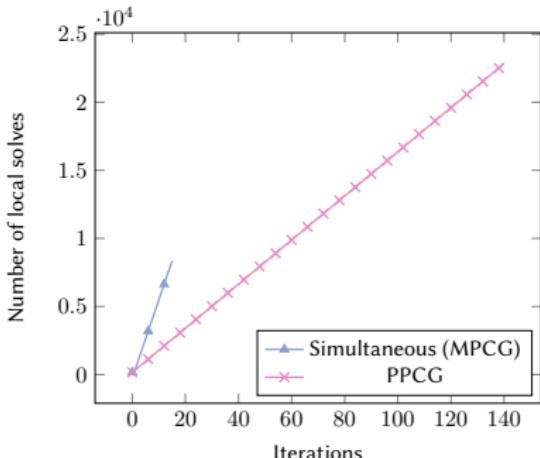
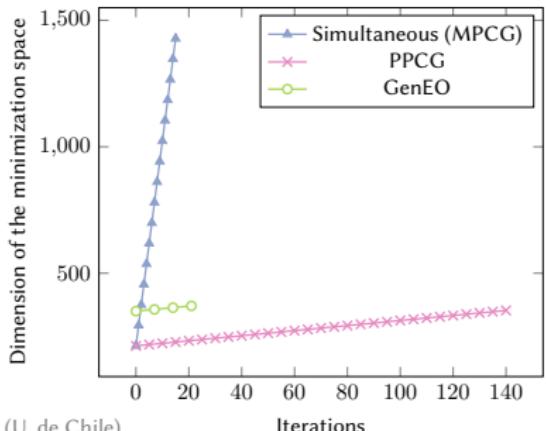
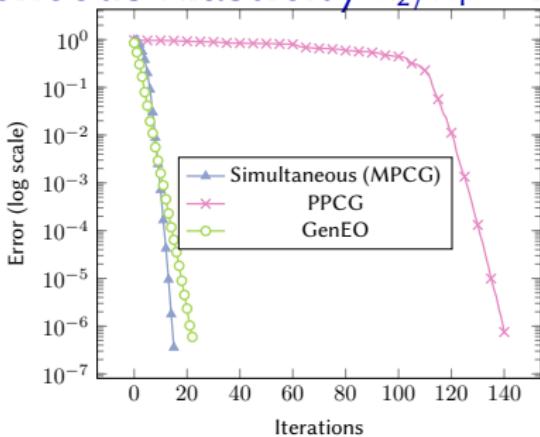
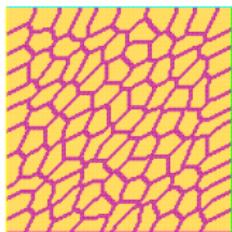
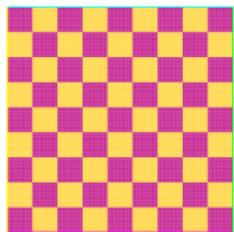
PPCG

```

 $\mathbf{x}_0 = \mathbf{U}(\mathbf{U}^\top \mathbf{A} \mathbf{U})^{-1} \mathbf{U}^\top \mathbf{b};$ 
 $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0;$ 
 $\mathbf{z}_0 = \mathbf{H}\mathbf{r}_0;$ 
 $\mathbf{p}_0 = \boldsymbol{\Pi} \mathbf{z}_0;$ 
for  $i = 0, 1, \dots$ , conv. do
   $\mathbf{q}_i = \mathbf{A}\mathbf{p}_i;$ 
   $\alpha_i = (\mathbf{q}_i^\top \mathbf{p}_i)^{-1} (\mathbf{p}_i^\top \mathbf{r}_i);$ 
   $\mathbf{x}_{i+1} = \mathbf{x}_i + \alpha_i \mathbf{p}_i;$ 
   $\mathbf{r}_{i+1} = \mathbf{r}_i - \alpha_i \mathbf{q}_i;$ 
   $\mathbf{z}_{i+1} = \mathbf{H}\mathbf{r}_{i+1};$ 
   $\beta_i = (\mathbf{q}_i^\top \mathbf{p}_i)^{-1} (\mathbf{q}_i^\top \mathbf{z}_{i+1});$ 
   $\mathbf{p}_{i+1} = \boldsymbol{\Pi} \mathbf{z}_{i+1} - \beta_i \mathbf{p}_i;$ 
end
Return  $\mathbf{x}_{i+1};$ 

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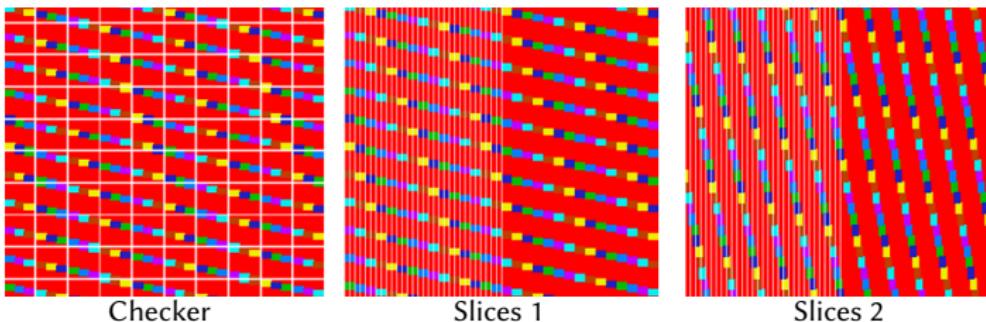
Numerical Illustration (Heterogeneous Elasticity $E_2/E_1 = 10^5$)



Simultaneous FETI: Tests with CPU time (F.-X. Roux)

100 subdomains, 17×10^6 dofs, $\nu = 0.45$ or 0.4999 , $1 \leq E \leq 10^5$.

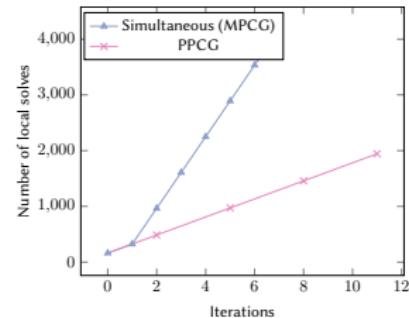
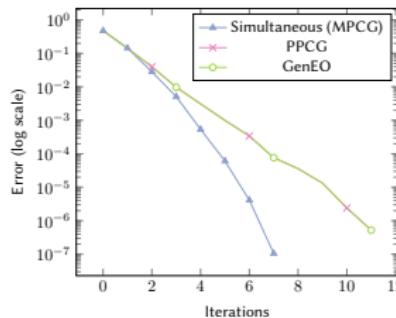
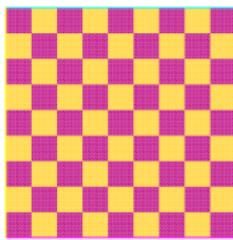
2.6 GHz 8-core Xeon processors, Intel fortran, MKL-pardiso.



Decomp.	ν	Solver	#it	dim	Max solves	Time (s)	
Slices 1	0.45	FETI S-FETI	> 800 48	> 800 4800	> 1600 192	> 7300 493	✗ ✓
Slices2	0.45	FETI S-FETI	409 36	409 3600	818 144	1979 363	✓ ✓
Checker	0.4999	FETI S-FETI	233 46	233 4600	466 276	991 320	✓ ✓
Slices 1	0.4999	FETI S-FETI	> 800 152	> 800 15200	> 1600 608	> 7300 4653	✗ ✓
Slices2	0.4999	FETI S-FETI	> 800 144	> 800 14400	> 1600 576	> 7300 4455	✗ ✓

Good convergence but two possible limitations

- ✓ Local contributions $\mathbf{H}^s \mathbf{r}_i$ form a good minimization space.
- ✗ Cost of inverting $\mathbf{P}_i^\top \mathbf{A} \mathbf{P}_i \in \mathbb{R}^{N \times N}$ at each iteration in $\alpha_i = (\mathbf{P}_i^\top \mathbf{A} \mathbf{P}_i)^\dagger (\mathbf{P}_i^\top \mathbf{r}_i)$ and $\beta_{i,j} = (\mathbf{P}_j^\top \mathbf{A} \mathbf{P}_j)^\dagger (\mathbf{Q}_j^\top \mathbf{Z}_{i+1})$.
- ✗ Simultaneous BDD may work ‘too hard’ on ‘easy’ problems.



💡 Introduce adaptativity into multipreconditioned CG.

From the GenEO section we know that:

- ▶ a few local vectors should suffice to accelerate convergence.
- ▶ they are the low frequency eigenvectors of:

$$\mathbf{D}^{s-1} \mathbf{S}^s \mathbf{D}^{s-1} \mathbf{x}_k^s = \lambda_k^s \mathbf{R}^s \mathbf{A} \mathbf{R}^{s\top} \mathbf{x}_k^s.$$

Adaptive Multi Preconditioned CG for $\mathbf{A}\mathbf{x}_* = \mathbf{b}$ preconditioned by $\sum_{s=1}^N \mathbf{H}^s$ and projection $\mathbf{\Pi}$. ($\tau \in \mathbb{R}^+$ is chosen by the user)

```

1  $\mathbf{x}_0 = \mathbf{U}(\mathbf{U}^\top \mathbf{A} \mathbf{U})^{-1} \mathbf{U}^\top \mathbf{b};$ 
2  $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0; \mathbf{Z}_0 = \mathbf{H}\mathbf{r}_0; \mathbf{P}_0 = \mathbf{\Pi}\mathbf{Z}_0;$ 
3 for  $i = 0, 1, \dots$ , convergence do
4    $\mathbf{Q}_i = \mathbf{A}\mathbf{P}_i;$ 
5    $\boldsymbol{\alpha}_i = (\mathbf{Q}_i^\top \mathbf{P}_i)^\dagger (\mathbf{P}_i^\top \mathbf{r}_i);$ 
6    $\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{P}_i \boldsymbol{\alpha}_i;$ 
7    $\mathbf{r}_{i+1} = \mathbf{r}_i - \mathbf{Q}_i \boldsymbol{\alpha}_i;$ 
8    $t_i = \frac{(\mathbf{P}_i \boldsymbol{\alpha}_i)^\top \mathbf{A} (\mathbf{P}_i \boldsymbol{\alpha}_i)}{\mathbf{r}_{i+1}^\top \mathbf{H} \mathbf{r}_{i+1}};$ 
9   if  $t_i < \tau$  then ←  $\tau$ -test
10    |  $\mathbf{Z}_{i+1} = [\mathbf{H}^1 \mathbf{r}_{i+1} | \dots | \mathbf{H}^N \mathbf{r}_{i+1}]$ 
11   else
12    |  $\mathbf{Z}_{i+1} = \mathbf{H}\mathbf{r}_{i+1};$ 
13   end
14    $\beta_{i,j} = (\mathbf{Q}_j^\top \mathbf{P}_j)^\dagger (\mathbf{Q}_j^\top \mathbf{Z}_{i+1}), \quad j = 0, \dots, i;$ 
15    $\mathbf{P}_{i+1} = \mathbf{\Pi}\mathbf{Z}_{i+1} - \sum_{j=0}^i \mathbf{P}_j \beta_{i,j};$ 
16 end
17 Return  $\mathbf{x}_{i+1};$ 

```

Remark

$\mathbf{x}_i, \mathbf{r}_i \in \mathbb{R}^n,$
 $\mathbf{Z}_i, \mathbf{P}_i, \mathbf{Q}_i \in \mathbb{R}^{n \times N}$ or \mathbb{R}^n ,
 $\boldsymbol{\alpha}_i \in \mathbb{R}^N$ or \mathbb{R} ,
 $\beta_{i,j} \in \mathbb{R}^{N \times N}, \mathbb{R}^N, \mathbb{R}^{1 \times N}$ or \mathbb{R} ,
 $\mathbf{P}_i \boldsymbol{\alpha}_i \in \mathbb{R}^n.$

- ▶ n : size of problem,
- ▶ N : nb of precs.

Theoretical Result (1/3): PPCG like Properties

```

 $\mathbf{x}_0 = \mathbf{U}(\mathbf{U}^\top \mathbf{A}\mathbf{U})^{-1}\mathbf{U}^\top \mathbf{b};$ 
 $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0; \mathbf{Z}_0 = \mathbf{H}\mathbf{r}_0; \mathbf{P}_0 = \boldsymbol{\Pi}\mathbf{Z}_0;$ 
for  $i = 0, 1, \dots$ , convergence do
     $\mathbf{Q}_i = \mathbf{A}\mathbf{P}_i;$ 
     $\alpha_i = (\mathbf{Q}_i^\top \mathbf{P}_i)^\dagger (\mathbf{P}_i^\top \mathbf{r}_i);$ 
     $\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{P}_i \alpha_i;$ 
     $\mathbf{r}_{i+1} = \mathbf{r}_i - \mathbf{Q}_i \alpha_i;$ 
     $t_i = \frac{(\mathbf{P}_i \alpha_i)^\top \mathbf{A}(\mathbf{P}_i \alpha_i)}{\mathbf{r}_{i+1}^\top \mathbf{H}\mathbf{r}_{i+1}};$ 
    if  $t_i < \tau$  then
         $\mathbf{z}_{i+1} = [\mathbf{H}^1\mathbf{r}_{i+1} | \dots | \mathbf{H}^N\mathbf{r}_{i+1}]$ 
    else
         $\mathbf{z}_{i+1} = \mathbf{H}\mathbf{r}_{i+1};$ 
    end
     $\beta_{i,j} = (\mathbf{Q}_j^\top \mathbf{P}_j)^\dagger (\mathbf{Q}_j^\top \mathbf{z}_{i+1});$ 
     $\mathbf{P}_{i+1} = \boldsymbol{\Pi}\mathbf{Z}_{i+1} - \sum_{j=0}^i \mathbf{P}_j \beta_{i,j};$ 
end
Return  $\mathbf{x}_{i+1};$ 

```

Remark

No short recurrence property as soon as the minimization space has been augmented.

Theorem

- ▶ $\mathbf{x}_{n-n_0} = \mathbf{x}_*$.
- ▶ *Blocs of search directions are pairwise \mathbf{A} -orthogonal:*
 $\mathbf{P}_j^\top \mathbf{A} \mathbf{P}_i = \mathbf{0} (i \neq j).$
- ▶ *Residuals are pairwise \mathbf{H} -orthogonal:* $\langle \mathbf{H}\mathbf{r}_j, \mathbf{r}_i \rangle = 0 (i \neq j).$

$$\begin{aligned} \blacktriangleright \quad & \| \mathbf{x}_* - \mathbf{x}_i \|_{\mathbf{A}} = \\ & \min \left\{ \| \mathbf{x}_* - \mathbf{x} \|_{\mathbf{A}}; \mathbf{x} \in \text{range}(\mathbf{U}) + \sum_{j=0}^{i-1} \text{range}(\mathbf{P}_j) \right\}. \end{aligned}$$

Theoretical Result (2/3): Two types of iterations

```

 $\mathbf{x}_0 = \mathbf{U}(\mathbf{U}^\top \mathbf{A}\mathbf{U})^{-1}\mathbf{U}^\top \mathbf{b};$ 
 $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0; \mathbf{Z}_0 = \mathbf{H}\mathbf{r}_0; \mathbf{P}_0 = \boldsymbol{\Pi}\mathbf{Z}_0;$ 
for  $i = 0, 1, \dots$ , convergence do
     $\mathbf{Q}_i = \mathbf{A}\mathbf{P}_i;$ 
     $\boldsymbol{\alpha}_i = (\mathbf{Q}_i^\top \mathbf{P}_i)^\dagger (\mathbf{P}_i^\top \mathbf{r}_i);$ 
     $\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{P}_i \boldsymbol{\alpha}_i;$ 
     $\mathbf{r}_{i+1} = \mathbf{r}_i - \mathbf{Q}_i \boldsymbol{\alpha}_i;$ 
     $t_i = \frac{(\mathbf{P}_i \boldsymbol{\alpha}_i)^\top \mathbf{A}(\mathbf{P}_i \boldsymbol{\alpha}_i)}{\mathbf{r}_{i+1}^\top \mathbf{H}\mathbf{r}_{i+1}};$ 
    if  $t_i < \tau$  then
         $\mathbf{Z}_{i+1} = [\mathbf{H}^1 \mathbf{r}_{i+1} \mid \dots \mid \mathbf{H}^N \mathbf{r}_{i+1}]$ 
    else
         $\mathbf{Z}_{i+1} = \mathbf{H}\mathbf{r}_{i+1};$ 
    end
     $\boldsymbol{\beta}_{i,j} = (\mathbf{Q}_j^\top \mathbf{P}_j)^\dagger (\mathbf{Q}_j^\top \mathbf{Z}_{i+1});$ 
     $\mathbf{P}_{i+1} = \boldsymbol{\Pi}\mathbf{Z}_{i+1} - \sum_{j=0}^i \mathbf{P}_j \boldsymbol{\beta}_{i,j};$ 
end
Return  $\mathbf{x}_{i+1};$ 

```

Theorem

If the τ -test returns $t_{i-1} \geq \tau$ then

$$\frac{\|\mathbf{x}_* - \mathbf{x}_i\|_{\mathbf{A}}}{\|\mathbf{x}_* - \mathbf{x}_{i-1}\|_{\mathbf{A}}} \leq \left(\frac{1}{1 + \lambda_{\min} \tau} \right)^{1/2},$$

$\lambda_{\min} = 1$ for BDD.

Theoretical Result (2/3): Two types of iterations

```

 $\mathbf{x}_0 = \mathbf{U}(\mathbf{U}^\top \mathbf{A} \mathbf{U})^{-1} \mathbf{U}^\top \mathbf{b};$ 
 $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0; \mathbf{Z}_0 = \mathbf{H}\mathbf{r}_0; \mathbf{P}_0 = \boldsymbol{\Pi}\mathbf{Z}_0;$ 
for  $i = 0, 1, \dots$ , convergence do
     $\mathbf{Q}_i = \mathbf{A}\mathbf{P}_i;$ 
     $\boldsymbol{\alpha}_i = (\mathbf{Q}_i^\top \mathbf{P}_i)^\dagger (\mathbf{P}_i^\top \mathbf{r}_i);$ 
     $\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{P}_i \boldsymbol{\alpha}_i;$ 
     $\mathbf{r}_{i+1} = \mathbf{r}_i - \mathbf{Q}_i \boldsymbol{\alpha}_i;$ 
     $t_i = \frac{(\mathbf{P}_i \boldsymbol{\alpha}_i)^\top \mathbf{A} (\mathbf{P}_i \boldsymbol{\alpha}_i)}{\mathbf{r}_{i+1}^\top \mathbf{H} \mathbf{r}_{i+1}};$ 
    if  $t_i < \tau$  then
         $\mathbf{Z}_{i+1} = [\mathbf{H}^1 \mathbf{r}_{i+1} | \dots | \mathbf{H}^N \mathbf{r}_{i+1}]$ 
    else
         $\mathbf{Z}_{i+1} = \mathbf{H}\mathbf{r}_{i+1};$ 
    end
     $\boldsymbol{\beta}_{i,j} = (\mathbf{Q}_j^\top \mathbf{P}_j)^\dagger (\mathbf{Q}_j^\top \mathbf{Z}_{i+1});$ 
     $\mathbf{P}_{i+1} = \boldsymbol{\Pi}\mathbf{Z}_{i+1} - \sum_{j=0}^i \mathbf{P}_j \boldsymbol{\beta}_{i,j};$ 
end
Return  $\mathbf{x}_{i+1};$ 

```

Theorem

If the τ -test returns $t_{i-1} \geq \tau$ then

$$\frac{\|\mathbf{x}_* - \mathbf{x}_i\|_{\mathbf{A}}}{\|\mathbf{x}_* - \mathbf{x}_{i-1}\|_{\mathbf{A}}} \leq \left(\frac{1}{1 + \lambda_{\min} \tau} \right)^{1/2},$$

$\lambda_{\min} = 1$ for BDD.

Proof

$$\begin{aligned}
 \mathbf{x}_* &= \mathbf{x}_0 + \sum_{i=0}^{n-n_0} \mathbf{P}_i \boldsymbol{\alpha}_i = \mathbf{x}_i + \sum_{j=i}^{n-n_0} \mathbf{P}_j \boldsymbol{\alpha}_j \\
 \Rightarrow \|\mathbf{x}_* - \mathbf{x}_i\|_{\mathbf{A}}^2 &= \sum_{j=i}^{n-n_0} \|\mathbf{P}_j \boldsymbol{\alpha}_j\|_{\mathbf{A}}^2 \\
 \Rightarrow \|\mathbf{x}_* - \mathbf{x}_{i-1}\|_{\mathbf{A}}^2 &= \|\mathbf{x}_* - \mathbf{x}_i\|_{\mathbf{A}}^2 + \|\mathbf{P}_{i-1} \boldsymbol{\alpha}_{i-1}\|_{\mathbf{A}}^2.
 \end{aligned}$$

(Similar to [Axelsson and Kaporin, 2001].)

$$\begin{aligned}
 \frac{\|\mathbf{x}_* - \mathbf{x}_{i-1}\|_{\mathbf{A}}^2}{\|\mathbf{x}_* - \mathbf{x}_i\|_{\mathbf{A}}^2} &= 1 + \underbrace{\frac{\|\mathbf{r}_i\|_{\mathbf{H}}^2}{\|\mathbf{d}_i\|_{\mathbf{A}}^2}}_{= t_{i-1}} \frac{\|\mathbf{P}_{i-1} \boldsymbol{\alpha}_{i-1}\|_{\mathbf{A}}^2}{\|\mathbf{r}_i\|_{\mathbf{H}}^2} \geq 1 + \lambda_{\min} \underbrace{\frac{\|\mathbf{P}_{i-1} \boldsymbol{\alpha}_{i-1}\|_{\mathbf{A}}^2}{\|\mathbf{r}_i\|_{\mathbf{H}}^2}}_{= t_{i-1}} \geq 1 + \lambda_{\min} \tau.
 \end{aligned}$$

Theoretical Result (3/3): No extra work for ‘easy’ pbs.

```

 $x_0 = U(U^\top A U)^{-1} U^\top b;$ 
 $r_0 = b - Ax_0; Z_0 = Hr_0; P_0 = \Pi Z_0;$ 
for  $i = 0, 1, \dots$ , convergence do
     $Q_i = AP_i;$ 
     $\alpha_i = (Q_i^\top P_i)^\dagger (P_i^\top r_i);$ 
     $x_{i+1} = x_i + P_i \alpha_i;$ 
     $r_{i+1} = r_i - Q_i \alpha_i;$ 
     $t_i = \frac{(P_i \alpha_i)^\top A (P_i \alpha_i)}{r_{i+1}^\top H r_{i+1}};$ 
    if  $t_i < \tau$  then
         $Z_{i+1} = [H^1 r_{i+1} | \dots | H^N r_{i+1}]$ 
    else
         $Z_{i+1} = H r_{i+1};$ 
    end
     $\beta_{i,j} = (Q_j^\top P_j)^\dagger (Q_j^\top Z_{i+1});$ 
     $P_{i+1} = \Pi Z_{i+1} - \sum_{j=0}^i P_j \beta_{i,j};$ 
end
Return  $x_{i+1};$ 

```

Theorem

If $\lambda_{\max}(HA) \leq 1/\tau$ then the algorithm is the usual PPCG.

Theoretical Result (3/3): No extra work for ‘easy’ pbs.

```

 $x_0 = U(U^\top A U)^{-1} U^\top b;$ 
 $r_0 = b - Ax_0; Z_0 = Hr_0; P_0 = \Pi Z_0;$ 
for  $i = 0, 1, \dots$ , convergence do
     $Q_i = AP_i;$ 
     $\alpha_i = (Q_i^\top P_i)^\dagger (P_i^\top r_i);$ 
     $x_{i+1} = x_i + P_i \alpha_i;$ 
     $r_{i+1} = r_i - Q_i \alpha_i;$ 
     $t_i = \frac{(P_i \alpha_i)^\top A (P_i \alpha_i)}{r_{i+1}^\top H r_{i+1}};$ 
    if  $t_i < \tau$  then
         $Z_{i+1} = [H^1 r_{i+1} | \dots | H^N r_{i+1}]$ 
    else
         $Z_{i+1} = Hr_{i+1};$ 
    end
     $\beta_{i,j} = (Q_j^\top P_j)^\dagger (Q_j^\top Z_{i+1});$ 
     $P_{i+1} = \Pi Z_{i+1} - \sum_{j=0}^i P_j \beta_{i,j};$ 
end
Return  $x_{i+1};$ 

```

Theorem

If $\lambda_{\max}(HA) \leq 1/\tau$ then the algorithm is the usual PPCG.

Proof

We begin with $r_i = r_{i-1} - Q_{i-1} \alpha_{i-1}$ and take the inner product by Hr_i :

$$\begin{aligned} \langle Hr_i, r_i \rangle &= \cancel{\langle Hr_i, r_{i-1} \rangle} - \langle Hr_i, AP_{i-1} \alpha_{i-1} \rangle \\ &\leq \|r_i\|_{HAH}^{1/2} \|P_{i-1} \alpha_{i-1}\|_A^{1/2} \quad (C.S.), \end{aligned}$$

or equivalently:

$$\frac{\langle Hr_i, r_i \rangle}{\langle Hr_i, AHr_i \rangle} \leq \frac{\langle P_{i-1} \alpha_{i-1}, AP_{i-1} \alpha_{i-1} \rangle}{\langle Hr_i, r_i \rangle}.$$

Finally: $\tau \leq \frac{1}{\lambda_{\max}} \leq \frac{\langle Hr_i, r_i \rangle}{\langle Hr_i, AHr_i \rangle} \leq \frac{\langle P_{i-1} \alpha_{i-1}, AP_{i-1} \alpha_{i-1} \rangle}{\langle Hr_i, r_i \rangle} = t_{i-1}.$

Local Adaptive MPCG for $\sum_{s=1}^N \mathbf{A}^s \mathbf{x}_* = \mathbf{b}$ preconditioned by $\sum_{s=1}^N \mathbf{H}^s$ and projection $\boldsymbol{\Pi}$. ($\tau \in \mathbb{R}^+$ is chosen by the user)

```

1  $\mathbf{x}_0 = \mathbf{U}(\mathbf{U}^\top \mathbf{A}\mathbf{U})^{-1}\mathbf{U}^\top \mathbf{b}; \mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0; \mathbf{Z}_0 = \mathbf{H}\mathbf{r}_0;$   

 $\mathbf{P}_0 = \boldsymbol{\Pi}\mathbf{Z}_0;$ 
2 for  $i = 0, 1, \dots$ , convergence do
3    $\mathbf{Q}_i = \mathbf{A}\mathbf{P}_i;$ 
4    $\boldsymbol{\alpha}_i = (\mathbf{Q}_i^\top \mathbf{P}_i)^\dagger (\mathbf{P}_i^\top \mathbf{r}_i);$ 
5    $\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{P}_i \boldsymbol{\alpha}_i;$ 
6    $\mathbf{r}_{i+1} = \mathbf{r}_i - \mathbf{Q}_i \boldsymbol{\alpha}_i;$ 
7    $\mathbf{Z}_{i+1} = \mathbf{H}\mathbf{r}_{i+1};$             $\leftarrow$  initialize  $\mathbf{Z}_{i+1}$ 
8   for  $s = 1, \dots, N$  do
9      $t_i^s = \frac{\langle \mathbf{P}_i \boldsymbol{\alpha}_i, \mathbf{A}^s \mathbf{P}_i \boldsymbol{\alpha}_i \rangle}{\mathbf{r}_{i+1}^\top \mathbf{H}^s \mathbf{r}_{i+1}};$ 
10    if  $t_i^s < \tau$  then           $\leftarrow$  local  $\tau$ -test
11       $\mathbf{Z}_{i+1} = [\mathbf{Z}_{i+1} | \mathbf{H}^s \mathbf{r}_{i+1}];$ 
12    end
13  end
14   $\beta_{i,j} = (\mathbf{Q}_j^\top \mathbf{P}_j)^\dagger (\mathbf{Q}_j^\top \mathbf{Z}_{i+1}), \quad j = 0, \dots, i;$ 
15   $\mathbf{P}_{i+1} = \boldsymbol{\Pi}\mathbf{Z}_{i+1} - \sum_{j=0}^i \mathbf{P}_j \beta_{i,j};$ 
16 end
17 Return  $\mathbf{x}_{i+1};$ 

```

► $\mathbf{A} = \sum_{s=1}^N \underbrace{\mathbf{R}^s \top \mathbf{S}^s \mathbf{R}^s}_{:= \mathbf{A}^s}$

► Between 1 and N search directions per iteration.

► Reduces the cost of inverting $\mathbf{P}_i^\top \mathbf{A} \mathbf{P}_i$ (one limitation of MPCG)

Theorem

If the τ -test returns $t_{i-1}^s \geq \tau$ for all $s = 1, \dots, N$ then

$$\frac{\|\mathbf{x}_* - \mathbf{x}_i\|_{\mathbf{A}}}{\|\mathbf{x}_* - \mathbf{x}_{i-1}\|_{\mathbf{A}}} \leq \left(\frac{1}{1 + \lambda_{\min} \tau} \right)^{1/2}.$$

Implementation for BDD: Saving local solves

```

1  $\mathbf{x}_0 = \mathbf{U}(\mathbf{U}^\top \mathbf{A}\mathbf{U})^{-1}\mathbf{U}^\top \mathbf{b}; \mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0; \mathbf{Z}_0 = \mathbf{H}\mathbf{r}_0; \tilde{\mathbf{P}}_0 = \mathbf{Z}_0;$ 
2 for  $i = 0, 1, \dots$ , convergence do
3    $\mathbf{Q}_i = \sum_{s=1}^N \mathbf{Q}_i^s$  where  $\mathbf{Q}_i^s = \mathbf{A}^s \mathbf{Z}_i - \mathbf{A}^s \mathbf{U}(\mathbf{U}^\top \mathbf{A}\mathbf{U})^{-1}(\mathbf{A}\mathbf{U})^\top \mathbf{Z}_i - \sum_{j=0}^{i-1} \mathbf{Q}_j^s \beta_{i-1,j};$ 
4    $\alpha_i = (\mathbf{Q}_i^\top \tilde{\mathbf{P}}_i)^\dagger (\tilde{\mathbf{P}}_i^\top \mathbf{r}_i); \mathbf{x}_{i+1} = \mathbf{x}_i + \boldsymbol{\Pi} \tilde{\mathbf{P}}_i \alpha_i; \mathbf{r}_{i+1} = \mathbf{r}_i - \mathbf{Q}_i \alpha_i;$ 
5    $\mathbf{Z}_{i+1} = \mathbf{H}\mathbf{r}_{i+1};$ 
6   for  $s = 1, \dots, N$  do
7      $t_i^s = \frac{\langle \boldsymbol{\Pi} \tilde{\mathbf{P}}_i \alpha_i, \mathbf{Q}_i^s \alpha_i \rangle}{\mathbf{r}_{i+1}^\top \mathbf{H}^s \mathbf{r}_{i+1}};$ 
8     if  $t_i^s < \tau$  then
9        $\mathbf{Z}_{i+1} = [\mathbf{Z}_{i+1} | \mathbf{H}^s \mathbf{r}_{i+1}];$ 
10      Subtract  $\mathbf{H}^s \mathbf{r}_{i+1}$  from the first column in  $\mathbf{Z}_{i+1};$ 
11    end
12  end
13   $\beta_{i,j} = (\mathbf{Q}_i^\top \tilde{\mathbf{P}}_i)^\dagger (\mathbf{Q}_j^\top \mathbf{Z}_{i+1}) (j = 0, \dots, i); \tilde{\mathbf{P}}_{i+1} = \mathbf{Z}_{i+1} - \sum_{j=0}^i \tilde{\mathbf{P}}_j \beta_{i,j};$ 
14 end
15 Return  $\mathbf{x}_{i+1};$ 

```

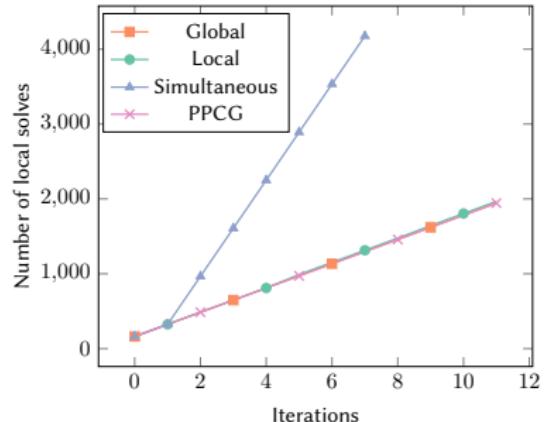
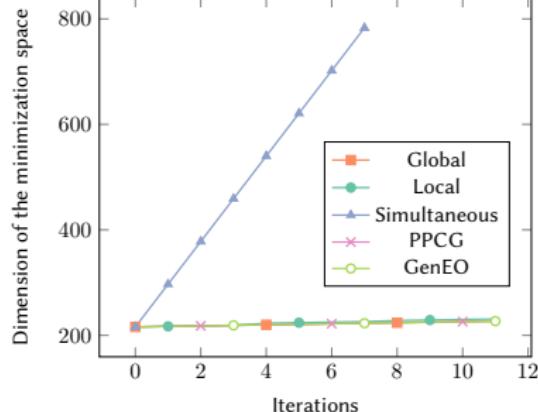
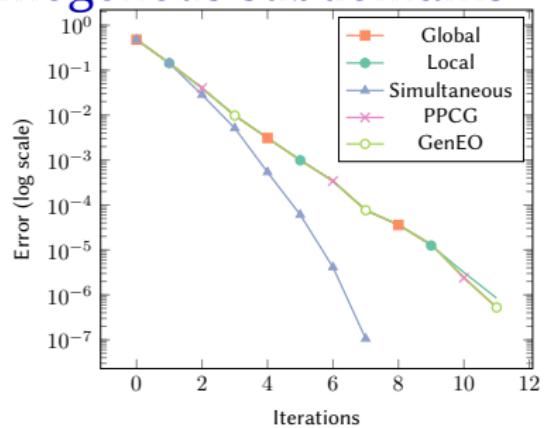
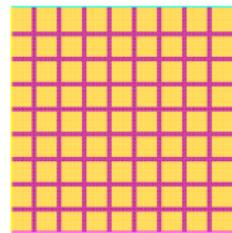
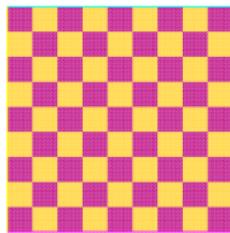
Same ‘trick’ as in :

 P. Gosselet, D. J. Rixen, F.-X. Roux, and N. S.

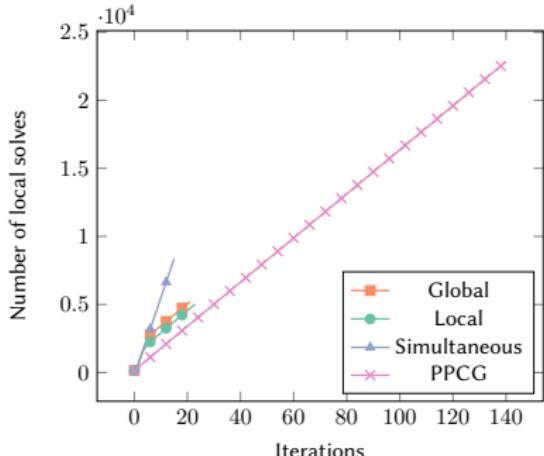
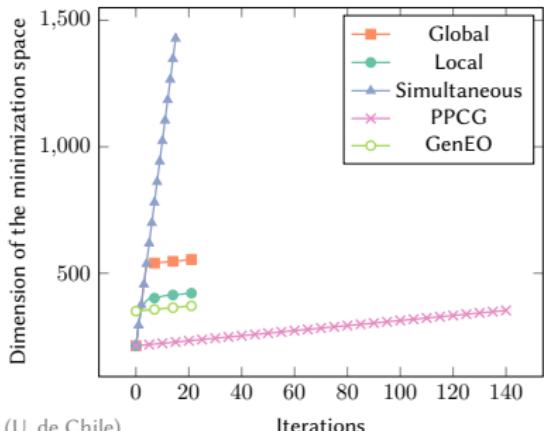
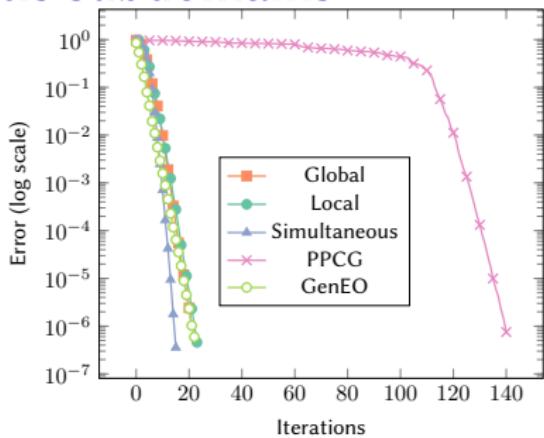
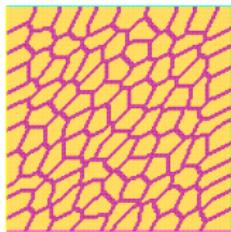
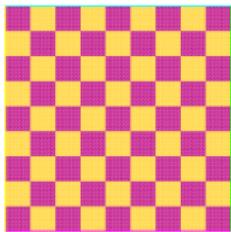
Simultaneous FETI and block FETI: Robust domain decomposition with multiple search directions.

International Journal for Numerical Methods in Engineering, 2015.

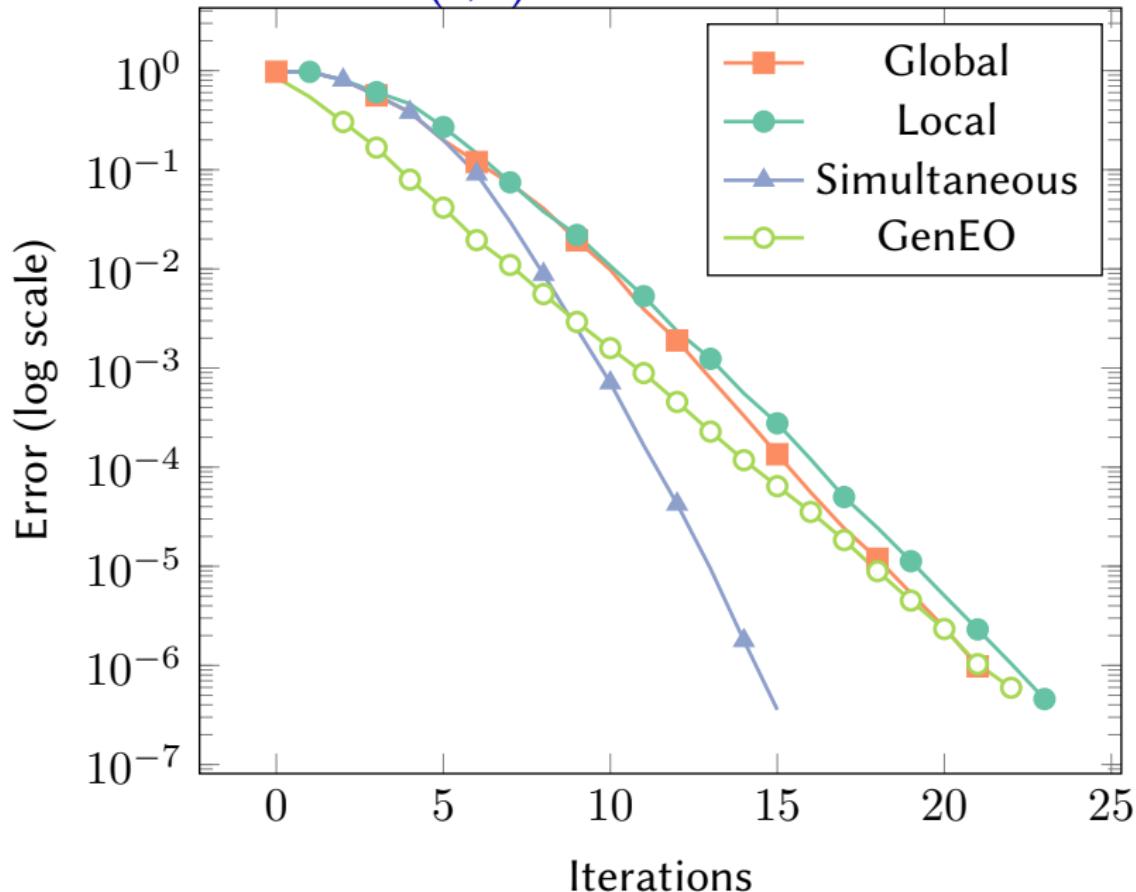
Numerical Illustration (1/4): Homogenous subdomains



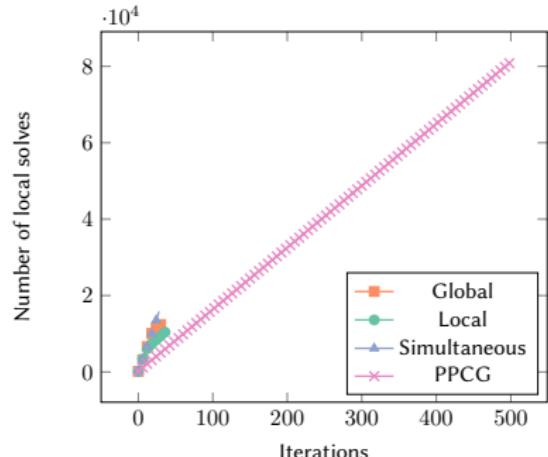
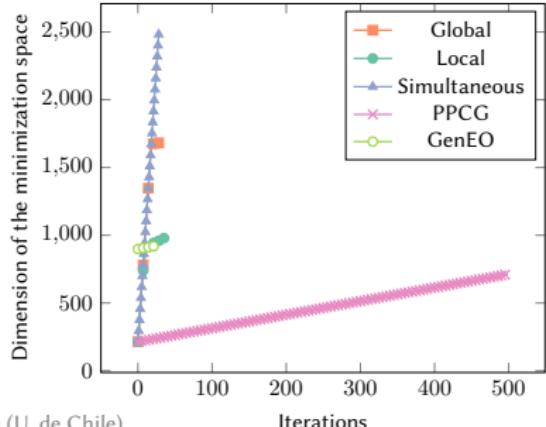
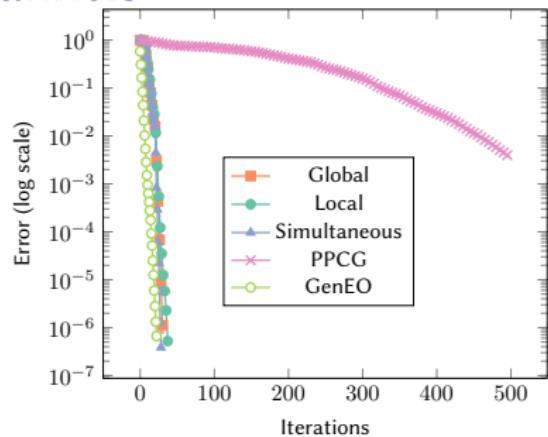
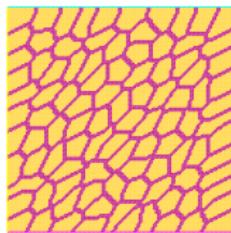
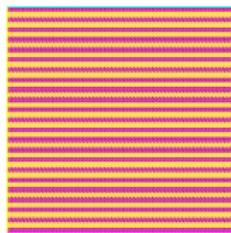
Numerical Illustration (2/4): Metis subdomains



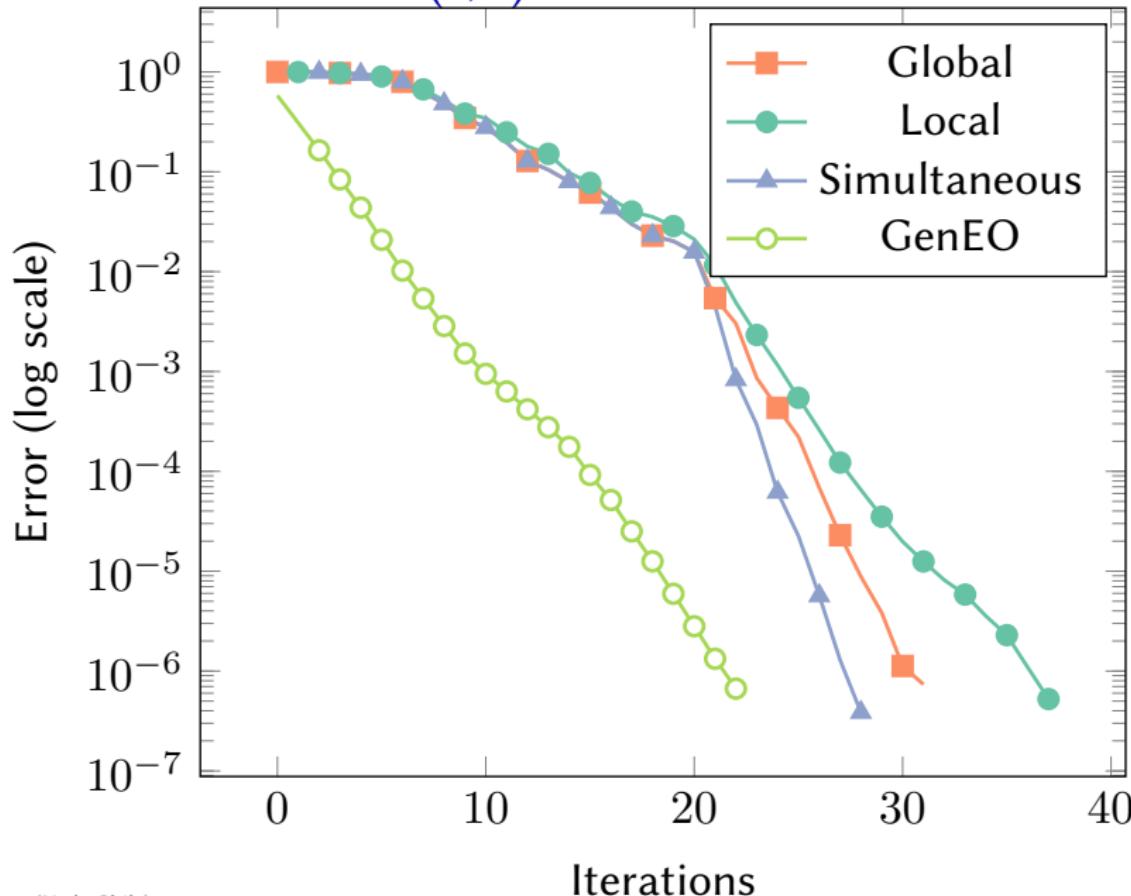
Numerical Illustration (2/4): Zoom on new methods



Numerical Illustration (3/4): Channels



Numerical Illustration (3/4): Zoom on new methods



Numerical Illustration (4/4)

Variable heterogeneity for $N = 81$ (k-scaling) :

E_2/E_1	Global τ -test it	Local τ -test solves	Simultaneous it	usual BDD it	GenEO it				
1	26	4624	25	4602	14	7212	36	5832	23
10	26	5036	28	5213	14	7212	44	7128	23
10^2	30	6096	25	5164	15	7786	76	12312	21
10^3	23	5374	25	5133	16	8360	126	20412	22
10^4	22	5212	25	5176	16	8360	139	22518	22
10^5	22	5212	24	5041	16	8360	141	22842	23

$dim < 554$ $dim < 423$ $dim < 1428$ $dim < 353$ $dim < 372$

Variable number of subdomains for $E_2/E_1 = 10^5$ (k scaling) :

N	Global τ -test it	Local τ -test solves	Simultaneous it	usual BDD it	GenEO it				
25	20	1784	22	1447	17	2530	69	3450	20
36	24	2392	23	2150	16	3476	87	6264	20
49	20	3364	24	3146	16	4844	110	10780	20
64	21	5264	24	4137	17	7006	152	19456	20

$dim < 693$ $dim < 379$ $dim < 1193$ $dim < 320$ $dim < 327$

Numerical Illustration (4/4)

Variable heterogeneity for $N = 81$ (k-scaling) :

E_2/E_1	Global τ -test		Local τ -test		Simultaneous		usual BDD		GenEO it
	it	solves	it	solves	it	solves	it	solves	
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Conclusion

Reliability, Efficiency and Simplicity through adaptive coarse spaces and adaptive multiple search directions.

Perspectives

- ▶ Test on industrial test cases and measure CPU times.
- ▶ Use the τ -test to recycle part of the minimization spaces.
- ▶ Simultaneous BDD: Theoretical Analysis at the PDE level.
- ▶ Adaptive Multi PCG for other DD methods: when λ_{\max} is known or neither λ_{\min} or λ_{\max} .



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