Adaptive Multipreconditioning and its Application to Domain Decomposition

github.com/gouarin/GenEO

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'Never believe *anything*, unless you can run it.' (Matt)

Download the code from: `https://github.com/gouarin/GenEO`
Or run it on Binder.

What's in the code ?

- A Domain Decomposition (DD) preconditioner
  - BNN by default
  - Additive Schwarz with option -PCBNN_switchtoASM
- GenEO coarse space
- Adaptive Multipreconditioned Conjugate Gradient Solver

At this stage all subdomains are non-overlapping

Introduction to DD

Domain Decomposition: Abstract Schwarz Framework

$\mathbf{A}\mathbf{x}_* = \mathbf{b}$ with $\mathbf{A}$ symmetric positive definite (spd)

1. Partition the domain:

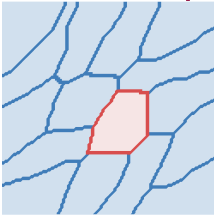
$$\Omega = \bigcup_{s=1}^{N} \Omega^s$$

2. Define interpolation operators:

$$\Omega^s \underset{\mathbf{R}^s}{\overset{\mathbf{R}^{s\top}}{\rightleftarrows}} \Omega,$$

3. Choose local solvers:

$$\tilde{\mathbf{A}}^s : \Omega^s \to \Omega^s.$$



Ω Ω^s

A. Toselli and O. Widlund.
Domain decomposition methods—algorithms and theory
Springer-Verlag, Berlin, 2005.

Preconditioner is $\mathbf{H} := \sum_{s=1}^{N} \mathbf{R}^{s\top} \tilde{\mathbf{A}}^{s\,-1} \mathbf{R}^s$.

Domain Decomposition: Abstract Schwarz Framework

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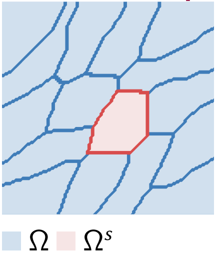


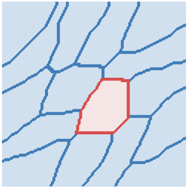
A. Toselli and O. Widlund. *Domain decomposition methods—algorithms and theory* Springer-Verlag, Berlin, 2005.

In PETSc:

```
ksp.pc.setType("asm")
localksp=
ksp.pc.getASMSubKSP()[0]
localksp.setType("Ã^s")
```

Domain Decomposition ($\mathbf{A}\mathbf{x}_* = \mathbf{b}$ with $\mathbf{A}$ spd)

Possible choices for the local solver $\tilde{\mathbf{A}}^s$



Notation from previous slide:

- $\mathbf{R}_s: \Omega \to \Omega^s$ (Restriction).
- $\mathbf{R}_s^T: \Omega_s \to \Omega$ (Extension).
- $\mathbf{H} = \sum_{s=1}^N \mathbf{R}^{s\top} \tilde{\mathbf{A}}^{s\,-1} \mathbf{R}^s$ (Preconditioner).

- Additive Schwarz Preconditioner

$$\tilde{\mathbf{A}}^s = \mathbf{R}^s \mathbf{A} \mathbf{R}^{s\top} \text{ (exact local solver).}$$

- Balancing Neumann Neumann (BNN)

$$\tilde{\mathbf{A}}^s = (\mathbf{D}^s)^{-1} \mathbf{A}_{|\Omega^s} (\mathbf{D}^s)^{-1};$$

$$(\mathbf{A}_{|\Omega^s})_{ij} := \int_{\Omega^s} a(\phi_i, \phi_j) \text{ if } \mathbf{A}_{ij} := \int_\Omega a(\phi_i, \phi_j),$$

$$\sum_{s=1}^N \mathbf{R}^{s\top} \mathbf{D}^s \mathbf{R}^s = \mathbf{I} \text{ (partition of unity).}$$

- Inexact local solver

$$\tilde{\mathbf{A}}^s = \text{ilu}(\mathbf{R}^s \mathbf{A} \mathbf{R}^{s\top}) \text{ (default choice in PETSc).}$$

Two-level Domain Decomposition ($(\mathbf{H})\mathbf{A}\mathbf{x}_* = (\mathbf{H})\mathbf{b}$ with $\mathbf{A}$ spd)

also known as deflation [Nicolaides, 1987], projection preconditioning [Dostál, 1988] and Balancing [Mandel]:

(i) Choose $\mathbf{U} := (\mathbf{u}_1 | \dots | \mathbf{u}_{n_0})$ (span($\mathbf{U}$) is the **coarse space**)

(ii) Let $\mathbf{\Pi} := \mathbf{I} - \mathbf{U}(\mathbf{U}^\top \mathbf{A}\mathbf{U})^{-1}\mathbf{U}^\top \mathbf{A}$
then $(\mathbf{I} - \mathbf{\Pi})$: $\mathbf{A}$-orthogonal projection onto span($\mathbf{U}$)

$$\mathbf{A}\mathbf{x}_* = \mathbf{b} \Leftrightarrow \mathbf{\Pi}^\top \mathbf{A}\mathbf{x}_* = \mathbf{\Pi}^\top \mathbf{b} \text{ and } (\mathbf{I} - \mathbf{\Pi}^\top)\mathbf{A}\mathbf{x}_* = (\mathbf{I} - \mathbf{\Pi}^\top)\mathbf{b}$$

(iii) Solve $\underbrace{(\mathbf{H})\mathbf{\Pi}^\top \mathbf{A}\mathbf{x}_* = (\mathbf{H})\mathbf{\Pi}^\top b}_{\text{DD solver (PCG)}}$ and $\underbrace{(\mathbf{I} - \mathbf{\Pi}^\top)\mathbf{A}\mathbf{x}_* = (\mathbf{I} - \mathbf{\Pi})^\top \mathbf{b}}_{\text{direct solver : setup step}}$.

Related PETSc concept:
`PETScMatnullspace` and `PETScMatnearnullspace`.

Two main reasons to use a coarse space

$\big((\mathbf{H})\mathbf{A}(\mathbf{\Pi})\mathbf{x}_* = (\mathbf{H})(\mathbf{\Pi}^\top)\mathbf{b}$ with $\mathbf{A}$, $\mathbf{H}$ spd and $\mathbf{\Pi}$ an $\mathbf{A}$-orthogonal projection$\big)$

- Make operations well defined,*e.g.*, BNN:

$$\mathbf{H} = \sum_{s=1}^{N} \mathbf{R}^{s\top} \underbrace{\mathbf{D}^s \mathbf{A}_{|\Omega^s}{}^{\dagger} \mathbf{D}^s}_{\tilde{\mathbf{A}}^{s\,\dagger}} \mathbf{R}^s \text{ where } (\mathbf{A}_{|\Omega^s})_{ij} := \int_{\Omega^s} a(\phi_i, \phi_j).$$

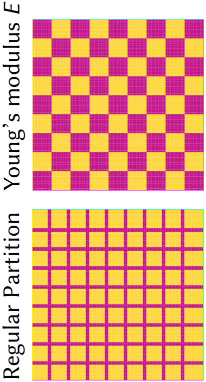
  Natural coarse space:

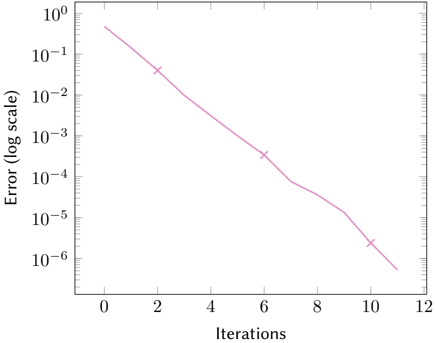
$$\mathbf{U} = \left(\mathbf{R}^{1\top}\mathbf{Z}^1 \quad | \quad \dots \quad | \quad \mathbf{R}^{N\top}\mathbf{Z}^N \right) \text{ where } \mathbf{Z}^s \text{ is a basis for } \operatorname{Ker}(\tilde{\mathbf{A}}^s).$$

- Improve convergence of PCG.

Elasticity with **homogeneous** subdomains **Fast** convergence with the natural coarse space.

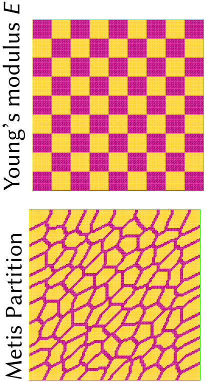
$N = 81$ subdomains, $\nu = 0.4$, $E_1 = 10^7$ and $E_2 = 10^{12}$.

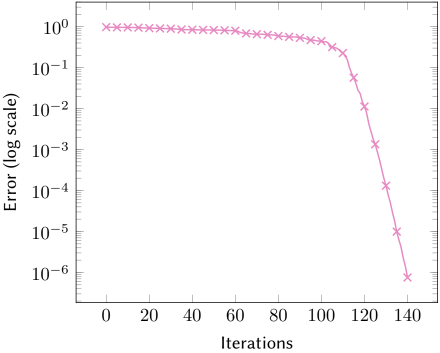




Elasticity with **heterogeneous** subdomains: **Slow** convergence with the natural coarse space.

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





GenEO coarse space

Ideal Coarse Space

PPCG convergence bound:

$$\frac{\|\mathbf{x}_* - \mathbf{x}_m\|_\mathbf{A}}{\|\mathbf{x}_* - \mathbf{x}_0\|_\mathbf{A}} \leqslant 2\left[\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right]^m, \quad \kappa = \frac{\lambda_{\max}(\mathbf{HA\Pi})}{\lambda_{\min}(\mathbf{HA\Pi})} \leftarrow \text{excluding zero}$$

An unrealistic way to guarantee fast convergence:

(i) Compute $(\lambda_k, \mathbf{x}_k)$ such that $\mathbf{HAx}_k = \lambda_k \mathbf{x}_k$.

(ii) Define $\mathbf{U} := \left\{\mathbf{x}_k; \lambda_k \geqslant \lambda_{\max}^{\text{target}} \text{ or } \lambda_k \leqslant \lambda_{\min}^{\text{target}}\right\}$
$(\mathbf{I}-\mathbf{\Pi})$: $\mathbf{A}$-orthogonal projection onto span$(\mathbf{U})$.

(iii) Solve $\underbrace{\mathbf{HA\Pi x}_* = \mathbf{H\Pi}^\top b}_{\text{fast converging PCG}}$ and $\underbrace{(\mathbf{I}-\mathbf{\Pi}^\top)\mathbf{Ax}_* = (\mathbf{I}-\mathbf{\Pi})^\top \mathbf{b}}_{\text{coarse problem (direct solver)}}$.

$$\frac{\|\mathbf{x}_* - \mathbf{x}_m\|_\mathbf{A}}{\|\mathbf{x}_* - \mathbf{x}_0\|_\mathbf{A}} \leqslant 2\left[\frac{\sqrt{\kappa^{\text{target}}}-1}{\sqrt{\kappa^{\text{target}}}+1}\right]^m, \quad \kappa^{\text{target}} = \frac{\lambda_{\max}^{\text{target}}}{\lambda_{\min}^{\text{target}}}$$

GenEO Coarse Space :Generalized Eigenvalues in the Overlaps

- $\mathbf{H} = \sum_{s=1}^{N} \mathbf{R}^{s\top} \tilde{\mathbf{A}}^{s\,-1} \mathbf{R}^{s}$ is the preconditioner.
- Let $\mathcal{N}$ bet the maximal multiplicity of a dof.

Upper bound for the spectrum of HAΠ

If $\langle \mathbf{x}^s, \mathbf{R}^s \mathbf{A} \mathbf{R}^{s\top} \mathbf{x}^s \rangle \leqslant \omega \langle \mathbf{x}^s, \tilde{\mathbf{A}}^s \mathbf{x}^s \rangle; \forall\, \mathbf{x}^s$ then $\lambda_{\max} \leqslant \mathcal{N}\omega$.

A coarse space that guarantees $\lambda_{\max}^{\text{target}}$

1. Solve $\tilde{\mathbf{A}}^s \mathbf{p}_k^s = \lambda_k^s \mathbf{R}^s \mathbf{A} \mathbf{R}^{s\top} \mathbf{p}_k^s$
2. Let $\mathbf{U} = \left\{ \mathbf{R}^{s\top} \mathbf{p}_k^s ; \lambda_k^s \leqslant \mathcal{N} / \lambda_{\max}^{\text{target}} \right\}$.

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Upper bound for the spectrum of $\mathbf{HA\Pi}$

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1. Solve $\tilde{\mathbf{A}}^s \mathbf{p}_k^s = \lambda_k^s \mathbf{R}^s\mathbf{A}\mathbf{R}^{s\top}\mathbf{p}_k^s$
2. Let $\mathbf{U} = \left\{ \mathbf{R}^{s\top}\mathbf{p}_k^s ; \lambda_k^s \leqslant \mathcal{N}/\lambda_{\max}^{\text{target}} \right\}$.

Remark for Additive Schwarz

- Additive Schwarz is $\tilde{\mathbf{A}}^s = \mathbf{R}^s\mathbf{A}\mathbf{R}^{s\top}$ so $\lambda_{\max} \leqslant \mathcal{N}$ for free.

GenEO Coarse Space :Generalized Eigenvalues in the Overlaps

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Lower bound for the spectrum of $\mathbf{HA\Pi}$ (excluding 0)

$$\text{If } \langle \mathbf{x}^s, \tilde{\mathbf{A}}^s\mathbf{x}^s \rangle \leqslant C_0^2 \langle \mathbf{x}^s, (\mathbf{D}^s)^{-1}\mathbf{A}_{|\Omega^s}(\mathbf{D}^s)^{-1}\mathbf{x}^s \rangle\,;\forall\, \mathbf{x}^s \text{ then } \lambda_{\min} \geqslant C_0^{-2}.$$

A coarse space that guarantees $\lambda_{\max}^{\text{target}}$ and $\lambda_{\min}^{\text{target}}$

1. Solve $\tilde{\mathbf{A}}^s\mathbf{p}_k^s = \lambda_k^s\mathbf{R}^s\mathbf{A}\mathbf{R}^{s\top}\mathbf{p}_k^s$, and $(\mathbf{D}^s)^{-1}\mathbf{A}_{|\Omega^s}(\mathbf{D}^s)^{-1}\mathbf{q}_k^s = \mu_k^s\tilde{\mathbf{A}}^s\mathbf{q}_k^s$.
2. Let $\mathbf{U} = \left\{\mathbf{R}^{s\top}\mathbf{p}_k^s; \lambda_k^s \leqslant \mathcal{N}/\lambda_{\max}^{\text{target}}\right\} \bigcup \left\{\mathbf{R}^{s\top}\mathbf{q}_k^s; \mu_k^s \leqslant \lambda_{\min}^{\text{target}}\right\}$.

Remark for Additive Schwarz

- Additive Schwarz is $\tilde{\mathbf{A}}^s = \mathbf{R}^s\mathbf{A}\mathbf{R}^{s\top}$ so $\lambda_{\max} \leqslant \mathcal{N}$ for free.

GenEO Coarse Space :Generalized Eigenvalues in the Overlaps

- $\mathbf{H} = \sum_{s=1}^{N} \mathbf{R}^{s\top} \tilde{\mathbf{A}}^{s\,-1} \mathbf{R}^s$ is the preconditioner.
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Upper bound for the spectrum of $\mathbf{HA\Pi}$

If $\langle \mathbf{x}^s, \mathbf{R}^s \mathbf{A} \mathbf{R}^{s\top} \mathbf{x}^s \rangle \leqslant \omega \langle \mathbf{x}^s, \tilde{\mathbf{A}}^s \mathbf{x}^s \rangle$; $\forall\, \mathbf{x}^s$ then $\lambda_{\text{max}} \leqslant \mathcal{N}\omega$.

Lower bound for the spectrum of $\mathbf{HA\Pi}$ (excluding 0)

If $\langle \mathbf{x}^s, \tilde{\mathbf{A}}^s \mathbf{x}^s \rangle \leqslant C_0^2 \langle \mathbf{x}^s, (\mathbf{D}^s)^{-1} \mathbf{A}_{|\Omega^s} (\mathbf{D}^s)^{-1} \mathbf{x}^s \rangle$; $\forall\, \mathbf{x}^s$ then $\lambda_{\text{min}} \geqslant C_0^{-2}$.

A coarse space that guarantees $\lambda_{\text{max}}^{\text{target}}$ and $\lambda_{\text{min}}^{\text{target}}$

1. Solve $\tilde{\mathbf{A}}^s \mathbf{p}_k^s = \lambda_k^s \mathbf{R}^s \mathbf{A} \mathbf{R}^{s\top} \mathbf{p}_k^s$, and $(\mathbf{D}^s)^{-1} \mathbf{A}_{|\Omega^s} (\mathbf{D}^s)^{-1} \mathbf{q}_k^s = \mu_k^s \tilde{\mathbf{A}}^s \mathbf{q}_k^s$.
2. Let $\mathbf{U} = \left\{ \mathbf{R}^{s\top} \mathbf{p}_k^s ; \lambda_k^s \leqslant \mathcal{N} / \lambda_{\text{max}}^{\text{target}} \right\} \bigcup \left\{ \mathbf{R}^{s\top} \mathbf{q}_k^s ; \mu_k^s \leqslant \lambda_{\text{min}}^{\text{target}} \right\}$.

Remark for Additive Schwarz and BNN

- Additive Schwarz is $\tilde{\mathbf{A}}^s = \mathbf{R}^s \mathbf{A} \mathbf{R}^{s\top}$ so $\lambda_{\text{max}} \leqslant \mathcal{N}$ for free.
- BNN is $\tilde{\mathbf{A}}^s = (\mathbf{D}^s)^{-1} \mathbf{A}_{|\Omega^s} (\mathbf{D}^s)^{-1}$ so $\lambda_{\text{min}} \geqslant 1$ for free.

References

N. S., V. Dolean, P. Hauret, F. Nataf, C. Pechstein, and R. Scheichl.
Abstract robust coarse spaces for systems of PDEs via generalized eigenproblems in the overlaps.
Numer. Math., 2014.

N. S. and D. J. Rixen.
Automatic spectral coarse spaces for robust FETI and BDD algorithms.
Int. J. Numer. Meth. Engng., 2013.

Related work

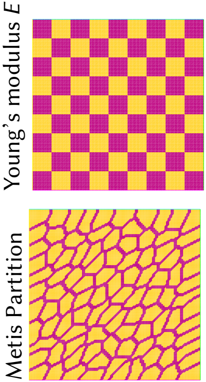
- BDDC with adaptive selection of constraints (S. Zampini),
- GenEO is part of HPDDM (P. Jolivet and F. Nataf).

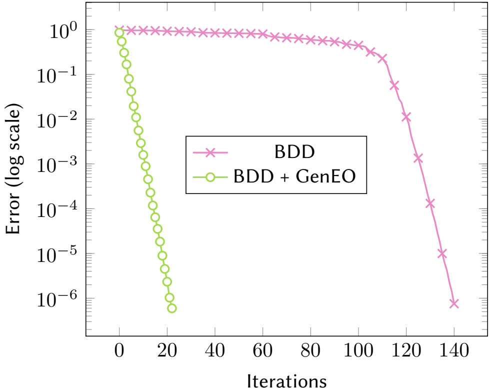
Important remark: PETSc Matis format is needed

since all these methods need to assemble $\mathbf{A}_{|\Omega^s}$ " = " $\int_{\Omega^s} a(\phi_i, \phi_j)$.

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.

Run codes

`demo_GenEO_2d.py` and `demo_elasticity_2d.py`.

Multipreconditioned BNN

What is multipreconditioning ? $(\mathbf{H})\mathbf{A}\mathbf{x}_* = (\mathbf{H})\mathbf{b}$

PCG : Minimize $\|\mathbf{x}_* - \mathbf{x}_{i+1}\|_\mathbf{A}$ over $\mathbf{x}_i + \widetilde{\operatorname{span}}(\mathbf{H}\mathbf{r}_i)$.

An enlarged minimization space implies better convergence:

- deflation (*e.g.* with a spectral coarse space),
- block methods,

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- deflation (*e.g.* with a spectral coarse space),
- block methods,
- or **multipreconditioning !**

MPCG: Minimize $\|\mathbf{x}_* - \mathbf{x}_{i+1}\|_\mathbf{A}$ over $\mathbf{x}_i + \widetilde{\text{span}}(\mathbf{H}^1\mathbf{r}_i, \dots, \mathbf{H}^N\mathbf{r}_i)$
where $\mathbf{H}^1, \dots, \mathbf{H}^N$ are N preconditioners.

R. Bridson and C. Greif.
A multipreconditioned conjugate gradient algorithm. *SIAM J. Matrix Anal. Appl.*, 2006.

Very natural for DD: one preconditioner per subdomain

$$\mathbf{H} = \sum_{s=1}^{N} \underbrace{\mathbf{R}^{s\top}(\tilde{\mathbf{A}}^s)^\dagger\mathbf{R}^s}_{:=\mathbf{H}^s}.$$

What is multipreconditioning ? $(\mathbf{H})\mathbf{A}\mathbf{x}_* = (\mathbf{H})\mathbf{b}$

PCG : Minimize $\|\mathbf{x}_* - \mathbf{x}_{i+1}\|_{\mathbf{A}}$ over $\mathbf{x}_i + \widetilde{\text{span}}(\mathbf{H}\mathbf{r}_i)$.

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D. J. Rixen.
Substructuring and Dual Methods in Structural Analysis. PhD thesis, 1997.

R. Bridson and C. Greif.
A multipreconditioned conjugate gradient algorithm. *SIAM J. Matrix Anal. Appl.*, 2006.

C. Greif, T. Rees, and D. Szyld.
MPGMRES: a generalized minimum residual method with multiple preconditioners. *Technical report*, 2011 (now published in SeMA Journal).

C. Greif, T. Rees, and D. Szyld.
Additive Schwarz with variable weights. *DD21 proceedings*, 2014.

P. Gosselet, D. J. Rixen, F.-X. Roux, and N. S.
Simultaneous FETI and block FETI… *International Journal for Numerical Methods in Engineering*, 2015.

Multipreconditioned CG for $\mathbf{A}\mathbf{x}_* = \mathbf{b}$ prec. by $\{\mathbf{H}^s\}_{s=1,\dots,N}$

- $\mathbf{A}, \mathbf{H} \in \mathbb{R}^{n \times n}$ spd,
- $\mathbf{H} = \sum_{s=1}^{N} \mathbf{H}^s$, where $\mathbf{H}^s$ spsd.

MPCG

$\mathbf{x}_0$ given ; ⇽ *Initial Guess*

$\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$;

$\mathbf{Z}_0 = \left[\mathbf{H}^1\mathbf{r}_0 \mid \dots \mid \mathbf{H}^N\mathbf{r}_0\right]$;

$\mathbf{P}_0 = \mathbf{Z}_0$; ⇽ *Initial search directions*

for $i = 0, 1, \dots,$ *convergence* **do**

  $\mathbf{Q}_i = \mathbf{A}\mathbf{P}_i$;

  $\boldsymbol{\alpha}_i = (\mathbf{Q}_i^\top \mathbf{P}_i)^\dagger (\mathbf{P}_i^\top \mathbf{r}_i)$;

  $\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{P}_i\boldsymbol{\alpha}_i$; ⇽ *Update approximate solution*

  $\mathbf{r}_{i+1} = \mathbf{r}_i - \mathbf{Q}_i\boldsymbol{\alpha}_i$; ⇽ *Update residual*

  $\mathbf{Z}_{i+1} = \left[\mathbf{H}^1\mathbf{r}_{i+1} \mid \dots \mid \mathbf{H}^N\mathbf{r}_{i+1}\right]$; ⇽ *Multiprecondition*

  $\boldsymbol{\beta}_{i,j} = (\mathbf{Q}_j^\top \mathbf{P}_j)^\dagger (\mathbf{Q}_j^\top \mathbf{Z}_{i+1}), \quad j = 0, \dots, i$;

  $\mathbf{P}_{i+1} = \mathbf{Z}_{i+1} - \sum_{j=0}^{i} \mathbf{P}_j\boldsymbol{\beta}_{i,j}$; ⇽ *Orthogonalize*

end

Return $\mathbf{x}_{i+1}$;

PCG

$\mathbf{x}_0$ given ;

$\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$;

$\mathbf{z}_0 = \mathbf{H}\mathbf{r}_0$;

$\mathbf{p}_0 = \mathbf{z}_0$;

for $i = 0, 1, \dots,$ *conv.* **do**

  $\mathbf{q}_i = \mathbf{A}\mathbf{p}_i$;

  $\alpha_i = (\mathbf{q}_i^\top \mathbf{p}_i)^{-1}(\mathbf{p}_i^\top \mathbf{r}_i)$;

  $\mathbf{x}_{i+1} = \mathbf{x}_i + \alpha_i\mathbf{p}_i$;

  $\mathbf{r}_{i+1} = \mathbf{r}_i - \alpha_i\mathbf{q}_i$;

  $\mathbf{z}_{i+1} = \mathbf{H}\mathbf{r}_{i+1}$;

  $\beta_i = (\mathbf{q}_i^\top \mathbf{p}_i)^{-1}(\mathbf{q}_i^\top \mathbf{z}_{i+1})$;

  $\mathbf{p}_{i+1} = \mathbf{z}_{i+1} - \beta_i\mathbf{p}_i$;

end

Return $\mathbf{x}_{i+1}$;

Multipreconditioned CG for $\mathbf{Ax}_* = \mathbf{b}$ prec. by $\{\mathbf{H}^s\}_{s=1,\dots,N}$

- $\mathbf{A}, \mathbf{H} \in \mathbb{R}^{n\times n}$ spd,
- $\mathbf{H} = \sum_{s=1}^{N} \mathbf{H}^s$, where $\mathbf{H}^s$ spsd.

MPCG

$\mathbf{x}_0$ given ; ← *Initial Guess*

$\mathbf{r}_0 = \mathbf{b} - \mathbf{Ax}_0$;

$\mathbf{Z}_0 = [\mathbf{H}^1\mathbf{r}_0 \mid \dots \mid \mathbf{H}^N\mathbf{r}_{i+1}]$; ← *Multiprecondition*

$\mathbf{P}_0 = \mathbf{Z}_0$; ← *Initial search directions*

for $i = 0, 1, \dots,$ *convergence* **do**

- $\mathbf{Q}_i = \mathbf{AP}_i$;
- $\boldsymbol{\alpha}_i = (\mathbf{Q}_i^\top \mathbf{P}_i)^\dagger (\mathbf{P}_i{}^\top \mathbf{r}_i)$;
- $\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{P}_i\boldsymbol{\alpha}_i$; ← *Update approximate solution*
- $\mathbf{r}_{i+1} = \mathbf{r}_i - \mathbf{Q}_i\boldsymbol{\alpha}_i$; ← *Update residual*
- $\mathbf{Z}_{i+1} = [\mathbf{H}^1\mathbf{r}_{i+1} \mid \dots \mid \mathbf{H}^N\mathbf{r}_{i+1}]$; ← *Multiprecondition*
- $\boldsymbol{\beta}_{i,j} = (\mathbf{Q}_j^\top \mathbf{P}_j)^\dagger(\mathbf{Q}_j^\top \mathbf{Z}_{i+1}), \quad j = 0, \dots, i$;
- $\mathbf{P}_{i+1} = \mathbf{Z}_{i+1} - \sum_{j=0}^{i} \mathbf{P}_j\boldsymbol{\beta}_{i,j}$; ← *Orthogonalize*

end

Return $\mathbf{x}_{i+1}$;

Remark

$$\mathbf{x}_i, \mathbf{r}_i \in \mathbb{R}^n.$$

$$\mathbf{Z}_i,\ \mathbf{P}_i, \in \mathbb{R}^{n\times N}$$

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

Properties

1. Global minimization over

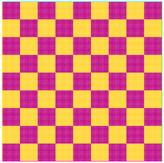
$$\mathbf{x}_0 + \bigoplus_{j=0}^{i-1} \text{range}(\mathbf{P}_j)$$

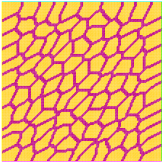
of dimension: $i \times N$.

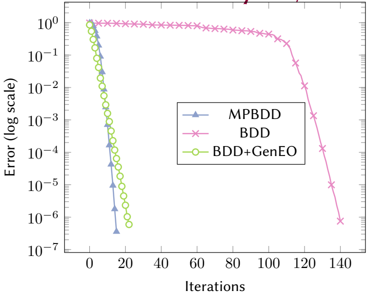
2. $\mathbf{P}_i^\top \mathbf{AP}_j = 0 \ (i \neq j)$, but **no** short recurrence.

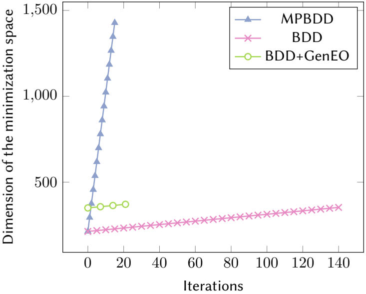
Numerical Illustration (Heterogeneous Elasticity $E_2/E_1 = 10^5$)

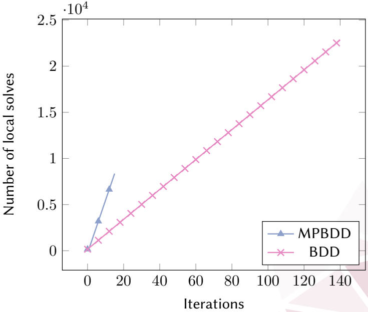
All algorithms deflate the natural coarse space.





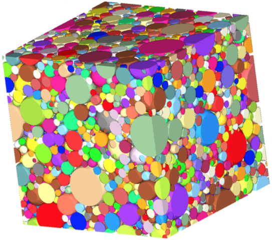


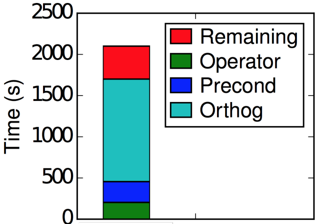


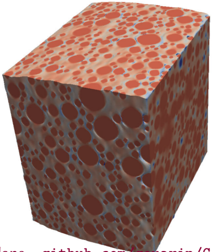


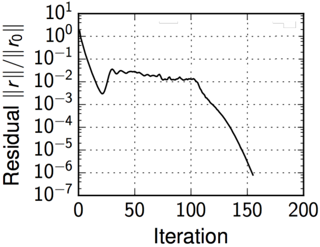
Solid propellant (linear elasticity with FETI) – in collaboration with C. Bovet (ONERA)

6721 stiff inclusions, $E_2/E_1 \leqslant 10^6$, 57 Mdofs, 360 subdomains on 1440 cores









Adaptive Multipreconditioned BNN

Good convergence of MPBDD but a possible limitation

- ✓ Local contributions $\mathbf{H}^s \mathbf{r}_i$ form a good minimization space.
- ✗ Not adaptive: invert $\mathbf{P}_i^\top \mathbf{A} \mathbf{P}_i \in \mathbb{R}^{N \times N}$ at **each** iteration in $\boldsymbol{\alpha}_i = (\mathbf{P}_i^\top \mathbf{A} \mathbf{P}_i)^\dagger (\mathbf{P}_i{}^\top \mathbf{r}_i)$.

💡 Introduce adaptativity into multipreconditioned CG.

- a few local vectors should suffice to accelerate convergence (previous work on GenEO).

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Introduce adaptativity into multipreconditioned CG.

- a few local vectors should suffice to accelerate convergence (previous work on GenEO).

An important assumption for the adaptive process :

$$\lambda_{\min}(\mathbf{H} \mathbf{A} \mathbf{\Pi}) \geqslant 1,$$

where eigenvalue 0 is excluded.

Assumption satisfied by BNN.

Adaptive Multipreconditioned CG for $\mathbf{A}\mathbf{x}_* = \mathbf{b}$ preconditioned by $\sum_{s=1}^{N} \mathbf{H}^s$.

($\tau \in \mathbb{R}^+$ is chosen by the user – *e.g.*, $\tau = 0.1$)

$\mathbf{x}_0$ chosen;
$\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$; $\mathbf{Z}_0 = \mathbf{H}\mathbf{r}_0$; $\mathbf{P}_0 = \mathbf{Z}_0$;
for $i = 0, 1, \dots,$ *convergence* **do**
  $\mathbf{Q}_i = \mathbf{A}\mathbf{P}_i$;
  $\boldsymbol{\alpha}_i = (\mathbf{Q}_i^\top \mathbf{P}_i)^\dagger (\mathbf{P}_i^\top \mathbf{r}_i)$;
  $\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{P}_i \boldsymbol{\alpha}_i$;
  $\mathbf{r}_{i+1} = \mathbf{r}_i - \mathbf{Q}_i \boldsymbol{\alpha}_i$;
  $t_i = \dfrac{(\mathbf{P}_i\boldsymbol{\alpha}_i)^\top \mathbf{A}(\mathbf{P}_i\boldsymbol{\alpha}_i)}{\mathbf{r}_{i+1}^\top \mathbf{H}\mathbf{r}_{i+1}}$;
  if $t_i < \tau$ **then** ← *τ-test*
    $\mathbf{Z}_{i+1} = \left[\mathbf{H}^1\mathbf{r}_{i+1} \mid \dots \mid \mathbf{H}^N\mathbf{r}_{i+1}\right]$; ← *Multiprec.*
  else
    $\mathbf{Z}_{i+1} = \mathbf{H}\mathbf{r}_{i+1}$; ← *Precondition*
  end
  $\boldsymbol{\beta}_{i,j} = (\mathbf{Q}_j^\top \mathbf{P}_j)^\dagger (\mathbf{Q}_j^\top \mathbf{Z}_{i+1})$, $\quad j = 0, \dots, i$;
  $\mathbf{P}_{i+1} = \mathbf{Z}_{i+1} - \sum_{j=0}^{i} \mathbf{P}_j \boldsymbol{\beta}_{i,j}$;
end
Return $\mathbf{x}_{i+1}$;

Remark

$\mathbf{x}_i, \mathbf{r}_i \in \mathbb{R}^n$.

$\mathbf{Z}_i, \mathbf{P}_i \in \mathbb{R}^{n \times N}$ or $\mathbb{R}^n$,

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

Properties

1. Global minimization over
$$\mathbf{x}_0 + \bigoplus_{j=0}^{i-1} \operatorname{range}(\mathbf{P}_j)$$
of dim $i \leqslant dim \leqslant i \times N$.
2. $\mathbf{P}_i^\top \mathbf{A}\mathbf{P}_j = 0$ $(i \neq j)$, but **no** short recurrence.

Theoretical Result: Choice of the τ-test ?

Theorem

If the τ–test returns $t_i \geqslant \tau$ then

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

$\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{P}_i \boldsymbol{\alpha}_i$;

$t_i = \dfrac{(\mathbf{P}_i\boldsymbol{\alpha}_i)^\top \mathbf{A}(\mathbf{P}_i\boldsymbol{\alpha}_i)}{\mathbf{r}_{i+1}^\top \mathbf{H}\mathbf{r}_{i+1}}$;

if $t_i < \tau$ **then**

  $\mathbf{Z}_{i+1} = \left[\mathbf{H}^1\mathbf{r}_{i+1} \mid \dots \mid \mathbf{H}^N\mathbf{r}_{i+1}\right]$

else

  $\mathbf{Z}_{i+1} = \mathbf{H}\mathbf{r}_{i+1}$;

end

Proof (inspired by [Axelsson, Kaporin, '01]):

$$\mathbf{x}_* = \mathbf{x}_0 + \sum_{i=0}^{n} \mathbf{P}_i\boldsymbol{\alpha}_i = \mathbf{x}_i + \sum_{j=i}^{n} \mathbf{P}_j\boldsymbol{\alpha}_j$$

$$\Rightarrow \|\mathbf{x}_* - \mathbf{x}_i\|_{\mathbf{A}}^2 = \sum_{j=i}^{n} \|\mathbf{P}_j\boldsymbol{\alpha}_j\|_{\mathbf{A}}^2 \Rightarrow \|\mathbf{x}_* - \mathbf{x}_{i-1}\|_{\mathbf{A}}^2 = \|\mathbf{x}_* - \mathbf{x}_i\|_{\mathbf{A}}^2 + \|\mathbf{P}_{i-1}\boldsymbol{\alpha}_{i-1}\|_{\mathbf{A}}^2.$$

$$\Rightarrow \frac{\|\mathbf{x}_* - \mathbf{x}_{i-1}\|_{\mathbf{A}}^2}{\|\mathbf{x}_* - \mathbf{x}_i\|_{\mathbf{A}}^2} = 1 + \underbrace{\frac{\|\mathbf{r}_i\|_{\mathbf{H}}^2}{\|\mathbf{x}_* - \mathbf{x}_i\|_{\mathbf{A}}^2}}_{= \|\mathbf{x}_* - \mathbf{x}_i\|_{\mathbf{AHA}}^2 / \|\mathbf{x}_* - \mathbf{x}_i\|_{\mathbf{A}}^2 \geqslant \lambda_{min} \geqslant 1} \frac{\|\mathbf{P}_{i-1}\boldsymbol{\alpha}_{i-1}\|_{\mathbf{A}}^2}{\|\mathbf{r}_i\|_{\mathbf{H}}^2} \geqslant 1 + \underbrace{\frac{\|\mathbf{P}_{i-1}\boldsymbol{\alpha}_{i-1}\|_{\mathbf{A}}^2}{\|\mathbf{r}_i\|_{\mathbf{H}}^2}}_{= t_{i-1}} \geqslant 1 + \tau.$$

Local Adaptive MPCG for $\sum_{s=1}^{N} \mathbf{A}^s \mathbf{x}_* = \mathbf{b}$ preconditioned by $\sum_{s=1}^{N} \mathbf{H}^s$.

($\tau \in \mathbb{R}^+$ is chosen by the user)

$\mathbf{x}_0$ chosen; $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$; $\mathbf{Z}_0 = \mathbf{H}\mathbf{r}_0$; $\mathbf{P}_0 = \mathbf{Z}_0$;
for $i = 0, 1, \dots,$ *convergence* **do**
  $\mathbf{Q}_i = \mathbf{A}\mathbf{P}_i$;
  $\boldsymbol{\alpha}_i = (\mathbf{Q}_i^\top \mathbf{P}_i)^\dagger (\mathbf{P}_i^\top \mathbf{r}_i)$;
  $\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{P}_i \boldsymbol{\alpha}_i$;
  $\mathbf{r}_{i+1} = \mathbf{r}_i - \mathbf{Q}_i \boldsymbol{\alpha}_i$;
  $\mathbf{Z}_{i+1} = \mathbf{H}\mathbf{r}_{i+1}$; ◁ *initialize* $\mathbf{Z}_{i+1}$
  for $s = 1, \dots, N$ **do**
    $t_i^s = \dfrac{\langle \mathbf{P}_i \boldsymbol{\alpha}_i, \mathbf{A}^s \mathbf{P}_i \boldsymbol{\alpha}_i \rangle}{\mathbf{r}_{i+1}^\top \mathbf{H}^s \mathbf{r}_{i+1}}$;
    if $t_i^s < \tau$ **then** ◁ *local* τ*-test*
      $\mathbf{Z}_{i+1} = \left[\mathbf{Z}_{i+1} \mid \mathbf{H}^s \mathbf{r}_{i+1} \right]$;
    end
  end
  $\boldsymbol{\beta}_{i,j} = (\mathbf{Q}_j^\top \mathbf{P}_j)^\dagger (\mathbf{Q}_j^\top \mathbf{Z}_{i+1}), \quad j = 0, \dots, i$;
  $\mathbf{P}_{i+1} = \mathbf{Z}_{i+1} - \sum_{j=0}^{i} \mathbf{P}_j \boldsymbol{\beta}_{i,j}$;
end
Return $\mathbf{x}_{i+1}$;

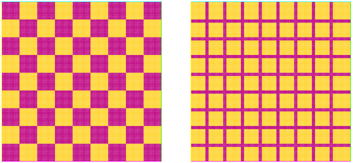
An additional assumption

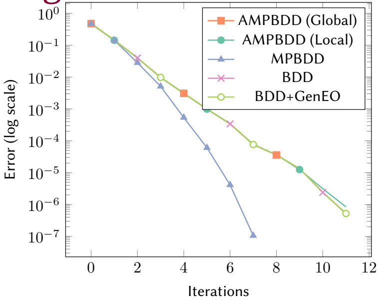
$$\mathbf{A} = \sum_{s=1}^{N} \mathbf{A}^s.$$

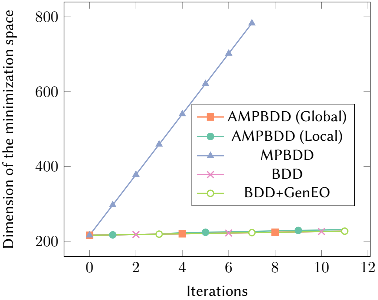
Benefits

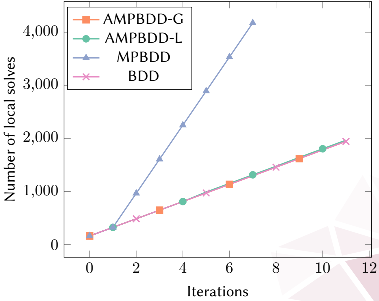
- Between 1 and N search directions per iteration.
- Reduces the cost of storage and of inverting $\mathbf{P}_i^\top \mathbf{A} \mathbf{P}_i$.

Numerical Illustration (0/4): Homogenous subdomains





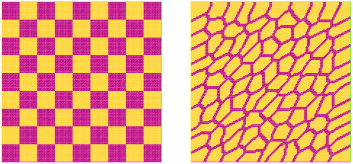


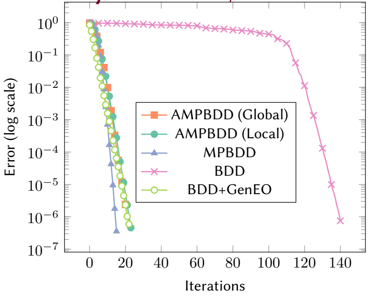


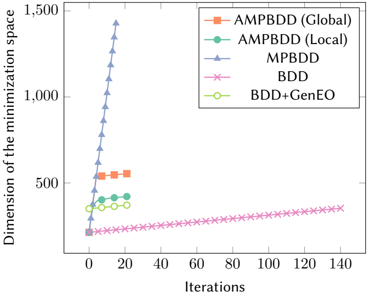
Numerical Illustration (1/4) – Elasticity with $E_2/E_1 = 10^5$

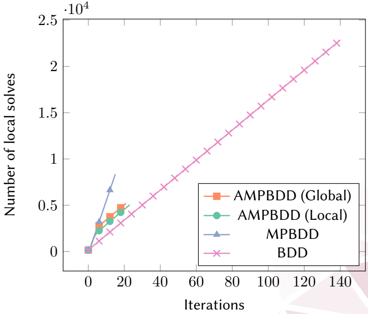
Also run:

`demo_elasticity_2d.py`.





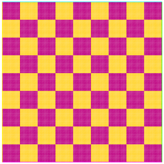


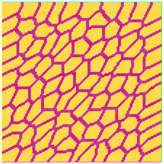


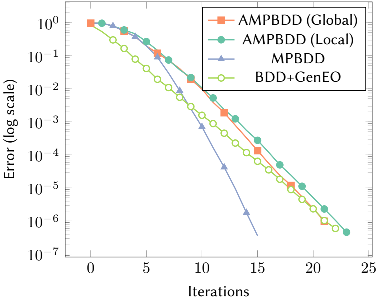
Numerical Illustration (2/4): Zoom on new methods

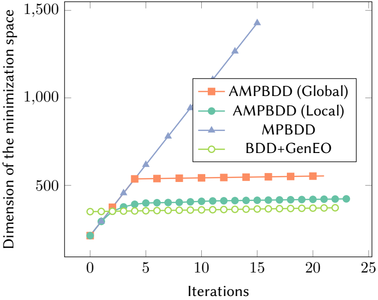
Also run:

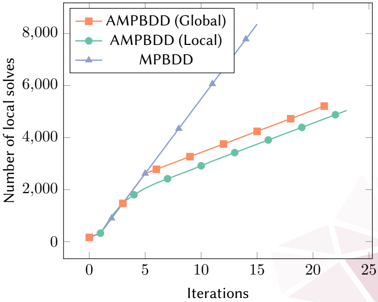
`demo_elasticity_2d.py`.



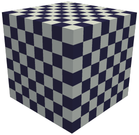


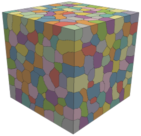




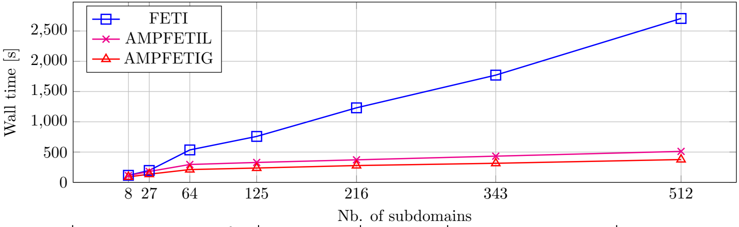


Numerical Illustration (3/4): Weak Scalability – FETI





- Software: Z-Set
- Cluster: Cobalt at CCRT/TGCC
- 1422 computational nodes with Intel Broadwell Processors: 2.4 GHz, 28 cores
- 128 Go SDRAM, infiniband Mellanox network
- 7 cores per subdomain and local factorizations are performed with mumps.

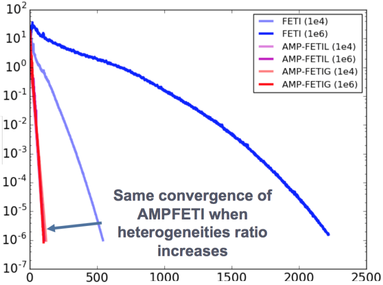


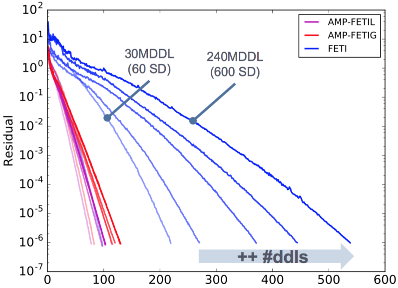
N	#DOFs ($\times 10^6$)	#cores	#iter.	# min. space	time (s)
8	1.6	56	69	132	89.58
64	12.5	448	112	742	210.80
216	42.0	1512	107	2257	277.30
512	99.2	3584	108	5729	376.30

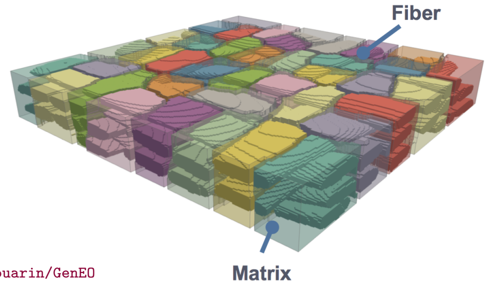
C. Bovet, P. Gosselet, A. Parret Freaud, and N. S.
Adaptive multi preconditioned FETI: scalability results and robustness assessment.
Computers and Structures, 2017.

Numerical Illustration (4/4): Composite Weave Pattern

FETI – in collaboration with A. Parret Freaud (Safran Tech)







Conclusion

GenEO coarse space and AMPDD $\rightarrow$ Robustness and Efficiency.

Perspectives

- Move from PETSc4py to PETSc
- Best adaptation process in non symmetric cases ? Best adaptation process in a fully algebraic context ?
- Restart ! Recycle ! within AMPDD Krylov subspace solvers.

N. S.
An Adaptive Multipreconditioned Conjugate Gradient
SISC, 2016.

N. S.
Algebraic Adaptive Multi Preconditioning applied to Restricted Additive Schwarz.
DD23 Proceedings, 2016.

C. Bovet, P. Gosselet, A. Parret Freaud, and N. S.
Adaptive multi preconditioned FETI: scalability results and robustness assessment.
Computers and Structures, 2017.

C. Bovet, P. Gosselet, and N. S.
Multipreconditioning for nonsymmetric problems: the case of orthomin and biCG.
Note au CRAS, 2017.