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Helmut Schmidt University, Hamburg

Adaptive GDSW (AGDSW)

A Coarse Space for the Overlapping Schwarz Domain Decomposition Method and Highly Heterogeneous Positive Semidefinite Problems in Trilinos

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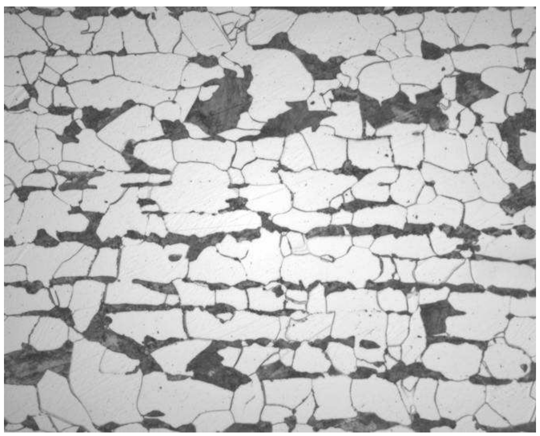
Motivation

Adaptive Coarse Spaces

Overview

In many areas of modern science and engineering **multiscale problems** appear, e.g., **composite materials**, porous media, and plate tectonics.

Example: **dual-phase steel**

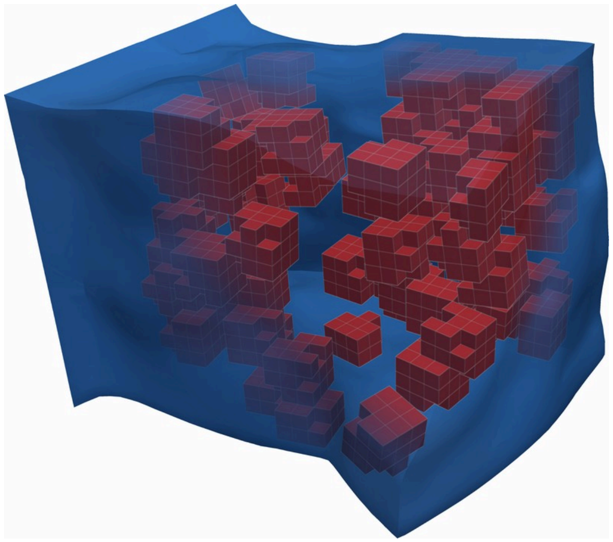


(Courtesy of Jörg Schröder, University of Duisburg-Essen, Germany; originating from a cooperation with ThyssenKrupp Steel.)

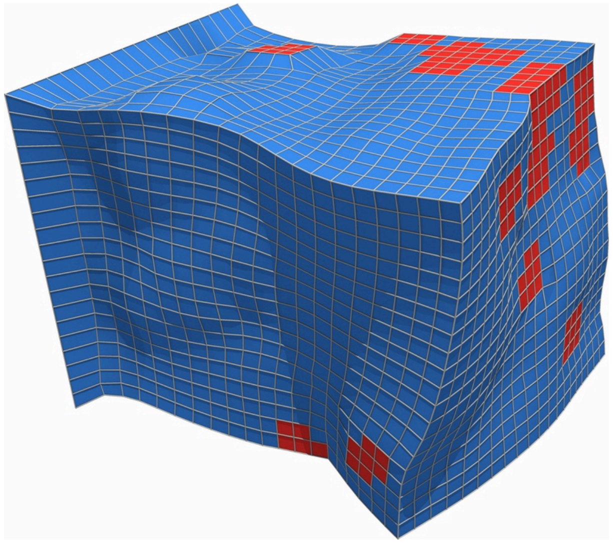
1. **Partial differential equation:** elliptic with a highly heterogeneous coefficient function.
2. **Discretization:** finite element discretization $\rightarrow Ku = b$. Stiffness matrix K is symmetric, positive definite.
3. **Solver:** very large system $Ku = b \rightarrow$ iterative solver (conjugate gradient method) $\rightarrow$ requires a preconditioner for fast convergence.
4. **Preconditioner:** additive overlapping Schwarz domain decomposition method.
5. **Numerical scalability:** Solve coarse problem in each iter.
6. **Heterogeneities:** can drastically reduce convergence speed.
7. **Recover fast convergence:** Use adaptive coarse functions Φ_{coarse} to construct $K_{\text{coarse}} := \Phi_{\text{coarse}}^T K \Phi_{\text{coarse}}$ (coarse stiffness matrix).

(8.) **Parallel scalability:** In each iteration, we need to evaluate $\Phi_{\text{coarse}} K_{\text{coarse}}^{-1} \Phi_{\text{coarse}}^T x \rightarrow$ reduce coarse space dimension to reduce computational cost $\rightarrow$ Reduced AGDSW & ACMS-type coarse space (*not part of this talk*).

Motivational Example: "Simple" Problem



Taken from [3, Fig. 1.1].



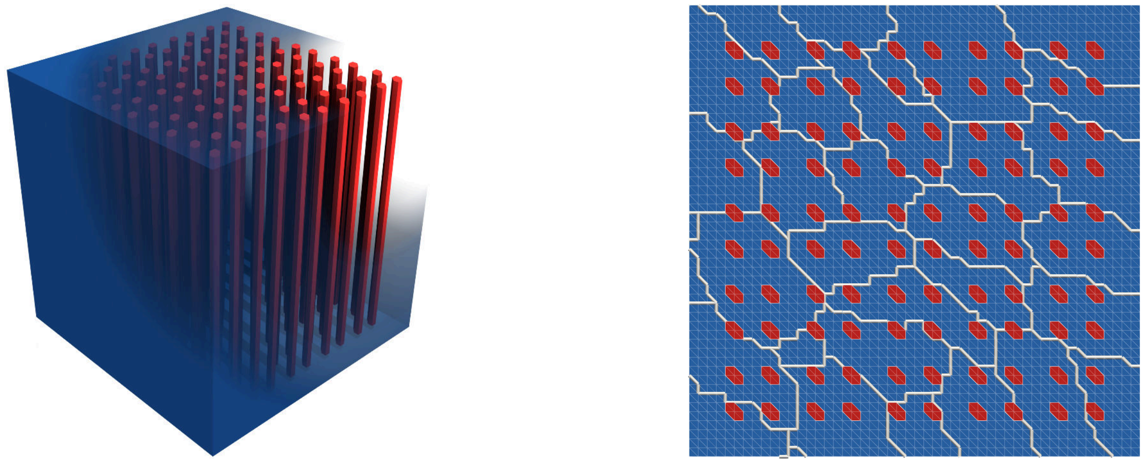
Setting: compressible linear elasticity

- cube $[0,1]^3$, 20^3 trilinear finite elements, 4^3 subdomains
- body force $f = (1.5, 0, 0)$
- body clamped on the left, no traction on the remaining boundary
- compressible (Poisson's ration $\nu = 0.4$)
- Young's modulus (stiffness) $E = 10\,000$ in red, remainder $E = 1$

Results: Iterations using additive overlapping Schwarz method

- without coarse problem: 3 504
- with nonadaptive coarse space (GDSW): 803
- with adaptive coarse space (AGDSW–S): 104

Motivational Example: Difficult Problem



Taken from [3, Fig. 2.2].

Setting: compressible linear elasticity (Poisson's ration $\nu = 0.4$)

- cube $[0,1]^3$, $3 \cdot 132\,651$ degrees of freedom, 125 subdomains
- body force $f = (1,1,1)$
- zero displacement on boundary
- Young's modulus (stiffness) $E = 10^6$ in red, remainder $E = 1$

	GDSW	AGDSW–S
its.	$>2\,000$	94
$\dim(V_0)$	9 996	11 316
adaptive	no	yes

$\dim(V_0)$: size of the coarse problem

Preliminaries

A Highly Heterogeneous Model Problem and the Two-Level Additive Overlapping Schwarz Method

Highly Heterogeneous Model Problem

- Explanations and visualizations in this talk for stationary scalar diffusion problem.
- Numerical results: diffusion problem and compressible linear elasticity with Young's modulus $E(x)$.

Let $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$) be the domain. For $f \in L^2(\Omega)$, find $u \in V^h(\Omega)$ such that $\forall v \in V^h(\Omega)$ we have

$$a_\Omega(u, v) := \int_\Omega \mathbf{E} \nabla u \cdot \nabla v \, \mathrm{d}x \stackrel{!}{=} \int_\Omega f v \, \mathrm{d}x,$$

where $E_{\text{max}} \geq \mathbf{E}(x) \geq E_{\text{min}} > 0$ is a **highly heterogeneous**, piecewise constant diffusion coefficient.

- Finite element space $V^h(\Omega)$:
  - ⋆ Piecewise linear (or bi- or trilinear) basis functions.
  - ⋆ Zero Dirichlet boundary condition on $\partial\Omega_D \subset \partial\Omega$.
- $\partial\Omega_N := \partial\Omega \setminus \partial\Omega_D$: zero Neumann boundary condition.
- K: stiffness matrix corresponding to $a_\Omega(\cdot, \cdot)$.

Since K is symmetric, positive definite, we can solve $M^{-1}Ku = M^{-1}b$ with the preconditioned conjugate gradient method using a suitable preconditioner M^{-1}.

Two-Level Additive Overlapping Schwarz Method

- $\Omega_1', \ldots, \Omega_N'$: overlapping subdomains of Ω
- δ: size of the overlap; H: maximum subdomain diameter
- Restriction operators $R_i : V^h(\Omega) \rightarrow V_0^h(\Omega_i')$
- $\Phi = (\Phi_1, \ldots, \Phi_n)$: basis vectors of the coarse space V_0

Two-level overlapping additive Schwarz preconditioner:

$$M_{\text{OS-2}}^{-1} = \underbrace{\Phi\left(\Phi^T K \Phi\right)^{-1}\Phi^T}_{\text{coarse level}} + \underbrace{\sum_{i=1}^{N} R_i^T\left(R_i K R_i^T\right)^{-1} R_i}_{\text{first level}}$$

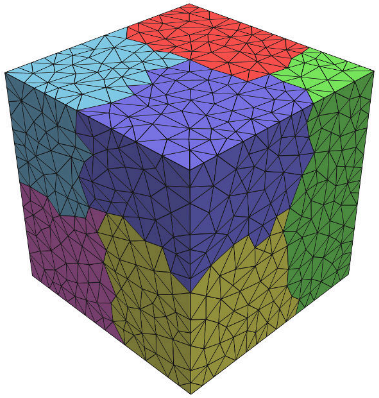
Condition number bound using **nonadaptive coarse functions**:

$$\kappa\left(M_{\text{OS-2}}^{-1} K\right) \leq C \frac{E_{\max}}{E_{\min}}\left(1 + \frac{H}{\delta}\right)$$

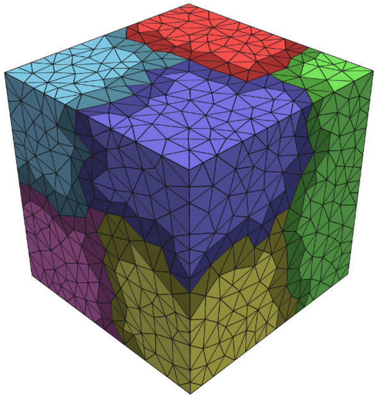
$\Longrightarrow$ The convergence speed of the employed preconditioned Krylov method generally depends on the coefficient contrast.
We will define **adaptive coarse functions** such that

$$\kappa\left(M_{\text{OS-2}}^{-1} K\right) \leq C\left(1 + \frac{1}{tol}\right),$$

where tol is a user-prescribed tolerance, and C is independent of the coefficient function and of the mesh parameters H and h.



nonoverlapping subdomains
Ω_i



overlapping subdomains
Ω_i'

Taken from [1, Fig. 1].

Generalized Dryja–Smith–Widlund (GDSW) Coarse Space

Dohrmann, Klawonn, Widlund (2008), *A Family of Energy Minimizing Coarse Spaces for Overlapping Schwarz Preconditioners*

GDSW Coarse Space

How to define $\mathbf{\Phi} = \left(\Phi_1, \ldots, \Phi_n\right)$ in

$$M_{\text{OS-2}}^{-1} = \mathbf{\Phi}\left(\mathbf{\Phi}^T K \mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^T + \sum_{i=1}^{N} R_i^T \left(R_i K R_i^T\right)^{-1} R_i$$

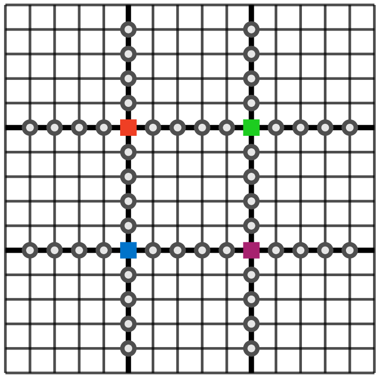
?

1. **Specify null space** of the (non-overlapping) subdomain matrices K_i on the domain decomposition interface Γ.
   - *Example for diffusion problem:* Set $\Phi|_\Gamma = 1$.
2. **Partition domain decomposition interface** Γ into vertices, edges, and faces (3D) $\rightarrow$ partition of unity.
3. **Multiply partition of unity with nullspace**:

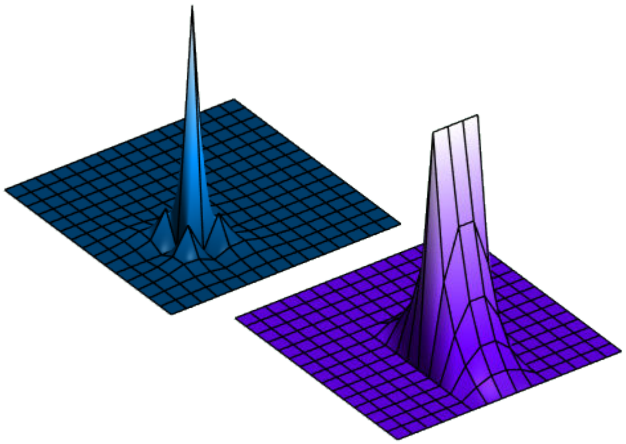
$$\Phi|_\Gamma \rightarrow \Phi_{\Gamma,1}, \ldots, \Phi_{\Gamma,n}.$$

4. **Extend** $\Phi_{\Gamma,i}$ **energy-minimally**:

$$\Phi_i := \begin{pmatrix} -K_{II}^{-1} K_{\Gamma I}^T \Phi_{\Gamma,i} \\ \Phi_{\Gamma,i} \end{pmatrix}, \quad K = \begin{pmatrix} K_{II} & K_{I\Gamma} \\ K_{\Gamma I} & K_{\Gamma\Gamma} \end{pmatrix}.$$



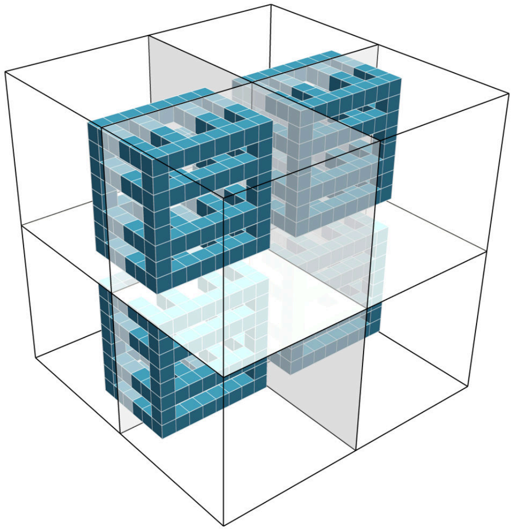
vertices & edges

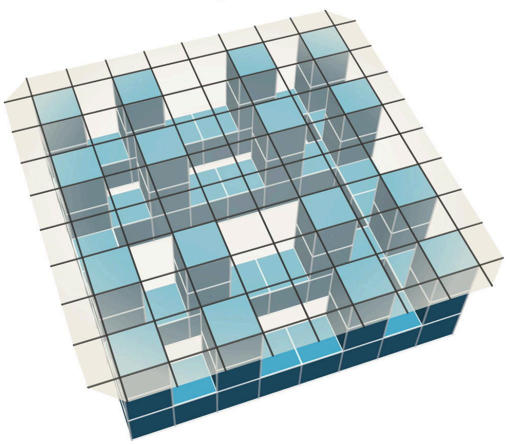


vertex & edge function for a 2D diffusion problem

Taken from [2, Fig. 1].

GDSW: Robust for Some Heterogeneous Problems





- Diffusion problem, $E_{\max} = 10^6$
- Ω: cube, solution zero on $\partial\Omega$
- Structured mesh (voxels)
- $4 \times 4 \times 4$ subdomains
- $(H/h)^3 = 10^3$ finite elements per subdomain
- Overlap of two finite elements

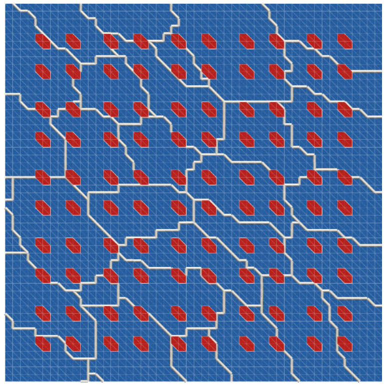
Iterations	49
Condition number	26.2
Coarse space dim.	279

GDSW robust for this difficult problem!

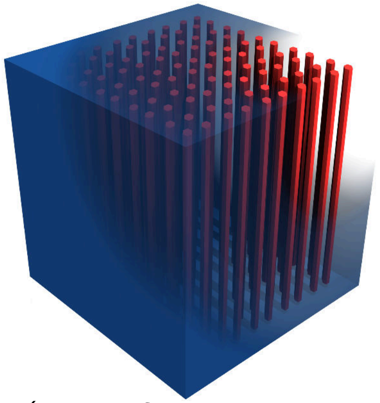
GDSW: Not Robust in All Cases

- Diffusion problem, $E_{\max} = 10^6$
- Ω: cube, solution zero on $\partial\Omega$
- Structured mesh (tetrahedra): 132 651 nodes
- Unstructured domain decomposition (METIS): 125 subdomains
- Overlap of two finite elements

Iterations	$>1\,000$
Condition number	$4.7 \cdot 10^5$
Coarse space dim.	1 980



(cross section)



(view of partially peeled beams)

Taken from [2, Fig. 1].

Adaptivity is required to obtain a robust preconditioner for this coefficient function.

Adaptive GDSW

A robust extension of the GDSW coarse space

Heinlein, Klawonn, Knepper, Rheinbach (2019), *Adaptive GDSW Coarse Spaces for Overlapping Schwarz Methods in Three Dimensions*

Overview of AGDSW Coarse Space Construction & FROSch

1)	Create partition $\mathcal{P}$ of the domain decomposition interface Γ: vertices, edges, faces.	*Implemented in FROSch: Yes.*
2)	**Set up generalized eigenvalue problem** $$S_\xi \tau = \lambda K_\xi \tau$$ for each interface component $\xi \in \mathcal{P}$. • S_ξ is a local Schur complement. • K_ξ is submatrix of K (global stiffness matrix).	*Implemented in FROSch: (Yes)*
3)	**Solve generalized eigenvalue problem** and select all eigenvectors with eigenvalue $\lambda \leq tol$, where tol is a user-prescribed tolerance.	*Implemented in FROSch: (Yes)*
4)	Coarse functions: Extend selected eigenvectors by zero to Γ and then energy-minimally to the domain.	*Implemented in FROSch: Yes.*

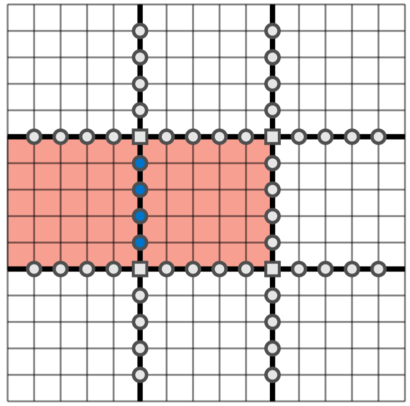
Schur Complement for AGDSW & AGDSW-S

$$S_\xi \tau = \lambda K_\xi \tau, \quad \xi \in \mathcal{P}$$

Notation

- Ω_ξ: union of subdomains adjacent to ξ
- K^{Ω_ξ}: assembly of $a_{\Omega_\xi}(\cdot,\cdot)$ that incorporates the zero Dirichlet boundary on $\partial\Omega_D$
  $\rightarrow$ Neumann matrix if Ω_ξ and $\partial\Omega_D$ do not share nodes
- Partition of Ω_ξ by nodes of ξ and the remaining ones, R:

$$K^{\Omega_\xi} = \begin{pmatrix} K^{\Omega_\xi}_{RR} & K^{\Omega_\xi}_{R\xi} \\ K^{\Omega_\xi}_{\xi R} & K^{\Omega_\xi}_{\xi\xi} \end{pmatrix}$$

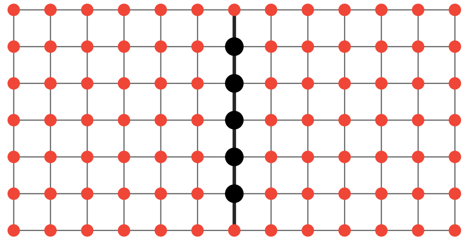


highlighted edge: ξ
highlighted domain: Ω_ξ

Definition of S_ξ:

$$S_\xi := S^{\Omega_\xi}_{\xi\xi} = K^{\Omega_\xi}_{\xi\xi} - K^{\Omega_\xi}_{\xi R}\left(K^{\Omega_\xi}_{RR}\right)^+ K^{\Omega_\xi}_{R\xi} \qquad \text{(AGDSW)}$$

$$S_\xi := \sum_{\Omega_i \subset \Omega_\xi} S^{\Omega_i}_{\xi\xi} = \sum_{\Omega_i \subset \Omega_\xi} \left(K^{\Omega_i}_{\xi\xi} - K^{\Omega_i}_{\xi R}\left(K^{\Omega_i}_{RR}\right)^+ K^{\Omega_i}_{R\xi}\right) \qquad \text{(AGDSW-S)}$$



Red: R; Black: ξ
Taken from [3, Fig. 3.5].

Implementation of Pseudoinverse of Local Stiffness Matrix

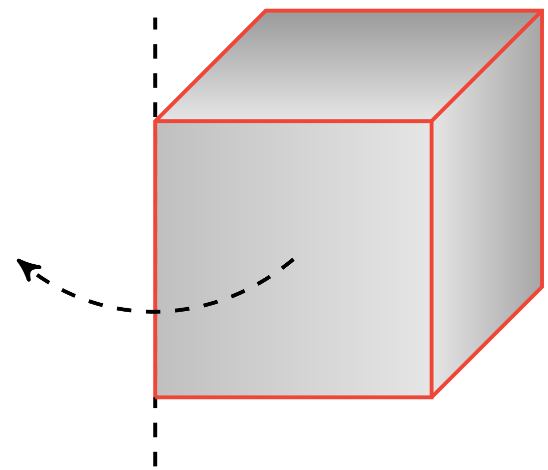
$$K^{\Omega_\xi} = \begin{pmatrix} \boxed{K_{RR}^{\Omega_\xi}} & K_{\xi R}^{\Omega_\xi} \\ K_{\xi R}^{\Omega_\xi} & K_{\xi\xi}^{\Omega_\xi} \end{pmatrix} \qquad K^{\Omega_i} = \begin{pmatrix} \boxed{K_{RR}^{\Omega_i}} & K_{\xi R}^{\Omega_i} \\ K_{\xi R}^{\Omega_i} & K_{\xi\xi}^{\Omega_i} \end{pmatrix}$$

- Diffusion problem: $K_{RR}^{\Omega_\xi}$ and $K_{RR}^{\Omega_i}$ are invertible $\rightarrow$ Pseudoinverse not required.
- Linear elasticity problem: $K_{RR}^{\Omega_\xi}$ and $K_{RR}^{\Omega_i}$ are singular if ξ is a straight edge.

If a pseudoinverse is required, multiple approaches are possible. Simple and algebraic approach:

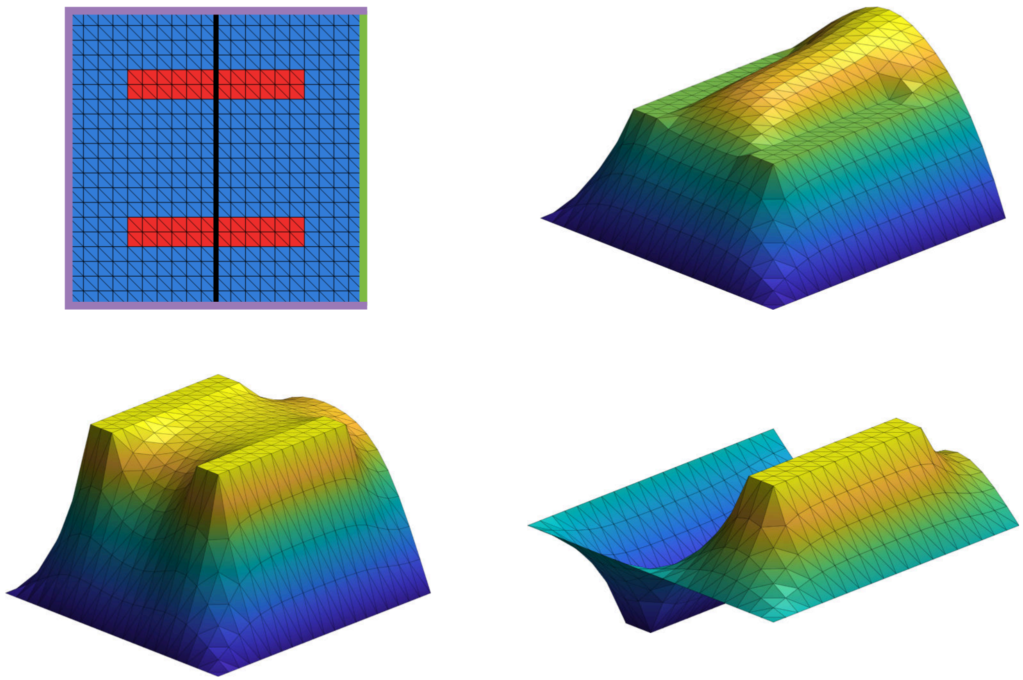
- Add a regularization term $K_{II}^{\Omega_\xi} \leftarrow K_{II}^{\Omega_\xi} + 10^{-13}\,\mathrm{diag}(K_{II}^{\Omega_\xi})$.

Then $K_{II}^{\Omega_\xi}$ is invertible and standard solvers can be used. But, the regularization may affect the coarse space (was not observed in our tests).



Taken from [3, Fig. 1.3].

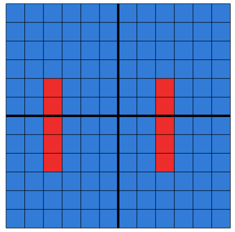
MATLAB Code of a Simple Problem



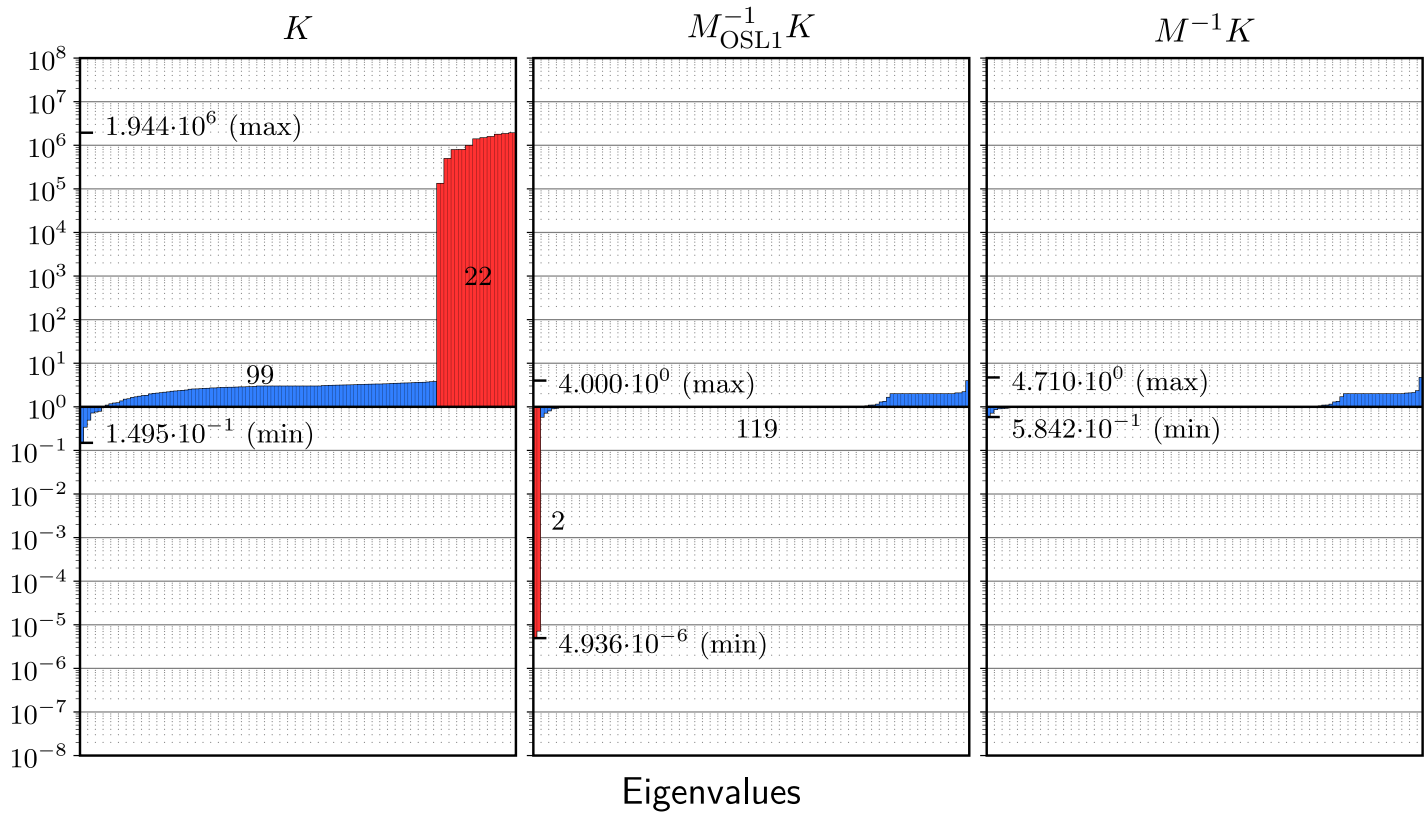
Taken from [3, Fig. 3.2].

- **(Top left)** Two subdomains, $E_{\text{max}} = 10^6$, Dirichlet boundary in purple, Neumann boundary in green.
- **(Top right)** Finite element solution to the corresponding diffusion problem using $\mathcal{P}_1$ basis functions.
- **(Bottom)** AGDSW coarse functions.

Simple Problem: Spectrum of the Preconditioned Operators



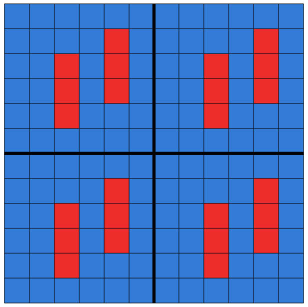
- Diffusion problem
- $E_{\text{max}} = 10^6$



Taken from [3, Fig. 1.5 & 1.6].

Coefficient Functions and Coarse Functions: Example A

- Domain decomposition with 4 subdomains.
- Coefficient function with $E = 10^6$ (red) and $E = 1$ (blue).



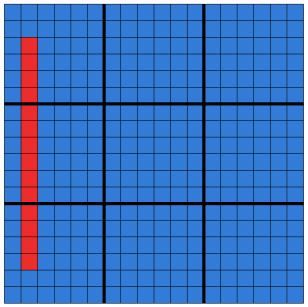
Taken from [3, Fig. 1.10].

- No coarse functions are required to obtain a well-conditioned problem.
- All difficult components are contained in one of the local problems of the first level of the preconditioner.

$$M_{\text{OS-2}}^{-1} = \underbrace{\Phi\left(\Phi^T K \Phi\right)^{-1} \Phi^T}_{\text{coarse level}} + \underbrace{\sum_{i=1}^{N} R_i^T \left(R_i K R_i^T\right)^{-1} R_i}_{\text{first level}}$$

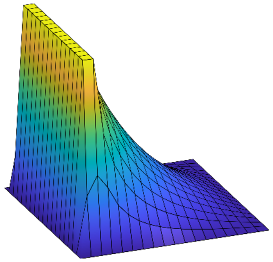
Coefficient Functions and Coarse Functions: Example B

- Domain decomposition with 9 subdomains.
- Coefficient function with $E = 10^6$ (red) and $E = 1$ (blue).



Taken from [3, Fig. 1.8].

- Select the entire interface as the only interface component: $\mathcal{P} = \{\Gamma\}$.
- $S_\xi \tau = \lambda K_\xi \tau$, $\xi = \Gamma$, has only one small eigenvalue. Corresponding coarse function Φ_Γ:

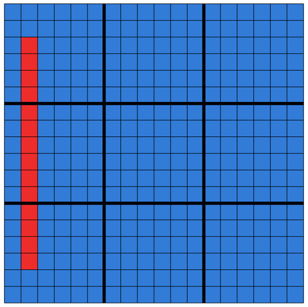


Taken from [3, Fig. 1.8].

- Solving an eigenvalue problem on the entire interface is too expensive.

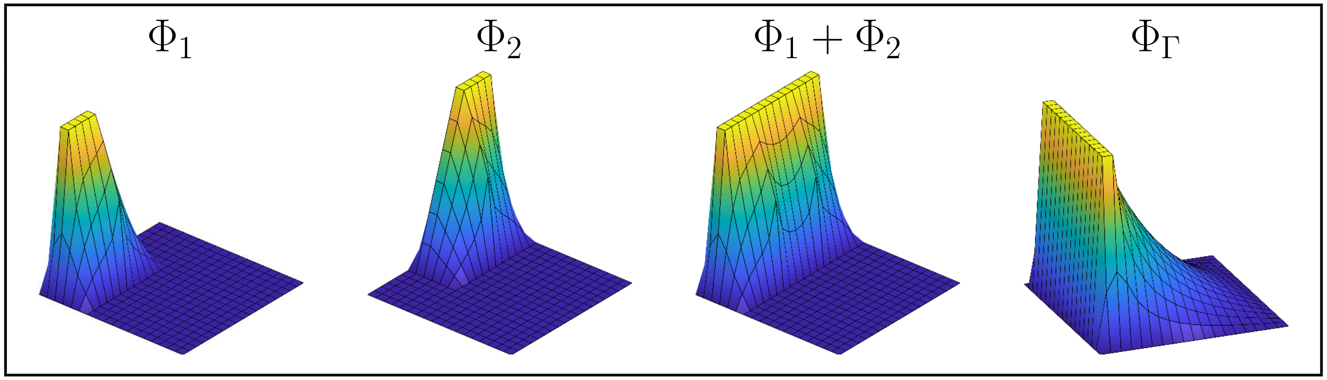
Coefficient Functions and Coarse Functions: Example B

- Domain decomposition with 9 subdomains.
- Coefficient function with $E = 10^6$ (red) and $E = 1$ (blue).



Taken from [3, Fig. 1.8].

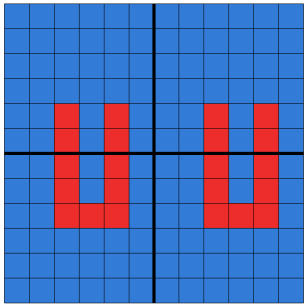
- Partition the interface into 12 edges and 4 vertices.
- Let ξ be a horizontal edge on the left, then $S_\xi \tau = \lambda K_\xi \tau$ has only one small eigenvalue for each ξ. The corresponding coarse functions are Φ_1 and Φ_2:



Taken from [3, Fig. 1.8 & 1.9].

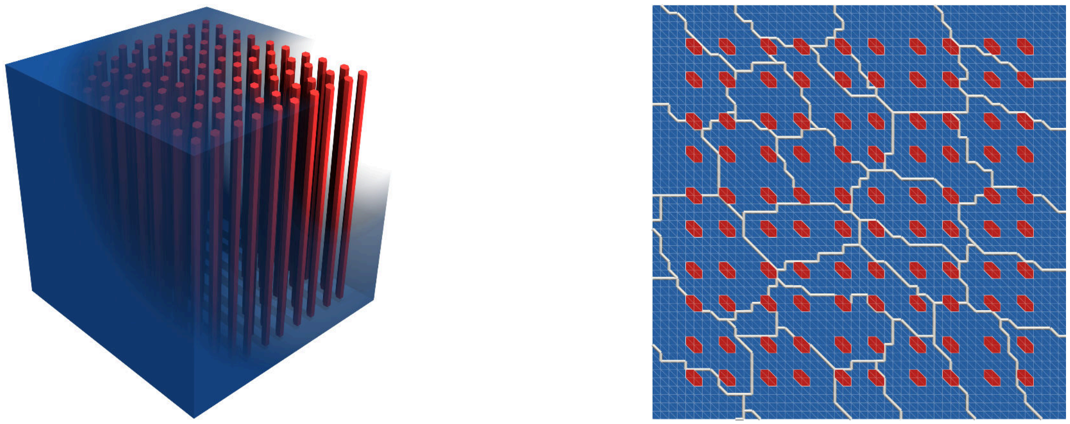
Coefficient Functions and Coarse Functions: Example C

- Domain decomposition with 4 subdomains.
- Coefficient function with $E = 10^6$ (red) and $E = 1$ (blue).



Taken from [3, Fig. 1.5].

- Although the interface is intersected four times, we only require two coarse functions to obtain a well-conditioned problem: there are only two connected components of large coefficients.



Taken from [3, Fig. 2.2].

Setting: compressible linear elasticity (Poisson's ration $\nu = 0.4$)

- cube $[0,1]^3$, $3 \cdot 132\,651$ degrees of freedom, 125 subdomains
- body force $f = (1,1,1)$
- zero displacement on boundary
- Young's modulus (stiffness) $E = 10^6$ in red, remainder $E = 1$

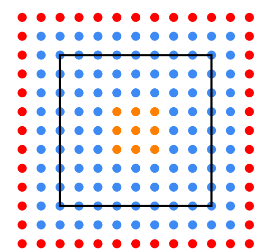
	GDSW	AGDSW–S
tol	/	0.005
its.	$>2\,000$	94
κ	$3.1 \cdot 10^5$	126.7
$\dim(V_0)$	9 996	11 316

Overlap: two layers of finite elements

List of Ad- and Disadvantages and Difficulties

- If theoretical assumptions are met: provably robust solver
- Apart from local Neumann matrices: few addional requirements
- Algorithmically fairly simple setup
- Small eigenvalue problems $\rightarrow$ Direct eigensolver feasible if Schur complement is available
- Each degree of freedom on the interface appears in exactly one eigenvalue problem $\rightarrow$ no unnecessary work or large coarse space

	Faces	Edges	Vertices	GenEO (subdomains)
# evp	515	750	328	100
mean dof(evp)	344.9	22.3	3	8 697.1
max dof(evp)	1 140	78.0	3	12 111
sum(dof(evp))	177 624	16 731	984	869 712

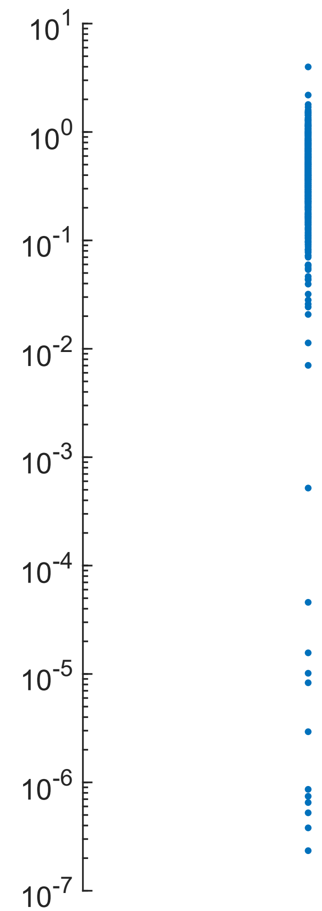


blue: nodes of GenEO evp
red: bnd. of overl. subd.
—: nonoverl. subd.

- Three-level version (theoretically) straight-forward
- Extended framework exists that allows many variants
- Only uses stiffness matrix
- Robust for different interface partitions ($\rightarrow$ RAGDSW)
  But: noncontiguous sets of interface components can lead to an increase in the coarse space dimension

Difficulties

- Setup computationally expensive → Intended for very difficult problems
- Local (Neumann) stiffness matrices required (for some problems, Dirichlet matrices can be used)
  - ⋆ For Neumann matrices, we use `Tpetra FECrsMatrix`.
  - ⋆ After `endAssembly` (like `fillComplete`), the matrix can be used like a `CrsMatrix`.
  - ⋆ Before `endAssembly`, currently we create a copy of the `FECrsMatrix`.
- Setup of full Schur complements expensive
  Can we leverage the GPU for the computation of Schur complements?
- No theory yet for higher order elements (probably unproblematic)
- A large coarse space may become the bottleneck → Consider a three-level version
- Pseudoinverse sometimes required. If regularization fails, nonstandard solvers or less algebraic algorithms required.
- So far, indefinite problems not supported. Also for some problems, the coarse space dimension may grow too quickly (almost incompressible linear elasticity).
- Tolerance for the selection of eigenvectors: difficult to prove anything with practical implications → based on experience



Spectrum of face eigenvalue problem (linear elasticity)

Summary

- Brief overview of the construction of Adaptive GDSW, which makes use of a generalized eigenvalue problem of the type
$$S_\xi \tau = \lambda K_\xi \tau.$$
- Interface partitioning and extension of interface functions already implemented in FROSch (ShyLU).
- Focus of this talk was on AGDSW. There are many more related coarse spaces and variants (reduce coarse space dimension!).
- Rudimentary implementation in FROSch done.

Thank you for your attention

References of Figures

[1] Alexander Heinlein, Axel Klawonn, Jascha Knepper, and Oliver Rheinbach (2019) *"Adaptive GDSW Coarse Spaces for Overlapping Schwarz Methods in Three Dimensions,"* SIAM J. Sci. Comp., 41(5), pp. A3045–A3072. DOI: 10.1137/18M1220613.

[2] Alexander Heinlein, Axel Klawonn, Jascha Knepper, and Oliver Rheinbach (2022) *"Adaptive GDSW Coarse Spaces of Reduced Dimension for Overlapping Schwarz Methods,"* SIAM J. Sci. Comp., 44(3), pp. A1176–A1204. DOI: 10.1137/20M1364540.

[3] Jascha Knepper (2022) *"Adaptive Coarse Spaces for the Overlapping Schwarz Method and Multiscale Elliptic Problems,"* dissertation, University of Cologne, Cologne, Germany. URN: urn:nbn:de:hbz:38-620024.