Advances of FROSch Preconditioners for Multiphysics and Multiscale Simulations

Alexander Heinlein[1]

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[1]Delft University of Technology

Outline

1. The FROSch Package – Algebraic and Parallel Schwarz Preconditioners in Trilinos

2. Monolithic Coarse Spaces Multiphysics Problems

   Based on joint work with

Axel Klawonn, **Jascha Knepper**, and **Lea Saßmannshausen**	(University of Cologne)
Mauro Perego, **Siva Rajamanickam**, and **Ichitaro Yamazaki**	(Sandia National Laboratories)

3. Robust Coarse Spaces for Heterogeneous Problems

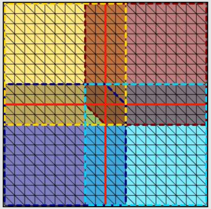
   Based on joint work with

Filipe Cumaru and **Hadi Hajibeygi**	(Delft University of Technology)
Axel Klawonn and **Jascha Knepper**	(University of Cologne)
Ichitaro Yamazaki	(Sandia National Laboratories)

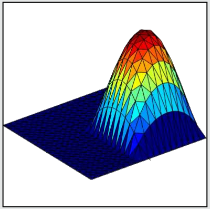
The FROSch Package – Algebraic and Parallel Schwarz Preconditioners in Trilinos

One-level Schwarz preconditioner

Overlap $\delta = 2h$



Solution of local problem



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

$$M_{\text{OS-1}}^{-1} A = \sum_{i=1}^{N} R_i^\top A_i^{-1} R_i A,$$

where R_i and $R_i^\top$ are restriction and prolongation operators corresponding to Ω_i', and $A_i := R_i A R_i^\top$.

Condition number estimate:

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

with subdomain size H and overlap width δ.

Lagrangian coarse space

Coarse triangulation

Coarse solution

The **two-level overlapping Schwarz operator** reads

$$M_{\text{OS-2}}^{-1} A = \underbrace{\Phi A_0^{-1} \Phi^\top A}_{\text{coarse level -- global}} + \underbrace{\sum_{i=1}^{N} R_i^\top A_i^{-1} R_i A}_{\text{first level -- local}},$$

where Φ contains the coarse basis functions and $A_0 := \Phi^\top A \Phi$; cf., e.g., **Toselli, Widlund (2005)**. The construction of a Lagrangian coarse basis requires a coarse triangulation.

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Two-Level Schwarz Preconditioners

One-level Schwarz preconditioner

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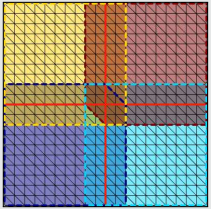

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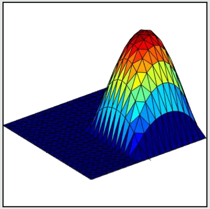

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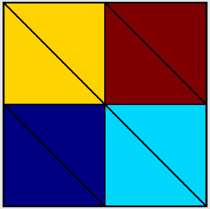
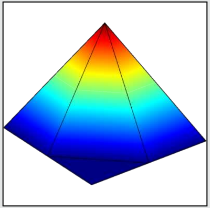
Coarse triangulation



Coarse solution



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One-level Schwarz preconditioner

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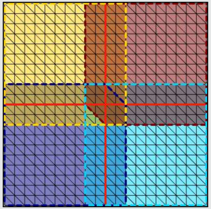

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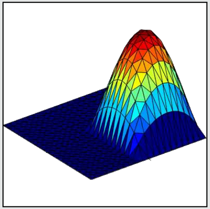

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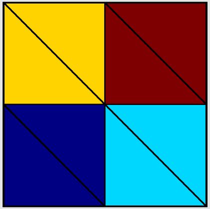

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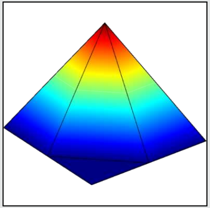
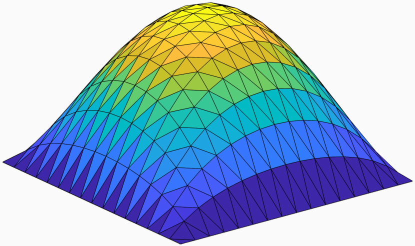
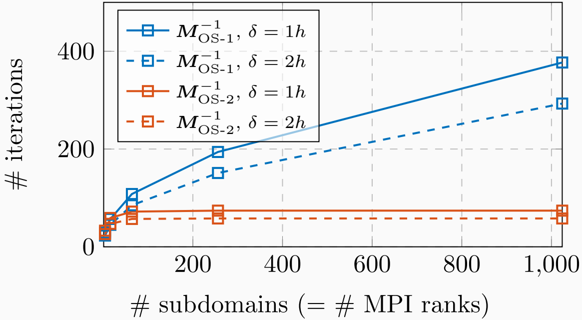


Diffusion model problem in two dimensions,
$H/h = 100$





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 the parallel linear algebra based on TPETRA
- Node-level parallelization and performance portability on CPU and GPU architectures through KOKKOS and KOKKOSKERNELS
- Accessible through unified TRILINOS solver interface STRATIMIKOS

Methodology

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

Team (active)

- Filipe Cumaru (TU Delft)
- Alexander Heinlein (TU Delft)
- Kyrill Ho (UCologne)
- Sebastian Kinnewig (LUH)
- Axel Klawonn (UCologne)
- Jascha Knepper (UCologne)
- Stephan Köhler (TUBAF)
- Friederike Röver (TUBAF)
- Siva Rajamanickam (SNL)
- Oliver Rheinbach (TUBAF)
- Lea Saßmannshausen (UCologne)
- Ichitaro Yamazaki (SNL)

Partition of Unity

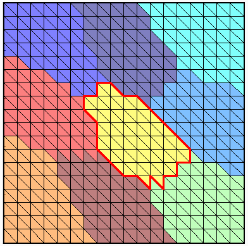
The **energy-minimizing extension** $v_i = H_{\partial\Omega_i \to \Omega_i}(v_{i,\partial\Omega_i})$ solves

$$\begin{aligned} -\Delta v_i &= 0 && \text{in } \Omega_i, \\ v_i &= v_{i,\partial\Omega_i} && \text{on } \partial\Omega_i. \end{aligned}$$

Hence, $v_i = E_{\partial\Omega_i \to \Omega_i}(\mathbb{1}_{\partial\Omega_i}) = \mathbb{1}.$

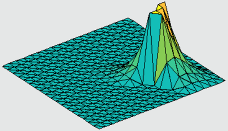
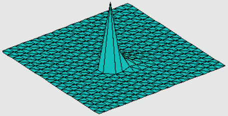
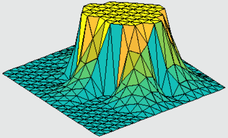
Due to **linearity of the extension operator**, we have

$$\sum_i \varphi_i = \mathbb{1}_{\partial\Omega_i} \Rightarrow \sum_i E_{\partial\Omega_i \to \Omega_i}(\varphi_i) = \mathbb{1}_{\Omega_i}$$



Null space property

Any extension-based coarse space built from a partition of unity on the domain decomposition interface satisfies the **null space property necessary for numerical scalability**:

$\sum$ edges $\subset \partial\Omega_i$  $+ \sum$ vertices $\subset \partial\Omega_i$  $=$ 

Algebraicity of the energy-minimizing extension

The computation of energy-minimizing extensions only requires $\boldsymbol{K}_{II}$ and $\boldsymbol{K}_{I\Gamma}$, **submatrices of the fully assembled matrix** $\boldsymbol{K}_i$.

$$\boldsymbol{v} = \begin{bmatrix} -\boldsymbol{K}_{II}^{-1}\boldsymbol{K}_{I\Gamma} \\ \boldsymbol{I}_\Gamma \end{bmatrix} \boldsymbol{v}_\Gamma,$$

Overlapping domain decomposition

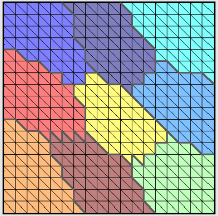
The **overlapping subdomains** are constructed by **recursively adding layers of elements** via the sparsity pattern of $\boldsymbol{K}$.

The corresponding matrices

$$\boldsymbol{K}_i = \boldsymbol{R}_i \boldsymbol{K} \boldsymbol{R}_i^T$$

can easily be extracted from $\boldsymbol{K}$.

Nonoverlapping DD



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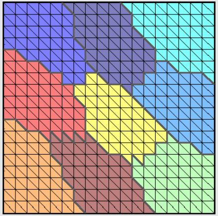
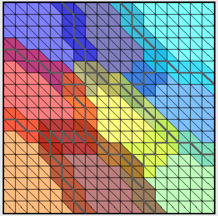


Overlap $\delta = 1h$



Algorithmic Framework for FROSch Preconditioners

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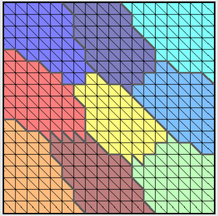

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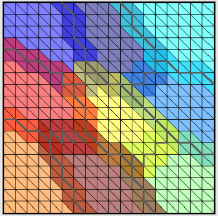
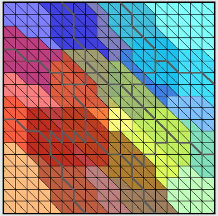


Overlap $\delta = 2h$



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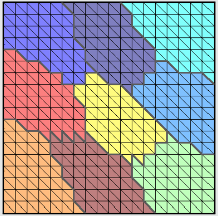

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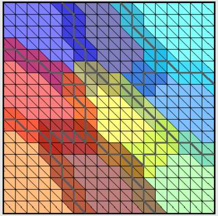

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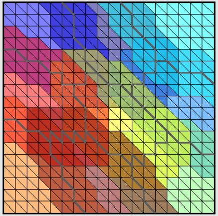
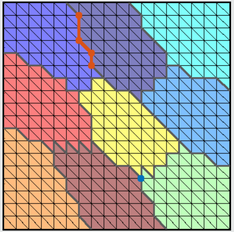


Coarse space

1. Interface components



Algorithmic Framework for FROSch Preconditioners

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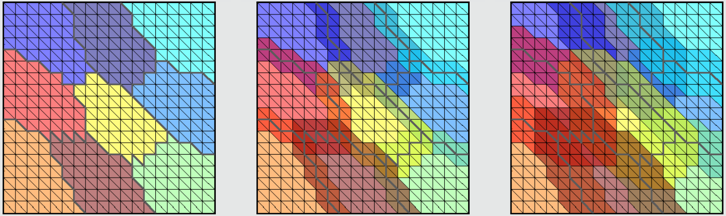

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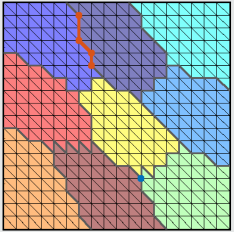
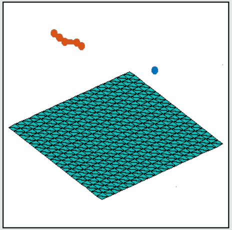


2. Interface basis (partition of unity $\times$ null space)



For **scalar elliptic problems**, the **null space** consists only of **constant functions**.

Algorithmic Framework for FROSch Preconditioners

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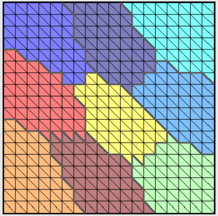

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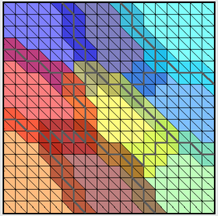

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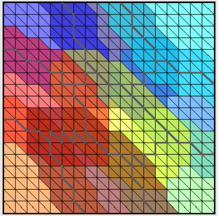

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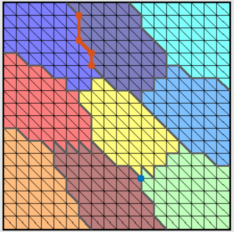

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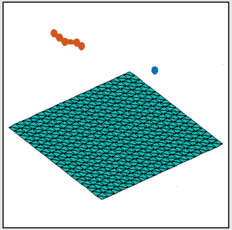

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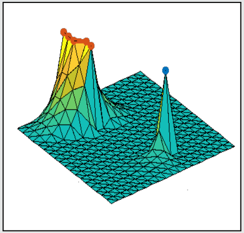
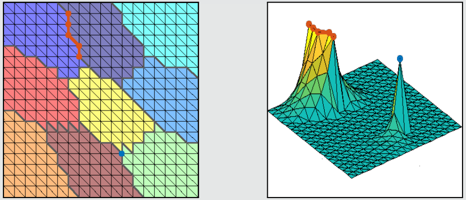
3. Extension



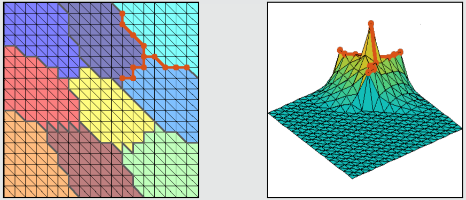
Examples of FROSch Coarse Spaces

GDSW (Generalized Dryja–Smith–Widlund)



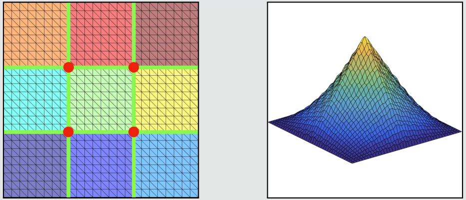
- Dohrmann, Klawonn, Widlund (2008)
- Dohrmann, Widlund (2009, 2010, 2012)

RGDSW (Reduced dimension GDSW)



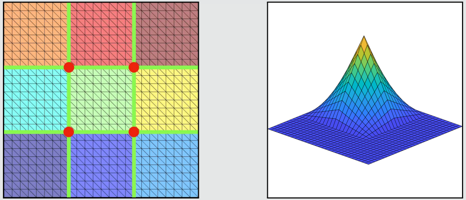
- Dohrmann, Widlund (2017)
- H., Klawonn, Knepper, Rheinbach, Widlund (2022)

MsFEM (Multiscale Finite Element Method)



- Hou (1997), Efendiev and Hou (2009)
- Buck, Iliev, and Andrä (2013)
- H., Klawonn, Knepper, Rheinbach (2018)

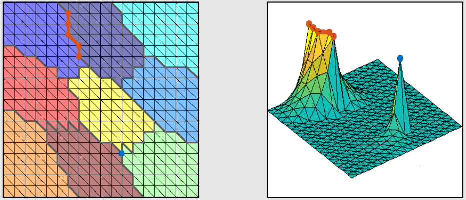
Q1 Lagrangian / piecewise bilinear



Piecewise linear interface partition of unity functions and a **structured domain decomposition**.

Examples of FROSch Coarse Spaces

GDSW (Generalized Dryja–Smith–Widlund)



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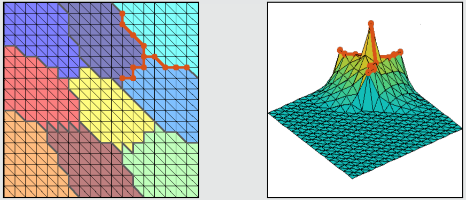


- Dohrmann, Widlund (2017)
- H., Klawonn, Knepper, Rheinbach, Widlund (2022)

For elliptic model problems, the **condition number of the (R)GDSW two-level Schwarz operator** is bounded by

$$\kappa \left(\boldsymbol{M}^{-1}_{\text{(R)GDSW}} \boldsymbol{K} \right) \leq C \left(1 + \frac{H}{\delta} \right) \left(1 + \log \left(\frac{H}{h} \right) \right)^{\alpha},$$

where

C	constant (does not depend on h, H, or δ),
H	subdomain diameter,
h	element size,
δ	width of the overlap,
$\alpha \in \{0, 1, 2\}$	power (depends on problem dimension, regularity of the subdomains, and variant of the algorithm).

Monolithic Coarse Spaces Multiphysics Problems

Consider the discrete saddle point problem

$$\mathcal{A}x = \begin{bmatrix} \boldsymbol{K} & \boldsymbol{B}^\top \\ \boldsymbol{B} & \boldsymbol{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{0} \end{bmatrix} = \mathscr{b}.$$

Monolithic GDSW preconditioner

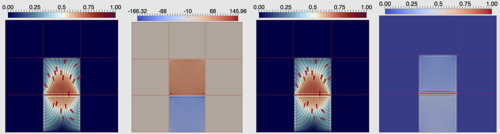
We construct a **monolithic GDSW preconditioner**

$$\mathcal{M}_{\mathrm{GDSW}}^{-1} = \phi \mathcal{A}_0^{-1} \phi^\top + \sum_{i=1}^{N} \mathcal{R}_i^\top \overline{\mathcal{P}}_i \mathcal{A}_i^{-1} \mathcal{R}_i,$$

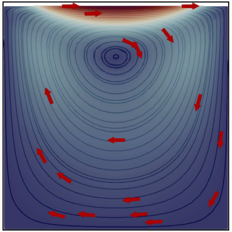
with block matrices $\mathcal{A}_0 = \phi^\top \mathcal{A} \phi$, $\mathcal{A}_i = \mathcal{R}_i \mathcal{A} \mathcal{R}_i^\top$, local pressure projections $\overline{\mathcal{P}}_i$, and

$$\mathcal{R}_i = \begin{bmatrix} \mathcal{R}_{u,i} & \boldsymbol{0} \\ \boldsymbol{0} & \mathcal{R}_{p,i} \end{bmatrix} \quad \text{and} \quad \phi = \begin{bmatrix} \Phi_{u,u_0} & \Phi_{u,p_0} \\ \Phi_{p,u_0} & \Phi_{p,p_0} \end{bmatrix}.$$

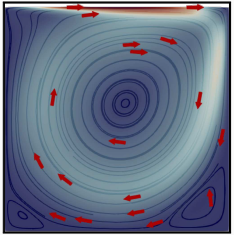
Using $\mathcal{A}$ to compute extensions: $\phi_I = -\mathcal{A}_{II}^{-1} \mathcal{A}_{I\Gamma} \phi_\Gamma$; cf. **Heinlein, Hochmuth, Klawonn (2019, 2020)**.



Φ_{u,u_0} Φ_{p,u_0} Φ_{u,p_0} Φ_{p,p_0}



Stokes flow



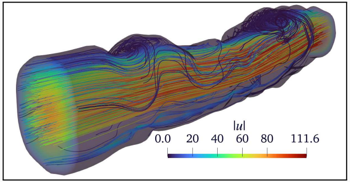
Navier–Stokes flow

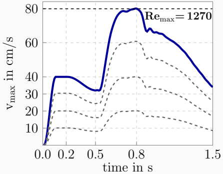
Related work:

- Original work on monolithic Schwarz preconditioners: **Klawonn and Pavarino (1998, 2000)**
- Other publications on monolithic Schwarz preconditioners: e.g., **Hwang and Cai (2006)**, **Barker and Cai (2010)**, **Wu and Cai (2014)**, and the presentation **Dohrmann (2010)** at the *Workshop on Adaptive Finite Elements and Domain Decomposition Methods* in Milan.

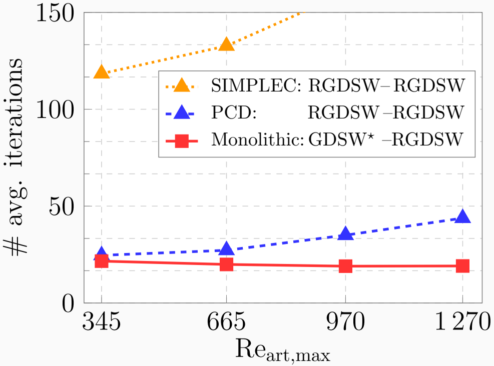
Results for Blood Flow Simulations

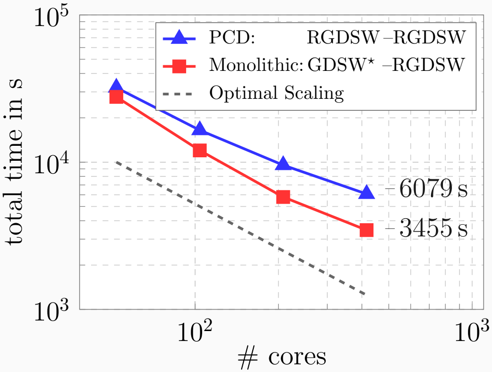
- **3D unsteady flow simulation** within the **geometry of a realistic artery** (from **Balzani et al. (2012)**) and kinematic viscosity $\nu = 0.03\,\text{cm}^2/\text{s}$
- **Parabolic inflow profile** at inlet
- **Time discretization**: BDF-2; **space discretization**: P2-P1 elements





Cf. **Heinlein, Klawonn, Knepper, Saßmannshausen (arXiv 2025)**

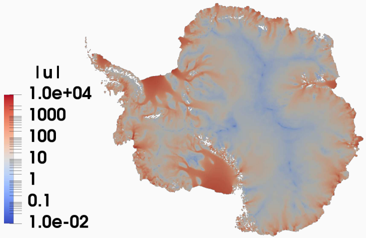




More details in the **talk by Lea Saßmannshausen** in MS24, Thursday, 2.40pm.

FROSch Preconditioners for Land Ice Simulations

https://github.com/SNLComputation/Albany



The velocity of the ice sheet in Antarctica and Greenland is modeled by a **first-order-accurate Stokes approximation model**,

$$-\nabla \cdot (2\mu \dot{\epsilon}_1) + \rho g \frac{\partial s}{\partial x} = 0, \quad -\nabla \cdot (2\mu \dot{\epsilon}_2) + \rho g \frac{\partial s}{\partial y} = 0,$$

with a **nonlinear viscosity model** (Glen's law); cf., e.g., **Blatter (1995)** and **Pattyn (2003)**.

MPI ranks	Antarctica (**velocity**) 4 km resolution, 20 layers, 35 m dofs			Greenland (**multiphysics vel. & temperature**) 1-10 km resolution, 20 layers, 69 m dofs		
	avg. its	avg. setup	avg. solve	avg. its	avg. setup	avg. solve
512	**41.9** (11)	25.10 s	12.29 s	**41.3** (36)	18.78 s	4.99 s
1024	**43.3** (11)	9.18 s	5.85 s	**53.0** (29)	8.68 s	4.22 s
2048	**41.4** (11)	4.15 s	2.63 s	**62.2** (86)	4.47 s	4.23 s
4096	**41.2** (11)	1.66 s	1.49 s	**68.9** (40)	2.52 s	2.86 s
8192	**40.2** (11)	1.26 s	1.06 s	-	-	-

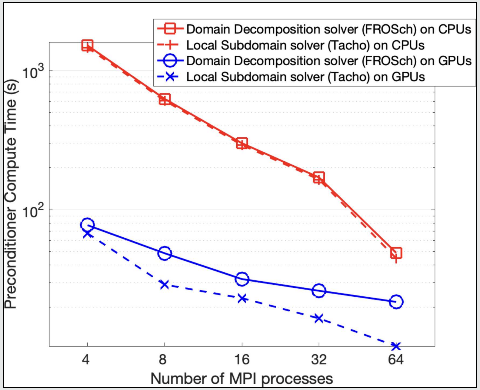
Computations performed on Cori (NERSC). **Heinlein, Perego, Rajamanickam (2022)**

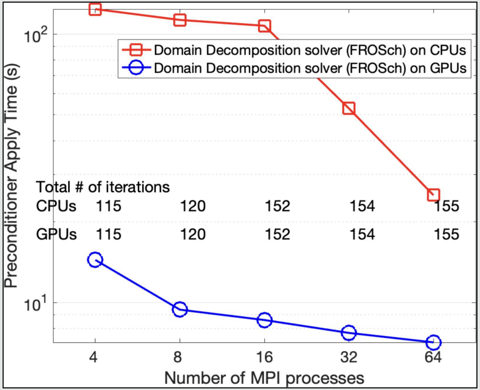
Tacho

- Multifrontal factorization with pivoting
- Impl. using KOKKOS and level-set scheduling

Cf. **Kim, Edwards, Rajamanickam (2018)**.

Strong scaling results on a single compute node of Perlmutter (NERSC)





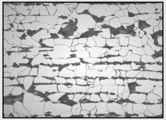
Cf. **Yamazaki, Ellingwood, and Rajamanickam (subm. 2025)**.

Robust Coarse Spaces for Heterogeneous Problems

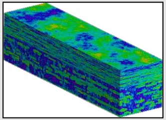
Spectral Extension-Based Coarse Spaces for Schwarz Preconditioners

Highly heterogeneous problems . . .

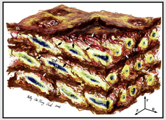
. . . appear in most areas of modern science and engineering:



Micro section of a dual-phase steel. Courtesy of **J. Schröder**.



Groundwater flow (SPE10); cf. **Christie and Blunt (2001)**.



Composition of arterial walls; taken from **O'Connell et al. (2008)**.

Spectral coarse spaces

The coarse space is **enhanced** by eigenfunctions of **local edge and face eigenvalue problems** with eigenvalues below tolerances $tol_{\mathcal{E}}$ and $tol_{\mathcal{F}}$:

$$\kappa\left(\boldsymbol{M}_*^{-1}\boldsymbol{K}\right) \leq C\left(1 + \frac{1}{tol_{\mathcal{E}}} + \frac{1}{tol_{\mathcal{F}}} + \frac{1}{tol_{\mathcal{E}} \cdot tol_{\mathcal{F}}}\right);$$

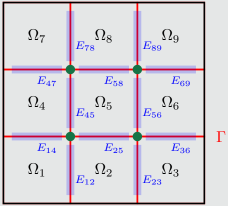
C does not depend on h, H, or the coefficients.
OS-ACMS & adaptive GDSW (AGDSW) (**Heinlein, Klawonn, Knepper, Rheinbach (2018, 2018, 2019)**).

Local eigenvalue problems

Local generalized eigenvalue problems corresponding to the edges $\mathcal{E}$ and faces $\mathcal{F}$ of the domain decomposition:

$$\forall E \in \mathcal{E}: \qquad \boldsymbol{S}_{EE}\tau_{*,E} = \lambda_{*,E}\boldsymbol{K}_{EE}\tau_{*,E}, \quad \forall \tau_{*,E} \in V_E,$$

$$\forall F \in \mathcal{F}: \qquad \boldsymbol{S}_{FF}\tau_{*,F} = \lambda_{*,F}\boldsymbol{K}_{FF}\tau_{*,F}, \quad \forall \tau_{*,F} \in V_F,$$

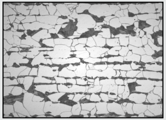


with **Schur complements** S_{EE}, S_{FF} with **Neumann boundary conditions** and **submatrices** K_{EE}, K_{FF} of K. We select eigenfunctions corresponding to **eigenvalues below tolerances** $tol_{\mathcal{E}}$ and $tol_{\mathcal{F}}$.

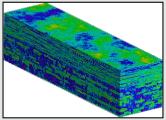
$\rightarrow$ The corresponding coarse basis functions are **energy-minimizing extensions** into the interior of the subdomains.

Highly heterogeneous problems . . .

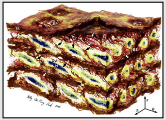
. . . appear in most areas of modern science and engineering:



Micro section of a dual-phase steel. Courtesy of **J. Schröder**.



Groundwater flow (SPE10); cf. **Christie and Blunt (2001)**.



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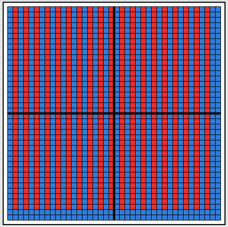
C does not depend on h, H, or the coefficients.

OS-ACMS & adaptive GDSW (AGDSW) (**Heinlein, Klawonn, Knepper, Rheinbach (2018, 2018, 2019)**).

FROSch – Channel coefficient function example



Example: 2×2 subd.'s and $H/h = 20$

Red: $\alpha = 10^6$; **blue:** $\alpha = 1$

- 2D Diffusion problem on unit square discretized Q1 finite elements
- $N \times N$ subdomains, $H/h = 20$, minimal algebraic overlap

# subdomains = # MPI ranks	# iterations GDSW	# iterations AGDSW
2×2	105	13
4×4	502	17
8×8	1451	19
16×16	2981	19

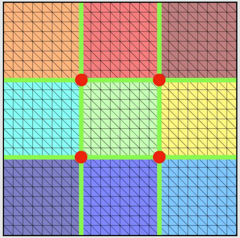
Joint work with **Axel Klawonn**, **Jascha Knepper**, and **Ichitaro Yamazaki**.

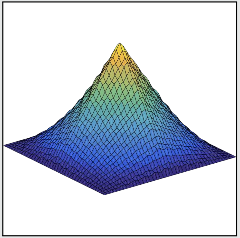
Algebraic Multiscale Coarse Space

Multiscale Finite Element Method (MsFEM) (Hou and Wu, 1997)

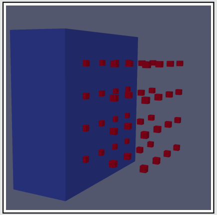
MsFEM defines a set of coarse basis functions as the solution of the local boundary condition problem:

$$
\begin{aligned}
-\nabla \cdot (\alpha(x)\nabla\varphi_i(x)) &= 0 \quad \text{in } \Omega_k,\\
\varphi_i &= 0 \quad \text{on } \partial\Omega,\\
\nabla_{||}\left(\alpha(x)\varphi_i(x)\right)_{||} &= 0 \quad \text{on } \Gamma = \partial\Omega_k \setminus \partial\Omega,\\
\varphi_i(x_j) &= \delta_{ij} \quad \text{for a coarse node } x_j.
\end{aligned}
$$

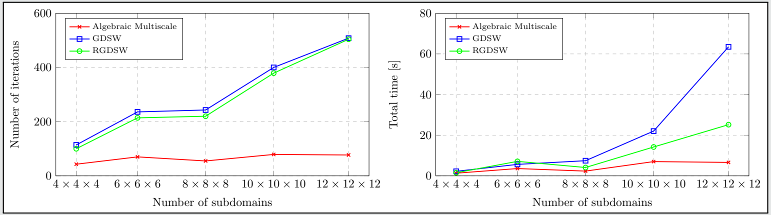




3D heterogeneous problem on DelftBlue (TU Delft)



Red: $\alpha = 10^5$; **blue:** $\alpha = 1$



Comparison of coarse spaces with $H/h = 16$, one layer of overlap

More details in the **talk by Filipe Cumaru** in MS05, Tuesday, 12.00pm.

Summary

Advances of FROSch Preconditioners for Multiphysics and Multiscale Simulations

- FROSch leverages the **Schwarz framework** and **extension-based coarse spaces** to achieve **robustness** and **scalability** while relying mostly on **algebraic information**.
- **Monolithic coarse spaces** ensure robust performance for **multiphysics problems**, e.g., strong convergence in **CFD** and scalability in **land ice** simulations.
- Robust convergence for **heterogeneous problems** requires tailored coarse spaces; recent advances include **robust multiscale** and **spectral coarse spaces** in FROSch.

Further talks on FROSch

- **Kyrill Ho** in MS27, Monday, 2.20pm (Room T23)
- **Filipe Cumaru** in MS05, Tuesday, 12.00pm (Room T04)
- **Thomas Wick** in MS06, Tuesday, at 3.00pm (Room 16B11)
- **Lea Saßmannshausen** in MS24, Thursday, 2.40pm (16B21)
- **Sebastian Kinnewig** in MS17, Thursday, at 11.40am (Room T23)

Thank you for your attention!