

A fully algebraic spectral coarse space for overlapping Schwarz methods

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Based on joint work with Axel Klawonn, Jascha Knepper, Martin Lanser, Janine Weber (University of Cologne), Oliver Rheinbach (TU Bergakademie Freiberg), Kathrin Smetana (Stevens Institute of Technology), and Olof Widlund (New York University)

Highly Heterogeneous Multiscale Problems

Highly heterogeneous multiscale problems appear in most areas of modern science and engineering, e.g., composite materials, porous media, and turbulent transport in high Reynolds number flow.



Microsection of a dual-phase steel. (Courtesy of Jörg Schröder, University of Duisburg-Essen, Germany; cooperation with ThyssenKrupp Steel.)



Groundwater flow: model 2 from the Tenth SPE Comparative Solution Project; cf. Christie and Blunt (2001).



Representation of the composition of a small segment of arterial walls; taken from O'Connell et al. (2008).

 \rightarrow The solution of such problems requires a **high spatial and temporal resolution** but also poses **challenges to the solvers**.

Highly Heterogeneous Model Problem

Consider the diffusion boundary value problem: find u such that

$$-\nabla \cdot (\alpha(x)\nabla u(x)) = f(x) \quad \text{in } \Omega,$$
$$u = 0 \qquad \text{on } \partial\Omega,$$

with a highly varying coefficient function α . The corresponding weak formulation is: find $u \in H_0^1(\Omega)$, such that

 $a_{\Omega}(u, v) = f(v) \qquad \forall v \in H^1_0(\Omega)$

with the bilinear form and linear functional

$$a_{\Omega}(u,v) := \int_{\Omega} \alpha(x) (\nabla u(x))^T \nabla v(x) \, dx \text{ and } f(v) := \int_{\Omega} f(x) v(x) \, dx.$$

Discretization using finite elements yields the linear system

Au = f

with stiffness matrix A, discrete solution u, and right hand side f.

Original microsection of a dual-phase steel



Binary coefficient function





Schwarz Domain Decomposition Preconditioners

Homogeneous Model Problem & Overlapping Domain Decomposition



Consider a homogeneous diffusion model problem $(\alpha(x) = 1)$:

$$-\Delta u = f \quad \text{in } \Omega = [0, 1]^2,$$
$$u = 0 \quad \text{on } \partial \Omega.$$

Discretization using finite elements yields the linear equation system

$$Au = f$$
.

Overlapping Domain Decomposition Overlapping Schwarz methods are based on overlapping decompositions of the computational domain Ω .

Overlapping subdomains $\Omega'_1, ..., \Omega'_N$ can be constructed by **recursively adding layers of elements** to nonoverlapping subdomains $\Omega_1, ..., \Omega_N$.



Nonoverlap. DD

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Two-Level Schwarz Preconditioners



Based on an overlapping domain decomposition, we define a one-level Schwarz operator

$$\boldsymbol{M}_{\text{OS-1}}^{-1}\boldsymbol{A} = \sum_{i=1}^{N} \boldsymbol{R}_{i}^{T} \boldsymbol{A}_{i}^{-1} \boldsymbol{R}_{i} \boldsymbol{A}$$

where \mathbf{R}_i and \mathbf{R}_i^T are restriction and prolongation operators corresponding to Ω'_i , and $\mathbf{A}_i := \mathbf{R}_i \mathbf{A} \mathbf{R}_i^T$.

Condition number estimate:

$$\kappa\left(\boldsymbol{M}_{\mathsf{OS-1}}^{-1}\boldsymbol{A}
ight)\leq C\left(1+rac{1}{H\delta}
ight)$$

with subdomain size H and the width of the overlap δ .

Adding a Lagrangian Coarse Space

The two-level overlapping Schwarz operator reads

$$\boldsymbol{M}_{\text{OS-2}}^{-1}\boldsymbol{A} = \underbrace{\boldsymbol{\Phi}\boldsymbol{A}_{0}^{-1}\boldsymbol{\Phi}^{\mathsf{T}}\boldsymbol{A}}_{\text{coarse level - global}} + \underbrace{\sum_{i=1}^{N}\boldsymbol{R}_{i}^{\mathsf{T}}\boldsymbol{A}_{i}^{-1}\boldsymbol{R}_{i}\boldsymbol{A}}_{\text{first level - local}},$$

where Φ contains the coarse basis functions and $A_0 := \Phi^T A \Phi$; cf., e.g., Toselli, Widlund (2005).

A Lagrangian coarse basis requires a coarse triangulation (geometric information) \rightarrow not algebraic

$$\Rightarrow \kappa \left(\textit{M}_{\mathsf{OS-2}}\textit{A}
ight) \leq C \left(1 + rac{\textit{H}}{\delta}
ight)$$

Extension-Based GDSW Coarse Spaces





In GDSW (Generalized–Dryja–Smith–Widlund) coarse spaces, the coarse basis functions are chosen as energy minimizing extensions of functions Φ_{Γ} that are defined on the interface Γ :

$$\boldsymbol{\Phi} = \left[\begin{array}{c} -\boldsymbol{A}_{II}^{-1} \boldsymbol{A}_{\Gamma I}^{T} \boldsymbol{\Phi}_{\Gamma} \\ \boldsymbol{\Phi}_{\Gamma} \end{array} \right] = \left[\begin{array}{c} \boldsymbol{\Phi}_{I} \\ \boldsymbol{\Phi}_{\Gamma} \end{array} \right]$$

The functions Φ_{Γ} are restrictions of the null space of global Neumann matrix to the edges, vertices, and, in 3D, faces (partition of unity) of the non-overlapping decomposition.



The condition number of the GDSW operator is bounded by

$$\kappa\left(\pmb{M}_{ ext{GDSW}}^{-1}\pmb{A}
ight) \leq C\left(1+rac{\pmb{H}}{\delta}
ight)\left(1+\log\left(rac{\pmb{H}}{\pmb{h}}
ight)
ight)^2;$$

cf. Dohrmann, Klawonn, Widlund (2008), Dohrmann, Widlund (2009, 2010, 2012).

 \rightarrow We only obtain the exponent 2 for very irregular subdomains.

\rightarrow Scalable and algebraic!

Weak Scalability up to 64 k MPI Ranks / 1.7 b Unknowns (3D Poisson; Juqueen)

GDSW vs RGDSW (Reduced Dimension)

Heinlein, Klawonn, Rheinbach, Widlund (2019).





FROSch (Fast and Robust Overlapping Schwarz) Framework in Trilinos





Software

- Object-oriented C++ domain decomposition solver framework with MPI-based distributed memory parallelization
- Part of Trilinos with support for both parallel linear algebra packages Epetra and Tpetra
- Node-level parallelization and performance portability on CPU and GPU architectures through Kokkos
- Accessible through unified Trilinos solver interface Stratimikos

Methoddology

- Parallel scalable multi-level Schwarz domain decomposition preconditioners
- Algebraic construction based on the parallel distributed system matrix
- Extension-based coarse spaces

Team (Active)

- Alexander Heinlein (TU Delft)
- Siva Rajamanickam (Sandia)
- Friederike Röver (TUBAF)

- Axel Klawonn (Uni Cologne)
- Oliver Rheinbach (TUBAF)
- Ichitaro Yamazaki (Sandia)

Observations for Heterogeneous Problems

Heterogeneous Problem – Random Distribution

Problem Configuration

Diffusion problem with random binary coefficient α : find u such that

$$-\nabla \cdot (\alpha(x)\nabla u(x)) = f(x)$$
 in Ω ,

u = 0 on $\partial \Omega$.

Domain decomposition into 10×10 subdomains with H/h = 10and overlap 1*h*.



Prec.	its.	κ		
-	>2 000	$4.51\cdot 10^8$		
$M_{ m OS-1}^{-1}$	>2 000	$4.51\cdot 10^8$		
$M_{ m OS-2}^{-1}$	586	$5.56\cdot 10^5$		

Observations

→ For heterogeneous coefficients, the condition number clearly deteriorates. It depends on the contrast of the coefficient function

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Observations

→ For heterogeneous coefficients, the condition number clearly deteriorates. It depends on the contrast of the coefficient function

Let us consider some **pathological cases** to better understand the behavior of overlapping Schwarz methods for heterogeneous coefficient distributions.

Heterogeneous Problem – Heterogeneities Only Inside Subdomains

Problem Configuration

Diffusion problem with random binary coefficient α without high coefficients touching the interface: find u such that

$$-\nabla \cdot (\alpha(x)\nabla u(x)) = f(x)$$
 in Ω ,

u = 0 on $\partial \Omega$.

Domain decomposition into 10×10 subdomains with H/h = 10and overlap 1h.



Prec.	its.	к		
-	>2 000	$7.99\cdot 10^8$		
$M_{ m OS-1}^{-1}$	64	133.16		
$M_{ m OS-2}^{-1}$	78	139.15		

- $\rightarrow\,$ In the first level, we solve the subdomain problems exactly
 - \Rightarrow Jumps inside the subdomains are **not problematic**
- $\rightarrow\,$ Classical one- and two-level methods are robust for jumps within the subdomains

Heterogeneous Problem – Channels Across the Interface

Problem Configuration

Diffusion problem with binary coefficient α with high contrast channels: find u such that

$$-\nabla \cdot (\alpha(x)\nabla u(x)) = f(x)$$
 in Ω ,

u = 0 on $\partial \Omega$.

Domain decomposition into 10×10 subdomains with H/h = 10and overlap 1*h*.



Prec.	δ	its.	κ
-		987	$8.03 \cdot 10^8$
	1h	259	$83.34\cdot 10^6$
$M_{ m OS-1}^{-1}$	2h	216	$5.56\cdot 10^6$
	3h	37	91.97
	1h	163	$4.70\cdot 10^5$
$M_{\rm OS-2}^{-1}$	2h	128	$3.24\cdot 10^5$
	3h	44	91.94

- → In case the channels with high coefficient lie completely within the overlapping subdomains, the method is again robust. Otherwise, the convergence deteriorates.
- → In general, it is not practical to extend the overlap until each high coefficient component lies completely within one overlapping subdomain.

Heterogeneous Problem – Inclusions at the Vertices

Problem Configuration

Diffusion problem with **binary coefficient** α with **high coefficient inclusions at the vertices**: find u such that

$$-\nabla \cdot (\alpha(x)\nabla u(x)) = f(x) \quad \text{in } \Omega,$$

u = 0 on $\partial \Omega$.

Domain decomposition into 10×10 subdomains with H/h = 10 and overlap 1*h*.



Prec.	its.	κ
-	874	$1.35\cdot 10^9$
$M_{ m OS-1}^{-1}$	163	$4.06\cdot 10^7$
$M_{\rm OS-2}^{-1}$	138	$1.07\cdot 10^6$
M_{MsFEM}^{-1}	24	8.05

- → In general, one- or two-level Schwarz methods are not robust for high coefficient inclusions at the vertices
- → Robustness can be retained by using multiscale finite element method (MsFEM) type functions instead; cf. Hou (1997), Efendiev and Hou (2009)



Heterogeneous Problem – Channels & Inclusions

Problem Configuration

Diffusion problem with **binary coefficient** α with **channels and vertex inclusions**: find u such that

$$-\nabla \cdot (\alpha(x)\nabla u(x)) = f(x)$$
 in Ω ,

u = 0 on $\partial \Omega$.

Domain decomposition into 10×10 subdomains with H/h = 10and overlap 1*h*.



Prec.	its.	κ
-	1708	$1.16\cdot 10^9$
$M_{\rm OS-1}^{-1}$	447	$4.17\cdot 10^7$
$M_{\rm OS-2}^{-1}$	268	$1.10\cdot 10^6$
M_{MsFEM}^{-1}	117	$4.34\cdot 10^5$

- \rightarrow All of the aforementioned approaches fail for this example.
- → Since we were able to deal with the vertex inclusions, the problem has to be related to the edges. How can we construct suitable coarse basis functions to deal with coefficient jumps at the edges?

Heterogeneous Problem – Channels & Inclusions

Problem Configuration

Diffusion problem with **binary coefficient** α with **channels and vertex inclusions**: find u such that

$$-\nabla \cdot (\alpha(x)\nabla u(x)) = f(x)$$
 in Ω ,

u = 0 on $\partial \Omega$.

Domain decomposition into 10×10 subdomains with H/h = 10and overlap 1*h*.



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Observations

- → All of the aforementioned approaches fail for this example.
- → Since we were able to deal with the vertex inclusions, the problem has to be related to the edges. How can we construct suitable coarse basis functions to deal with coefficient jumps at the edges?

Let us now discuss the **Schwarz theory** in order to construct a **robust coarse space for arbitrary heterogeneous problems**.

Influence of Heterogeneities on the Schwarz Theory

Schwarz Theory

In order to establish a condition number bound for $\kappa \left(M_{ad}^{-1} A \right)$ based on the abstract Schwarz framework, we have to verify the following three assumptions:

Assumption 1: Stable Decomposition

There exists a constant C_0 such that, for every $u \in V$, there exists a decomposition $u = \sum_{i=0}^{N} \mathbf{R}_i^T u_i$, $u_i \in V_i$, with

$$\sum_{i=0}^{N} a_i(u_i, u_i) \le C_0^2 a(u, u).$$

Assumption 2: Strengthened Cauchy-Schwarz Inequality

There exist constants $0 \le \epsilon_{ij} \le 1$, $1 \le i, j \le N$, such that

$$\left| \mathsf{a}(\mathbf{R}_{i}^{\mathsf{T}}u_{i},\mathbf{R}_{j}^{\mathsf{T}}u_{j}) \right| \leq \epsilon_{ij} \left(\mathsf{a}(\mathbf{R}_{i}^{\mathsf{T}}u_{i},\mathbf{R}_{i}^{\mathsf{T}}u_{j}) \right)^{1/2} \left(\mathsf{a}(\mathbf{R}_{j}^{\mathsf{T}}u_{j},\mathbf{R}_{j}^{\mathsf{T}}u_{j}) \right)^{1/2}$$

for $u_i \in V_i$ and $u_j \in V_j$. (Consider $\mathcal{E} = (\varepsilon_{ij})$ and $\rho(\mathcal{E})$ its spectral radius)

Assumption 3: Local Stability

There exists $\omega < 0$, such that

$$a(\mathbf{R}_i^T u_i, \mathbf{R}_i^T u_i) \leq \omega a_i(u_i, u_i), \quad u_i \in \operatorname{range}\left(\tilde{P}_i\right), \quad 0 \leq i \leq N.$$

Schwarz Theory

General Condition Number Bound

With Assumption 1-3, we have

$$\kappa\left(\boldsymbol{M}_{\mathrm{ad}}^{-1}\boldsymbol{A}\right) \leq C_{0}^{2}\omega\left(\rho\left(\boldsymbol{\varepsilon}\right)+1\right)$$

for

$$\mathbf{M}_{\mathrm{ad}}\mathbf{A} = \sum_{0=1}^{N} \mathbf{R}_{i}^{\mathsf{T}} \mathbf{A}_{i}^{-1} \mathbf{R}_{i} \mathbf{A};$$

see, e.g., Toselli, Wildund (2005).

To obtain a condition number bound for a specific additive Schwarz preconditioner, we have to estimate ω , $\rho(\&)$, and C_0^2 .

The constants ω and $\rho(\mathcal{E})$ can often easily be bounded.

Exact Solvers

If we choose the local bilinear forms as

$$a_i(u_i, u_i) := a(\mathbf{R}_i^T u_i, \mathbf{R}_i^T u_i)$$

we obtain $\boldsymbol{A}_i = \boldsymbol{R}_i \boldsymbol{A} \boldsymbol{R}_i^T$ and $\omega = 1$.

 \rightarrow For exact exact local and coarse solvers, ω does not depend on the coefficient.

Coloring Constant



The spectral radius $\rho(\mathcal{E})$ is bounded by the number of colors N^c of the domain decomposition.

 $\rightarrow N^c$ depends only on the domain decomposition but not on the coefficient function.

Stable Decomposition – GDSW Coarse Space

In order to prove the existence of a stable decomposition

$$u = \sum_{i=0}^{N} \boldsymbol{R}_i^{\mathsf{T}} u_i$$
 and $\sum_{i=0}^{N} a_i(u_i, u_i) \leq C_0^2 \boldsymbol{a}(u, u)$

for a specific coarse space, the most essential estimate is

$$a_0(u_0, u_0) \leq C_0^2 a(u, u).$$

 $\Rightarrow C_0^2$ will arise in the condition number estimate.

Homogeneous Diffusion

In the case of a diffusion problem with a constant coefficient,

$$-\Delta u = f \quad \text{in } \Omega,$$
$$u = 0 \quad \text{on } \partial \Omega$$

this just corresponds to proving

$$|u_0|^2_{H^1(\Omega)} \le C_0^2 |u|^2_{H^1(\Omega)}$$

GDSW Coarse Space

In the proof for the GDSW preconditioner, we have $u_0(x) = \sum_{U} u(V)\theta_V(x) + \sum_{e} \bar{u}_{\mathcal{E}}\theta_{\mathcal{E}}(x).$

Then, using an inverse inequality for θ_V and a discrete Sobolev inequality for $u - \bar{u}_{\Omega_i}$,

$$\left|\left(u(\mathcal{V})-\bar{u}_{\Omega_{i}}
ight) heta_{\mathcal{V}}
ight|_{a,\Omega_{i}}^{2}\leq C(1+\log(H/h))\left|\left|u-\bar{u}_{\Omega_{i}}
ight|
ight|_{H^{1}(\Omega_{i})}^{2}
ight|$$

and, similarly (estimating θ_{δ} adds another $(1 + \log(H/h)))$,

$$\left| \left(\bar{u}_{\delta} - \bar{u}_{\Omega_i} \right) \theta_{\delta} \right|_{\mathfrak{a},\Omega_i}^2 \leq C (1 + \log(H/h))^2 \left\| u - \bar{u}_{\Omega_i} \right\|_{H^1(\Omega_i)}^2.$$

Using a Poincaré inequality, we then obtain $|u|^2_{a,\Omega_i}$.



Discrete harmonic GDSW basis functions θ_V and θ_δ .

Stable Decomposition – GDSW Coarse Space

In order to prove the existence of a stable decomposition

$$u = \sum_{i=0}^N \textbf{\textit{R}}_i^{\mathcal{T}} u_i ext{ and } \sum_{i=0}^N a_i(u_i,u_i) \leq C_0^2 a(u,u)$$

for a specific coarse space, the most essential estimate is

$$a_0(u_0, u_0) \leq C_0^2 a(u, u).$$

 $\Rightarrow C_0^2$ will arise in the condition number estimate.

Heterogeneous Diffusion

In the case of a heterogeneous diffusion problem,

$$-\nabla \cdot (A(x) \cdot \nabla u) = f \quad \text{in } \Omega,$$
$$u = 0 \quad \text{on } \partial \Omega$$

we have $a(u, v) = \int_{\Omega} A(x) \nabla u \cdot \nabla v \, dx$ and the constants may depend on the contrast $\alpha_{\max} / \alpha_{\min}$.

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In the proof for the GDSW preconditioner, we have $u_0(x) = \sum_{U} u(V)\theta_V(x) + \sum_{e} \bar{u}_{\mathcal{E}}\theta_{\mathcal{E}}(x).$

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ight) heta_{\mathcal{V}}
ight|_{a,\Omega_{i}}^{2}\leq C(1+\log(H/h))\left|\left|u-\bar{u}_{\Omega_{i}}
ight|
ight|_{H^{1}(\Omega_{i})}^{2}
ight|$$

and, similarly (estimating θ_{δ} adds another $(1 + \log(H/h)))$,

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Using a Poincaré inequality, we then obtain $|u|^2_{a,\Omega_i}$.



Discrete harmonic GDSW basis functions θ_V and $\theta_{\mathcal{E}}$.

Stable Decomposition – Adaptive Coarse Spaces

In order to prove the existence of a stable decomposition

$$u = \sum_{i=0}^{N} \boldsymbol{R}_i^{\mathsf{T}} u_i$$
 and $\sum_{i=0}^{N} a_i(u_i, u_i) \leq C_0^2 \boldsymbol{a}(u, u)$

for a specific coarse space, the most essential estimate is

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 $\Rightarrow C_0^2$ will arise in the condition number estimate.

Heterogeneous Diffusion

In the case of a heterogeneous diffusion problem,

 $-\nabla \cdot (A(x) \cdot \nabla u) = f \quad \text{in } \Omega,$ $u = 0 \quad \text{on } \partial \Omega,$

we have $a(u, v) = \int_{\Omega} A(x) \nabla u \cdot \nabla v \, dx$ and the constants may depend on the contrast $\alpha_{\max}/\alpha_{\min}$. \Rightarrow Remove dependence

Idea of Adaptive Coarse Spaces

Ensure

$$a(u_0, u_0) \leq C_0^2 a(u, u)$$

by introducing two bilinear forms $c(\cdot, \cdot)$ and $d(\cdot, \cdot)$ with

$$a(u_0, u_0) \leq C_1 d(u_0, u_0)$$
 (high energy)

and

 $c(u_0, u_0) \leq C_2 a(u, u)$, (low energy)

where C_1 and C_2 are independent of the coefficient function and $u_0 := l_0 u$ is a suitable coarse function. Then, we enhance the coarse space by all eigenvectors with eigenvalues below a tolerance *tol* of the generalized eigenvalue problem

$$d(v,w) = \lambda c(v,w)$$

and obtain

 $a(u_0, u_0) \leq C_1 \ d(u_0, u_0) \leq C_1 \ tol \ c(u_0, u_0) \leq C_1 \ C_2 \ tol \ a(u, u)$

without applying a Poincaré inequality. In practice, eigenvalue problem is partitioned into many local eigenvalue problems \rightarrow parallelization!

Stable Decomposition – Adaptive Coarse Spaces

In order to prove the existence of a stable decomposition

$$u = \sum_{i=0}^N \textit{R}_i^{\mathcal{T}} u_i ext{ and } \sum_{i=0}^N a_i(u_i, u_i) \leq C_0^2 \textit{a}(u, u)$$

for a specific coarse space, the most essential estimate is

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Heterogeneous Diffusion

In the case of a heterogeneous diffusion problem,

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we have $a(u, v) = \int_{\Omega} A(x) \nabla u \cdot \nabla v \, dx$ and the constants may depend on the contrast $\alpha_{\max} / \alpha_{\min}$.

Idea of Adaptive Coarse Spaces

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$$a(u_0, u_0) \leq C_0^2 a(u, u)$$

by introducing two bilinear forms $c(\cdot, \cdot)$ and $d(\cdot, \cdot)$ with

$$a(u_0, u_0) \leq C_1 d(u_0, u_0)$$
 (high energy)

and

$$c(u_0, u_0) \leq C_2 a(u, u),$$
 (low energy)

where C_1 and C_2 are independent of the coefficient function and $u_0 := I_0 u$ is a suitable coarse function. Then, In practice, it is sufficient if C_1 and C_2 depend on either

- α_{\min} or
- α_{max}.

 \rightarrow In the algebraic variant, C_2 depends only on α_{\min} .

 $\mathsf{a}(u_0, u_0) \leq C_1 \, \mathsf{d}(u_0, u_0) \leq C_1 \, \mathsf{tol} \, \mathsf{c}(u_0, u_0) \leq C_1 \, C_2 \, \mathsf{tol} \, \mathsf{a}(u, u)$

without applying a Poincaré inequality. In practice, eigenvalue problem is partitioned into many local eigenvalue problems \rightarrow parallelization!

Adaptive Coarse Spaces – OS-ACMS, AGDSW, and a Fully Algebraic Adaptive Coarse Space This list is not exhaustive:

- FETI & Neumann-Neumann: Bjørstad and Krzyzanowski (2002); Bjørstad, Koster, and Krzyzanowski (2001); Rixen and Spillane (2013); Spillane (2015, 2016)
- BDDC & FETI-DP: Mandel and Sousedík (2007); Sousedík (2010); Sístek, Mandel, and Sousedík (2012); Dohrmann and Pechstein (2013, 2016); Klawonn, Radtke, and Rheinbach (2014, 2015, 2016); Klawonn, Kühn, and Rheinbach (2015, 2016, 2017); Kim and Chung (2015); Kim, Chung, and Wang (2017); Beirão da Veiga, Pavarino, Scacchi, Widlund, and Zampini (2017); Calvo and Widlund (2016); Oh, Widlund, Zampini, and Dohrmann (2017)
- Overlapping Schwarz: Galvis and Efendiev (2010, 2011); Nataf, Xiang, Dolean, and Spillane (2011); Spillane, Dolean, Hauret, Nataf, Pechstein, and Scheichl (2011); Gander, Loneland, and Rahman (preprint 2015); Eikeland, Marcinkowski, and Rahman (preprint 2016); Marcinkowski and Rahman (2018); Al Daas, Grigori, Jolivet, Tournier (2021); Bastian, Scheichl, Seelinger, and Strehlow (2022); Spillane (preprint 2021, preprint 2021); Bootland, Dolean, Graham, Ma, Scheichl (preprint 2021)
- Approaches for overlapping Schwarz methods in this talk:
 - OS-ACMS: Heinlein, Klawonn, Knepper, Rheinbach (2018)
 - AGDSW: Heinlein, Klawonn, Knepper, Rheinbach (2019, 2019), Heinlein, Klawonn, Knepper, Rheinbach Widlund (2022)
 - Fully Algebraic Coarse Space: Heinlein and Smetana (Preprint: arXiv:2207.05559)

There is also related work on multigrid methods, such as AMGe by Brezina, Cleary, Falgout, Henson, Jones, Manteuffel, McCormick, Ruge (2000).

OS-ACMS – An Adaptive Coarse Space Based on the ACMS Discretization

As in the ACMS finite element space, we construct a coarse space composed of **MsFEM-type nodal and coupling basis functions**. However, in order to obtain a robust coarse space, the construction has to be slightly **modified**; see **Heinlein**, **Klawonn**, **Knepper**, **Rheinbach** (2018).



We define the interface values as follows:

$$\begin{split} \varphi_{\mathbf{v}}(\mathbf{v}') &= \delta_{\mathbf{v},\mathbf{v}'} & \forall \mathbf{v}' \in \mathcal{V} \quad (\textit{Kronecker property}) \\ \varphi_{\mathbf{v}}|_{e} &= E_{\partial e \to \Omega_{e}} \left(\varphi_{\mathbf{v}}|_{\partial e}\right) \quad \forall e \in \mathcal{E} \quad (\textit{Energy min. ext.}) \end{split}$$

The interior values are then obtained by an energy minimizing extension into the interior:

$$\varphi_{\mathsf{v}} = \mathit{E}_{\Gamma \to \Omega}\left(\varphi_{\mathsf{v}}|_{\Gamma}\right)$$

Energy Minimizing Extensions

The energy minimizing extension $E_{\partial\Omega\to\Omega}(v)$ of the function v defined on $\partial\Omega$ is given by the solution of the boundary value problem:

$$\begin{aligned} a_{\Omega}(E_{\partial\Omega\to\Omega}\left(v\right),w) &= & 0 \quad \forall w\in V_{\Omega}^{0}, \\ E_{\partial\Omega\to\Omega}\left(v\right) &= & v \qquad \text{on } \partial\Omega. \end{aligned}$$

This is equivalent to solving

$$E_{\partial\Omega\to\Omega}\left(v\right) = \arg\min_{\substack{w\in V_{\Omega}\\ w_{\partial\Omega}=v}} a_{\Omega}\left(w,w\right).$$

OS-ACMS – An Adaptive Coarse Space Based on the ACMS Discretization

OS-ACMS Edge Basis Functions

Low energy extension $E_{\overline{e} \to \Omega_e}(\cdot)$



High energy extension $R_{e \to \Omega_e}(\cdot)$



Ext. into the interior



First, we solve the following eigenvalue problem for each edge $e \in \mathcal{E}$:

$$a_{\Omega_{e}}\left(E_{\overline{e}\rightarrow\Omega_{e}}\left(\tau_{e,*}\right),E_{\overline{e}\rightarrow\Omega_{e}}\left(\theta\right)\right)=\lambda_{e,*}a_{\Omega_{e}}\left(R_{e\rightarrow\Omega_{e}}\left(\tau_{e,*}\right),R_{e\rightarrow\Omega_{e}}\left(\theta\right)\right)\quad\forall\theta\in V_{e}^{0}$$

Then, we select all eigenfunctions $\tau_{e,*}$ with $\lambda_{e,*}$ below a **user-chosen threshold** *TOL*. We then extend $\tau_{e,*}$ by zero onto Γ and with minimum energy into Ω to obtain the corresponding basis functions:

$$\varphi_{e,*} = E_{\Gamma \to \Omega} \left(R_{e \to \Gamma} \left(\tau_{e,*} \right) \right)$$

Condition Number Bound

Using the coarse space $V_{\text{OS-ACMS}} = \{\varphi_v\} \cup \{\varphi_e\}$ in the two-level Schwarz preconditioner, we obtain

$$\kappa\left(\boldsymbol{M}_{ ext{OS-ACMS}}^{-1} \boldsymbol{A}
ight) \leq C\left(1/ ext{TOL}
ight),$$

where C is independent of H, h, and the contrast of the coefficient function α .

AGDSW – An Adaptive GDSW Coarse Space

The adaptive GDSW (AGDSW) coarse space is a related approach, which also depends on a partition of the domain decomposition interface into edges and vertices. It differs from OS-ACMS as follows:

- Instead of MsFEM functions, we use the much simpler and cheaper GDSW vertex basis functions
- The edge eigenvalue problem has to be modified accordingly

As a result, the AGDSW coarse space

always contains the classical GDSW coarse space.

Cf. Heinlein, Klawonn, Knepper, Rheinbach (2019, 2019, 2022).

AGDSW Vertex Basis Function

The interior values are then obtained by extending 1 be zero onto the remainder of the interface followed by an energy minimizing extension into the interior:

$$\varphi_{v} = E_{\Gamma \to \Omega} \left(R_{v \to \Gamma} \left(\mathbb{1}_{v} \right) \right)$$



AGDSW – An Adaptive GDSW Coarse Space

AGDSW Edge Basis Functions Low energy extension $E_{e \to \Omega_e}(\cdot)$ High energy extension $R_{e \to \Omega_e}(\cdot)$ Ext. into the interior Image: Colspan="2">Image: Colspan="2" Image: Colspan="2">Image: Colspan="2" Image: Colspan="2">Image: Colspan="2" Image: Colspan="2" Image: Colspan="2">Image: Colspan="2" Image: Colspan="2" Image

First, we solve the following eigenvalue problem for each edge $e \in \mathcal{E}$:

$$a_{\Omega_{e}}\left(E_{e \to \Omega_{e}}\left(\tau_{e,*}\right), E_{e \to \Omega_{e}}\left(\theta\right)\right) = \lambda_{e,*} a_{\Omega_{e}}\left(R_{e \to \Omega_{e}}\left(\tau_{e,*}\right), R_{e \to \Omega_{e}}\left(\theta\right)\right) \quad \forall \theta \in V_{e}$$

Then, we select eigenfunctions using the threshold *TOL* and extend the edge values to Ω :

$$\varphi_{e,*} = E_{\Gamma \to \Omega} \left(R_{e \to \Gamma} \left(\tau_{e,*} \right) \right)$$

Condition Number Bound

Using the coarse space $V_{\text{OS-ACMS}} = \{\varphi_v\} \cup \{\varphi_e\}$ in the two-level Schwarz preconditioner, we obtain

$$\kappa\left(\boldsymbol{M}_{\text{AGDSW}}^{-1}\boldsymbol{A}\right) \leq C\left(1/\text{TOL}\right),$$

where C is independent of H, h, and the contrast of the coefficient function α .

Numerical Results of Adaptive Coarse Spaces (2D)



SHEM by Gander, Loneland, Rahman (TR 2015), OS-ACMS from H., Klawonn, Knepper, Rheinbach (2018), AGDSW from H., Klawonn, Knepper, Rheinbach (2019)

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dim V_0

9

33

93

45

к

13.2

6.4

16.5

Extensions of the AGDSW Approach



As in the reduced dimension GDSW (RGDSW) approach, we partition the interface into **interface components centered around the vertices**. On these interface components, we solve (slightly modified) eigenvalue problems.

Cf. Heinlein, Klawonn, Knepper, Rheinbach (2021) and Heinlein, Klawonn, Knepper, Rheinbach, Widlund (2022).

Extension to Three Dimensions





- In AGDSW, we have to solve face and edge eigenvalue problems
- In RAGDSW, only the interface components change



RGDSW interface component

Reduced Dimension (Adaptive) GDSW – 3D Numerical Example



detailed view of partially peeled



Heterogeneous linear elasticity problem

- Ω : cube; Dirichlet boundary condition on $\partial \Omega$.
- Structured tetrahedral mesh; 132 651 nodes (397 953 DOFs); unstructured domain decomposition (METIS); 125 subdomains.
- Poisson ration $\nu = 0.4$.
- Young modulus: elements with E(T) = 10⁶ in light blue (beams); remainder set to E(T) = 1.
- Right hand side $f \equiv 1$.
- Overlap: two layers of finite elements.

V ₀	tol	iter	κ	dim V ₀	$\frac{\dim V_0}{\dim V^h}$
GDSW	_	>2000	$3.1 \cdot 10^{5}$	9 996	2.51%
RGDSW	_	>2000	$3.9 \cdot 10^5$	3 358	0.84%
AGDSW	0.100	71	41.1	14 439	3.63%
AGDSW	0.050	90	59.5	13945	3.50%
AGDSW	0.010	132	161.1	13763	3.46%
RAGDSW	0.100	67	34.6	8 2 4 9	2.07%
RAGDSW	0.050	88	61.3	7 683	1.93%
RAGDSW	0.010	114	117.4	7 501	1.88%

- RAGDSW: 45% reduction of coarse space dimension compared to AGDSW (highlighted line).
- RAGDSW: smaller coarse space dimension compared to GDSW and even robust!

The low energy property

 $c(u_0, u_0) \leq C_2 a(u, u)$

of the **left hand side in the eigenvalue problems** of the OS-ACMS and AGDSW methods is satisfied due to the use of **Neumann boundary conditions**:

$$\begin{aligned} a_{\Omega_{e}}\left(E_{\overline{e}\to\Omega_{e}}\left(\tau_{e,*}\right),E_{\overline{e}\to\Omega_{e}}\left(\theta\right)\right) &= \lambda_{e,*}a_{\Omega_{e}}\left(R_{e\to\Omega_{e}}\left(\tau_{e,*}\right),R_{e\to\Omega_{e}}\left(\theta\right)\right) \quad \forall \theta\in V_{e}^{0} \qquad (OS-ACMS) \\ a_{\Omega_{e}}\left(E_{e\to\Omega_{e}}\left(\tau_{e,*}\right),E_{e\to\Omega_{e}}\left(\theta\right)\right) &= \lambda_{e,*}a_{\Omega_{e}}\left(R_{e\to\Omega_{e}}\left(\tau_{e,*}\right),R_{e\to\Omega_{e}}\left(\theta\right)\right) \quad \forall \theta\in V_{e}^{0} \qquad (AGDSW) \end{aligned}$$

In both approaches, the right hand side matrix just corresponds to the submatrix A_{ee} of A corresponding to the edge e, whereas the Neumann matrices on the left hand sides cannot be extracted from the fully assembled matrix A.

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In both approaches, the right hand side matrix just corresponds to the submatrix A_{ee} of A corresponding to the edge e, whereas the Neumann matrices on the left hand sides cannot be extracted from the fully assembled matrix A.

 \rightarrow Both approaches are **not algebraic**

Fully Algebraic Adaptive Coarse Space

We can make use of the a-orthogonal decomposition

$$V_{\Omega_e} = V_{\Omega_e}^0 \oplus \underbrace{\{E_{\partial\Omega_e o \Omega_e}(v) : v \in V_{\partial\Omega_e}\}}_{=:V_{\Omega_e, harm}}$$

to "split the AGDSW eigenvalue problem" into two:

- Dirichlet eigenvalue problem on V⁰_{Ω_e}
- Transfer eigenvalue problem on $V_{\Omega_e,harm}$; cf. Smetana, Patera (2016)



We solve the eigenvalue problem, choose $\lambda_{e,*} < TOL_1$, and extend the basis functions to Ω as before:

$$\mathsf{a}_{\Omega_{e}}\left(\mathsf{E}_{e \to \Omega_{e}}^{\partial \Omega_{e}}\left(\tau_{e,*}\right), \mathsf{E}_{e \to \Omega_{e}}^{\partial \Omega_{e}}\left(\theta\right)\right) = \lambda_{e,*} \mathsf{a}_{\Omega_{e}}\left(\mathsf{R}_{e \to \Omega_{e}}\left(\tau_{e,*}\right), \mathsf{R}_{e \to \Omega_{e}}\left(\theta\right)\right) \quad \forall \theta \in V_{e}^{0}$$



Transfer Operator

Solution Space of Elliptic PDEs is Locally Low-Dimensional

- Consider $\omega^{out} = (-2, 2) \times (0, 1)$ $-\Delta u = 0$ in ω^{out} , $u_{\chi}(x, 1) = u_{\chi}(x, 0) = 0.$
- plus arbitrary Dirichlet b.c. on $\partial \omega^{out}$.
- separation of variables: all local solutions on ω^{out} have the form

$$u(x,y) = a_0 + b_0 x + \sum_{n=1}^{\infty} \cos(n\pi y) [a_n \cosh(n\pi x) + b_n \sinh(n\pi x)]$$

• Solution $u(x, \frac{2}{3})$ for boundary cond. $-\cos(n\pi y)$ at x = -2, x = 2:



A very low-dimensional subspace on ω^{in} will already yield a very good approximation

, ,in

a wout

20,out

Cf. Smetana, Patera (2016)

Constructing Local Reduced Spaces via a Transfer Operator

Introduce transfer operator \mathcal{T} :

- ... acts on the space of local solutions of the PDE and maps values ζ on $\partial \omega^{out}$ to ω^{in}
- ... by solving the PDE locally with Dirichlet boundary values $\boldsymbol{\zeta}$
- ... and restricting the local solution to ω^{in}



Cf. Smetana, Patera (2016)

Fully Algebraic Adaptive Coarse Space – Transfer Eigenvalue Problem

Transfer Eigenvalue Problem



The transfer eigenvalue problem is based on **Smetana**, **Patera** (2016). Different from all the eigenvalue problems before, it is solved on the boundary of Ω_e :

$$a_{\Omega_{e}}\left(E_{\partial\Omega_{e}\to\Omega_{e}}\left(\eta_{e,*}\right),E_{\partial\Omega_{e}\to\Omega_{e}}\left(\theta\right)\right)=\lambda_{e,*}a_{\Omega_{e}}\left(R_{e\to\Omega_{e}}\left(E_{\partial\Omega_{e}\to\Omega_{e}}\left(\tau_{e,*}\right)\right),R_{e\to\Omega_{e}}\left(E_{\partial\Omega_{e}\to\Omega_{e}}\left(\theta\right)\right)\right)\quad\forall\theta\in V_{\partial\Omega_{e}}^{0}$$

We select all eigenfunctions $\eta_{e,*}$ with $\lambda_{e,*}$ above a second **user-chosen threshold** TOL_2 . Then, we first compute the edge values $\tau_{e,*} = E_{\partial\Omega_e \to \Omega_e} (\eta_{e,*})|_e$ and then extend them into the interior

$$\varphi_{e,*} = E_{\Gamma \to \Omega} \left(R_{e \to \Gamma} \left(\tau_{e,*} \right) \right)$$

Fully Algebraic Adaptive Coarse Space – Transfer Eigenvalue Problem

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$$\varphi_{e,*} = E_{\Gamma \to \Omega} \left(R_{e \to \Gamma} \left(\tau_{e,*} \right) \right)$$

 \rightarrow Even though no Neumann matrices are needed to compute $E_{\partial \Omega_e \rightarrow \Omega_e}(\theta)$, Neumann matrices are needed to evaluate $a_{\Omega_e}(\cdot, \cdot)$ for functions with nonnegative trace on $\partial \Omega_e$

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Fully Algebraic Adaptive Coarse Space – Transfer Eigenvalue Problem



Fully Algebraic Adaptive Coarse Space – Condition Number Bound

Condition Number Estimate (Non-Algebraic Variant)

Using the non-algebraic eigenvalue problem (transfer eigenvalue problem with $a_{\Omega_e}(\cdot, \cdot)$), we obtain a condition number of the form:

$$\kappa\left(\boldsymbol{M}_{\mathsf{DIR\&TR}}^{-1}\boldsymbol{A}
ight)\leq C\max\left(rac{1}{\mathcal{T}\mathcal{O}L_{1}},\mathcal{T}\mathcal{O}L_{2}
ight),$$

where C is independent of H, h, and the contrast of the coefficient function α .

Condition Number Estimate (Algebraic Variant)

Using the algebraic eigenvalue problem (transfer eigenvalue problem with $(\cdot, \cdot)_{l_2(\partial \Omega_e)}$), we obtain a condition number of the form:

$$\kappa\left(\boldsymbol{M}_{\mathsf{DIR\&TR}}^{-1}\boldsymbol{A}\right) \leq C \max\left\{\frac{1}{\mathsf{TOL}_1}, \frac{\mathsf{TOL}_2}{\alpha_{\min}}\right\},$$

where C is independent of H, h, and the contrast of the coefficient function α .

Cf. Heinlein and Smetana (Preprint: arXiv:2207.05559).

Fully Algebraic Adaptive Coarse Space – Condition Number Bound

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where C is independent of H, h, and the contrast of the coefficient function α .

 \rightarrow The α_{\min} arises from the fact that

$$\alpha_{\min} \|\theta\|_{l_{2}(\partial\Omega_{e})}^{2} \leq C \|E_{\partial\Omega_{e} \to \Omega_{e}}\left(\theta\right)\|_{a,\Omega_{e}}^{2} \quad \forall \theta \in V_{\partial\Omega_{e}}.$$

Cf. Heinlein and Smetana (Preprint: arXiv:2207.05559).

Numerical Results – Channel Coefficient Function



V ₀	variant	TOL _{DIR} TOL _{TR} TOL _{POD}	dim V ₀	κ	# its.
V _{GDSW}	-		33	$2.7\cdot 10^5$	118
V _{AGDSW}	-	$1.0 \cdot 10^{-2}$	57	7.4	24
V _{DIR&TR}	$a_{\Omega_{e}}\left(\cdot,\cdot ight)$	$1.0\cdot 10^{-3} \ 1.0\cdot 10^{1} \ 1.0\cdot 10^{-5}$	57	7.2	24
V _{DIR&TR}	$(\cdot, \cdot)_{l_2(\partial\Omega_e)}$	$1.0\cdot 10^{-3} \ 1.0\cdot 10^{1} \ 1.0\cdot 10^{-5}$	57	7.2	24

 \rightarrow In order to get rid of potential linear dependencies between the V_{DIR} and V_{TR} spaces, apply a **proper orthogonal decomposition (POD)** with threshold TOL_{POD} for each edge.

Numerical Results – Model 2, SPE10 Benchmark

Layer 70 from model 2 of the SPE10 benchmark; cf. Christie and Blunt (2001)



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Summary

- Using adaptive coarse spaces we are able to retain robustness of two-level Schwarz preconditioners for highly heterogeneous problems:
 - The support and computation of the coarse basis functions are local, however, the computation comes at substantial computational cost.
 - The condition number bound is independent of the contrast of the coefficient function.
- The algebraic variant requires the solution of **two eigenvalue problems**. The **minimum value of the coefficient function** appears in the condition number bound.

Outlook

- Efficient solution of the local eigenvalue problems, for instance, using inexact eigensolvers
- Parallel implementation of adaptive coarse spaces

Additional Results

Numerical Results – Comb Type Coefficient Function



V_0	Ω_e	TOL _{DI}	R TOL	rr TOL _{POD}	dim V_0	κ	# its.
	Ω_e^{2h}	10-3	-	-	57	7.1	24
V	Ω_e^{5h}	10-3	-	-	45	12.6	26
VAGDSW	Ω_e^H	10-3	-	-	33	24.1	31
	-	10-3	-	-	33	24.1	31
	Ω_e^{2h}	10-3	10 ⁶	10^{-5}	57	7.1	24
V _{DIR&TR}	Ω_e^{5h}	10-3	10 ⁵	10^{-5}	45	17.1	33
	Ω_e^H	10^{-3}	10 ⁵	10^{-5}	33	24.1	31

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Numerical Results – Variation of α_{\min}



$\alpha_{\sf min}$	V_0	tol _{dir} tol _{tr} TOL _O	dim V_0	κ	# its.
10-2	V _{GDSW}		33	$2.7\cdot 10^7$	142
10 -	V _{DIR&TR}	$10^- \ 10^4 \ 10^{-5}$	57	7.3	25
1	V _{GDSW}		33	$2.7\cdot 10^5$	118
1	V _{DIR&TR}	$10^- \ 10^4 \ 10^{-5}$	57	7.2	25
102	V _{GDSW}		33	$2.7\cdot 10^3$	95
10	V _{DIR&TR}	10^{-} 10^{4} 10^{-5}	57	7.4	24

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