University of Stuttgart
Germany

SAND2020-13743C

FROSch Preconditioners for Land Ice Simulations of Greenland and Antarctica

Alexander Heinlein[1] Mauro Perego[2] Sivasankaran Rajamanickam[2]

26th International Domain Decomposition Conference, December 9, 2020

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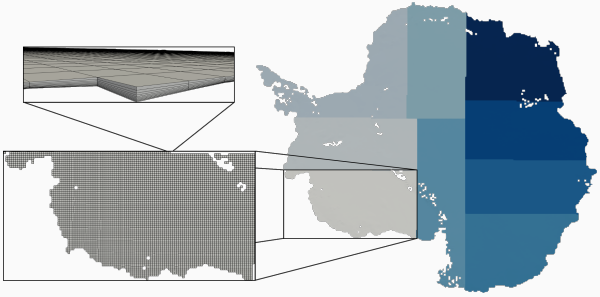
[2] Sandia National Laboratories

Land Ice Simulations of Greenland and Antarctica

Greenland and Antarctic ice sheets
- store most of the fresh water on earth and
- mass loss from these ice sheets significantly contributes to sea-level rise.

The simulation of temperature and velocity of the ice sheets gives rise to **large highly nonlinear systems of equations** with a **strong coupling** of the variables.

Taken from https://unsplash.com.



The simulations are also characterized by:
- The **mesh structure**:
  - Volume mesh is obtained by **extrusion** of the surface mesh $\Rightarrow$ **2D domain decomposition**.
  - **Highly anisotropic**.
- Specific combination of Dirichlet, Neumann, and Robin **boundary conditions**.

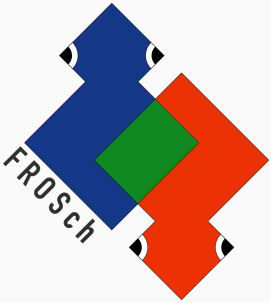
Domain Decomposition Methods in Trilinos

By Sandia National Laboratories

- Teko: **Block preconditioners** for multi-physics problems
- Ifpack/Ifpack2: **One-level overlapping Schwarz preconditioners**
  → **Algebraic** but **not scalable**
- ShyLU/BDDC: **BDDC** (Balancing Domain Decomposition by Constraints) **preconditioner**
  → **Scalable** but **less algebraic**

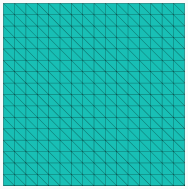
FROSch (**F**ast and **R**obust **O**verlapping **Sch**warz)

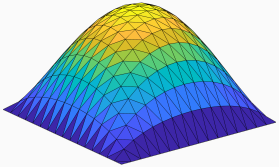
- **Schwarz preconditioners** with **algebraic coarse spaces** based on extension operators, e.g., **GDSW** (Generalized–Dryja–Smith–Widlund) coarse spaces
  → **Algebraic** and **scalable**
- Part of the package ShyLU:
  (Joint work with the Scalable Algorithms group of the **Sandia National Laboratories (SNL)**, Albuquerque, USA)
- Implementation based on Xpetra
  → Can be used with Epetra and Tpetra (linear algebra packages)
  Extension to current architectures, e.g., **GPUs**, *using the* Kokkos *programming model*



Easy access to FROSch through unified Trilinos solver interface Thyra.

Model Problem & Domain Decomposition





Consider a **Poisson model problem** on $[0,1]^2$:

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

Discretize (e.g., using finite elements)

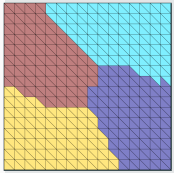
$$Kx = b.$$

$\Rightarrow$ Construct a **parallel scalable preconditioner** M^{-1} using **overlapping Schwarz domain decomposition methods**.

Overlapping domain decomposition

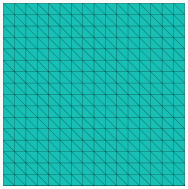
Overlapping Schwarz methods are based on **overlapping decompositions** of the computational domain Ω.

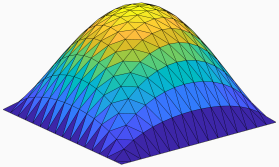
Overlapping subdomains $\Omega_1', ..., \Omega_N'$ can be constructed by **recursively adding layers of elements** to nonoverlapping subdomains $\Omega_1, ..., \Omega_N$.



Nonoverlap. DD

Model Problem & Domain Decomposition





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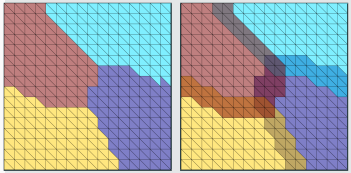
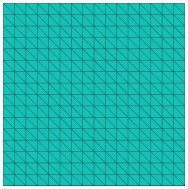
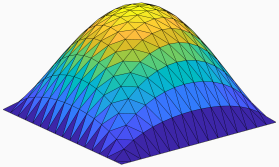


Nonoverlap. DD Overlap $\delta = 1h$

Model Problem & Domain Decomposition





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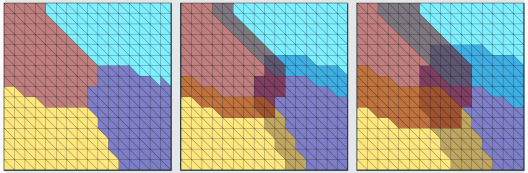
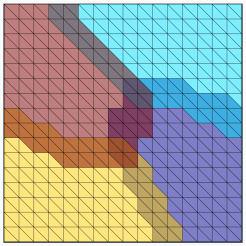


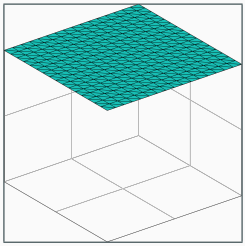
Nonoverlap. DD | Overlap $\delta = 1h$ | Overlap $\delta = 2h$

One-Level Schwarz Preconditioners

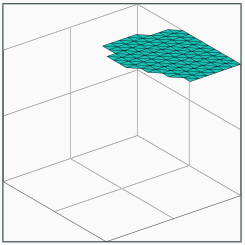
Overlapping domain decomposition



Function on Ω



Restriction to Ω_i'



Based on an **overlapping domain decomposition**, we define **local restriction operators** $R_i : V^h(\Omega) \to V_i := V^h(\Omega_i')$, for $i = 1, ..., N$, and obtain the **additive one-level Schwarz preconditioner**

$$M_{\mathrm{OS}-1}^{-1} = \underbrace{\sum_{i=1}^{N} R_i^T K_i^{-1} R_i}_{\textbf{local}},$$

where $K_i := R_i K R_i^T$.

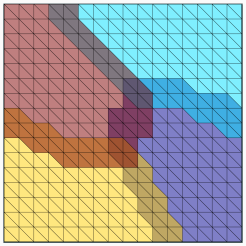
Condition number estimate:

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

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

One-Level Schwarz Preconditioners

Overlapping domain decomposition



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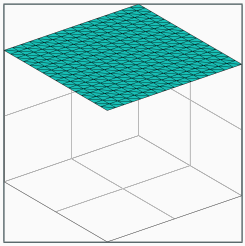

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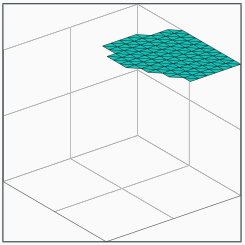

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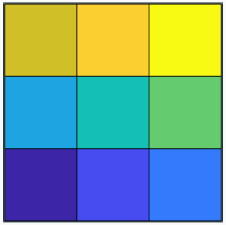
with the typical subdomain size H and the width of the overlap δ.

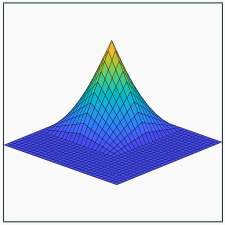
$\rightarrow$ **Algebraic! but not scalable...**

Two-Level Schwarz Preconditioners – Lagrangian Coarse Space

Coarse triangulation



Nodal bilinear basis function



The **additive two-level Schwarz preconditioner** reads

$$M_{\mathrm{OS}-2}^{-1} = \underbrace{\Phi K_0^{-1} \Phi^T}_{\text{coarse level – global}} + \underbrace{\sum_{i=1}^{N} R_i^T K_i^{-1} R_i}_{\text{first level – local}},$$

where Φ contains the coarse basis functions and $K_0 := \Phi^T K \Phi$; cf., e.g., **Toselli, Widlund (2005)**.

In the **classical Lagrangian coarse space**, the coarse basis functions are a **nodal finite element basis on the coarse triangulation**. Their construction **relies on geometric information and cannot be performed algebraically**.

The **condition number of the two-level Schwarz operator with classical Lagrangian coarse space** is bounded by

$$\kappa\left(M_{\mathrm{OS}-2}^{-1} K\right) \leq C\left(1 + \frac{H}{\delta}\right);$$

cf., e.g., **Toselli, Widlund (2005)**. The constant C is **independent of h, δ, and H**.

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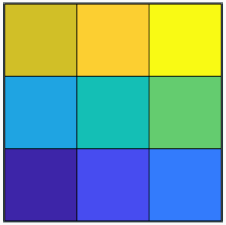

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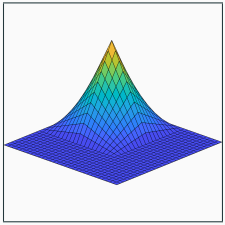

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→ **Scalable! But not algebraic...**

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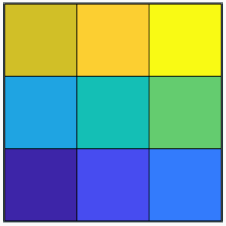

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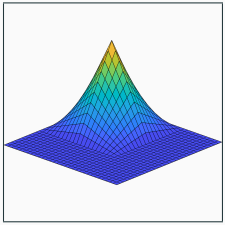

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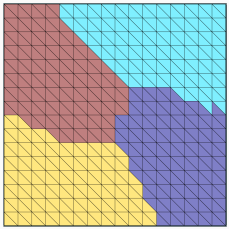
cf., e.g., **Toselli, Widlund (2005)**. The constant C is **independent of h, δ, and H.**

→ **Scalable! But not algebraic...**

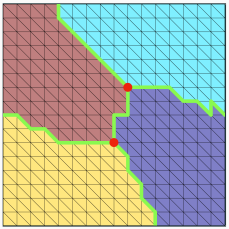
Can we construct a coarse space **algebraically**? → **GDSW coarse spaces**

Two-Level Schwarz Preconditioners – GDSW Coarse Space

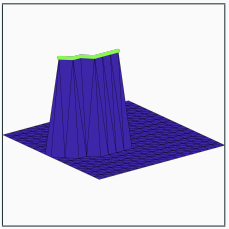
Non-overlapping DD



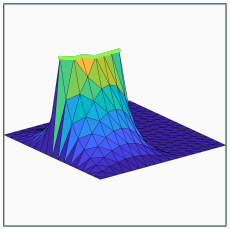
Ident. vertices & edges



Restr. of the null space



Energy minimizing ext.



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:

$$\Phi = \begin{bmatrix} -K_{II}^{-1} K_{\Gamma I}^T \Phi_\Gamma \\ \Phi_\Gamma \end{bmatrix} = \begin{bmatrix} \Phi_I \\ \Phi_\Gamma \end{bmatrix}$$

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

$$\kappa\left(M_{\mathrm{GDSW}}^{-1} K\right) \leq C \left(1 + \frac{H}{\delta}\right) \left(1 + \log\left(\frac{H}{h}\right)\right)^2;$$

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

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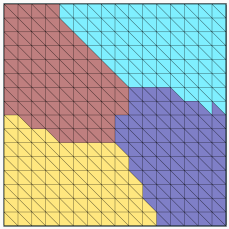

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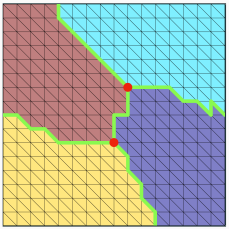

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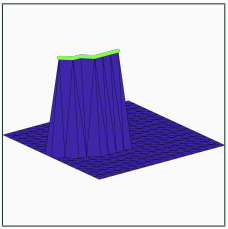

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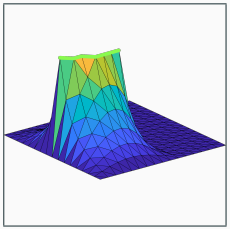

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cf. **Dohrmann, Klawonn, Widlund (2008)**, **Dohrmann, Widlund (2009, 2010, 2012)**.

→ We only obtain the exponent 2 for very irregular subdomains.

Two-Level Schwarz Preconditioners – GDSW Coarse Space

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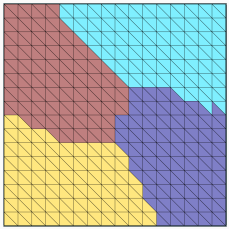

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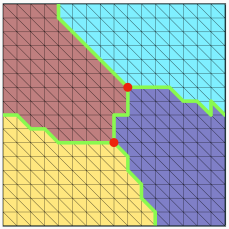

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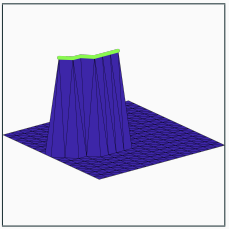
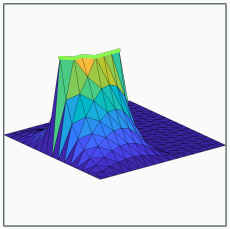


Energy minimizing ext.



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:

$$\Phi = \begin{bmatrix} -K_{II}^{-1} K_{\Gamma I}^T \Phi_\Gamma \\ \Phi_\Gamma \end{bmatrix} = \begin{bmatrix} \Phi_I \\ \Phi_\Gamma \end{bmatrix}$$

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

$$\kappa\left(M_{\mathrm{GDSW}}^{-1} K\right) \leq C \left(1 + \frac{H}{\delta}\right) \left(1 + \log\left(\frac{H}{h}\right)\right)^2;$$

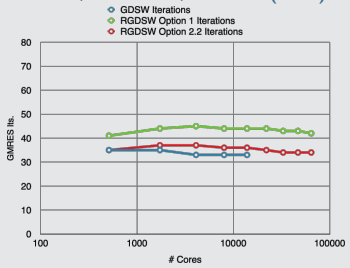
cf. **Dohrmann, Klawonn, Widlund (2008)**, **Dohrmann, Widlund (2009, 2010, 2012)**.

→ **Scalable and algebraic!**

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

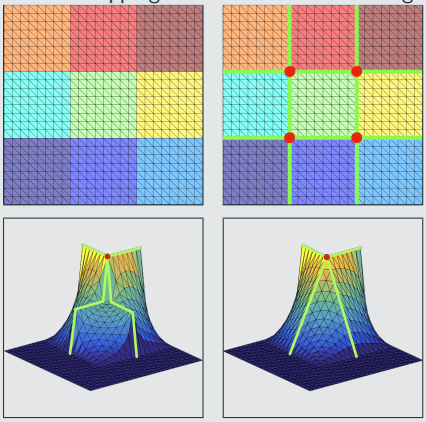
GDSW vs RGDSW (reduced dimension)

Heinlein, Klawonn, Rheinbach, Widlund (2019)



RGDSW (Reduced dimension GDSW)

Non-overlapping DD Ident. vertices & edges



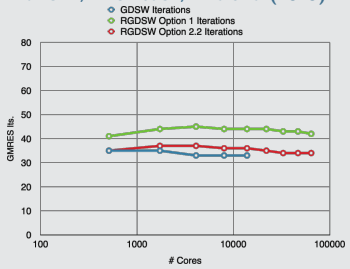
RGDSW option 1 RGDSW option 2.2

Reduced dimension GDSW coarse spaces are constructed from **nodal interface functions (different partition of unity)**; cf. **Dohrmann, Widlund (2017)**.

Weak Scalability up to $64\,\mathrm{k}$ MPI Ranks / $1.7\,\mathrm{b}$ Unknowns (3D Poisson; Juqueen)

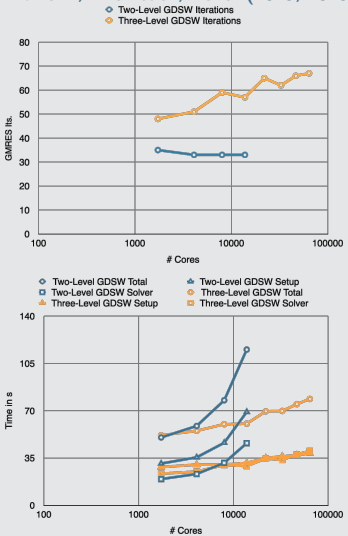
GDSW vs RGDSW (reduced dimension)

Heinlein, Klawonn, Rheinbach, Widlund (2019)



Two-level vs Three-level GDSW

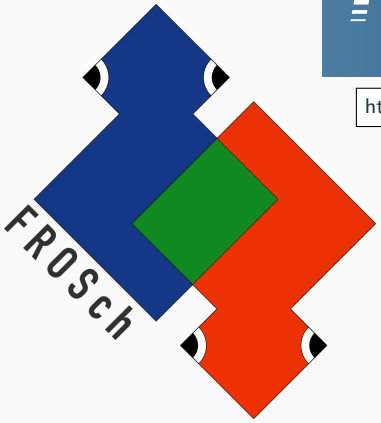
Heinlein, Klawonn, Rheinbach, Röver (2019, 2020)



→ Talk by **F. Röver** in **MS11-01 (earlier today)**

Software Framework

https://github.com/trilinos/Trilinos

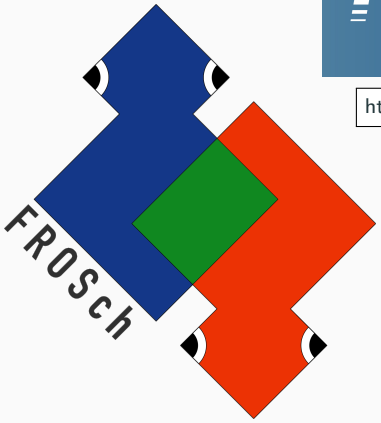


Part of `Trilinos`.
→ `MKL Pardiso` as the subdomain and coarse solver.

https://github.com/SNLComputation/Albany

Software Framework

https://github.com/trilinos/Trilinos



Part of `Trilinos`.
→ `MKL Pardiso` as the subdomain and coarse solver.

https://github.com/SNLComputation/Albany

Hardware

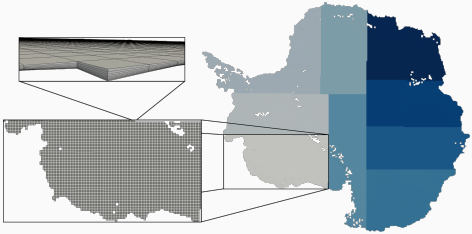
All simulations performed on Cori supercomputer (NERSC).

Velocity Problem

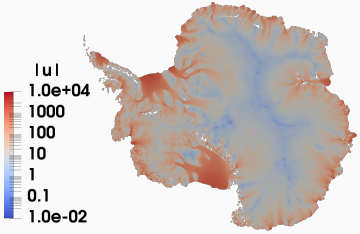
We use the so called **first-order (or Blatter-Pattyn) approximation of the Stokes equations**

$$\begin{cases} -\nabla \cdot (2\mu\,\dot{\boldsymbol{\epsilon}}_1) &= -\rho_i\,|\boldsymbol{g}|\,\partial_x s, \\ -\nabla \cdot (2\mu\,\dot{\boldsymbol{\epsilon}}_2) &= -\rho_i\,|\boldsymbol{g}|\,\partial_y s, \end{cases}$$

with the ρ_i the ice density, the ice surface elevation $s(x, y)$, the gravity acceleration $\boldsymbol{g}$, and strain rates $\dot{\boldsymbol{\epsilon}}_1$ and $\dot{\boldsymbol{\epsilon}}_2$; cf. **Blatter (1995)** and **Pattyn (2003)**.



Antarctica mesh & domain decomposition.



Velocity u solution

Nonlinear viscosity model

The **ice viscosity** μ is modeled using **Glen's law**

$$\mu \;=\; \frac{1}{2} A(T)^{-\frac{1}{n}}\, \dot{\epsilon}_e^{\frac{1-n}{n}},$$

where $A(T) = \alpha_1 e^{\alpha_2 T}$ is a temperature-dependent rate factor, $n = 3$ is the power-law exponent, and the effective strain rate $\dot{\epsilon}$.

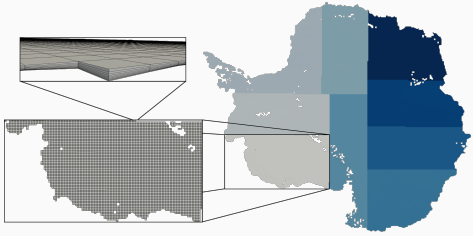
See **Perego, Gunzburger, Burkardt (2012)** and **Tezaur, Perego, Salinger, Tuminaro, Price (2015)** for more details.

Velocity Problem

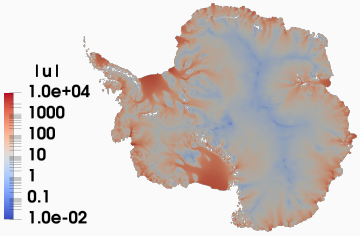
We use the so called **first-order (or Blatter-Pattyn) approximation of the Stokes equations**

$$\begin{cases} -\nabla \cdot (2\mu\,\dot{\boldsymbol{\epsilon}}_1) &= -\rho_i\,|\boldsymbol{g}|\,\partial_x s, \\ -\nabla \cdot (2\mu\,\dot{\boldsymbol{\epsilon}}_2) &= -\rho_i\,|\boldsymbol{g}|\,\partial_y s, \end{cases}$$

with the ρ_i the ice density, the ice surface elevation $s(x, y)$, the gravity acceleration $\boldsymbol{g}$, and strain rates $\dot{\boldsymbol{\epsilon}}_1$ and $\dot{\boldsymbol{\epsilon}}_2$; cf. **Blatter (1995)** and **Pattyn (2003)**.



Antarctica mesh & domain decomposition.



Velocity u solution

Boundary conditions

- *Upper surface*: $\dot{\boldsymbol{\epsilon}}_j = 0$, $j = 1, 2$ (**stress-free Neumann condition**)
- *Lower surface*: $2\mu_e\dot{\boldsymbol{\epsilon}}_j \cdot \boldsymbol{n} + \beta u = 0$, $j = 1, 2$ (**sliding Robin condition** with friction coefficient β)
- *Lateral boundary*: $2\mu\dot{\boldsymbol{\epsilon}}_j \cdot \boldsymbol{n} = \frac{1}{2} g H \left(\rho_i - \rho_w r^2\right) n_1$, $j = 1, 2$ (**open-ocean Neumann condition** with density of ocean water ρ_w and ratio of submerged ice thickness r)

See **Perego, Gunzburger, Burkardt (2012)** and **Tezaur, Perego, Salinger, Tuminaro, Price (2015)** for more details.

Antarctica Velocity Problem – Coarse Spaces

Without rotational coarse basis functions (2 rigid body modes)								
	GDSW				**RGDSW**			
MPI ranks	dim V_0	avg. its (nl its)	avg. setup	avg. solve	dim V_0	avg. its (nl its)	avg. setup	avg. solve
512	4 598	**40.8** (11)	15.36 s	**12.38 s**	1 834	42.6 (11)	**14.99 s**	12.50 s
1 024	9 306	**43.3** (11)	5.80 s	6.27 s	3 740	44.5 (11)	**5.65 s**	**6.08 s**
2 048	18 634	**41.7** (11)	3.27 s	2.91 s	7 586	42.7 (11)	**3.11 s**	**2.79 s**
4 096	37 184	**41.4** (11)	2.59 s	2.07 s	15 324	42.5 (11)	**1.07 s**	**1.54 s**
8 192	72 964	**39.5** (11)	1.51 s	1.84 s	30 620	42.0 (11)	**1.20 s**	**1.16 s**
With rotational coarse basis functions (3 rigid body modes)								
	GDSW				**RGDSW**			
MPI ranks	dim V_0	avg. its (nl its)	avg. setup	avg. solve	dim V_0	avg. its (nl its)	avg. setup	avg. solve
512	6 897	**35.5** (11)	15.77 s	**11.21 s**	2 751	40.7 (11)	**15.23 s**	12.22 s
1 024	13 959	**35.6** (11)	6.16 s	**5.78 s**	5 610	42.9 (11)	**5.65 s**	6.04 s
2 048	27 951	**33.5** (11)	3.78 s	3.45 s	11 379	42.2 (11)	**3.17 s**	**2.81 s**
4 096	55 776	**31.8** (11)	2.21 s	3.80 s	22 986	44.3 (11)	**1.95 s**	**2.70 s**
8 192	109 446	**29.3** (11)	2.49 s	5.33 s	45 930	40.8 (11)	**1.19 s**	**3.13 s**

Problem: Velocity **Mesh:** Antarctica, 4 km hor. resolution 20 vert. layers **Size:** 35.3 m degrees of freedom (P1 FE)

Antarctica Velocity Problem – Reuse

We employ different **reuse strategies** to **reduce the setup costs** of the two-level preconditioner

$$M_{\mathrm{OS}-2}^{-1} = \Phi \mathbf{K_0}^{-1} \Phi^T + \sum_{i=1}^{N} \mathbf{R_i}^T K_i^{-1} \mathbf{R_i}.$$

	restriction operators + symbolic fact. (1st level)			**+ coarse basis + symbolic fact. (2nd level)**			**+ coarse matrix**		
MPI ranks	avg. its (nl its)	avg. setup	avg. solve	avg. its (nl its)	avg. setup	avg. solve	avg. its (nl its)	avg. setup	avg. solve
512	**41.9** (11)	25.10 s	**12.29 s**	42.6 (11)	14.99 s	12.50 s	46.7 (11)	**14.94 s**	13.81 s
1 024	**43.3** (11)	9.18 s	**5.85 s**	44.5 (11)	**5.65 s**	6.08 s	49.2 (11)	5.75 s	6.78 s
2 048	**41.4** (11)	4.15 s	**2.63 s**	42.7 (11)	3.11 s	2.79 s	47.7 (11)	**2.92 s**	3.10 s
4 096	**41.2** (11)	1.66 s	**1.49 s**	42.5 (11)	1.07 s	1.54 s	48.9 (11)	**0.95 s**	1.75 s
8 192	**40.2** (11)	1.26 s	**1.06 s**	42.0 (11)	1.20 s	1.16 s	50.1 (11)	**0.63 s**	1.35 s

Problem: Velocity **Mesh:** Antarctica, 4 km hor. resolution, 20 vert. layers **Size:** 35.3 m degrees of freedom (P1 FE) **Coarse space:** RGDSW

Antarctica Velocity Problem – OpenMP VS MPI Parallelization

We can make use of **OpenMP parallelization**:

- `Tpetra` linear algebra stack in `FROSch` and `Albany` ⇒ **OpenMP parallelization of the linear algebra operations**.
- **OpenMP parallelization** of the **subdomain and coarse solver** `Pardiso MKL` used in `FROSch`.

	OpenMP parallelization (512 MPI ranks)				MPI parallelization			
cores	OpenMP threads	avg. its (nl its)	avg. setup	avg. solve	MPI ranks	avg. its (nl its)	avg. setup	avg. its solve
512	1	**42.6** (11)	**14.99 s**	**12.50 s**	512	**42.6** (11)	**14.99 s**	**12.50 s**
1 024	2	**42.6** (11)	9.43 s	6.80 s	1 024	44.5 (11)	**5.65 s**	**6.08 s**
2 048	4	**42.6** (11)	5.50 s	4.02 s	2 048	42.7 (11)	**3.11 s**	**2.79 s**
4 096	8	42.6 (11)	3.65 s	2.71 s	4 096	**42.5** (11)	**1.07 s**	**1.54 s**
8 192	16	42.6 (11)	2.56 s	2.32 s	8 192	**42.0** (11)	**1.20 s**	**1.16 s**

Problem: Velocity **Mesh:** Antarctica, 4 km hor. resolution 20 vert. layers **Size:** 35.3 m degrees of freedom (P1 FE) **Coarse space:** RGDSW

Antarctica Velocity Problem – OpenMP VS MPI Parallelization

We can make use of **OpenMP parallelization**:

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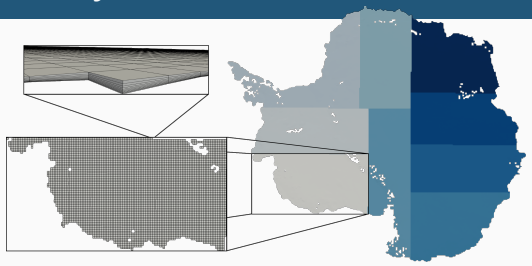
	OpenMP parallelization (512 MPI ranks)				MPI parallelization			
cores	OpenMP threads	avg. its (nl its)	avg. setup	avg. solve	MPI ranks	avg. its (nl its)	avg. setup	avg. its solve
512	1	**42.6** (11)	**14.99 s**	**12.50 s**	512	**42.6** (11)	**14.99 s**	**12.50 s**
1 024	2	**42.6** (11)	9.43 s	6.80 s	1 024	44.5 (11)	**5.65 s**	**6.08 s**
2 048	4	**42.6** (11)	5.50 s	4.02 s	2 048	42.7 (11)	**3.11 s**	**2.79 s**
4 096	8	42.6 (11)	3.65 s	2.71 s	4 096	**42.5** (11)	**1.07 s**	**1.54 s**
8 192	16	42.6 (11)	2.56 s	2.32 s	8 192	**42.0** (11)	**1.20 s**	**1.16 s**

Problem: Velocity **Mesh:** Antarctica, 4 km hor. resolution 20 vert. layers **Size:** 35.3 m degrees of freedom (P1 FE) **Coarse space:** RGDSW

→ **MPI parallelization** is more efficient than **OpenMP parallelization**. However, **for large numbers of MPI ranks** and a **large dimension of the coarse problem**, **OpenMP parallelization may be useful**.

Antarctica Velocity Problem – Weak Scalability

- Weak scalability study for in increasing horizontal mesh resolution.
  - **1 OpenMP thread:** From 32 to 8 192 processor cores
  - **4 OpenMP threads:** From 128 to 32 768 processor cores
- The number of vertical layers is fixed to 20.
- P1 FEM spatial discretization.



Antarctica mesh & domain decomposition.

MPI ranks	mesh	# dofs	1 OpenMP thread: avg. its (nl its)	1 OpenMP thread: avg. setup	1 OpenMP thread: avg. solve	4 OpenMP threads: avg. its (nl its)	4 OpenMP threads: avg. setup	4 OpenMP threads: avg. solve
32	16 km	2.2 m	24.1 (11)	11.97 s	9.47 s	23.5 (11)	4.15 s	3.25 s
128	8 km	8.8 m	32.0 (10)	14.08 s	8.71 s	32.0 (10)	4.97 s	2.85 s
512	4 km	35.3 m	42.6 (11)	14.99 s	12.50 s	42.6 (11)	5.50 s	4.02 s
2 048	2 km	141.5 m	61.0 (11)	22.83 s	19.76 s	61.0 (11)	7.36 s	6.55 s
8 192	1 km	566.1 m	67.1 (14)	17.36 s	22.91 s	67.1 (14)	6.20 s	7.39 s

Problem: Velocity **Mesh:** Antarctica, 20 vert. layers **Coarse space:** RGDSW (P1 FE)

Temperature Problem

The **steady state enthalpy equation** reads

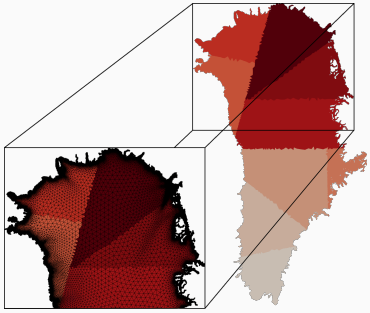
$$\nabla \cdot \boldsymbol{q}(h) + \boldsymbol{u} \cdot \nabla h = 4\mu\,\epsilon_e^2$$

with the enthalpy growing linearly with the water content ϕ

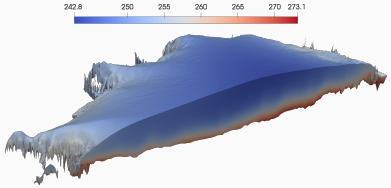
$$h = \begin{cases} \rho_i c\,(T - T_0), & \text{for cold ice } (h \le h_m), \\ h_m + \rho_w L\,\phi, & \text{for temperate ice.} \end{cases}$$

the **melting enthalpy** $h_m := \rho_w c(T_m - T_0)$, the **uniform reference temperature** T_0, and the **enthalpy flux**

$$\boldsymbol{q}(h) = \begin{cases} \frac{k}{\rho_i c_i}\nabla h, & \text{for cold ice } (h \le h_m), \\ \frac{k}{\rho_i c_i}\nabla h_m + \rho_w L \boldsymbol{j}(h), & \text{for temperate ice.} \end{cases}$$



Greenland mesh & domain decomposition.



Temperature T solution

Water flux term

The **water flux term**

$$\boldsymbol{j}(h) := \frac{1}{\eta_w}(\rho_w - \rho_i)k_0\phi^\gamma \boldsymbol{g}$$

describes the percolation of water driven by gravity; cf. **Schoof and Hewitt (2016, 2017)**.

See **Perego et al. (in preparation)** and **Heinlein et. al (in preparation)** for more details.

Temperature Problem

The **steady state enthalpy equation** reads

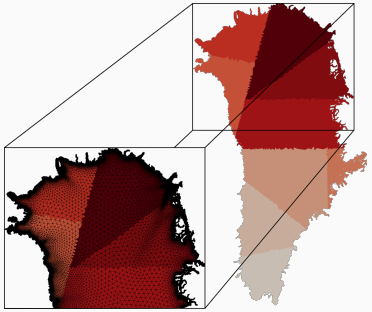
$$\nabla \cdot \boldsymbol{q}(h) + \boldsymbol{u} \cdot \nabla h = 4\mu\,\epsilon_e^2$$

with the enthalpy growing linearly with the water content ϕ

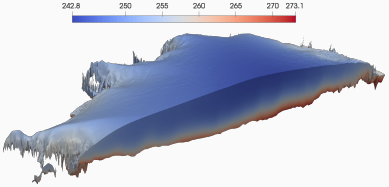
$$h = \begin{cases} \rho_i c\,(T - T_0), & \text{for cold ice } (h \le h_m), \\ h_m + \rho_w L\,\phi, & \text{for temperate ice.} \end{cases}$$

the **melting enthalpy** $h_m := \rho_w c(T_m - T_0)$, the **uniform reference temperature** T_0, and the **enthalpy flux**

$$\boldsymbol{q}(h) = \begin{cases} \frac{k}{\rho_i c_i}\nabla h, & \text{for cold ice } (h \le h_m), \\ \frac{k}{\rho_i c_i}\nabla h_m + \rho_w L \boldsymbol{j}(h), & \text{for temperate ice.} \end{cases}$$



Greenland mesh & domain decomposition.



Temperature T solution

Boundary conditions

- *Upper surface*: $h = \rho_i c(T_s - T_0)$
  (**Dirichlet boundary condition**)
- *Bed*: $m = G + \beta\sqrt{u^2 + v^2} - k\nabla T \cdot \boldsymbol{b}$,
  $m(T - T_m) = 0,\ T_m \le 0.$
  (**Stefan boundary condition**)

See **Perego et al. (in preparation)** and **Heinlein et. al (in preparation)** for more details.

Greenland Temperature Problem – One-Level Schwarz VS Two-Level Schwarz

One-level Schwarz						
	one layer of algebraic overlap			two layers of algebraic overlap		
MPI ranks	avg. its	avg. setup	avg. solve	avg. its	avg. setup	avg. solve
512	18.1 (11)	**0.42 s**	**0.35 s**	**17.1** (11)	0.51 s	0.40 s
1 024	23.7 (11)	**0.25 s**	**0.25 s**	**22.1** (11)	0.27 s	0.27 s
2 048	29.6 (11)	**0.16 s**	**0.17 s**	**27.6** (11)	0.23 s	0.20 s
4 096	39.8 (11)	**0.15 s**	**0.15 s**	**35.6** (11)	0.17 s	0.17 s
RGDSW						
	one layer of algebraic overlap			two layers of algebraic overlap		
MPI ranks	avg. avg. its	avg. setup	avg. solve	avg. avg. its	avg. setup	avg. solve
512	19.5 (11)	**0.44 s**	**0.41 s**	**18.7** (11)	0.55 s	0.46 s
1 024	25.2 (11)	**0.28 s**	**0.29 s**	**23.9** (11)	0.35 s	0.33 s
2 048	31.5 (11)	0.26 s	**0.24 s**	**29.5** (11)	**0.25 s**	0.27 s
4 096	42.2 (11)	**0.25 s**	**0.27 s**	**38.2** (11)	**0.25 s**	0.29 s

Problem: Temperature **Mesh:** Greenland, 1-10 km hor. resolution, 20 vert. layers **Size:** 1.9 m degrees of freedom (P1 FE)

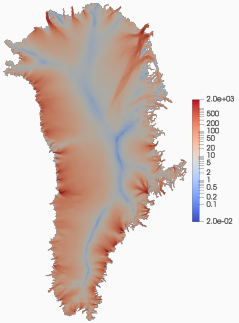
Coupled Problem

Couple the velocity and temperature problems. Therefore, compute the vertical velocity w using the incompressibility condition

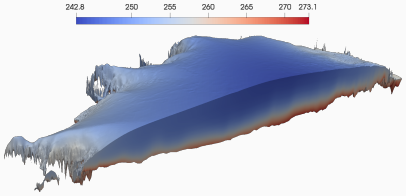
$$\partial_x u + \partial_y v + \partial_z w = 0,$$

with the **Dirichlet boundary condition at the ice lower surface**

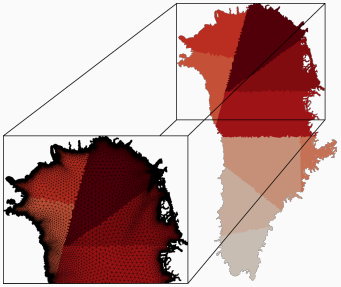
$$\boldsymbol{u} \cdot \boldsymbol{n} = \frac{m}{L\left(\rho_i - \rho_w \phi\right)}.$$



Velocity u solution



Temperature T solution



Greenland mesh & domain decomposition.

Then, the **tangent matrix** of the coupled problem has the structure

$$\begin{bmatrix} A_u & C_{uT} \\ C_{Tu} & A_T \end{bmatrix} \begin{bmatrix} x_u \\ x_T \end{bmatrix} = \begin{bmatrix} \tilde{r}_u \\ \tilde{r}_T \end{bmatrix}.$$

See **Perego et al. (in preparation)** and **Heinlein, Perego, Rajamanickam (in preparation)** for more details.

Monolithic GDSW preconditioner

Consider the discrete saddle point problem

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

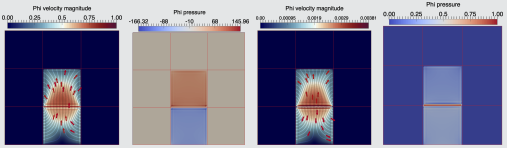
We construct a **monolithic GDSW preconditioner**

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

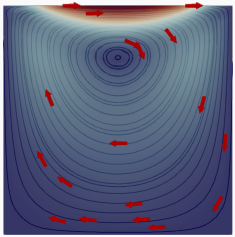
with block matrices $\mathcal{A}_0 = \phi^T \mathcal{A} \phi$, $\mathcal{A}_i = \mathcal{R}_i \mathcal{A} \mathcal{R}_i^T$, and

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

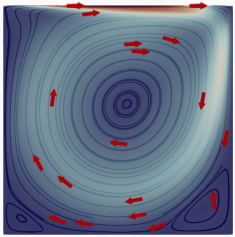
Using $\mathcal{A}$ to compute extensions: $\phi_I = -\mathcal{A}_{II}^{-1} \mathcal{A}_{I\Gamma} \phi_\Gamma$; cf. **Heinlein, Hochmuth, Klawonn (2019, 2020)**.



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.

Monolithic (R)GDSW Preconditioners for CFD Simulations

Monolithic GDSW preconditioner

Consider the discrete saddle point problem

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

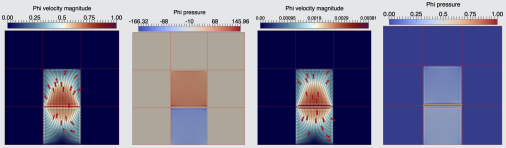
We construct a **monolithic GDSW preconditioner**

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

with block matrices $\mathcal{A}_0 = \phi^T \mathcal{A} \phi$, $\mathcal{A}_i = \mathcal{R}_i \mathcal{A} \mathcal{R}_i^T$, and

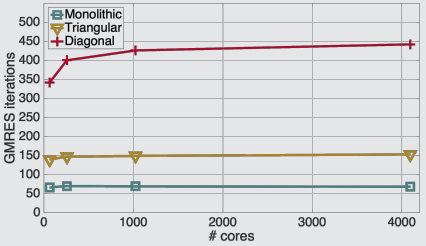
$$\mathcal{R}_i = \begin{bmatrix} \mathcal{R}_{u,i} & 0 \\ 0 & \mathcal{R}_{p,i} \end{bmatrix} \quad \text{and} \quad \phi = \begin{bmatrix} \Phi_{u,u_0} & \Phi_{u,p_0} \\ \Phi_{p,u_0} & \Phi_{p,p_0} \end{bmatrix}.$$

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}

Monolithic vs Block Preconditioners



Prec.	MPI ranks	64	256	1 024	4 096
Monolithic	time	154.7s	170.0s	175.8s	188.7s
	effic.	**100 %**	**91 %**	**88 %**	**82 %**
Triangular	time	309.4s	329.1s	359.8s	396.7s
	effic.	50 %	47 %	43 %	39 %
Diagonal	time	736.7s	859.4s	966.9s	1105.0s
	effic.	21 %	18 %	16 %	14 %

Computations performed on magnitUDE, University Duisburg-Essen.

Monolithic GDSW preconditioner

Consider the discrete saddle point problem

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

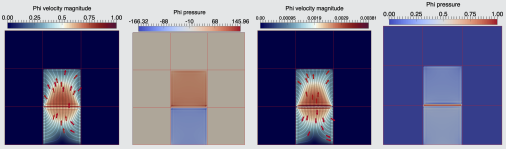
We construct a **monolithic GDSW preconditioner**

$$\mathcal{M}_{\text{GDSW}}^{-1} = \phi \mathcal{A}_0^{-1} \phi^T + \sum_{i=1}^{N} \mathcal{R}_i^T \mathcal{A}_i^{-1} \mathcal{R}_i,$$

with block matrices $\mathcal{A}_0 = \phi^T \mathcal{A} \phi$, $\mathcal{A}_i = \mathcal{R}_i \mathcal{A} \mathcal{R}_i^T$, and

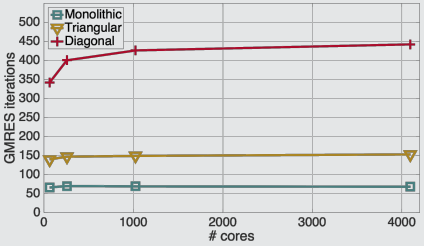
$$\mathcal{R}_i = \begin{bmatrix} \mathcal{R}_{u,i} & 0 \\ 0 & \mathcal{R}_{p,i} \end{bmatrix} \quad \text{and} \quad \phi = \begin{bmatrix} \Phi_{u,u_0} & \Phi_{u,p_0} \\ \Phi_{p,u_0} & \Phi_{p,p_0} \end{bmatrix}.$$

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}

Monolithic vs Block Preconditioners



Prec.	MPI ranks	64	256	1 024	4 096
Monolithic	time	154.7s	170.0s	175.8s	188.7s
	effic.	**100 %**	**91 %**	**88 %**	**82 %**
Triangular	time	309.4s	329.1s	359.8s	396.7s
	effic.	50 %	47 %	43 %	39 %
Diagonal	time	736.7s	859.4s	966.9s	1105.0s
	effic.	21 %	18 %	16 %	14 %

Computations performed on magnitUDE, University Duisburg-Essen.

→ Talk by **C. Hochmuth** in **MS11-02 (right after this talk)** for more details.

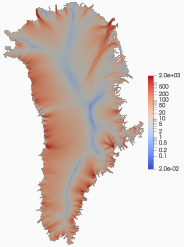
Monolithic (R)GDSW Preconditioners for Multiphysics Land Ice Simulations

We construct a **monolithic two-level GDSW preconditioner**

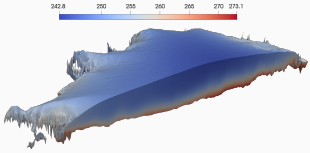
$$\mathcal{M}_{\mathrm{GDSW}}^{-1} = \phi \mathcal{A}_0^{-1} \phi^T + \sum_{i=1}^{N} \mathcal{R}_i^T \mathcal{A}_i^{-1} \mathcal{R}_i,$$

for the tangent matrix of the coupled problem

$$\mathcal{A}x := \begin{bmatrix} A_u & C_{uT} \\ C_{Tu} & A_T \end{bmatrix} \begin{bmatrix} x_u \\ x_T \end{bmatrix} = \begin{bmatrix} \tilde{r}_u \\ \tilde{r}_T \end{bmatrix} =: r.$$



Velocity u solution



Temperature T solution

Null space

We use an **equal-order P1 finite element discretization in space** for all variables.
Therefore, the null space in each finite element node is given by:

$$r_{u,1} := \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \; r_{u,2} := \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \; r_{u,3} := \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \; r_{u,4} := \begin{bmatrix} y \\ -x \\ 0 \\ 0 \end{bmatrix}, \text{ and } r_T := \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}.$$

See **Heinlein, Perego, Rajamanickam (in preparation)** for more details.

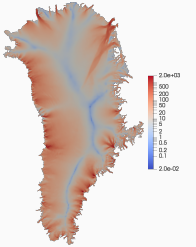
Monolithic (R)GDSW Preconditioners for Multiphysics Land Ice Simulations

We construct a **monolithic two-level GDSW preconditioner**

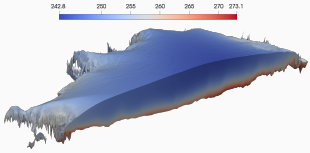
$$\mathcal{M}_{\mathrm{GDSW}}^{-1} = \phi \mathcal{A}_0^{-1} \phi^T + \sum_{i=1}^{N} \mathcal{R}_i^T \mathcal{A}_i^{-1} \mathcal{R}_i,$$

for the tangent matrix of the coupled problem

$$\mathcal{A}x := \begin{bmatrix} A_u & C_{uT} \\ C_{Tu} & A_T \end{bmatrix} \begin{bmatrix} x_u \\ x_T \end{bmatrix} = \begin{bmatrix} \tilde{r}_u \\ \tilde{r}_T \end{bmatrix} =: r.$$



Velocity u solution



Temperature T solution

Fully coupled extensions

We compute coarse basis function using extensions

$$\phi = \begin{bmatrix} -\mathcal{A}_{II}^{-1} \mathcal{A}_{\Gamma I}^T \Phi_\Gamma \\ \Phi_\Gamma \end{bmatrix} = \begin{bmatrix} \phi_I \\ \phi_\Gamma \end{bmatrix}$$

based on the coupled matrix $\mathcal{A}$.

See **Heinlein, Perego, Rajamanickam (in preparation)** for more details.

Decoupled extensions

We compute coarse basis function using extensions

$$\phi = \begin{bmatrix} -\tilde{\mathcal{A}}_{II}^{-1} \tilde{\mathcal{A}}_{\Gamma I}^T \Phi_\Gamma \\ \Phi_\Gamma \end{bmatrix} = \begin{bmatrix} \phi_I \\ \phi_\Gamma \end{bmatrix}$$

based on the decoupled matrix

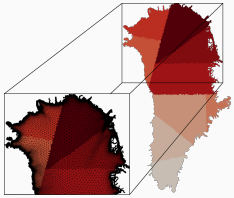
$$\tilde{\mathcal{A}} = \begin{bmatrix} A_u & 0 \\ 0 & A_T \end{bmatrix}.$$

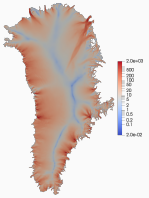
Greenland Coupled Problem – Coarse Spaces

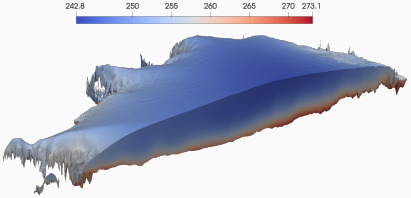
fully coupled extensions							
		no reuse			reuse coarse basis		
MPI ranks	dim V_0	avg. its (nl its)	avg. setup	avg. solve	avg. its (nl its)	avg. setup	avg. solve
256	1 400	100.1 (27)	4.10 s	6.40 s	**18.5** (70)	**2.28 s**	**1.07 s**
512	2 852	129.1 (28)	1.88 s	4.20 s	**24.6** (38)	**1.04 s**	**0.70 s**
1 024	6 036	191.2 (65)	1.21 s	4.76 s	**34.2** (32)	**0.66 s**	**0.70 s**
2 048	12 368	237.4 (30)	0.96 s	4.06 s	**37.3** (30)	**0.60 s**	**0.58 s**
decoupled extensions							
		no reuse			reuse coarse basis		
MPI ranks	dim V_0	avg. its (nl its)	avg. setup	avg. solve	avg. its (nl its)	avg. setup	avg. solve
256	1 400	23.6 (29)	3.90 s	1.32 s	**21.5** (34)	**2.23 s**	**1.18 s**
512	2 852	27.5 (30)	1.83 s	0.78 s	**26.4** (33)	**1.13 s**	**0.78 s**
1 024	6 036	30.1 (29)	1.19 s	**0.60 s**	**28.6** (43)	**0.66 s**	0.61 s
2 048	12 368	36.4 (30)	0.69 s	0.56 s	**31.2** (50)	**0.57 s**	**0.55 s**

Problem: Coupled **Mesh:** Greenland, 3-30 km hor. resolution 20 vert. layers **Size:** 7.5 m degrees of freedom (P1 FE) **Coarse space:** RGDSW

Greenland Coupled Problem – Large Problem







	decoupled (no reuse)			**fully coupled** (reuse coarse basis)			**decoupled** (reuse 1st level symb. fact. + coarse basis)		
MPI ranks	avg. (nl its)	avg. setup	avg. solve	avg. (nl its)	avg. setup	avg. solve	avg. (nl its)	avg. setup	avg. solve
512	**41.3** (36)	18.78 s	**4.99** s	45.3 (32)	11.84 s	5.35 s	45.0 (35)	**10.53** s	5.36 s
1 024	53.0 (29)	8.68 s	4.22 s	**47.8** (37)	5.36 s	**3.82 s**	54.3 (32)	**4.59 s**	4.31 s
2 048	62.2 (86)	4.47 s	4.23 s	66.7 (38)	2.81 s	4.53 s	**59.1** (38)	**2.32 s**	**3.99 s**
4 096	**68.9** (40)	2.52 s	**2.86 s**	79.1 (36)	1.61 s	3.30 s	78.7 (38)	**1.37 s**	3.30 s

Problem: Coupled **Mesh:** Greenland, 1-10 km hor. resolution 20 vert. layers **Size:** 7.5 m degrees of freedom (P1 FE) **Coarse space:** RGDSW

Thank you for your attention!

Summary

- Scalable FROSch preconditioners
  - for the single physics **velocity and temperature problems**,
  - for the **coupled multi physics problem**. (**monolithic (R)GDSW preconditioners**)

Outlook

- The solver time is dominated by the direct subdomain and coarse solvers
  $\rightarrow$ Speedup due to the use of **inexact solvers** & of **GPUs**.

Acknowledgements

- **Financial support:** DFG (KL2094/3-1, RH122/4-1), DOE (SciDAC projects FASTMath, ProSPect)
- **Computing ressources:** Cori (NERSC), JUQUEEN (JSC), magnitUDE (UDE), Piz Daint (CSCS)