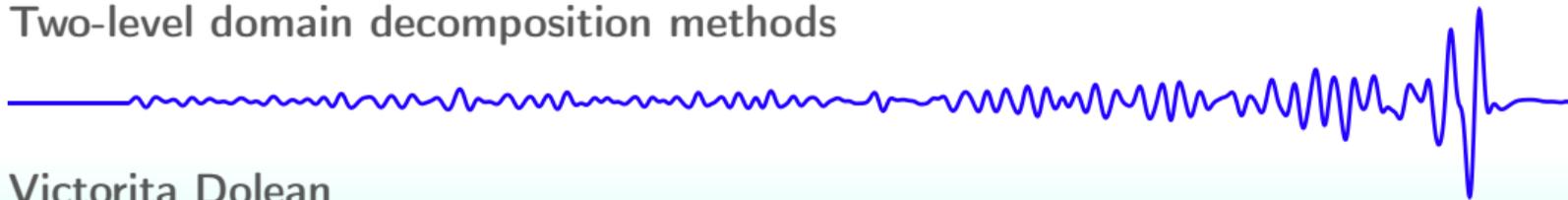


Two-level domain decomposition methods



Victorita Dolean

in collaboration with: F. Nataf, P. Jolivet, P.-H. Tournier

2-3 June 2021



Coarse Space correction

Coarse grids for heterogeneous problems

- Spectral coarse spaces

- Theoretical background

- Scalability tests

Conclusion

Numerics on a toy problem

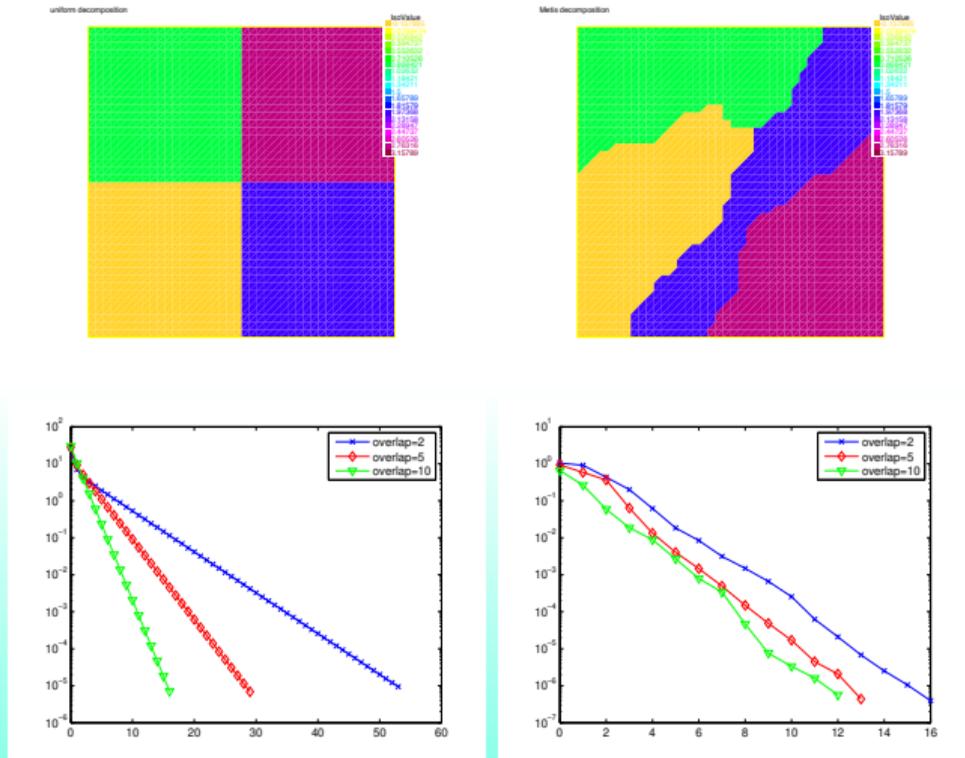


Figure 1: Schwarz convergence as a solver (left) and as a preconditioner (right) for different overlaps

Coarse Space correction

Coarse grids for heterogeneous problems

Conclusion

Strong scalability (Amdahl)

"How the solution time varies with the number of processors for a fixed *total* problem size"

Weak scalability (Gustafson)

"How the solution time varies with the number of processors for a fixed problem size *per processor*."

The one level method Schwarz is not scalable

Number of subdomains	8	16	32	64
AS	18	35	66	128

The iteration number increases linearly with the number of subdomains in one direction.

Condition number estimates: preconditioned system

Lemma

If there exist the constants C_1 and C_2 such that

$$C_1(M_{AS}\mathbf{x}, \mathbf{x}) \leq (A\mathbf{x}, \mathbf{x}) \leq C_2(M_{AS}\mathbf{x}, \mathbf{x}), \forall \mathbf{x} \in \mathbb{R}^n$$

then $\lambda_{max}(M_{AS}^{-1}A) \leq C_2$, $\lambda_{min}(M_{AS}^{-1}A) \geq C_1$ and thus $\kappa(M_{AS}^{-1}A) \leq C_2/C_1$.

If $\kappa(M_{AS}^{-1}A)$ independent of N (number of subdomains) \Rightarrow the solution time will be independent of the number of processors \Rightarrow weak scalability.

Why the algorithm is not scalable?

Lemma (Estimate of the largest eigenvalue)

Let $col(j) \in \{1, \dots, \mathcal{N}^c\}$ be the color of the domain j defined such that $col(k) = col(l)$ if $(AR_k^T \mathbf{x}_k, R_l^T \mathbf{x}_l) = 0$. Then $\lambda_{max}(M_{AS}^{-1}A) \leq \mathcal{N}^c$.

Proof. Useful result (Toselli, Widlund '05)

$$(M_{AS}\mathbf{x}, \mathbf{x}) = \min_{\{\mathbf{x}_j \in \mathbb{R}^{n_j}; \mathbf{x} = \sum_{j=1}^N R_j^T \mathbf{x}_j\}} \sum_{j=1}^N (A_j \mathbf{x}_j, \mathbf{x}_j), \quad A_j = R_j A R_j^T. \quad (1)$$

Let $(\mathbf{x}_j)_{1 \leq j \leq N}$ which achieves the minimum in (1). Then we have

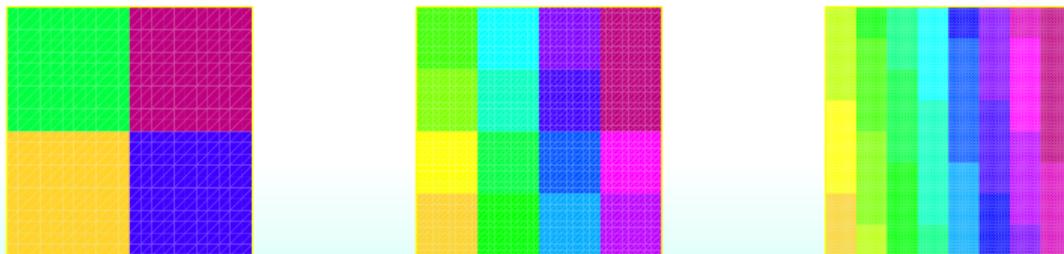
$$\begin{aligned} (M_{AS}\mathbf{x}, \mathbf{x}) &= \sum_{j=1}^N (AR_j^T \mathbf{x}_j, R_j^T \mathbf{x}_j) = \sum_{c=1}^{\mathcal{N}^c} \left(A \sum_{\{i; col(i)=c\}} R_i^T \mathbf{x}_i, \sum_{\{i; col(i)=c\}} R_i^T \mathbf{x}_i \right) \\ &\geq \frac{1}{\mathcal{N}^c} \left(A \sum_{j=1}^N R_j^T \mathbf{x}_j, \sum_{j=1}^N R_j^T \mathbf{x}_j \right) = \frac{1}{\mathcal{N}^c} (A\mathbf{x}, \mathbf{x}). \end{aligned} \quad (2)$$

Therefore $\lambda_{max}(M_{AS}^{-1}A) \leq \mathcal{N}^c$.

Why the algorithm is not scalable?

We have that $\lambda_{max}(M_{AS}^{-1}A) \leq \mathcal{N}_c \ll N$ (usual decomposition) BUT $\lambda_{min}(M_{AS}^{-1}A)$ depends on N (and decreases when N increases).

Numerical experiment: subdomain = square with 20×20 discretisation points with two layers of overlap.

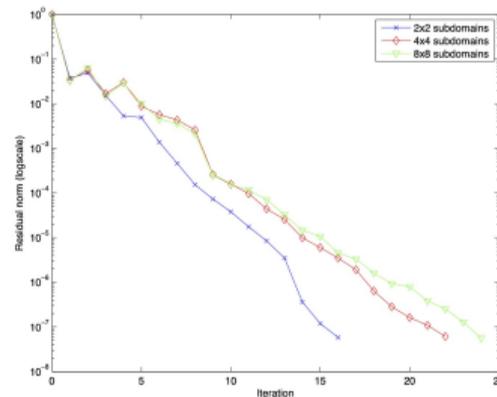
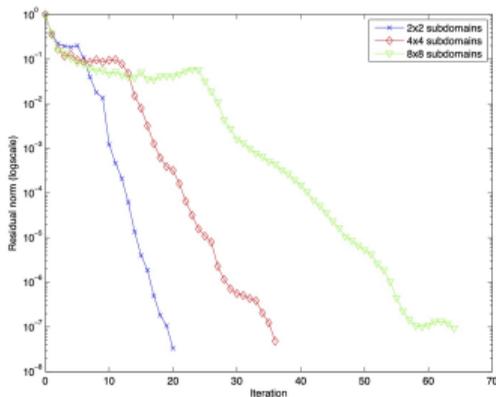


Solution of a Poisson problem $-\Delta u = f$

Number of subdomains	2×2	4×4	8×8
Number of iterations	20	36	64

How to achieve scalability

- Stagnation correspond to a few small eigenvalues from the spectrum of the preconditioned problem.
- They are due to the lack of global exchange of the information in the preconditioner.



A classical remedy : introduction of a **coarse problem** coupling all the subdomains.

Suppose we have identified the modes corresponding to the slow convergence of the iterative method used to solve the linear system:

$$M^{-1}Ax = M^{-1}\mathbf{b}$$

Examples:

- Constant functions that are in the null space (kernel) of the Laplace operators.
- Rigid body motions in the case of linear elasticity

Let us call Z the rectangular matrix whose columns correspond to these slow modes.

Consider the minimisation problem (finding the best correction to an approximate solution \mathbf{y} by a vector $Z\beta$)

$$\min_{\beta} \|A(\mathbf{y} + Z\beta) - \mathbf{b}\|_{A^{-1}} .$$

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and whose solution is:

$$\beta = (Z^T AZ)^{-1} Z^T (\mathbf{b} - A\mathbf{y}) .$$

Adding a coarse space: the Galerkin correction

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Thus, the correction term is:

$$Z\beta = Z (Z^T AZ)^{-1} Z^T \underbrace{(\mathbf{b} - A\mathbf{y})}_{\mathbf{r}} .$$

This kind of correction is called a **Galerkin correction**.

Let $R_0 := Z^T$ and $\mathbf{r} = \mathbf{b} - A\mathbf{y}$ be the residual associated to the approximate solution \mathbf{y} . Then the **coarse correction** is:

$$Z\beta = R_0^T \beta = R_0^T (R_0 A R_0^T)^{-1} R_0 \mathbf{r}.$$

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and we can define

$$M_{AS,2}^{-1} := R_0^T \underbrace{(R_0 A R_0^T)^{-1}}_{\text{coarse problem}} R_0 + \underbrace{\sum_{i=1}^N R_i^T (R_i A R_i^T)^{-1} R_i}_{M_{AS}^{-1}} \quad (3)$$

A two-level Schwarz preconditioner

Let $R_0 := Z^T$ and $\mathbf{r} = \mathbf{b} - A\mathbf{y}$ be the residual associated to the approximate solution \mathbf{y} . Then the **coarse correction** is:

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Remark

- The structure of the two level preconditioner $M_{AS,2}^{-1}$ is the same that of the one level method.
- There is not a unique way to choose R_0 (or Z)!!
- The coarse problem is a small $O(n_C \times n_C)$ square matrix and the extra cost is negligible.

The Nicolaides coarse space (1987)

We define Z as the matrix whose i -th column is

$$Z_i := R_i^T D_i R_i \mathbf{1} \quad \text{for } 1 \leq i \leq N \quad (4)$$

where $\mathbf{1}$ is the vector of dimension \mathcal{N} full of ones. The global structure of Z is:

$$Z = \begin{bmatrix} D_1 R_1 \mathbf{1} & 0 & \cdots & 0 \\ 0 & D_2 R_2 \mathbf{1} & \ddots & \\ \vdots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & D_N R_N \mathbf{1} \end{bmatrix}. \quad (5)$$

where

$$D_i : \mathbb{R}^{\#\mathcal{N}_i} \mapsto \mathbb{R}^{\#\mathcal{N}_i} \quad (6)$$

so that we have:

$$\sum_{i=1}^N R_i^T D_i R_i = Id.$$

Theorem (Widlund, Dryija)

Let $M_{AS,2}^{-1}$ be the two-level additive Schwarz method:

$$\kappa(M_{AS,2}^{-1} A) \leq C \left(1 + \frac{H}{\delta} \right)$$

where δ is the size of the overlap between the subdomains and H the subdomain size.

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This does indeed work very well

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Fails for highly heterogeneous problems → We need a larger and adaptive coarse space

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Conclusion

Large discretized system of PDEs
strongly heterogeneous coefficients
(high contrast, nonlinear, multiscale)

E.g. Darcy pressure equation, P^1 -finite elements:

$$\mathbf{A}u = \mathbf{f}$$

$$\text{cond}(\mathbf{A}) \sim \frac{\alpha_{\max}}{\alpha_{\min}} h^{-2}$$

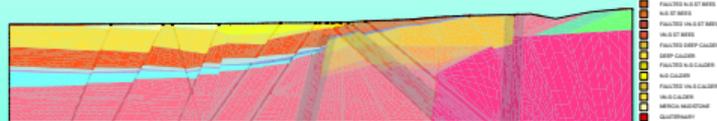
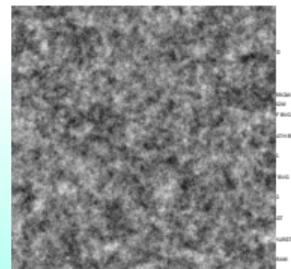
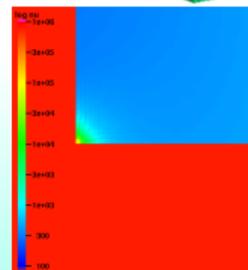
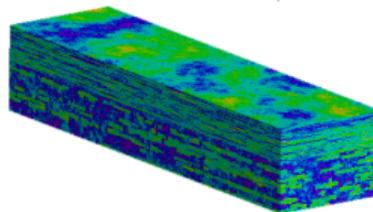
Goal:

iterative solvers

robust in size and heterogeneities

Applications:

flow in heterogeneous stochastic / layered media
structural mechanics, electromagnetics



Adaptive Coarse space for highly heterogeneous Darcy
and (compressible) elasticity problems

Geneo EVP per subdomain:

Find $V_{j,k} \in \mathbb{R}^{\mathcal{N}_j}$ and $\mu_{j,k} \geq 0$:

$$D_j R_j A R_j^T D_j V_{j,k} = \mu_{j,k} A_j^{Neu} V_{j,k}$$

Adaptive Coarse space for highly heterogeneous Darcy and (compressible) elasticity problems

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In the two-level AS let τ be a user chosen parameter:

Choose eigenvectors $\mu_{j,k} \geq \tau$ per subdomain:

$$Z := (R_j^T D_j V_{j,k})_{\substack{j=1,\dots,N \\ \mu_{j,k} \geq \tau}}$$

This automatically includes Nicolaides CS (Zero Energy Modes).

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Theorem (Spillane, D., Hauret, Nataf, Pechstein, Scheichl, 2014)

Under some technical assumptions... If for all j : $0 < \mu_{j,m_{j+1}} < \infty$:

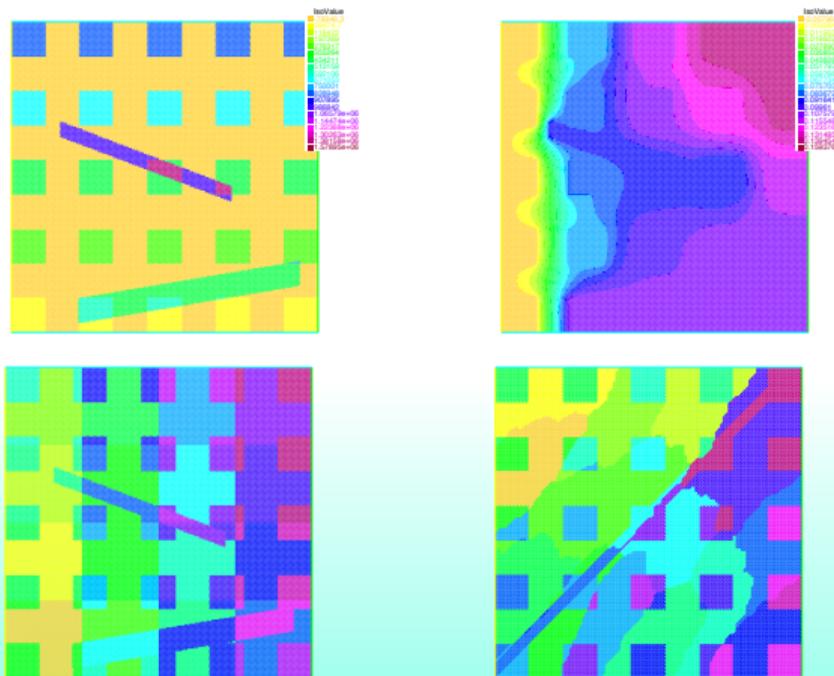
$$\kappa(M_{AS,2}^{-1}A) \leq (1 + k_0) \left[2 + k_0 (2k_0 + 1) (1 + \tau) \right]$$

Possible criterion for picking τ :

(used in our Numerics)

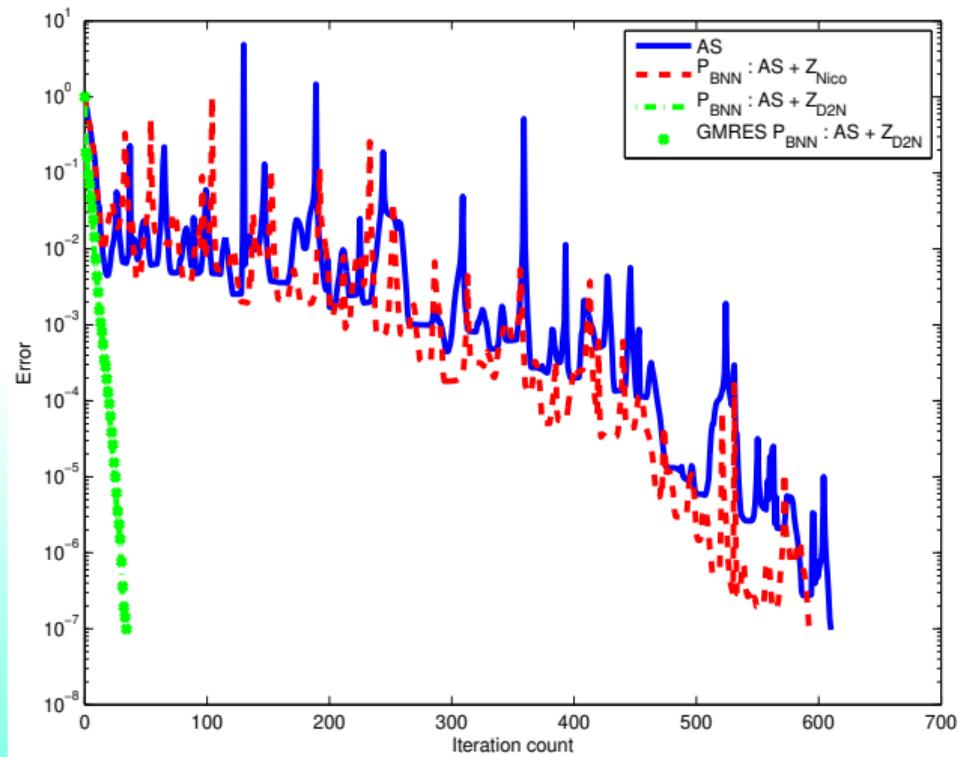
$$\tau := \min_{j=1,\dots,N} \frac{H_j}{\delta_j}$$

Numerical results (Darcy)



Channels and inclusions: $1 \leq \alpha \leq 1.5 \times 10^6$, the solution and partitionings (Metis or not)

Convergence

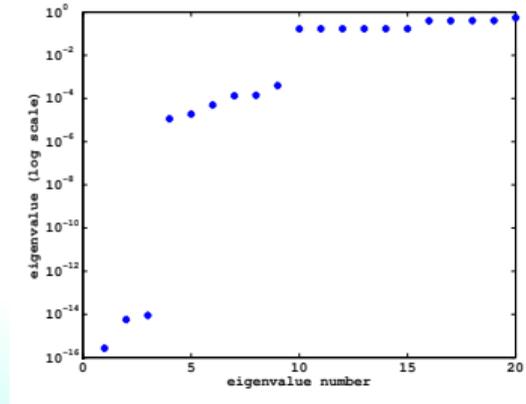


Eigenvalues and eigenvectors (Elasticity)



m_i is given automatically by the chosen criterion and is optimal

#Z per subd.	AS	AS+Z _{Nico}	AS+Z _{Geneo}
$\max(m_i - 1, 1)$			273
m_i	614	543	36
$m_i + 1$			32



Logarithmic scale



- $H := \mathbb{R}^{\#\mathcal{N}}$ and the a -bilinear form:

$$a(\mathbf{U}, \mathbf{V}) := \mathbf{V}^T A \mathbf{U}. \quad (7)$$

where A is the matrix of the problem we want to solve.

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- H_D is a product space and b a bilinear form defined by

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- The linear operator \mathcal{R}_{AS} is defined as

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We have: $M_{AS}^{-1} = \mathcal{R}_{AS} B^{-1} \mathcal{R}_{AS}^*$.

Lemma (Fictitious Space Lemma, Nepomnyaschikh 1991)

Let H and H_D be two *Hilbert spaces*. Let a be a *symmetric positive* bilinear form on H and b on H_D . Suppose that there exists a linear operator $\mathcal{R} : H_D \rightarrow H$, such that

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$$c_T \cdot a(u, u) \leq a(\mathcal{R}B^{-1}\mathcal{R}^*Au, u) \leq c_R \cdot a(u, u), \quad \forall u \in H \quad (12)$$

which proves that the **eigenvalues of operator** $\mathcal{R}B^{-1}\mathcal{R}^*A$ are bounded from below by c_T and from above by c_R .

Application of the FSL

Application of the FSL

Let k_0 be the maximum number of neighbors of a subdomain. We can take $c_R := k_0$.

Let k_1 be the maximum multiplicity of the intersection between subdomains and :

$$\tau_1 := \min_{1 \leq i \leq N} \min_{U_i \in \mathbb{R}^{\#\mathcal{N}_i} \setminus \{0\}} \frac{\mathbf{U}_i^T A_i^{Neu} \mathbf{U}_i}{\mathbf{U}_i^T (D_i R_i A R_i^T D_i) \mathbf{U}_i} .$$

We can take $c_T := \frac{\tau_1}{k_1}$.

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We can take $c_T := \frac{\tau_1}{k_1}$. Then

$$\frac{\tau_1}{k_1} \leq \lambda(M_{ASM}^{-1} A) \leq k_0 .$$

Issue: τ_1 can be very small.

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Definition (Generalized Eigenvalue Problem for the lower bound)

For each subdomain $1 \leq j \leq N$, we introduce the generalized eigenvalue problem

Find $(\mathbf{V}_{jk}, \lambda_{jk}) \in \mathbb{R}^{\#\mathcal{N}_j} \setminus \{0\} \times \mathbb{R}$ such that

$$A_j^{Neu} \mathbf{V}_{jk} = \lambda_{jk} (D_j R_j A R_j^T D_j) \mathbf{V}_{jk} .$$

Let $\tau > 0$ be a user-defined threshold, we define $Z_{geneo,ASM}^\tau \subset \mathbb{R}^{\#\mathcal{N}}$ as the vector space spanned by the family of vectors $(R_j^T D_j \mathbf{V}_{jk})_{\lambda_{jk} < \tau, 1 \leq j \leq N}$ corresponding to eigenvalues smaller than τ .

ASM theory for a SPD matrix A (summary)

- Algebraic reformulation

$$M_{RAS}^{-1} := \sum_{i=1}^N R_i^T D_i A_i^{-1} R_i$$

- Symmetric variant

$$M_{AS}^{-1} := \sum_{i=1}^N R_i^T A_i^{-1} R_i$$

- Adaptive Coarse space with prescribed targeted convergence rate.

Aim: develop a similar theory and computational framework for Optimised variants of RAS (ORAS)

et B_i be the matrix of the Robin subproblem in each subdomain $1 \leq i \leq N$

Optimized multiplicative, additive, and restricted additive Schwarz preconditioning (St Cyr et al, 2007)

$$M_{ORAS}^{-1} := \sum_{i=1}^N R_i^T D_i B_i^{-1} R_i$$

- Symmetric variants:

$$M_{OAS}^{-1} := \sum_{i=1}^N R_i^T B_i^{-1} R_i \text{ (Natural but K.O.)}$$

$$M_{SORAS}^{-1} := \sum_{i=1}^N R_i^T D_i B_i^{-1} D_i R_i \text{ (O.K.)}$$

ASM theory for a SPD matrix A (summary)

- Algebraic reformulation

$$M_{RAS}^{-1} := \sum_{i=1}^N R_i^T D_i A_i^{-1} R_i$$

- Symmetric variant

$$M_{AS}^{-1} := \sum_{i=1}^N R_i^T A_i^{-1} R_i$$

- Adaptive Coarse space with prescribed targeted convergence rate.

Aim: develop a similar theory and computational framework for Optimised variants of RAS (ORAS)

Let B_i be the matrix of the Robin subproblem in each subdomain $1 \leq i \leq N$

Optimized multiplicative, additive, and restricted additive Schwarz preconditioning (St Cyr et al, 2007)

$$M_{ORAS}^{-1} := \sum_{i=1}^N R_i^T D_i B_i^{-1} R_i$$

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Application of FSL

- Let $H := \mathbb{R}^{\#\mathcal{N}}$ and the a -bilinear form:

$$a(\mathbf{U}, \mathbf{V}) := \mathbf{V}^T A \mathbf{U}.$$

where A is the matrix of the problem we want to solve.

- H_D is a product space and b a bilinear form

$$H_D := \prod_{i=1}^N \mathbb{R}^{\#\mathcal{N}_i} \text{ and } b(\mathcal{U}, \mathcal{V}) := \sum_{i=1}^N \mathbf{V}_i^T B_i \mathbf{U}_i, .$$

- The linear operator \mathcal{R}_{SORAS} is defined as

$$\mathcal{R}_{SORAS} : H_D \longrightarrow H, \mathcal{R}_{SORAS}(\mathcal{U}) := \sum_{i=1}^N R_i^T D_i \mathbf{U}_i.$$

We have: $M_{SORAS}^{-1} = \mathcal{R}_{SORAS} B^{-1} \mathcal{R}_{SORAS}^*$.

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Estimate for the one level SORAS

- Let k_0 be the maximum number of neighbours of a subdomain and γ_1 be defined as:

$$\gamma_1 := \max_{1 \leq i \leq N} \max_{\mathbf{U}_i \in \mathbb{R}^{\#\mathcal{N}_i} \setminus \{0\}} \frac{(R_i^T D_i \mathbf{U}_i)^T A (R_i^T D_i \mathbf{U}_i)}{\mathbf{U}_i^T B_i \mathbf{U}_i}$$

We can take $c_R := k_0 \gamma_1$.

- Let k_1 be the maximum multiplicity of the intersection between subdomains and τ_1 be defined as:

$$\tau_1 := \min_{1 \leq i \leq N} \min_{\mathbf{U}_i \in \mathbb{R}^{\#\mathcal{N}_i} \setminus \{0\}} \frac{\mathbf{U}_i^T A_i^{Neu} \mathbf{U}_i}{\mathbf{U}_i^T B_i \mathbf{U}_i}.$$

We can take $c_T := \frac{\tau_1}{k_1}$.

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We can take $c_T := \frac{\tau_1}{k_1}$. Then

$$\frac{\tau_1}{k_1} \leq \lambda(M_{SORAS}^{-1} A) \leq k_0 \gamma_1.$$

Control of the upper bound

Definition (Generalised Eigenvalue Problem for the upper bound)

Find $(\mathbf{U}_{ik}, \mu_{ik}) \in \mathbb{R}^{\#\mathcal{N}_i} \setminus \{0\} \times \mathbb{R}$ such that

$$D_i R_i A R_i^T D_i \mathbf{U}_{ik} = \mu_{ik} B_i \mathbf{U}_{ik} .$$

Let $\gamma > 0$ be a user-defined threshold, we define $Z_{geneo}^\gamma \subset \mathbb{R}^{\#\mathcal{N}}$ as the vector space spanned by the family of vectors

$(R_i^T D_i \mathbf{U}_{ik})_{\mu_{ik} > \gamma, 1 \leq i \leq N}$ corresponding to eigenvalues larger than γ .

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Control of the lower bound

Definition (Generalised Eigenvalue Problem for the lower bound)

For each subdomain $1 \leq j \leq N$, we introduce the generalised eigenvalue problem

Find $(\mathbf{V}_{jk}, \lambda_{jk}) \in \mathbb{R}^{\#\mathcal{N}_j} \setminus \{0\} \times \mathbb{R}$ such that

$$A_j^{Neu} \mathbf{V}_{jk} = \lambda_{jk} B_j \mathbf{V}_{jk} .$$

Let $\tau > 0$ be a user-defined threshold, we define $Z_{geneo}^\tau \subset \mathbb{R}^{\#\mathcal{N}}$ as the vector space spanned by the family of vectors

$(R_j^T D_j \mathbf{V}_{jk})_{\lambda_{jk} < \tau, 1 \leq j \leq N}$ corresponding to eigenvalues smaller than τ .

Let P_0 denote the a -orthogonal projection on the SORAS-GENEO-2 coarse space

$$Z_{\text{GenEO-2}} := Z_{\text{geneo}}^\tau \oplus Z_{\text{geneo}}^\gamma,$$

the two-level SORAS-GENEO-2 preconditioner is:

$$M_{\text{SORAS},2}^{-1} := P_0 A^{-1} + (I - P_0) M_{\text{SORAS}}^{-1} (I - P_0^T)$$

where $P_0 A^{-1} = R_0^T (R_0 A R_0^T)^{-1} R_0$, (J. Mandel, 1992).

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where $P_0 A^{-1} = R_0^T (R_0 A R_0^T)^{-1} R_0$, (J. Mandel, 1992).

Theorem (Haferssas, Jolivet and Nataf)

Let γ and τ be user-defined targets. Then, the eigenvalues of the two-level SORAS-GenEO-2 preconditioned system satisfy the following estimate

$$\frac{1}{1 + \frac{k_1}{\tau}} \leq \lambda(M_{\text{SORAS},2}^{-1} A) \leq \max(1, k_0 \gamma)$$

Material properties: Young modulus E and Poisson ratio ν or alternatively by its Lamé coefficients λ and μ :

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} \quad \text{and} \quad \mu = \frac{E}{2(1+\nu)}.$$

For ν close to $1/2$, the variational problem consists in finding $(\mathbf{u}_h, p_h) \in \mathcal{V}_h := \mathbb{P}_2^d \cap H_0^1(\Omega) \times \mathbb{P}_1$ such that for all $(\mathbf{v}_h, q_h) \in \mathcal{V}_h$

$$\begin{cases} \int_{\Omega} 2\mu \underline{\underline{\varepsilon}}(\mathbf{u}_h) : \underline{\underline{\varepsilon}}(\mathbf{v}_h) dx & - \int_{\Omega} p_h \operatorname{div}(\mathbf{v}_h) dx = \int_{\Omega} \mathbf{f} \mathbf{v}_h dx \\ - \int_{\Omega} \operatorname{div}(\mathbf{u}_h) q_h dx & - \int_{\Omega} \frac{1}{\lambda} p_h q_h = 0 \end{cases}$$
$$\implies A\mathbf{U} = \begin{bmatrix} H & B^T \\ B & -C \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ 0 \end{bmatrix} = \mathbf{F}.$$

A is symmetric but no longer positive.



Figure 2: 2D Elasticity: Sandwich of steel $(E_1, \nu_1) = (210 \cdot 10^9, 0.3)$ and rubber $(E_2, \nu_2) = (0.1 \cdot 10^9, 0.4999)$.

Metis partitioning

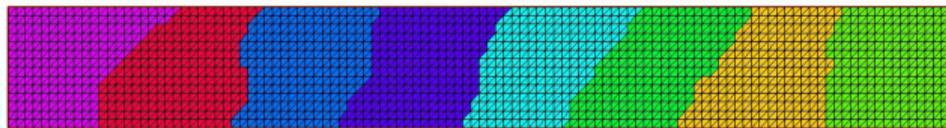


Table 1: 2D Elasticity. GMRES iteration counts

		AS	SORAS	AS+CS(ZEM)	SORAS +CS(ZEM)	AS-GenEO	SORAS -GenEO-2				
Nb DOFs	Nb subdom	iteration	iteration	iteration	dim	iteration	dim	iteration	dim	iteration	dim
35841	8	150	184	117	24	79	24	110	184	13	145
70590	16	276	337	170	48	144	48	153	400	17	303
141375	32	497	++1000	261	96	200	96	171	800	22	561
279561	64	++1000	++1000	333	192	335	192	496	1600	24	855
561531	128	++1000	++1000	329	384	400	384	++1000	2304	29	1220
1077141	256	++1000	++1000	369	768	++1000	768	++1000	3840	36	1971

Strong scalability in two and three dimensions (with FreeFem++ and HPDDM)

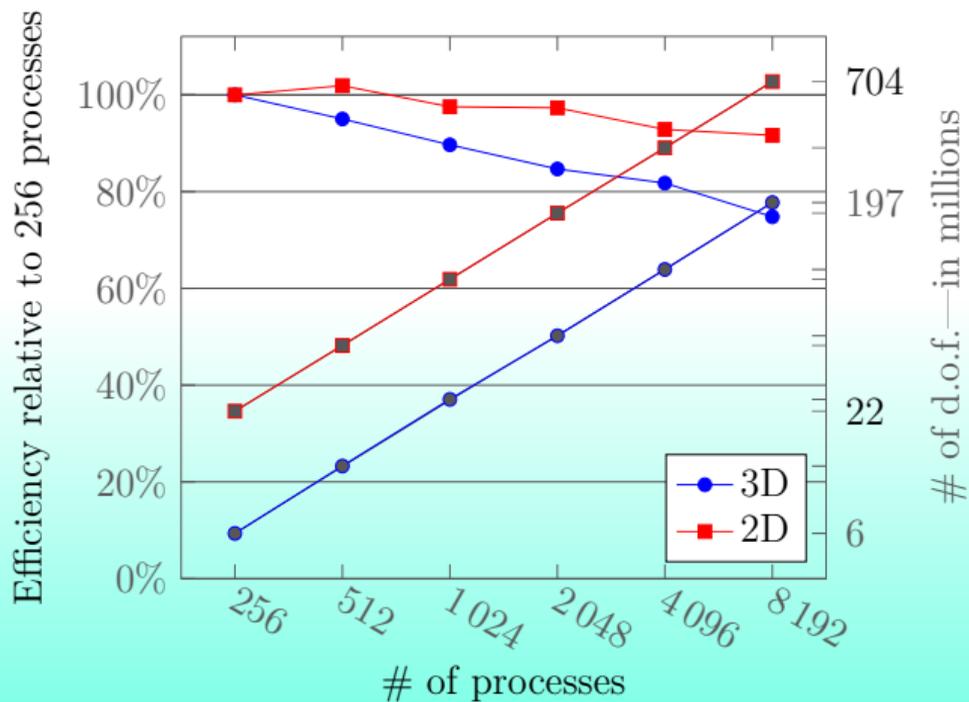
Stokes problem with automatic mesh partition. Driven cavity problem

	N	Factorization	Deflation	Solution	# of it.	Total	# of d.o.f.
3D	1 024	79.2 s	229.0 s	76.3 s	45	387.5 s	$50.63 \cdot 10^6$
	2 048	29.5 s	76.5 s	34.8 s	42	143.9 s	
	4 096	11.1 s	45.8 s	19.8 s	42	80.9 s	
	8 192	4.7 s	26.1 s	14.9 s	41	56.8 s	
2D	1 024	5.2 s	37.9 s	51.5 s	51	95.6 s	$100.13 \cdot 10^6$
	2 048	2.4 s	19.3 s	22.1 s	42	44.5 s	
	4 096	1.1 s	10.4 s	10.2 s	35	22.6 s	
	8 192	0.5 s	4.6 s	6.9 s	38	12.7 s	

Peak performance: 50 millions d.o.f's in 3D in 57 sec.

IBM/Blue Gene Q machine with 1.6 GHz Power A2 processors. Hours provided by an IDRIS-GENCI project.

Rubber Steel sandwich with automatic mesh partition



(a) Timings of various simulations

Coarse Space correction

Coarse grids for heterogeneous problems

Conclusion

Summary

Using generalised eigenvalue problems and projection preconditioning we are able to achieve a targeted convergence rate for

- Additive Schwarz method (AS)
- Optimised Schwarz method (OAS, SORAS)
- BNN methods (see Lecture Notes)
- Available in HPDDM C++/MPI library
- Available in the public release of FreeFem++ (ffddm)

Further and ongoing work

- Non symmetric, indefinite problems
- Time-harmonic wave propagation problems.

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