

Sparse Days 2016



Coarse Correction for Generalized Abstract Schwarz Solvers

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joint work with

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Goal

- Solve $\mathcal{A}x = b$, where \mathcal{A} is a large sparse SPD matrix, on a distributed platform

How?

- Use Domain Decomposition :
 - Geometric partition of a domain & Mathematical transformation of the PDE

Focus of the talk

- Coarse Correction for the MaPHyS solver
- Coarse Space for Generalized Abstract Schwarz methods
 - Need access to local matrices

Installing MaPHyS

- MaPHyS and its dependencies can be installed through spack in ≤ 15 minutes + coffee break

morse.gforge.inria.fr/spack/spack.html

- From a laptop to an heterogeneous supercomputer

Using MaPHyS

- Documented test cases
- Centralized/Distributed input
- CeCILL-C license

Motivation: Coarse Correction for MaPHyS

MaPHyS: a Massively Parallel Hybrid Solver

- Nested Dissection to distribute the unknowns (Scotch/Metis)
- Local direct solve in each subdomain (PaStiX/MUMPS)
- Iterative solve on the global interface

A Domain Decomposition Method

- Additive Schwarz on the Schur (AS/S)

Need for Coarse Correction

- Good scalability of the direct part ☺
- The size and condition number of the iterative problem increases with the number of subdomains ☹

Example: 2D Test problem

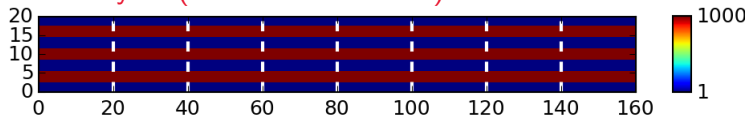
Heterogeneous diffusion

- $\nabla(K\nabla u) = q$
- 7 alternating conductivity layers
- Subdomain: 20×20 elements

Boundary conditions

- Dirichlet on the left
- Neumann elsewhere
- Source: $q = 1$

Conductivity K ($N = 8$ subdomains)



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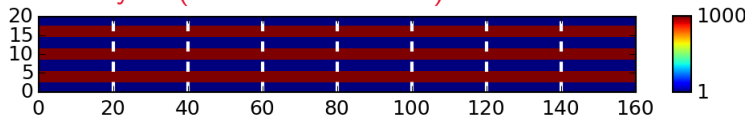
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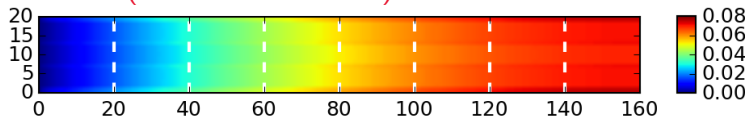
Boundary conditions

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- Neumann elsewhere
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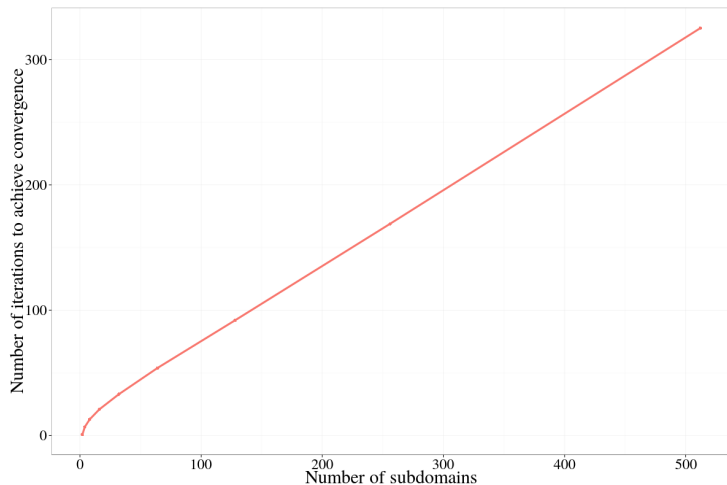
Conductivity K ($N = 8$ subdomains)



Solution x^* ($N = 8$ subdomains)



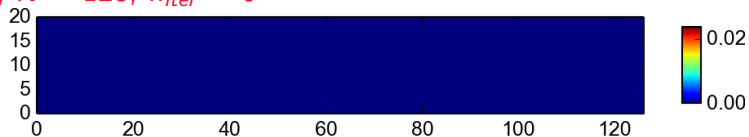
Weak Scalability



N	2	4	8	16	32	64	128	256	512
n_{iter}	1	7	13	21	33	54	92	169	325

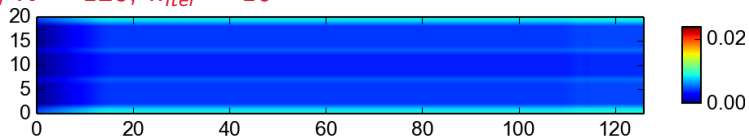
Convergence Behavior

x_Γ , $N = 128$, $n_{iter} = 0$



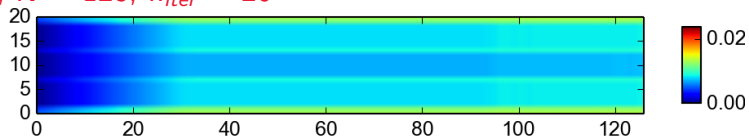
Convergence Behavior

x_Γ , $N = 128$, $n_{iter} = 10$



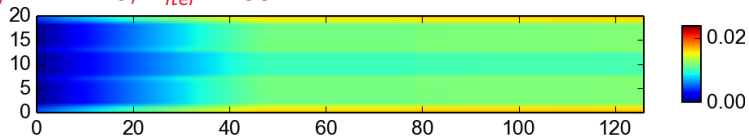
Convergence Behavior

x_Γ , $N = 128$, $n_{iter} = 20$



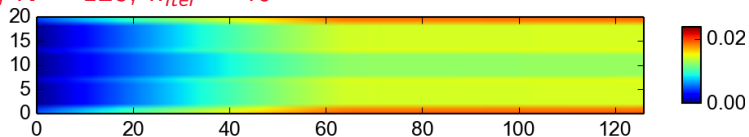
Convergence Behavior

x_Γ , $N = 128$, $n_{iter} = 30$



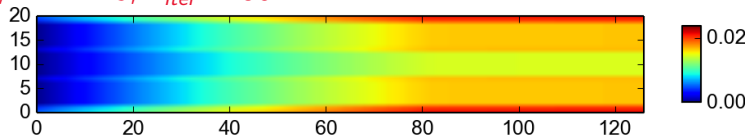
Convergence Behavior

x_Γ , $N = 128$, $n_{iter} = 40$



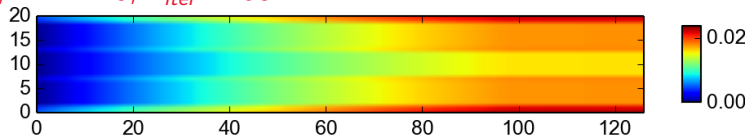
Convergence Behavior

x_Γ , $N = 128$, $n_{iter} = 50$



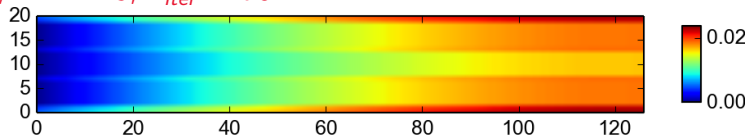
Convergence Behavior

x_Γ , $N = 128$, $n_{iter} = 60$



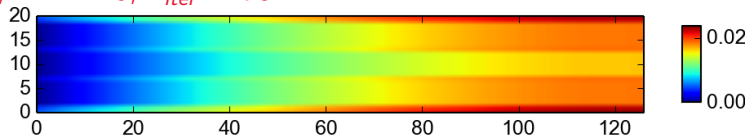
Convergence Behavior

x_Γ , $N = 128$, $n_{iter} = 70$



Convergence Behavior

x_Γ , $N = 128$, $n_{iter} = 70$

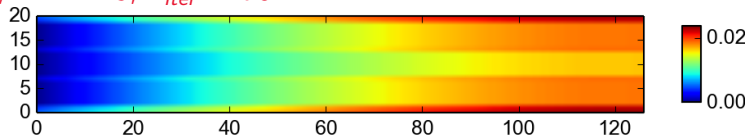


Problem

- No global exchange of information

Convergence Behavior

x_Γ , $N = 128$, $n_{iter} = 70$



Problem

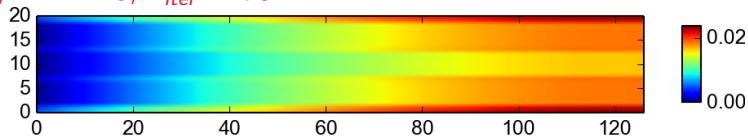
- No global exchange of information

Solution

- Use an exact direct solve on a coarse space V_0

Convergence Behavior

x_Γ , $N = 128$, $n_{iter} = 70$



Problem

- No global exchange of information

Solution

- Use an exact direct solve on a coarse space V_0

Contribution

- Coarse space for MaPHyS
 - but also for a wider class of methods
 - only in the SPD case

- 1 Generalized Abstract Schwarz (GAS) Methods
 - Domain Decomposition Methods
 - Generalized Abstract Schwarz

- 2 Coarse space for GAS
 - Convergence Theorem for GAS
 - Choosing the Coarse Space (GenEO)
 - Two-level Additive Schwarz on the Schur (AS,2)

- 3 Experimental results

- 1 Generalized Abstract Schwarz (GAS) Methods
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Geometric domain decomposition

Domain decomposition methods on boundary value problems

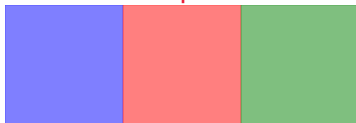
- Geometric partition of a domain
- Mathematical transformation of a PDE

With overlap



- Additive Schwarz method
- Multiplicative Schwarz method

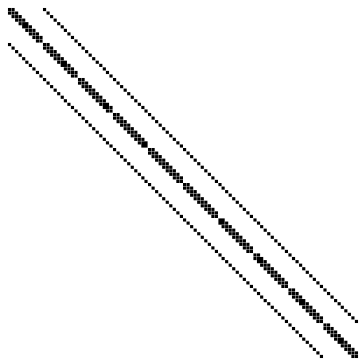
Without overlap



- Substructuring methods (Schur complement)
- Mortar methods (Lagrange multipliers)

Algebraic domain decomposition

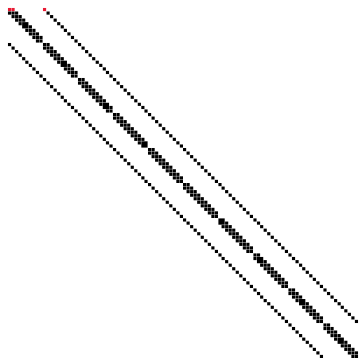
Global Matrix \mathcal{A}



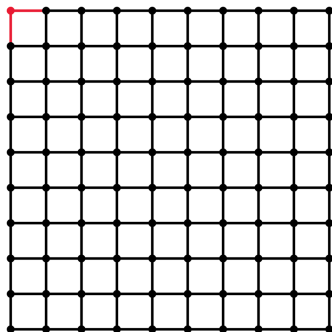
- \mathcal{A} is a sparse matrix. We want to solve $\mathcal{A}x = b$.

Algebraic domain decomposition

Global Matrix \mathcal{A}



Adjacency graph G



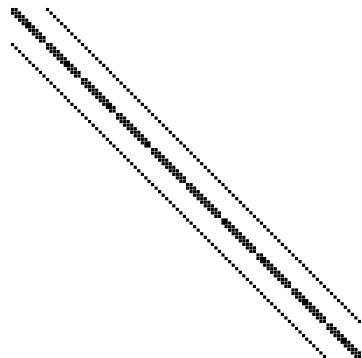
- The adjacency graph of \mathcal{A} ($n \times n$) is used as an algebraic mesh:

$$G = (\{1, \dots, n\}, \{(i, j), a_{ij} \neq 0 \mid a_{ji} \neq 0\})$$

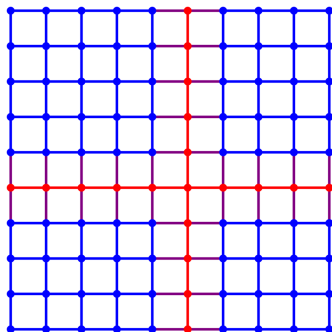
- On the first row of \mathcal{A} , $a_{1,1}$, $a_{1,2}$ and $a_{1,11} \neq 0$
 $\Rightarrow (1, 1)$, $(1, 2)$ and $(1, 11) \in G$

Algebraic domain decomposition

Global Matrix \mathcal{A}



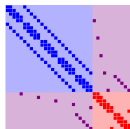
Adjacency graph G



- A graph partitioner is used to split the graph

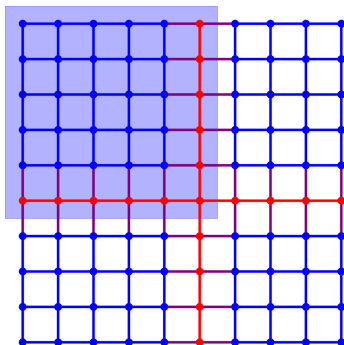
Algebraic domain decomposition

Local Matrices \mathcal{A}_i



$$\mathcal{A}_i = \begin{pmatrix} \mathcal{A}_{\mathcal{I}_i \mathcal{I}_i} & \mathcal{A}_{\mathcal{I}_i \Gamma_i} \\ \mathcal{A}_{\Gamma_i \mathcal{I}_i} & \mathcal{A}_{\Gamma_i \Gamma_i} \end{pmatrix}$$

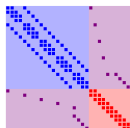
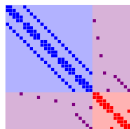
Adjacency graph G



$$\mathcal{A} = \sum_{i=1}^N \mathcal{R}_i^T \mathcal{A}_i \mathcal{R}_i$$

Algebraic domain decomposition

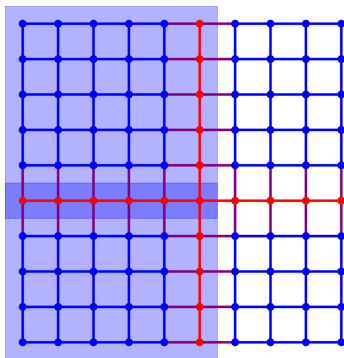
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- We have to split the interface non-zeros

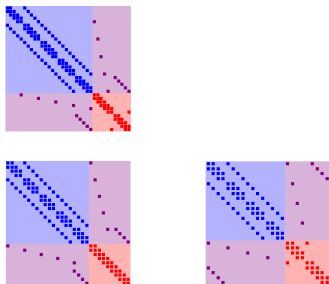
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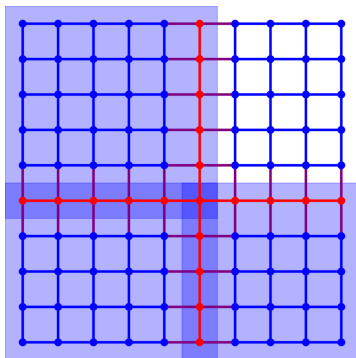
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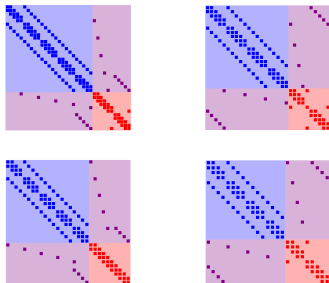
Adjacency graph G



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Algebraic domain decomposition

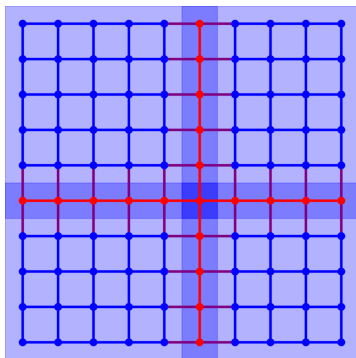
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Adjacency graph G

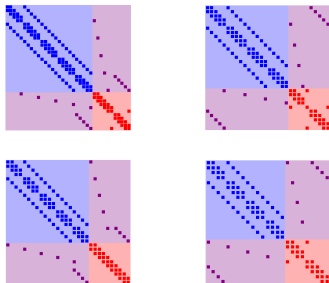


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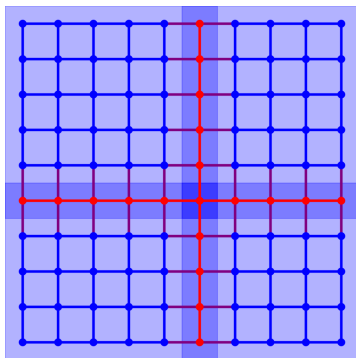
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Abstract Schwarz Preconditioners

Local Preconditioner \hat{A}_i



Adjacency graph G



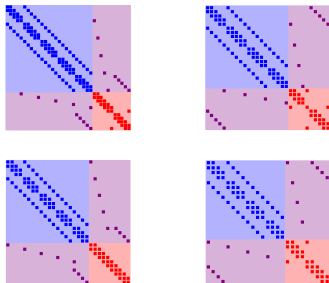
$$\mathcal{A} = \sum_{i=1}^N \mathcal{R}_i^T \mathcal{A}_i \mathcal{R}_i$$

$$\mathcal{A}^{-1} \approx \mathcal{M} = \sum_{i=1}^N \mathcal{R}_i^T \hat{\mathcal{A}}_i^\dagger \mathcal{R}_i$$

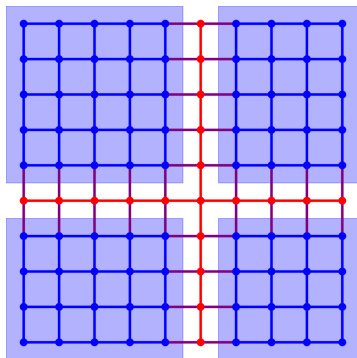
$\hat{\mathcal{A}}_i$ is a local SPSD matrix *close to* \mathcal{A} inside the subdomain.

Substructuring Methods

Local Matrix \mathcal{A}_i



Adjacency graph G

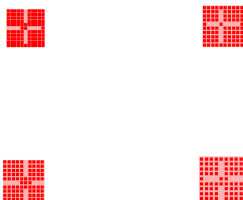


- We factorize $\mathcal{A}_{\mathcal{I}_i\mathcal{I}_i}$ and compute $\mathcal{S}_i = \mathcal{A}_{\Gamma_i\Gamma_i} - \mathcal{A}_{\Gamma_i\mathcal{I}_i}\mathcal{A}_{\mathcal{I}_i\mathcal{I}_i}^{-1}\mathcal{A}_{\mathcal{I}_i\Gamma_i}$

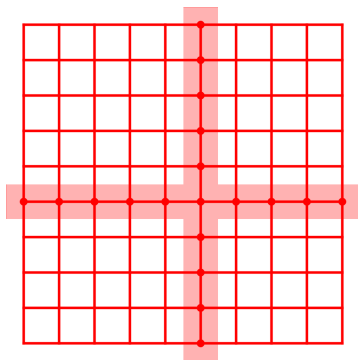
$$\mathcal{A}_i = \begin{pmatrix} \mathcal{A}_{\mathcal{I}_i\mathcal{I}_i} & \mathcal{A}_{\mathcal{I}_i\Gamma_i} \\ \mathcal{A}_{\Gamma_i\mathcal{I}_i} & \mathcal{A}_{\Gamma_i\Gamma_i} \end{pmatrix}$$

Substructuring Methods

Local Schur \mathcal{S}_i



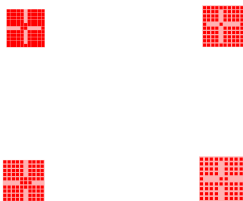
Adjacency graph G



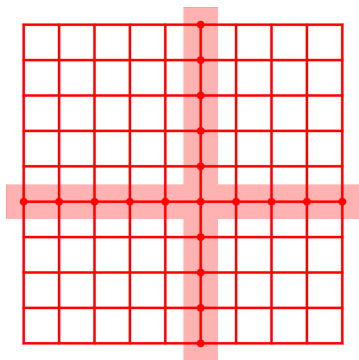
- We factorize $\mathcal{A}_{\mathcal{I}_i\mathcal{I}_i}$ and compute $\mathcal{S}_i = \mathcal{A}_{\Gamma_i\Gamma_i} - \mathcal{A}_{\Gamma_i\mathcal{I}_i}\mathcal{A}_{\mathcal{I}_i\mathcal{I}_i}^{-1}\mathcal{A}_{\mathcal{I}_i\Gamma_i}$
- Now, on each subdomain, the whole local problem is condensed onto the interface (dense matrix)

Substructuring Methods

Local Schur \mathcal{S}_i



Adjacency graph G



- We solve the interface problem $\mathcal{S}x_{\Gamma} = f = b_{\Gamma} - \mathcal{A}_{\Gamma I} \mathcal{A}_{II}^{-1} b_I$ with a **preconditioned** Krylov method
 - $x_{\mathcal{I}_i} = \mathcal{A}_{\mathcal{I}_i \mathcal{I}_i}^{-1} (b_{\mathcal{I}_i} - \mathcal{A}_{\mathcal{I}_i \Gamma_i} x_{\Gamma_i})$

Why use the Schur?

- \mathcal{S} is smaller than \mathcal{A} and better conditioned ☺

Problem

- $\mathcal{S}_i = \mathcal{A}_{\Gamma_i \Gamma_i} - \mathcal{A}_{\Gamma_i \mathcal{I}_i} \mathcal{A}_{\mathcal{I}_i \mathcal{I}_i}^{-1} \mathcal{A}_{\mathcal{I}_i \Gamma_i}$ is dense
 - increased memory consumption ☹

Solution

- don't compute \mathcal{S}_i explicitly & use sparsification/compression
- use an approximate Schur $\tilde{\mathcal{S}} = \sum_{i=1}^N \mathcal{R}_{\Gamma_i}^T \tilde{\mathcal{S}}_i \mathcal{R}_{\Gamma_i}$ where $\tilde{\mathcal{S}}_i$ is SPSD

$$\text{and } \exists \omega_-, \omega_+ > 0, \quad \forall v \in V \quad \omega_- \leq \frac{v^T \tilde{\mathcal{S}} v}{v^T \mathcal{S} v} \leq \omega_+.$$

Now, we search a preconditioner for $\tilde{\mathcal{S}}$ instead of \mathcal{S} .

Abstract Schwarz \rightarrow use any local preconditioner \hat{S}_i

- $\mathcal{M}_1 = \sum_{i=1}^N \mathcal{R}_{\Gamma_i}^T \hat{S}_i^\dagger \mathcal{R}_{\Gamma_i}$
 - $\hat{S}_i = \dots$ should be SPSD
 - $\hat{S}_i = D_i^{-1} S_i D_i^{-1}$ for Neumann-Neumann (NN)
 - $\hat{S}_i = \mathcal{R}_{\Gamma_i} S \mathcal{R}_{\Gamma_i}^T$ for Additive Schwarz (AS)

Generalized Abstract Schwarz Preconditioners

Abstract Schwarz \rightarrow use any local preconditioner \hat{S}_i

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2-level Abstract Schwarz

2-level tools

V_0	Coarse space
$\mathcal{M}_0 = V_0 (V_0^T \mathcal{S} V_0)^\dagger V_0^T$	Coarse solve
$\mathcal{P}_0 = \mathcal{M}_0 \mathcal{S}$	Projector onto the coarse space

- 2-level AS: $\mathcal{M}_D = \mathcal{M}_0 + (\mathcal{I} - \mathcal{P}_0) \mathcal{M}_1 (\mathcal{I} - \mathcal{P}_0)^T$

Generalized Abstract Schwarz Preconditioners

Abstract Schwarz \rightarrow use any local preconditioner \hat{S}_i

- $\mathcal{M}_1 = \sum_{i=1}^N \mathcal{R}_{\Gamma_i}^T \hat{S}_i^\dagger \mathcal{R}_{\Gamma_i}$
 - $\hat{S}_i = \dots$ should be SPSP
 - $\hat{S}_i = D_i^{-1} \tilde{S}_i D_i^{-1}$ for Neumann-Neumann (NN)
 - $\hat{S}_i = \mathcal{R}_{\Gamma_i} \tilde{S} \mathcal{R}_{\Gamma_i}^T$ for Additive Schwarz (AS)

Generalized \rightarrow use \tilde{S} instead of S

2-level tools

V_0	Coarse space
$\tilde{\mathcal{M}}_0 = V_0 (V_0^T \tilde{S} V_0)^\dagger V_0^T$	Coarse solve
$\tilde{\mathcal{P}}_0 = \tilde{\mathcal{M}}_0 \tilde{S}$	Projector onto the coarse space

- 2-level GAS: $\tilde{\mathcal{M}}_D = \tilde{\mathcal{M}}_0 + (\mathcal{I} - \tilde{\mathcal{P}}_0) \mathcal{M}_1 (\mathcal{I} - \tilde{\mathcal{P}}_0)^T$

Common GAS Preconditioners

Generalized Neumann-Neumann Preconditioner

[Le Tallec & Vidrascu 98]

$$\tilde{\mathcal{M}}_{NN} = \tilde{\mathcal{M}}_0 + (\mathcal{I} - \tilde{\mathcal{P}}_0) \sum_{i=1}^N \mathcal{R}_{\Gamma_i}^T (D_i^{-1} \tilde{\mathcal{S}}_i D_i^{-1})^\dagger \mathcal{R}_{\Gamma_i} (\mathcal{I} - \tilde{\mathcal{P}}_0)^T$$
$$\lambda_{\min}(\tilde{\mathcal{M}}_{NN} \mathcal{S}) \geq \frac{1}{\omega_+}$$

Generalized Additive Schwarz Preconditioner

[MaPHYs]

$$\tilde{\mathcal{M}}_{AS} = \tilde{\mathcal{M}}_0 + (\mathcal{I} - \tilde{\mathcal{P}}_0) \sum_{i=1}^N \mathcal{R}_{\Gamma_i}^T (\mathcal{R}_{\Gamma_i} \tilde{\mathcal{S}} \mathcal{R}_{\Gamma_i}^T)^{-1} \mathcal{R}_{\Gamma_i} (\mathcal{I} - \tilde{\mathcal{P}}_0)^T$$
$$\lambda_{\max}(\tilde{\mathcal{M}}_{AS} \mathcal{S}) \leq \frac{\max_{i \leq N} (N_i + 1)}{\omega_-} = \frac{N_c}{\omega_-}$$

$N_i = \#\{j \neq i, \mathcal{R}_{\Gamma_i} \tilde{\mathcal{S}} \mathcal{R}_{\Gamma_j}^T \neq 0\}$ is the number of neighbors of subdomain i .

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Convergence Theorem for GAS

Theorem

$$\kappa(\tilde{\mathcal{M}}_D \mathcal{S}) \leq \frac{\omega_+}{\omega_-} \left(1 + \max_{i \leq N} \sup_{v \in \tilde{V}_i^\perp} \frac{|v|_{\hat{\mathcal{S}}_i}^2}{|v|_{D_i^{-1} \tilde{\mathcal{S}}_i D_i^{-1}}^2} \right) \max_{i \leq N} (N_i + 1) \sup_{v \in \hat{V}_i^\perp} \frac{|v|_{\mathcal{R}_{\Gamma_i} \tilde{\mathcal{S}} \mathcal{R}_{\Gamma_i}^T}^2}{|v|_{\hat{\mathcal{S}}_i}^2}$$

where $\tilde{V}_i^\perp = (D_i^{-1} \tilde{\mathcal{S}}_i D_i^{-1} V_i^0)^\perp$, $\hat{V}_i^\perp = (\hat{\mathcal{S}}_i V_i^0)^\perp$, $V_0 = \sum_{i=1}^N \mathcal{R}_{\Gamma_i}^T V_i^0$ and

$$\tilde{\mathcal{M}}_D = \tilde{\mathcal{M}}_0 + (\mathcal{I} - \tilde{\mathcal{P}}_0) \sum_{i=1}^N \mathcal{R}_{\Gamma_i}^T \hat{\mathcal{S}}_i^\dagger \mathcal{R}_{\Gamma_i} (\mathcal{I} - \tilde{\mathcal{P}}_0)^T$$

Convergence Theorem for GAS

Theorem

$$\kappa(\tilde{\mathcal{M}}_D \mathcal{S}) \leq \frac{\omega_+}{\omega_-} \left(1 + \max_{i \leq N} \sup_{v \in \tilde{V}_i^\perp} \frac{|v|_{\hat{\mathcal{S}}_i}^2}{|v|_{D_i^{-1} \tilde{\mathcal{S}}_i D_i^{-1}}^2} \right) \max_{i \leq N} (N_i + 1) \sup_{v \in \hat{V}_i^\perp} \frac{|v|_{\mathcal{R}_{\Gamma_i} \tilde{\mathcal{S}} \mathcal{R}_{\Gamma_i}^T}^2}{|v|_{\hat{\mathcal{S}}_i}^2}$$

where $\tilde{V}_i^\perp = (D_i^{-1} \tilde{\mathcal{S}}_i D_i^{-1} V_i^0)^\perp$, $\hat{V}_i^\perp = (\hat{\mathcal{S}}_i V_i^0)^\perp$, $V_0 = \sum_{i=1}^N \mathcal{R}_{\Gamma_i}^T V_i^0$ and

$$\tilde{\mathcal{M}}_D = \tilde{\mathcal{M}}_0 + (\mathcal{I} - \tilde{\mathcal{P}}_0) \sum_{i=1}^N \mathcal{R}_{\Gamma_i}^T \hat{\mathcal{S}}_i^\dagger \mathcal{R}_{\Gamma_i} (\mathcal{I} - \tilde{\mathcal{P}}_0)^T$$

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Outline of the proof

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The (few) vectors where $\hat{\mathcal{S}}_i$ is far worse than AS or NN should be in the coarse space V_0 .

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Extending GenEO [Spillane 2012] for GAS

$$\kappa(\tilde{\mathcal{M}}_D \mathcal{S}) \leq \frac{\omega_+}{\omega_-} \left(1 + \max_{i \leq N} \sup_{v \in \tilde{V}_i^\perp} \frac{|v|_{\tilde{S}_i}^2}{|v|_{D_i^{-1} \tilde{S}_i D_i^{-1}}^2} \right) \max_{i \leq N} (N_i + 1) \sup_{v \in \hat{V}_i^\perp} \frac{|v|_{\mathcal{R}_{\Gamma_i} \tilde{S} \mathcal{R}_{\Gamma_i}^T}^2}{|v|_{\tilde{S}_i}^2}$$

- 1 Choose two thresholds $\alpha > 0$ and $\beta \geq 1$.

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- 1 Choose two thresholds $\alpha > 0$ and $\beta \geq 1$.
- 2 Solve locally the generalized eigenproblems

$$D_i^{-1} \tilde{S}_i D_i^{-1} p = \lambda \hat{S}_i p \quad \text{and} \quad \hat{S}_i p = \eta \mathcal{R}_{\Gamma_i} \tilde{S} \mathcal{R}_{\Gamma_i}^T p$$

for eigenvalues $\lambda \leq \alpha^{-1}$ and $\eta \leq (N_i + 1)\beta^{-1}$.

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- 3 Assemble the resulting coarse space $V_0 = \sum_{i=1}^N \mathcal{R}_{\Gamma_i}^T V_i^0$.

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Then:

$$\kappa(\tilde{\mathcal{M}}_D \mathcal{S}) \leq \frac{\omega_+}{\omega_-} (1 + \alpha) \beta.$$

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Convergence Theorem for AS,2

- In the Additive Schwarz case, we don't always need the projection step:

$$\tilde{\mathcal{M}}_{AS,2} = \tilde{\mathcal{M}}_0 + \sum_{i=1}^N \mathcal{R}_{\Gamma_i}^T (\mathcal{R}_{\Gamma_i} \tilde{\mathcal{S}} \mathcal{R}_{\Gamma_i}^T)^{-1} \mathcal{R}_{\Gamma_i}$$
$$\kappa(\tilde{\mathcal{M}}_{AS,2} \mathcal{S}) \leq \frac{\omega_+}{\omega_-} [N_c + 1 + \alpha(N_c + 2)] (N_c + 1)$$

where $N_c = \max N_i + 1$.

- The bound on the condition number is bigger (N_c^2 instead of N_c) ☺
- Each iteration is cheaper (one less matrix-vector product) ☺
- Possibility to overlap some computation and communications ☺

Step 1: Domain Decomposition

- $\mathcal{A} = \sum_{i=1}^N \mathcal{R}_i^T \mathcal{A}_i \mathcal{R}_i$

Step 2: Factorization

- Computation of $\mathcal{A}_{\mathcal{I}_i \mathcal{I}_i}^{-1}$ and $\mathcal{S}_i = \mathcal{A}_{\Gamma_i \Gamma_i} - \mathcal{A}_{\Gamma_i \mathcal{I}_i} \mathcal{A}_{\mathcal{I}_i \mathcal{I}_i}^{-1} \mathcal{A}_{\mathcal{I}_i \Gamma_i}$

Step 3: Preconditioner Setup

- $\mathcal{M}_{AS} = \sum_{i=1}^N \mathcal{R}_{\Gamma_i}^T (\mathcal{R}_{\Gamma_i} \mathcal{S} \mathcal{R}_{\Gamma_i}^T)^{-1} \mathcal{R}_{\Gamma_i}$

Step 4: Solve

- on Γ : *Krylov method* $\mathcal{S} x_\Gamma = f$ preconditioned with \mathcal{M}_{AS}

- on \mathcal{I} : *Direct method* $x_{\mathcal{I}_i} = \mathcal{A}_{\mathcal{I}_i \mathcal{I}_i}^{-1} (b_{\mathcal{I}_i} - \mathcal{A}_{\mathcal{I}_i \Gamma_i} x_\Gamma)$

Step 1: Domain Decomposition (Application level)

- $\mathcal{A} = \sum_{i=1}^N \mathcal{R}_i^T \mathcal{A}_i \mathcal{R}_i$

Step 2: Factorization

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Step 3: Preconditioner Setup

- $\mathcal{M}_{AS,2} = \mathcal{M}_0 + \sum_{i=1}^N \mathcal{R}_{\Gamma_i}^T (\mathcal{R}_{\Gamma_i} \mathcal{S} \mathcal{R}_{\Gamma_i}^T)^{-1} \mathcal{R}_{\Gamma_i}$

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3D Test problem

Heterogeneous diffusion

- $\nabla(K\nabla u) = 1$
- Alternating conductivity layers of 3 elements (ratio K between layers)
- Dirichlet on the left, Neumann elsewhere

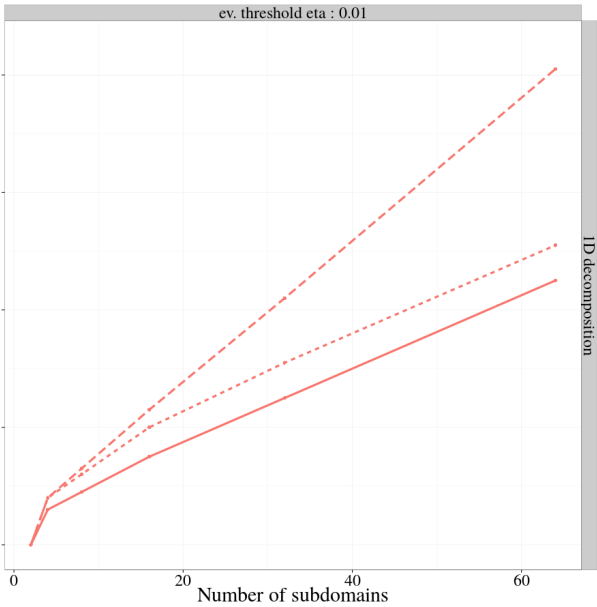
Domain decomposition

- $N \times 1 \times 1$ (1D decomposition)
- $N/2 \times 2 \times 1$ (2D decomposition)
- Constant subdomain size: $10 \times 10 \times 10$ elements

Implementation

- python/MPI

Number of iterations to achieve convergence

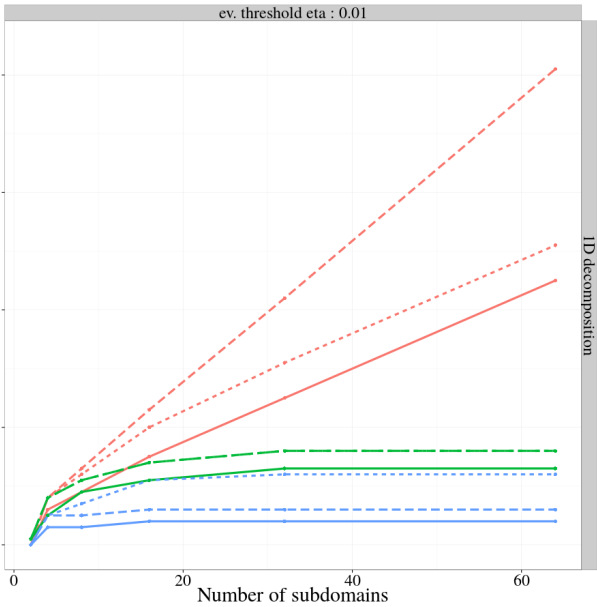


Number of subdomains

ID decomposition

- Heterogeneity K
- 1
- ⋯ 100
- - 10000
- Numerical method
- AS/S

Number of iterations to achieve convergence



ID decomposition

- Heterogeneity K
- 1
 - - - 100
 - - - 10000
- Numerical method
- AS/S
 - AS/S,2
 - AS/S,D

0

20

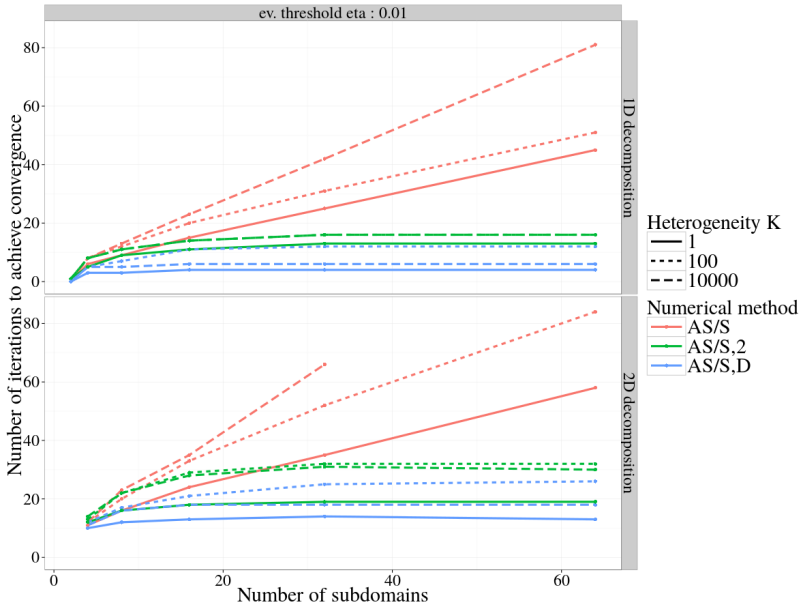
Number of subdomains

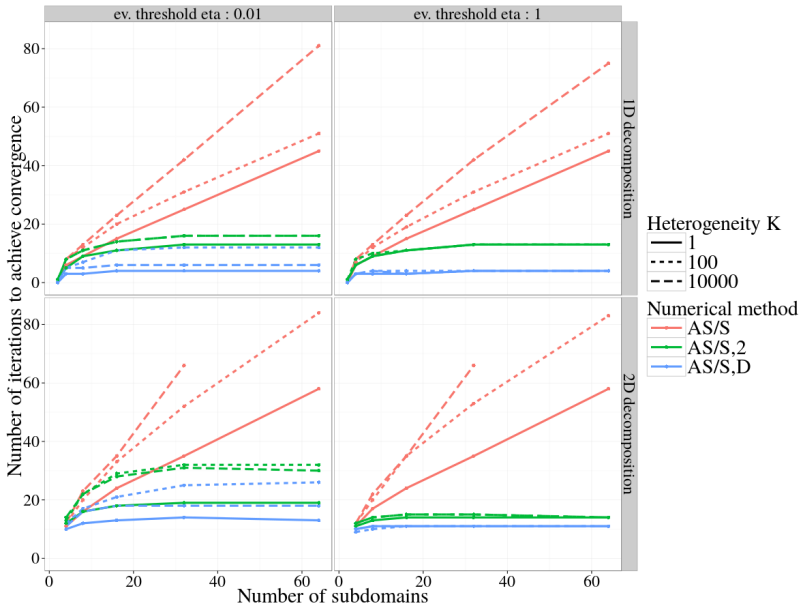
40

60

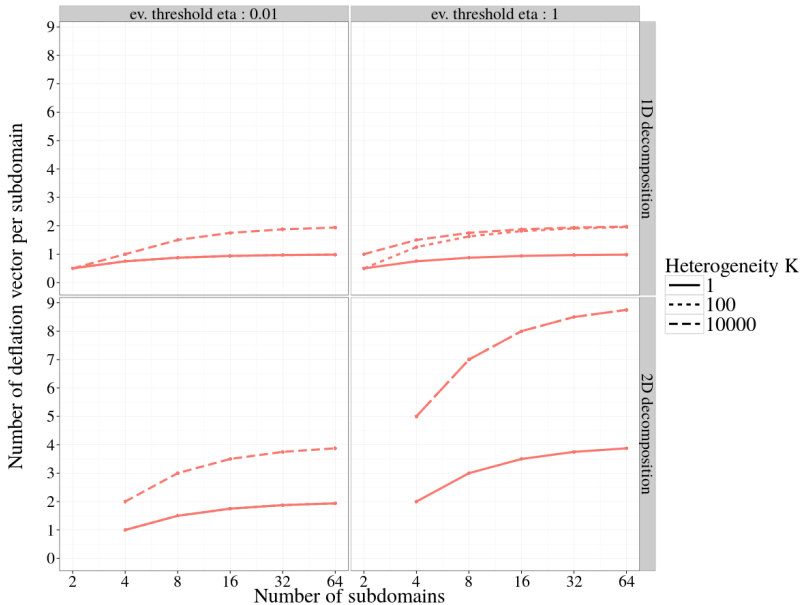
80

ev. threshold eta : 0.01

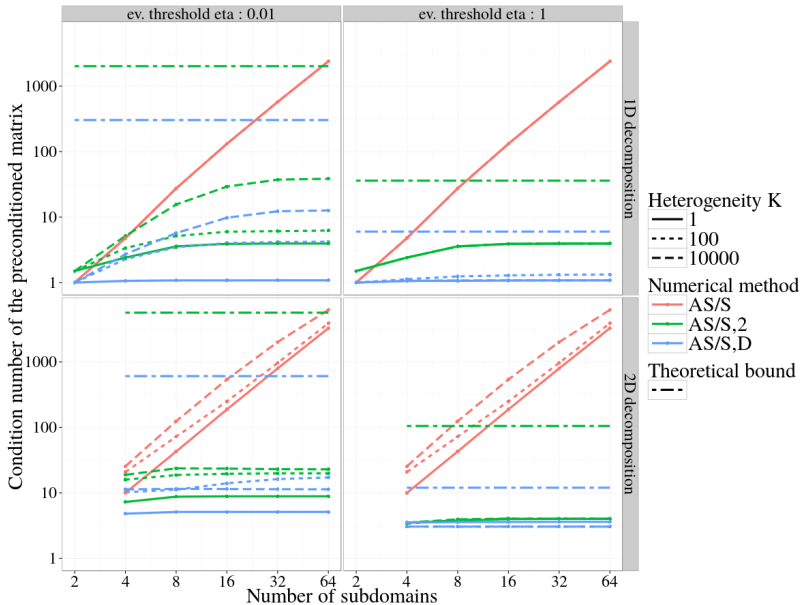


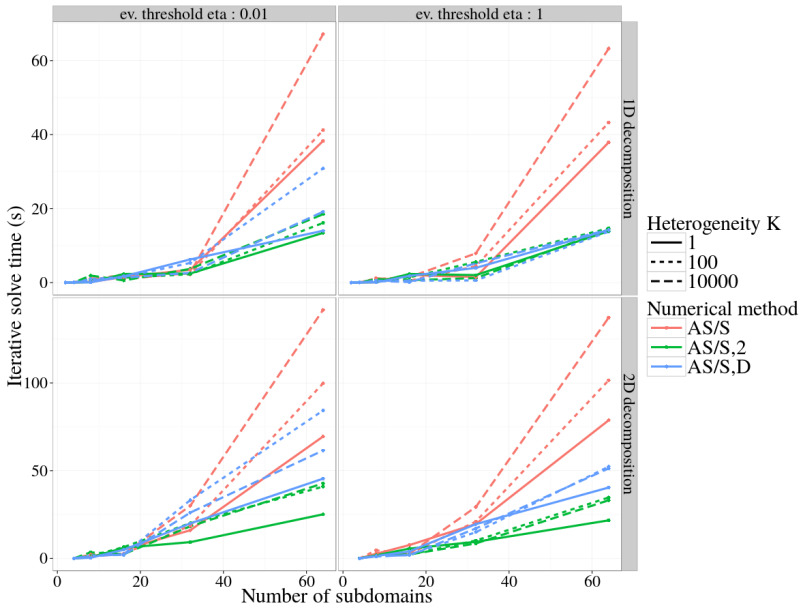


- The number of iterations is stabilized independently of K and N



- More difficult problems require a bigger coarse space





GenEO in MaPHyS

- Loosening the assumptions (\mathcal{A}_i SPSD and \mathcal{A} SPD)
- Implementation and test of the 2-level preconditioner on real applications

Other recent/ongoing efforts in MaPHyS

- Partitioning/balancing both interface and interior vertices (A. Casadei)
- Parallel analysis and dist. sub. API (M. Kuhn)
- \mathcal{H} -arithmetic for local solve (\mathcal{H} -PaStiX) and preconditioner (A. Falco, G. Pichon, Y. Harness)
- Numerical resilience policies (M. Zounon)
- Task-based implementation (S. Nakov)

Thanks for your attention!

Questions?

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