Two-level domain decomposition methods

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Outline

Coarse space corrections

Many Cores: Strong and Weak Scalability

Scalability Metrics

Strong scalability (Amdahl)
Measures how the solution time varies with the number of processors for a fixed total problem size.

Weak scalability (Gustafson)
Measures how the solution time varies with the number of processors when the problem size per processor is fixed.

One-Level Schwarz: Not Scalable

# Subdomains	8	16	32	64
AS	18	35	66	128

- Iteration count increases linearly with number of subdomains.
- Clear breakdown of scalability in one-level methods.

Numerics on a toy problem

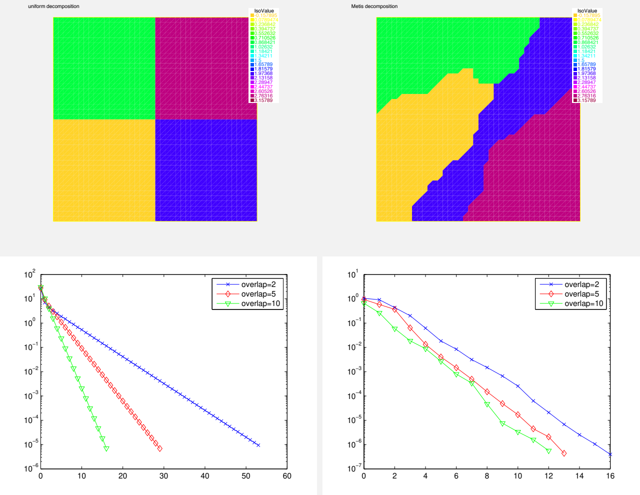


Figure 1: Schwarz convergence as a solver (left) and as a preconditioner (right) for different overlaps

Weak Scaling: A Mathematical Proof

Condition Number Estimates for the Preconditioned System

Lemma

If there exist constants C_1 and C_2 such that

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

then

$$\lambda_{\max}(M_{AS}^{-1}A) \leq C_2, \quad \lambda_{\min}(M_{AS}^{-1}A) \geq C_1, \quad \Rightarrow \quad \kappa(M_{AS}^{-1}A) \leq \frac{C_2}{C_1}.$$

- If $\kappa(M_{AS}^{-1}A)$ is independent of N, the solution time becomes independent of the number of subdomains.
- $\Rightarrow$ Weak scalability is achieved.

Why the algorithm is not scalable?

Lemma (Estimate of the largest eigenvalue)

Let $\mathrm{col}(j) \in \{1, \ldots, \mathcal{N}^c\}$ be the color of the domain j defined such that $\mathrm{col}(k) = \mathrm{col}(l)$ 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)

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

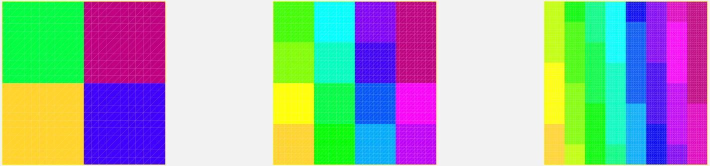
Let $(\mathbf{x}_j)_{1 \leq j \leq N}$ which achieves the minimum in (**??**). Then we have

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

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

Why the Algorithm is Not Scalable?

- We have that $\lambda_{\max}(M_{AS}^{-1}A) \leq \mathcal{N}_c \ll N$
- But $\lambda_{\min}(M_{AS}^{-1}A)$ decreases as N increases.
- $\Rightarrow$ Condition number grows with N, breaking weak scalability.



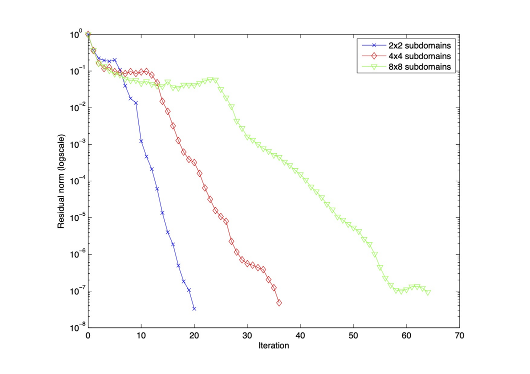
Poisson Problem $-\Delta u = f$ with 20×20 discretisation and 2-layer overlap

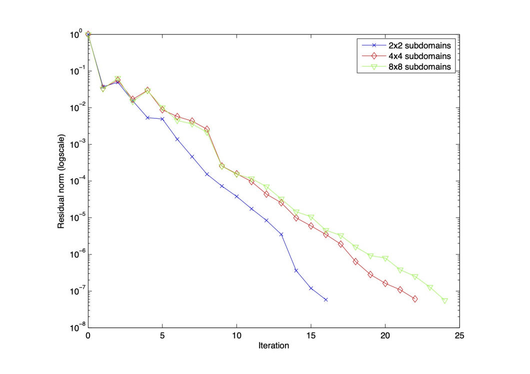
# Subdomains	2×2	4×4	8×8
Iterations	20	36	64

How to Achieve Scalability

Root Cause of Stagnation

- Stagnation is caused by a few small eigenvalues in the spectrum of the preconditioned system.
- These small eigenvalues arise due to the **lack of global information exchange** in the preconditioner.





Classical Remedy

Introduce a **coarse problem** that couples all subdomains and enables global information exchange.

Adding a Coarse Space

Targeting Slow Convergence Modes

Assume we have identified the slow modes of the preconditioned system:

$$M^{-1}A\mathbf{x} = M^{-1}\mathbf{b}$$

Examples of Slow Modes

- Constant functions in the **null space of the Laplace operator**.
- **Rigid body motions** in linear elasticity problems.

Notation

Let Z be the rectangular matrix whose columns span these slow modes.

Adding a Coarse Space: the Galerkin Correction

Correction by Minimization

We seek to correct an approximate solution $\mathbf{y}$ with $Z\beta$:

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

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Equivalent Formulation

$$\min_{\beta \in \mathbb{R}^{n_c}} \; 2(A\mathbf{y} - \mathbf{b}, Z\beta) + (AZ\beta, Z\beta)$$

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Optimal Coarse Coefficients

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

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$$\Rightarrow \quad Z\beta = {\color{blue} Z(Z^T A Z)^{-1} Z^T} \underbrace{(\mathbf{b} - A\mathbf{y})}_{\mathbf{r}}$$

Galerkin Correction

This term is known as the Galerkin correction.

A Two-Level Schwarz Preconditioner

Coarse Space Correction

Let $R_0 := Z^T$ and $\mathbf{r} = \mathbf{b} - A\mathbf{y}$.

Then the coarse correction is:

$$Z\beta = R_0^T\beta = R_0^T(R_0AR_0^T)^{-1}R_0\,\mathbf{r}$$

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Two-Level Preconditioner Definition

$$M_{AS,2}^{-1} := \underbrace{R_0^T(R_0AR_0^T)^{-1}R_0}_{\text{Coarse problem}} + \underbrace{\sum_{i=1}^{N} R_i^T(R_iAR_i^T)^{-1}R_i}_{M_{AS}^{-1}}$$

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Remarks

- The structure of $M_{AS,2}^{-1}$ mimics the one-level method.
- The choice of coarse basis R_0 (or Z) is not unique.
- The coarse problem is small ($O(n_C \times n_C)$); the added cost is negligible.

The Nicolaides Coarse Space (1987)

Definition. We define the coarse basis vectors Z_i as:

$$Z_i := R_i^T D_i R_i \mathbf{1}, \quad 1 \leq i \leq N$$

where **1** is the all-ones vector of length $\mathcal{N}$.

Global Structure of Z**.** Z contains blocks formed of one vector per subdomain:

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

Partition of Unity. The weights D_i form a partition of unity:

$$\sum_{i=1}^{N} R_i^T D_i R_i = \mathrm{Id}, \quad D_i : \mathbb{R}^{\#\mathcal{N}_i} \to \mathbb{R}^{\#\mathcal{N}_i} \text{ (diagonal)}$$

This construction ensures that each coarse basis vector is global while being defined locally

Theoretical Convergence Result

Theorem (Widlund - Dryja)

If $M_{AS,2}^{-1}$ is the two-level additive Schwarz preconditioner, then

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

where H = size of subdomains and δ = overlap size.

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Numerical Validation

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Limitation

Fails for highly heterogeneous problems.

$\Rightarrow$ **We need larger and possibly adaptive coarse spaces.**

Coarse spaces for heterogeneous problems

Motivation

Context

Solving large discretized PDE systems with strongly heterogeneous coefficients:

- High contrast
- Multiscale structure

Example

Darcy pressure equation with P^1 finite elements:

$$\mathbf{Au} = \mathbf{f}, \quad \mathrm{cond}(\mathbf{A}) \sim \frac{\alpha_{\mathrm{max}}}{\alpha_{\mathrm{min}}} \cdot h^{-2}$$

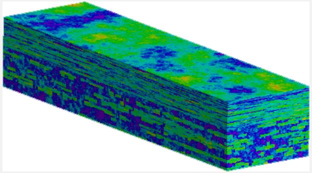
Goal: Robust Solvers

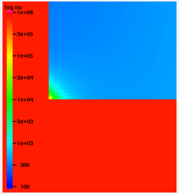
Iterative methods that remain effective:

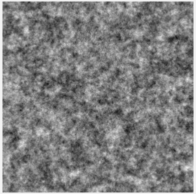
- As mesh size $h \to 0$
- For high coefficient contrast

Applications

- Flow in layered / stochastic media
- Structural mechanics
- Electromagnetics







GenEO: Adaptive Spectral Coarse Space

What is GenEO?

GenEO constructs an **adaptive coarse space** for:

- Highly heterogeneous **Darcy problems**
- Compressible **elasticity problems**

It uses local spectral analysis to capture slow-to-converge error modes.

Why?

To accelerate convergence of iterative solvers by improving global information flow.

Local Generalized Eigenproblem (EVP)

For each subdomain j, find:

$$A_j^{Neu} \phi_{j,k} = \lambda_{j,k} D_j R_j A R_j^T D_j \cdot \phi_{j,k}$$

where:

$$\phi_{j,k} \in \mathbb{R}^{\mathcal{N}_j}, \quad \lambda_{j,k} \geq 0$$

GenEO: Coarse Mode Selection and Convergence

Mode Selection (via Threshold τ)

Choose eigenmodes per subdomain with:

$$\lambda_{j,k} \leq \tau \quad \Rightarrow \quad Z := \left(R_j^T D_j\, \phi_{j,k}\right)$$

- $\lambda_{j,k} = 0 \Rightarrow$ **Nicolaides coarse space** (zero-energy modes)
- Smaller $\tau \rightsquigarrow$ fewer, high-impact modes
- Adaptivity to material contrast and geometry

Theoretical Guarantee (Spillane et al. - 2014)

Under mild assumptions, for all j with $0 < \mu_{j,m_{j+1}} < \infty$:

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

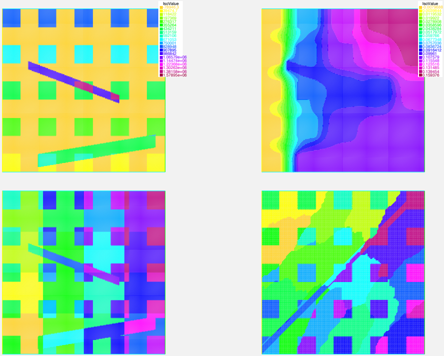
Recommended threshold:

$$\tau := \left(\max_j \frac{H_j}{\delta_j}\right)^{-1}$$

Numerical Results: Darcy Problem

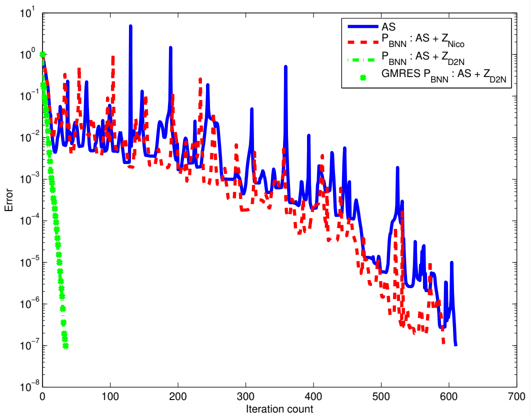
Test case: Channels and inclusions
Contrast: $1 \leq \alpha(x) \leq 1.5 \times 10^6$

- Highly heterogeneous permeability
- Two-level method with GenEO coarse space
- Comparison with and without Metis partitioning



Upper row: permeability $\alpha(x)$ and solution. Lower row: two domain decompositions (uniform and METIS).

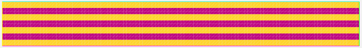
Convergence with and without Spectral Coarse Spaces



Key takeaway

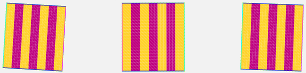
The GenEO coarse space drastically improves convergence and makes iteration robust w.r.t the heterogeneity.

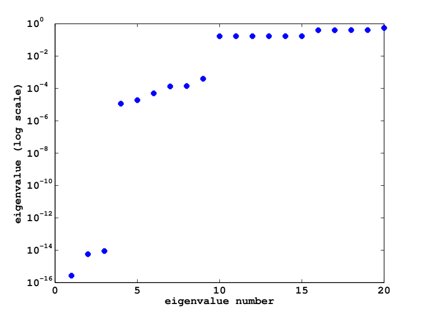
Eigenvalues and eigenvectors (Elasticity)



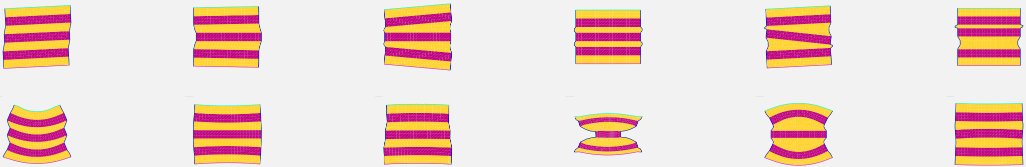
#Z per subd.	AS	AS+Z_{Nico}	AS+Z_{Geneo}
$\max(m_i - 1, 1)$			273
m_i	614	543	36
$m_i + 1$			32

m_i is given automatically by the chosen criterion





Logarithmic scale



Global Space and Bilinear Form

Let $\mathcal{H}_0 := \mathbb{R}^{\#\mathcal{N}}$ and A is the system matrix. Let:

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

Additive Schwarz – Abstract Finite Dimensional Reformulation

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Let $\mathcal{H}_0 := \mathbb{R}^{\#\mathcal{N}}$ and A is the system matrix. Let:

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Product Space and Local Bilinear Form

Define the product space:

$$\mathcal{H}_P := \prod_{i=1}^{N} \mathbb{R}^{\#\mathcal{N}_i} \quad \text{with} \quad b(\mathcal{U}, \mathcal{V}) := \sum_{i=1}^{N} \mathbf{V}_i^T (R_i A R_i^T) \mathbf{U}_i$$

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Assembly Operator

$$\mathcal{R}_{AS} : \mathcal{H}_P \to \mathcal{H}_0, \quad \mathcal{R}_{AS}(\mathcal{U}) := \sum_{i=1}^{N} R_i^T \mathbf{U}_i$$

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Conclusion

The additive Schwarz preconditioner is:

$$M_{AS}^{-1} = \mathcal{R}_{AS} \, B^{-1} \, \mathcal{R}_{AS}^*$$

Fictitious Space Lemma (FSL)

Let $\mathcal{H}_0, \mathcal{H}_P$ be Hilbert spaces with symmetric, positive definite bilinear forms

$$a : \mathcal{H}_0 \times \mathcal{H}_0 \to \mathbb{R}, \quad b : \mathcal{H}_P \times \mathcal{H}_P \to \mathbb{R},$$

and let $\mathcal{R} : \mathcal{H}_P \to \mathcal{H}_0$ be a linear operator.

(1) Surjectivity: $\mathcal{R}$ is onto $\mathcal{H}_0$, i.e.,

$$\forall u \in \mathcal{H}_0, \quad \exists u_P \in \mathcal{H}_P \text{ such that } \mathcal{R}u_P = u.$$

(2) Continuity (upper bound): There exists $c_R > 0$ such that

$$a(\mathcal{R}u_P, \mathcal{R}u_P) \leq c_R \cdot b(u_P, u_P) \quad \forall u_P \in \mathcal{H}_P.$$

(3) Stable Decomposition (lower bound): There exists $c_T > 0$ such that for every $u \in \mathcal{H}_0$,

$$\exists u_P \in \mathcal{H}_P \text{ with } \mathcal{R}u_P = u \quad \text{and} \quad c_T \cdot b(u_P, u_P) \leq a(u, u).$$

Then the following **spectral estimate** holds:

$$c_T \cdot a(u, u) \ \leq \ a(\mathcal{R}B^{-1}\mathcal{R}^* Au,\ u) \ \leq \ c_R \cdot a(u, u) \quad \forall u \in \mathcal{H}_0$$

In other words, the spectrum of the preconditioned operator $M^{-1} := \mathcal{R}B^{-1}\mathcal{R}^*$ with respect to A lies in the interval $\mathrm{Spec}(M^{-1}A) \subset [c_T,\ c_R]$

Estimate for the One-Level ASM

Goal

Use the Fictitious Space Lemma to bound the eigenvalues of the preconditioned operator $M_{ASM}^{-1}A$.

Upper bound (continuity constant c_R): Let $\mathcal{N}_c$ = max number of neighbors of a subdomain.

$$\Rightarrow \quad c_R := \mathcal{N}_c$$

Lower bound (stability constant c_T): Let $\mathcal{M}_c$ = max overlap multiplicity. Define:

$$\tau_1 := \min_i \min_{\mathbf{U}_i \neq 0} \frac{\mathbf{U}_i^T A_i^{Neu} \mathbf{U}_i}{\mathbf{U}_i^T D_i R_i A R_i^T D_i \mathbf{U}_i} \quad \Rightarrow \quad c_T := \frac{\tau_1}{\mathcal{M}_c}$$

Spectral Estimate

$$\frac{\tau_1}{\mathcal{M}_c} \leq \lambda(M_{ASM}^{-1}A) \leq \mathcal{N}_c$$

Caution: τ_1 can be very small for heterogeneous problems.

Analysis of other variants using FSL

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:

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

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

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One level SORAS

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

Estimate for the one level SORAS

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

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

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:

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

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

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

Numerical results and conclusion

Nearly Incompressible Elasticity

Material model:

- Young's modulus: E
- Poisson ratio: ν
- Lamé parameters:

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}, \qquad \mu = \frac{E}{2(1+\nu)}$$

Discretization: Mixed finite elements (Taylor–Hood: $\mathbb{P}_2^d$–$\mathbb{P}_1$)

Variational problem: Find $(\mathbf{u}_h, p_h) \in \mathcal{V}_h := \mathbb{P}_2^d \cap H_0^1(\Omega) \times \mathbb{P}_1$ such that for all $(\mathbf{v}_h, q_h) \in \mathcal{V}_h$:

$$\begin{cases} \int_\Omega 2\mu\, \varepsilon(\mathbf{u}_h) : \varepsilon(\mathbf{v}_h) - \int_\Omega p_h\, \nabla \cdot \mathbf{v}_h = \int_\Omega \mathbf{f} \cdot \mathbf{v}_h \\ -\int_\Omega \nabla \cdot \mathbf{u}_h\, q_h - \int_\Omega \frac{1}{\lambda} p_h q_h = 0 \end{cases}$$

Matrix form:

$$A\mathbf{U} = \begin{bmatrix} H & B^T \\ B & -C \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ 0 \end{bmatrix} = \mathbf{F}$$

Note: A is symmetric but **indefinite** due to the mixed formulation (saddle-point problem).

Numerical tests (with FreeFem++)

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

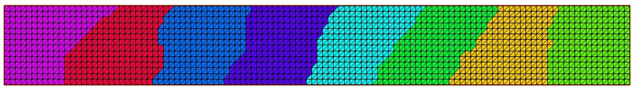


Table 1: 2D Elasticity. GMRES iteration counts

		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

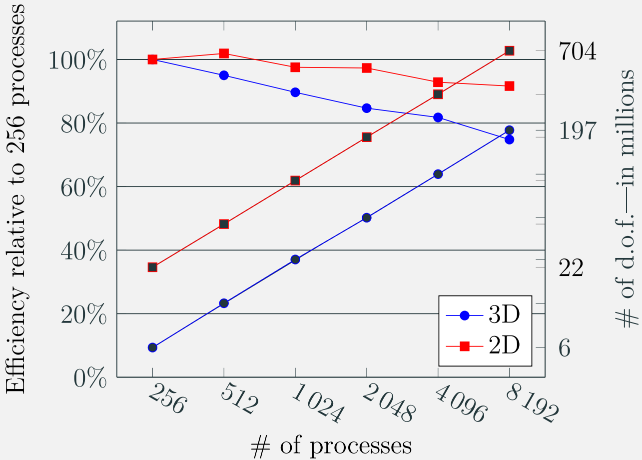
	N	Factorization	Deflation	Solution	# of it.	Total	# of d.o.f.
3D	1 024	79.2 s	229.0 s	76.3 s	45	387.5 s	$50.63 \cdot 10^6$
	2 048	29.5 s	76.5 s	34.8 s	42	143.9 s	
	4 096	11.1 s	45.8 s	19.8 s	42	80.9 s	
	8 192	4.7 s	26.1 s	14.9 s	41	56.8 s	
2D	1 024	5.2 s	37.9 s	51.5 s	51	95.6 s	$100.13 \cdot 10^6$
	2 048	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.

Weak scalability for heterogeneous elasticity (with FreeFem++ and HPDDM)

Rubber Steel sandwich with automatic mesh partition



(a) Timings of various simulations

Conclusion

Summary

We presented a unified spectral framework for domain decomposition:

- Projection-based coarse spaces from generalized eigenproblems
- Guaranteed convergence for:
  - Additive Schwarz (AS)
  - Optimized and Symmetric Optimized Schwarz (OAS, SORAS)
  - Block Newton–Neumann (BNN, see Lecture Notes)
- Fully implemented in:
  - **HPDDM** C++/MPI library
  - **FreeFem++** plugin `ffddm`

Ongoing Work

- Non-symmetric and indefinite problems
- Time-harmonic wave propagation
- Adaptive enrichment strategies and coarse space compression

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