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FROSCH PRECONDITIONERS FOR LAND ICE SIMULATIONS OF 2 **GREENLAND AND ANTARCTICA***

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Abstract. Numerical simulations of Greenland and Antarctic ice sheets involve the solution of 4 large-scale highly nonlinear systems of equations on complex shallow geometries. This work is con-5 6 cerned with the construction of Schwarz preconditioners for the solution of the associated tangent 7 problems, which are challenging for solvers mainly because of the strong anisotropy of the meshes and 8 wildly changing boundary conditions that can lead to poorly constrained problems on large portions of the domain. Here, two-level GDSW (Generalized Dryja-Smith-Widlund) type Schwarz precondi-9 tioners are applied to different land ice problems, i.e., a velocity problem, a temperature problem, as well as the coupling of the former two problems. We employ the MPI-parallel implementation 11 of multi-level Schwarz preconditioners provided by the package FROSch (Fast and Robust Schwarz) 12 13 from the Trilinos library. The strength of the proposed preconditioner is that it yields out-of-the-box 14scalable and robust preconditioners for the single physics problems.

To our knowledge, this is the first time two-level Schwarz preconditioners are applied to the 15 ice sheet problem and a scalable preconditioner has been used for the coupled problem. The pre-1617 conditioner for the coupled problem differs from previous monolithic GDSW preconditioners in the 18 sense that decoupled extension operators are used to compute the values in the interior of the sub-19domains. Several approaches for improving the performance, such as reuse strategies and shared 20 memory OpenMP parallelization, are explored as well.

21In our numerical study we target both uniform meshes of varying resolution for the Antarctic ice 22 sheet as well as non uniform meshes for the Greenland ice sheet are considered. We present several 23 weak and strong scaling studies confirming the robustness of the approach and the parallel scalability 24 of the FROSch implementation. Among the highlights of the numerical results are a weak scaling 25study for up to 32 K processor cores (8 K MPI-ranks and 4 OpenMP threads) and 566 M degrees of 26freedom for the velocity problem as well as a strong scaling study for up to 4K processor cores (and 27 MPI-ranks) and 68 M degrees of freedom for the coupled problem.

28Key words. domain decomposition methods, monolithic Schwarz preconditioners, GDSW 29coarse spaces, multiphysics simulations, parallel computing

AMS subject classifications. 65F08, 65Y05, 65M55, 65N55 30

1. Introduction. Greenland and Antarctic ice sheets store most of the fresh 31 32 water on earth and mass loss from these ice sheets significantly contributes to sea-33 level rise (see, e.g. [11]). In this work, we propose overlapping Schwarz domain decomposition preconditioners for efficiently solving the linear systems arising in the 34 context of ice sheet modeling.

We first consider the solution of the ice sheet momentum equations for com-36 puting the ice velocity. This problem is at the core of ice sheet modeling and 37 has been largely addressed in literature and several solvers have been considered 38 [40, 6, 18, 35, 50, 19, 10, 9]. Most solvers from the literature rely on Newton-39 Krylov methods, using, e.g., the conjugate gradient (CG) [31] or the generalized 40 minimal residual (GMRES) [44] method as the linear solver, and either one-level 41

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Schwarz preconditioners, hierarchical low-rank methods, or multigrid preconditioners 42 43 to accelerate the convergence. In particular, the ones that have been demonstrated on problems with hundreds of millions of unknowns [6, 35, 50, 19, 10] use tailored 44 multigrid preconditioners or hierarchical low-rank methods. Multigrid precondition-45ers [6, 35, 50, 19] require careful design of the grid transfer operators for properly 46 handling the anisotropy of the mesh and the basal boundary conditions that range 47 from no-slip to free-slip. Hierarchical low-rank approaches have also been used for the 48 velocity problem [10, 9]. Chen et al. [10] developed a parallel hiearchical low-rank 49 preconditioner that is aysmptotically scalable, but it has a large constant overhead 50and the trade-off between memory usage and solver convergence does not make it an ideal choice for the large problems considered here. The hierarchical low-rank approach that showed the most promise in terms of solver scalability is a sequential 53 implementation limiting its usage to small problems [9]. 54

In addition to the velocity problem, we also consider the problem of finding the 55temperature of an ice sheet using an enthalpy formulation ([1, 46, 32]) and the steady-56state thermo-mechanical problem coupling the velocity and the temperature problems. 58 The robust solution of this coupled problem is crucial for finding the initial thermomechanical state of the ice sheet under the assumption that the problem is almost at thermodynamic equilibrium. In fact, the initial state is estimated solving a PDE-60 constrained optimization problem where the loss function is the mismatch with ob-61 servations and the constraint is the coupled velocity-temperature problem considered 62 here. To our knowledge, while there are works in the literature targeting the solution 63 64 of unsteady versions of the coupled problem (5, 39, 43), none of them targets the steady thermo-mechanical problem at the ice sheet scale. 65

Both the velocity problem and the coupled velocity-temperature problem are characterized by strong nonlinearities and anisotropic meshes (due to the shallow nature of ice sheets). The coupled problem presents additional complexities due to the different nature of the velocity and temperature equations, the former being a purely diffusive elliptic problem, whereas the second is an advection dominated problem. In our experience, the naive use of multigrid methods leads to convergence failure for the coupled problem.

Our approach is to employ a preconditioning framework based on two-level Schwarz methods with GDSW (Generalized Dryja–Smith–Wildund) [12, 13, 22, 23] type coarse spaces. To our knowledge, scalable domain decomposition methods such as the GDSW preconditioner used in this work have not been shown to work on the ice sheet problems. The main contributions of this work are:

- We demonstrate that two-level Schwarz preconditioners such as GDSW (Generalized Dryja–Smith–Widlund) type preconditioners work out-of-the-box to solve two single physics problems (the velocity problem and the temperature problem) on land ice simulations.
 - We introduce a scalable two-level preconditioner for the coupled problem that is tailored for the coupled problem by decoupling the extension operators to compute the values in the interior of the subdomains.
 - We present results using an MPI-parallel implementation of multi-level Schwarz preconditioners provided by the package FROSch (Fast and Robust Schwarz) from the Trilinos software framework.
- Finally, we demonstrate the scalability of the approach with several weak
 and strong scaling studies confirming the robustness of the approach and
 the parallel scalability of the FROSch implementation. We conduct a weak
 scaling study for up to 32 K processor cores and 566 M degrees of freedom for

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86 87 the velocity problem as well as a strong scaling study for up to 4 K processor
cores and 68 M degrees of freedom for the coupled problem. We compare
against the multigrid method in [48, 50] for the velocity problem.

The remainder of the paper is organized as follows. Sections 2 and 3 introduces the ice sheet problems and the finite element discretization used in this study. We describe the Schwarz preconditioners, the reuse strategies for better performance and the way we tailor the preconditioner for the coupled problem in Section 4. Our software framework, which is based on Albany and FROSch, is briefly described in Section 5. Finally, the scalability and the performance of the proposed preconditioners are shown in Section 6.

102 2. Mathematical model. At the scale of glaciers and ice sheets, ice can be modeled as a very viscous shear-thinning fluid with a rheology that depends on the 103ice temperature. Complex phenomena like the formation of crevasses and ice calving 104would require more complex damage mechanics models, however the fluid descrip-105tion accounts for most of the large scale dynamics of ice sheets and it is adopted 106 by all ice sheet computational models. The ice temperature depends on ice flow 107(velocity/deformation). Given the large characteristic time scale of the temperature 108 evolution, it is reasonable to assume the temperature to be relatively constant over 109a few decades and solve the flow problem uncoupled from the temperature problem. 110 However, when finding the initial state of an ice sheet (by solving an inverse problem) 111 it is important to consider the coupled flow/temperature model, to find a self con-112113sistent initial thermo-mechanical state. In this case, we assume the ice temperature to be almost in steady-state. Therefore, in this paper, we consider a steady-state 114 temperature solver. In this section, we first introduce separately the flow model and 115116the temperature model and then the coupled model.

2.1. Flow model. We model the ice as a very viscous shear-thinning fluid with velocity \boldsymbol{u} and pressure p satisfying the Stokes equations:

$$\begin{cases} -\nabla \cdot \boldsymbol{\sigma}(\boldsymbol{u}, p) &= \rho_i \, \boldsymbol{g} \\ \nabla \cdot \boldsymbol{u} &= 0, \end{cases}$$

117 where \boldsymbol{g} is the gravity acceleration, ρ_i the ice density and σ the stress tensor. In what 118 follows, we use the so called first-order (FO) or Blatter-Pattyn approximation of the 119 Stokes equations derived using scaling arguments based on the fact that ice sheets are 120 shallow. Following [42] and [47], we have

121 (2.1)
$$\begin{cases} -\nabla \cdot (2\mu \dot{\boldsymbol{\epsilon}}_1) &= -\rho_i g \,\partial_x s, \\ -\nabla \cdot (2\mu \dot{\boldsymbol{\epsilon}}_2) &= -\rho_i g \,\partial_y s, \end{cases}$$

where x and y are the horizontal coordinate vectors in a Cartesian reference frame, s(x, y) is the ice surface elevation, $g = |\mathbf{g}|$, and $\dot{\boldsymbol{\epsilon}}_1$ and $\dot{\boldsymbol{\epsilon}}_2$ are given by

124 (2.2)
$$\dot{\boldsymbol{\epsilon}}_1 = \begin{pmatrix} 2\dot{\epsilon}_{xx} + \dot{\epsilon}_{yy}, \dot{\epsilon}_{xy}, \dot{\epsilon}_{xz} \end{pmatrix}^T$$
 and $\dot{\boldsymbol{\epsilon}}_2 = \begin{pmatrix} \dot{\epsilon}_{xy}, \dot{\epsilon}_{xx} + 2\dot{\epsilon}_{yy}, \dot{\epsilon}_{yz} \end{pmatrix}^T$.

125 Denoting with u and v the horizontal components of the velocity u, the stress com-126 ponents are defined as $\epsilon_{xx} = \partial_x u$, $\epsilon_{xy} = \frac{1}{2}(\partial_y u + \partial_x v)$, $\epsilon_{yy} = \partial_y v$, $\epsilon_{xz} = \frac{1}{2}\partial_z u$ and 127 $\epsilon_{yz} = \frac{1}{2}\partial_z v$. The ice viscosity μ in Eq. (2.1) is given by

128 (2.3)
$$\mu = \frac{1}{2}A(T)^{-\frac{1}{n}}\dot{\epsilon}_e^{\frac{1-n}{n}},$$

where $A(T) = \alpha_1 e^{\alpha_2 T}$ is a temperature-dependent rate factor (see [47] for the definition of coefficients α_1 and α_2), n = 3 is the power-law exponent, and the effective strain rate, $\dot{\epsilon}$, is defined as

132 (2.4)
$$\dot{\epsilon}_{e} \equiv \left(\dot{\epsilon}_{xx}^{2} + \dot{\epsilon}_{yy}^{2} + \dot{\epsilon}_{xx}\dot{\epsilon}_{yy} + \dot{\epsilon}_{xy}^{2} + \dot{\epsilon}_{xz}^{2} + \dot{\epsilon}_{yz}^{2}\right)^{\frac{1}{2}},$$

where $\dot{\epsilon}_{ij}$ are the corresponding strain-rate components. Given that the atmospheric pressure is negligible compared to the pressure in the ice, we prescribe stress-free conditions at the the upper surface:

136 (2.5)
$$\dot{\boldsymbol{\epsilon}}_1 \cdot \boldsymbol{n} = \dot{\boldsymbol{\epsilon}}_2 \cdot \boldsymbol{n} = 0,$$

137 where **n** is the outward pointing normal vector at the ice sheet upper surface, z = s(x, y). The lower surface can slide according to the following Robin-type boundary 139 condition

140
$$2\mu_e \dot{\boldsymbol{\epsilon}}_1 \cdot \boldsymbol{n} + \beta u = 0, \quad 2\mu \dot{\boldsymbol{\epsilon}}_2 \cdot \boldsymbol{n} + \beta v = 0,$$

141 where β is a spatially variable friction coefficient and u and v are the horizontal 142 components of the velocity u. The field β is set to zero beneath floating ice. On 143 lateral boundaries we prescribe the conditions

144 (2.6)
$$2\mu\dot{\boldsymbol{\epsilon}}_{1}\cdot\boldsymbol{n} = \frac{1}{2}gH\left(\rho_{i}-\rho_{w}r^{2}\right)n_{1}$$
 and $2\mu\dot{\boldsymbol{\epsilon}}_{2}\cdot\boldsymbol{n} = \frac{1}{2}gH\left(\rho_{i}-\rho_{w}r^{2}\right)n_{2},$

where **n** is the outward pointing normal vector to the lateral (i.e., parallel to the (x, y)plane), ρ_w is the density of ocean water, n_1 and n_2 are the x and y component of **n**, and r is the ratio of ice thickness that is submerged. On terrestrial ice margins r = 0, whereas on floating ice $r = \frac{\rho_i}{\rho_w}$. Additional details on the momentum balance solver can be found in [47].

2.2. Temperature model. As apparent from (2.3), the ice rheology depends on the ice temperature T. In order to model the ice sheet thermal state, we consider an enthalpy formulation similar to the one proposed by Aschwanded et al. in [1]. We assume that, for cold ice, the enthalpy h depends linearly on the temperature, whereas for temperate ice, the enthalpy grows linearly with the water content ϕ

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

150 Here, the melting enthalpy h_m is defined as $h_m := \rho_w c(T_m - T_0)$ and T_0 is a uniform

- 151 reference temperature.
- 152 The steady state enthalpy equation reads

153 (2.7)
$$\nabla \cdot \boldsymbol{q}(h) + \boldsymbol{u} \cdot \nabla h = 4\mu \epsilon_e^2.$$

Here, q(h) is the enthalpy flux, given by

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

 $\boldsymbol{u}\cdot \nabla h$ is the drift term, and $4\mu \epsilon_e^2$ is the heat associated to ice deformation. The water flux term

$$oldsymbol{j}(h) := rac{1}{\eta_w} (
ho_w -
ho_i) k_0 \phi^\gamma oldsymbol{g}$$

4

has been introduced by Schoof and Hewitt ([46, 32]), and it describes the percolation of water driven by gravity. The parameter c_i is the heat capacity of ice, k its thermal conductivity, and L is the latent heat of fusion. At the upper surface, the enthalpy is set to $h = \rho_i c(T_s - T_0)$, where T_s is the temperature of the air at the ice upper surface. At the bed, the ice is either in contact with a dry bed or with a film of water at the melting point temperature and, in first approximation, satisfies the Stefan condition:

$$m = G + \beta \sqrt{u^2 + v^2} - k \nabla T \cdot \boldsymbol{n}$$
 and $m (T - T_m) = 0$ and $T_m \leq 0$.

Here, *m* is the melting rate. Ice at the bed is melting when m > 0 and refreezing when m < 0. Moreover, *G* is the geothermal heat flux (positive if entering the ice domain), $\beta \sqrt{u^2 + v^2}$ is the frictional heat, and $-k\nabla T \cdot \mathbf{n}$ is the temperature heat flux exiting the domain as \mathbf{n} is the outer normal to the ice domain. Depending on whether the ice is cold at the bed, melting or refreezing, the Stefan condition translates into natural or essential boundary conditions for the enthalpy equation. Further details on the enthalpy formulation and its discretization are provided in [41].

161 **2.3. Coupled model.** The ice velocity depends on the temperature through 162 (2.4), and the enthalpy depends on the velocity field through the drift term $\boldsymbol{u} \cdot \nabla h$ 163 and the fractional heat term at the ice sheet lower surface. The first order problem 164 (2.1) only provides the horizontal velocities \boldsymbol{u} and \boldsymbol{v} , but we also need the vertical 165 velocity \boldsymbol{w} to solve the enthalpy equations. The vertical velocity \boldsymbol{w} is computed using 166 the incompressibility condition

167 (2.8)
$$\partial_x u + \partial_y v + \partial_z w = 0,$$

with the Dirichlet boundary condition at the ice lower surface

$$\boldsymbol{u}\cdot\boldsymbol{n}=rac{m}{L\left(
ho_{i}-
ho_{w}\phi
ight)}.$$

The coupled problem is formed by problems (2.1), (2.8) and (2.7) and their respective boundary conditions. For further details, see [41]. Figure 1 shows the ice velocity and temperature computed solving the coupled thermo-mechanical model. For details about the problem setting and the Greenland data set, see [41].

1723. Finite element discretization. The ice sheet mesh is generated by extruding in the vertical direction a two dimensional unstructured mesh of the ice sheet 173horizontal extension ([47]) and it is constituted of layers of prisms. The problems 174 described in section 2 are discretized with continuous piece-wise bi-linear (for trian-175gular prisms) or tri-linear (for hexahedra) finite elements using a standard Galerkin 176formulation, for each component of the velocity and for the enthalpy. We use up-177wind stabilization for the enthalpy equation. The nonlinear discrete problems can be 178written in the residual form 179

$$F(x) = 0,$$
 (3.1)

where x is the problem unknown (velocity, enthalpy, or both, depending on the problem). The nonlinear problems are then solved using a Newton-Krylov approach. More precisely, we linearize the problem using Newton's method, and solve the resulting linear tangent problems

$$\frac{186}{187} \quad (3.2) \qquad \qquad DF(x^{(k)})\Delta x^{(k)} = -F(x^{(k)})$$



FIG. 1. Solution of a Greenland ice sheet simulation. Left: ice surface speed in [m/yr], Right: ice temperature in [K] over a vertical section of the ice sheet.

using a Krylov subspace method. The Jacobian DF is computed through automatic differentiation. At each nonlinear iteration, we solve a problem of the form

$$199 \quad (3.3) \qquad \qquad Ax = r,$$

where A is the tangent matrix $DF(x^{(k)})$, and r is the residual vector $-F(x^{(k)})$. Using a block matrix notation, the tangent problem of the velocity problem can be written as

$$\begin{bmatrix} A_{uu} & A_{uv} \\ A_{vu} & A_{vv} \end{bmatrix} \begin{bmatrix} x_u \\ x_v \end{bmatrix} = \begin{bmatrix} r_u \\ r_v \end{bmatrix}$$

where the tangent matrix is symmetric positive definite. When considering also the vertical velocity w, the tangent problem becomes

$$\underbrace{ \begin{array}{c} 199 \quad (3.5) \\ 200 \end{array}}_{200} \underbrace{ \left[\begin{array}{c} A_{uu} & A_{uv} \\ A_{vu} & A_{vv} \\ =:A_{u} & A_{wu} \end{array} \right]}_{=:X_{u}} \underbrace{ \left[\begin{array}{c} x_{u} \\ x_{v} \\ x_{w} \end{array} \right]}_{=:x_{u}} = \underbrace{ \left[\begin{array}{c} r_{u} \\ r_{v} \\ r_{w} \end{array} \right]}_{=:r_{u}} \underbrace{ \left[\begin{array}{c} x_{u} \\ x_{v} \\ x_{w} \end{array} \right]}_{=:r_{u}} = \underbrace{ \left[\begin{array}{c} r_{u} \\ r_{v} \\ r_{w} \end{array} \right]}_{=:r_{u}} \underbrace{ \left[\begin{array}{c} x_{u} \\ x_{v} \\ x_{w} \end{array} \right]}_{=:r_{u}} \underbrace{ \left[\begin{array}{c} r_{u} \\ r_{v} \\ x_{w} \\ x_{w} \\ z_{w} \\ z_{w}$$

Note that the matrix is lower block-triangular because in the FO approximation, the horizontal velocities are independent of the vertical velocity. Similarly, the temperature equation reads

$$\frac{204}{204}$$
 (3.6) $A_T x_T = r_T.$

The coupled problem is a multiphysics problem coupling the velocity and the temperature problem. Hence, the tangent system can be written as

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



FIG. 2. Extending two-dimensional nonoverlapping subdomains (left) by layers of elements to obtain overlapping domain decompositions with an overlap of $\delta = 1h$ (middle) and $\delta = 2h$ (right).

where the blocks A_u and A_T and solution vectors $x_u x_T$ are the same as in the single physics problems; cf. (3.5) and (3.6). The residual vectors \tilde{r}_u and \tilde{r}_T differ from the single physics residuals r_u and r_T due to the coupling of velocity and temperature, which also results in the nonzero coupling blocks coupling blocks C_{uT} and C_{Tu} in the tangent matrix.

4. Preconditioners. In order to solve the tangent problems (3.2) in our Newton 215iteration, we apply the generalized minimal residual (GMRES) method [44] and speed 216up the convergence using generalized Dryja–Smith–Widlund (GDSW) type domain 217decomposition preconditioners. In particular, we will use classical GDSW and reduced 218 219 dimension GDSW (RGDSW) preconditioners, as described in subsection 4.1, as well as corresponding monolithic preconditioners, as introduced in subsection 4.3. In order 220 to improve the performance of the first level of the Schwarz preconditioners, we will 221 always apply scaled prolongation operators; cf. subsection 4.2. As we will describe 222 in subsection 4.4, domain decomposition preconditioners and, in particular, GDSW 223 224 type preconditioners are well-suited for the solution of land ice problems because 225 of the specific structure of the meshes. In order to improve the efficiency of the preconditioners in our Newton-Krylov algorithm, we will also apply strategies to reuse, 226in later Newton iterations, certain components of the preconditioners set up in the 227 first Newton iteration; see subsection 4.5. 228

For the sake of clarity, we will restrict ourselves to the case of uniform meshes with characteristic element size h for the description of the preconditioners. However, the methods can also be applied to non-uniform meshes as the ones for Greenland; see Figure 4.

4.1. GDSW type preconditioners. Let us consider the general linear system

$$234 (4.1) Ax = b$$

arising from a finite element discretization of an elliptic boundary value problem on Ω . Our aim is then to apply the preconditioners to the tangent problems (3.3) of the model problems described in section 2.

The GDSW preconditioner was originally introduced by Dohrmann, Klawonn, and Widlund in [13, 12] for elliptic problems. It is a two-level Schwarz preconditioner with energy minimizing coarse space and exact solvers. To describe the construction of the GDSW preconditioner, let Ω be partitioned into N nonoverlapping subdomains $\Omega_1, ..., \Omega_N$ with characteristic size H. We extend these subdomains by adding k layers of finite elements resulting in overlapping subdomains $\Omega'_1, ..., \Omega'_N$ with an overlap

 $\delta = kh$; cf. Figure 2 for a two-dimensional example. In general, two-level Schwarz 245preconditioners for (4.1) with exact solvers are of the form 246

247 (4.2)
$$M_{OS-2} = \underbrace{\Phi A_0^{-1} \Phi^T}_{\text{coarse level}} + \underbrace{\sum_{i=1}^N R_i^T A_i^{-1} R_i}_{\text{first level}}.$$

Here, $A_0 = \Phi^T A \Phi$ is the coarse matrix corresponding to a Galerkin projection onto 249the coarse space, which is spanned by the columns of matrix Φ . The local matrices A_i 250are submatrices of A corresponding to the overlapping subdomains $\Omega_1',...,\Omega_N'.$ They 251can be written as $A_i = R_i A R_i^T$, where $R_i : V^h \to V_i^h$ is the restriction operator from the global finite element space V^h to the local finite element space V_i^h on Ω_i' ; the R_i^T 252253is the corresponding prolongation. 254

255We first present the framework enabling the construction of energy-minimizing coarse spaces for elliptic problems based on a partition of unity on the interface 256

$$\Gamma = \left\{ x \in (\overline{\Omega}_i \cap \overline{\Omega}_j) \setminus \partial \Omega_D | i \neq j, 1 \le i, j \le N \right\}$$

of the nonoverlapping domain decomposition, where $\partial \Omega_D$ is the Dirichlet boundary. 259This will allow us to construct classical GDSW coarse spaces [13, 12] and reduced 260 dimension GDSW coarse spaces [16] as used in our simulations. Note that other 261types of coarse spaces can be constructed using this framework as well, e.g., coarse 262spaces based on the MsFEM (Multiscale Finite Element Method) [34]; see also [7]. 263 However, in our experiments, we restrict ourselves to the use of GDSW type coarse 264265spaces.

Let us first decompose Γ into connected components $\Gamma_1, ..., \Gamma_M$. This decom-266position of Γ may be overlapping or nonoverlapping. Furthermore, let R_{Γ_i} be the 267restriction from all interface degrees of freedom to the degrees of freedom of the in-268269 terface component Γ_i . In order to account for overlapping decompositions of the interface, we introduce diagonal scaling matrices D_{Γ_i} , such that 270

271 (4.4)
$$\sum_{i=1}^{M} R_{\Gamma_i}^T D_{\Gamma_i} R_{\Gamma_i} = I_{\Gamma},$$

where I_{Γ} is the identity matrix on Γ . This means that the scaling matrices correspond 273274 to a partition of unity on the interface Γ .

Using the scaling matrices D_{Γ_i} , we can now build a space which can represent the 275restriction of the null space of our problem to the interface. Therefore, let the columns 276of the matrix Z form a basis of the null space of the operator \hat{A} , which is the global 277matrix corresponding to A but with homogeneous Neumann boundary conditions on 278the full boundary, and let the Z_{Γ} be restriction of Z to the interface Γ . Because of 279280 (4.4), we have

281
$$\sum_{i=1}^{M} R_{\Gamma_i}^T D_{\Gamma_i} R_{\Gamma_i} Z_{\Gamma} = Z_{\Gamma}.$$

282

Now, for each Γ_i , we construct a matrix Φ_{Γ_i} such that its columns are a basis of 283the space spanned by the columns of $D_{\Gamma_i} R_{\Gamma_i} Z_{\Gamma}$. Then, the interface values of our 284coarse space are given by the matrix 285

286 (4.5)
$$\Phi_{\Gamma} = \begin{bmatrix} R_{\Gamma_1}^T \Phi_{\Gamma_1} & \dots & R_{\Gamma_M}^T \Phi_{\Gamma_M} \end{bmatrix}.$$

Based on these interface values, the coarse basis functions are finally computed as energy-minimizing extensions to the interior of the nonoverlapping subdomains. Therefore, we partition all degrees of freedom into interface (Γ) and interior (I) degrees of freedom. Then, the system matrix can written as

$$A = \begin{bmatrix} A_{II} & A_{I\Gamma} \\ A_{\Gamma I} & A_{\Gamma\Gamma} \end{bmatrix}$$

and the energy-minimizing extensions are computed as $\Phi_I = -A_{II}^{-1}A_{I\Gamma}\Phi_{\Gamma}$, resulting in the coarse basis

295 (4.6)
$$\Phi = \begin{bmatrix} \Phi_I \\ \Phi_{\Gamma} \end{bmatrix} = \begin{bmatrix} -A_{II}^{-1}A_{I\Gamma}\Phi_{\Gamma} \\ \Phi_{\Gamma} \end{bmatrix}$$

As mentioned earlier, this construction allows for a whole family of coarse spaces, depending on decomposition of the interface into components Γ_i and the choice of scaling matrices D_{Γ_i} .

299 GDSW coarse spaces. We obtain the interface components of the GDSW coarse 300 space $\Gamma_i^{(\text{GDSW})}$ by decomposing the interface Γ into the largest connected components 301 γ belonging to the same sets of subdomains \mathcal{N}_{γ} , i.e., into vertices, edges, and faces; 302 cf., e.g., [38]. More precisely,

303
$$\mathcal{N}_{\gamma} := \left\{ i : x \in \overline{\Omega_i} \ \forall x \in \gamma \right\}$$

Because these components are disjoint by construction, the scaling matrices $D_{\Gamma_i^{(\text{GDSW})}}$ have to be chosen as identity matrices $I_{\Gamma_i^{(\text{GDSW})}}$ in order to satisfy (4.4). Using this choice, we obtain the classical GDSW coarse space as introduced by Dohrmann, Klawonn, and Widlund in [13, 12]. If the boundaries of the subdomains are uniformly Lipschitz, the condition number estimate for the resulting two-level GDSW preconditioner,

holds for scalar elliptic and compressible linear elasticity model problems; the constant *C* is then independent of the geometrical parameters *H*, *h*, and δ . For the general case of $\Omega \subset \mathbb{R}^2$ being decomposed into John domains, we can obtain a condition number estimate with a second power logarithmic term, i.e., with $\left(1 + \log\left(\frac{H}{h}\right)\right)^2$ instead of $\left(1 + \log\left(\frac{H}{h}\right)\right)$; cf. [12, 13]. Please also refer to [14, 15] for other variants with linear logarithmic term.

318 RGDSW coarse spaces. Another choice of the Γ_i leads to reduced dimension 319 GDSW (RGDSW) coarse spaces; cf. [16]. In order to construct the interface com-320 ponents $\Gamma_i^{(RGDSW)}$, we first define a hierarchy of the previously defined $\Gamma_i^{(GDSW)}$. In 321 particular, we call an interface component γ ancestor of another interface compo-322 nent γ' if $\mathcal{N}_{\gamma'} \subset \mathcal{N}_{\gamma}$; conversely, we call γ offspring of γ' if $\mathcal{N}_{\gamma'} \supset \mathcal{N}_{\gamma}$. Now, let 323 $\{\hat{\Gamma}_i^{(GDSW)}\}_{i=1,...,M^{(RGDSW)}}$ be the set of all GDSW interface components which have 324 no ancestors; we call these coarse components. Now, we define the RGDSW interface 325 components as

326 (4.8)
$$\Gamma_i^{(\text{RGDSW})} := \bigcup_{\mathcal{N}_\gamma \subset \mathcal{N}_{\hat{\Gamma}_i^{(\text{GDSW})}}} \gamma, \quad \forall i = 1, ..., M^{(\text{RGDSW})}.$$

The $\Gamma_i^{(\text{RGDSW})}$ may overlap in nodes which do not belong to the coarse components. Hence, we have to introduce scaling operators $D_{\Gamma_i^{(\text{RGDSW})}} \neq I_{\Gamma_i^{(\text{RGDSW})}}$ to obtain a partition of unity on the interface; cf. (4.4). Different scaling operators D_{Γ_i} lead to different variants of RGDSW coarse spaces, e.g., Options 1, 2.1, and 2.2, introduced in [16] and another variant introduced in [25]. Here, we will only consider the algebraic variant, Option 1, where an inverse multiplicity scaling

$$\begin{array}{l} {}_{334} \qquad \qquad D_{\Gamma_i^{(\mathrm{RGDSW})}} = R_{\Gamma_i^{(\mathrm{RGDSW})}} \left(\sum_{j=1}^{M^{(\mathrm{RGDSW})}} R_{\Gamma_j^{(\mathrm{RGDSW})}}^T R_{\Gamma_i^{(\mathrm{RGDSW})}} \right)^{-1} R_{\Gamma_i^{(\mathrm{RGDSW})}}^T.$$

is employed. Under the condition that all subdomains are Lipschitz domains, we then obtain the same condition number estimate as previously for GDSW coarse spaces

$$\kappa(M_{\rm RGDSW}^{-1}A) \le C\left(1 + \frac{H}{\delta}\right)\left(1 + \log\left(\frac{H}{h}\right)\right);$$

³⁴⁰ for scalar elliptic and compressible linear elasticity model problems; cf. [16].

The only missing ingredient to construct the GDSW and RGDSW coarse spaces is the respective the null space Z of the global Neumann matrix corresponding to A. For the velocity and the temperature problem, the preconditioners can be directly constructed and applied using the corresponding null spaces spanned by

345
$$r_{u,1} := \begin{bmatrix} 1\\0 \end{bmatrix}, r_{u,2} := \begin{bmatrix} 0\\1 \end{bmatrix} \text{ and } r_{u,3} := \begin{bmatrix} y\\-x \end{bmatrix}$$

346 or

$$r_T := \begin{bmatrix} 1 \end{bmatrix},$$

respectively, on each finite element node. Here, $r_{u,1}$ and $r_{u,2}$ correspond to the translations and $r_{u,3}$ to the linearized rotation building the null space of the velocity problem.

350 The r_T is the constant null space element of the temperature problem.

351 *Remark* 4.1. Sometimes it may be beneficial to only consider a subspace Z of the full space Z. This results in a smaller coarse space, at the cost of slower convergence of 352 353 the linear solver. In particular, in theory, numerical scalability is not provided in this case. However, since the coarse solve is typically a parallel scaling bottleneck, it may 354still be faster to neglect a part of the coarse space for a large number of subdomains. 355 In our numerical results, we will actually observe that neglecting rotational rigid body 356 modes improves the parallel performance of our solver; see also [28, 24] for similar 357 experiments for elasticity problems. 358

Note that, if rotations are neglected, the GDSW and RGDSW coarse spaces are actually constructed in an algebraic way because the translational coarse basis functions can be computed without geometric information; see also the discussion in [24].

For the coupled problem described in subsection 2.3, we will describe an monolithic preconditioner in subsection 4.3, where we use the same construction but with decoupled extensions operators. Before that, however, we will describe the scaled prolongation operators used in the first level in our numerical experiments.

10

4.2. Scaled prolongation operators. As first shown in [8], the convergence of additive Schwarz preconditioners can often be improved using restricted or scaled variants of the prolongation operators R_i^T in (4.2); see also [17, 23]. For the sake of brevity, we will not compare the performance of the standard, the restricted, and the scaled variants for the different model problems considered in this paper. We only show results using the scaled variant because it performed best in preliminary tests. We construct the scaled prolongation operator \tilde{R}_i^T such that $\sum_{i=1}^N \tilde{R}_i^T R_i = I$:

$$\tilde{R}_i^T := \left(\sum_{j=1}^N R_j^T R_j\right)^{-1} R_i^T.$$

Note that the matrix $\sum_{i=1}^{N} R_i^T R_i$ is just a diagonal scaling matrix, and its inverse can therefore be specified directly. The two-level Schwarz preconditioner with scaled prolongations then reads

379
380
$$M_{OS-2} = \Phi A_0^{-1} \Phi^T + \sum_{i=1}^N \tilde{R}_i^T A_i^{-1} R_i.$$

 $\frac{380}{381}$

4.3. Monolithic preconditioning the coupled problem. For the coupled problem, *A* is structured as follows

$$\begin{array}{c} 384 \\ 385 \end{array} (4.10) \qquad \qquad A = \begin{bmatrix} A_{uu} & A_{uT} \\ A_{Tu} & A_{TT} \end{bmatrix}.$$

where the off-diagonal blocks formally account for the coupling of the different variables; cf. section 3. We will construct monolithic two-level Schwarz preconditioners as introduced in [36, 37] and extended to monothic GDSW preconditioners in [22, 23]. Formally, the monolithic preconditioners for the coupled problem can again be written as

391 (4.11)
$$M_{OS-2} = \Phi A_0^{-1} \Phi^T + \sum_{i=1}^N \tilde{R}_i^T A_i^{-1} R_i.$$

However, all matrices are now 2×2 block-matrices. In particular, the monolithic restriction and prolongation matrices are of the form

$$R_{i} = \begin{bmatrix} R_{i,u} & 0\\ 0 & R_{i,T} \end{bmatrix} \text{ and } \tilde{R}_{i} = \begin{bmatrix} \tilde{R}_{i,u} & 0\\ 0 & \tilde{R}_{i,T} \end{bmatrix}$$

where $R_{i,u}$ and $R_{i,T}$ are the restriction operators to the overlapping subdomain Ω'_i on the velocity and temperature degrees of freedom, and $\tilde{R}_{i,u}$ and $\tilde{R}_{i,T}$ are the respective prolongations operators.

The coarse space can be constructed in a similar way as in the single physics case. In particular, the interface components Γ_i and the scaling matrices D_{Γ_i} are constructed in the same way, and the null space Z of the multi physics problem is composed of the null spaces of the individual single physics problems. However, as we will observe in the numerical results, it is necessary to remove the coupling blocks between the velocity and the temperature problem before computing the extensions (4.6). Hence, instead of A, the matrix

is used in the computation of the harmonic extensions, i.e., $\Phi_I = -\dot{A}_{II}^{-1} \dot{A}_{I\Gamma} \Phi_{\Gamma}$. This can be viewed as applying a block Jacobi preconditioner with two blocks corresponding to the single physics problems instead of solving the systems corresponding to A_{II}^{-1} monolithically. Consequently, the coarse basis functions corresponding to the velocity and the temperature problem can be computed independently. Then, the matrix Φ is of the form

415 (4.13)
$$\Phi = \begin{bmatrix} \Phi_{u,u_0} & 0\\ 0 & \Phi_{T,T_0} \end{bmatrix},$$

where the row indices u and T indicate the finite element functions of the original 417 problem, and column indices u_0 and T_0 correspond to the basis functions of the coarse 418 space. A similar decoupling approach for the coarse basis functions was performed 419420 in [22, 23] for a monolithic preconditioner for fluid problems. However, it was necessary to first compute the fully coupled extensions (4.6) and to drop the off diagonal 421 422 blocks in the matrix Φ afterwards. This was due to the fact that the system matrix $\begin{bmatrix} B^T \\ 0 \end{bmatrix}$, such that the decoupled matrix would become singular. $\begin{bmatrix} A \\ B \end{bmatrix}$ was of the form 423 Here, the decoupled matrix (4.12) remains invertible since the individual blocks corre-424 spond to the single physics velocity and temperature problems. Therefore, our coarse 425basis matrix is also of the same structure for Lagrangian coarse spaces in [36, 37]. 426It is important to note that, even though the coarse basis functions do not contain 427

427 It is important to note that, even though the coarse basis functions do not contain
 428 any coupling blocks, the coarse problem is still a coupled problem with a coarse matrix
 429 of the form

430
$$A_0 = \begin{bmatrix} \Phi_{u,u_0} & 0\\ 0 & \Phi_{T,T_0} \end{bmatrix}^T \begin{bmatrix} A_{uu} & A_{uT}\\ A_{Tu} & A_{TT} \end{bmatrix} \begin{bmatrix} \Phi_{u,u_0} & 0\\ 0 & \Phi_{T,T} \end{bmatrix}$$

$$= \begin{bmatrix} \Phi_{u,u_0}^{I} A_{uu} \Phi_{u,u_0} & \Phi_{u,u_0}^{I} A_{uT} \Phi_{T,T_0} \\ \Phi_{T,T_0}^{T} A_{Tu} \Phi_{u,u_0} & \Phi_{T,T_0}^{T} A_{TT} \Phi_{T,T_0} \end{bmatrix}.$$

Because we use equal order discretizations for the velocity and temperature variables in the coupled problem, we can formally apply a node wise ordering to our degrees of freedom. Then, the monolithic preconditioner can be constructed exactly as in the elliptic case (see section 4), however, using the previously described decoupled matrix (4.12) to compute the extension.

We then obtain all three velocity degrees of freedom and one temperature degree of freedom for each finite element node. Therefore, the full null space is spanned by the null space corresponding to the three velocity degrees of freedom

441
$$r_{u,1} := \begin{bmatrix} 1\\0\\0\\0 \end{bmatrix}, r_{u,2} := \begin{bmatrix} 0\\1\\0\\0 \end{bmatrix}, r_{u,3} := \begin{bmatrix} 0\\0\\1\\0 \end{bmatrix}, \text{ and } r_{u,4} := \begin{bmatrix} y\\-x\\0\\0 \end{bmatrix}$$

442 as well as the null space on the temperature degree of freedom

443
$$r_T := \begin{bmatrix} 0\\0\\0\\1 \end{bmatrix}.$$

444 Here, $r_{u,4}$ corresponds to a linearized rotation, which will be neglected in some of our

⁴⁴⁵ numerical experiments to reduce the computing time on the coarse level.



FIG. 3. Uniform hexahedral mesh for the Antarctica ice sheet with a horizontal resolution of 16 km decomposed into nine subdomains. The domain decomposition is performed on the two-dimensional top surface mesh, and the subdomains are extruded in vertical direction to obtain three-dimensional subdomains with 10 layers height.



FIG. 4. Non-uniform triangulation of the top surface mesh for the Greenland ice sheet with a horizontal resolution of 3 km to 30 km decomposed into nine subdomains. The three-dimensional mesh is then obtained by extrusion in vertical direction.

4.4. Remarks on domain decomposition methods for land ice problems. The geometries for the ice sheets in Antarctica and Greenland are visualized in Figures 3 and 4. Generally, the horizontal extensions of the ice sheets are in the order of hundreds or thousands of kilometers, whereas their thickness is at maximum only a few kilometers. Therefore, the geometries and the corresponding meshes used in our simulations are clearly anisotropic; cf. section 3 for a description of the mesh generation procedure and Figure 3 for a visualization of a exemplary mesh of Antarctica

reuse strategy	short description
NR (no reuse)	Set up the preconditioner from scratch in each non-
	linear iteration.
IS (index sets)	Reuse the index sets for the overlapping subdomains
	and the interface components
SF1 (symb. fact. lvl 1)	Reuse the symbolic factorization of A_i .
SF2 (symb. fact. lvl 2)	Reuse the symbolic factorization of A_0 .
CB (coarse basis)	Reuse the coarse basis Φ .
CM (coarse matrix)	Reuse the coarse matrix A_0 .
5	TABLE 1

Reuse strategies for monolithic GDSW preconditioners (4.2) for nonlinear model problems.

453 with a horizontal mesh resolution of 16 km and 10 layers of elements in z direction.

Due to this specific structure of the meshes, we perform the domain decomposition 454into nonoverlapping subdomains as follows: First, we decompose the two-dimensional 455 mesh of the top surface. We extrude the two-dimensional subdomains in z direction 456 457 next resulting in a domain decomposition of the whole three-dimensional domain. Hence, the domain decomposition is essentially a two-dimensional domain decompo-458sition, and the partition of the domain decomposition interface Γ into the components 459 $\Gamma_i^{(\text{GDSW})}$ only yields edges and faces but no vertices. However, as can be seen in Fig-460 461 ures 3 and 4, the subdomain geometries can be very irregular due to the complex shape of the boundary of the ice sheets. Hence, the domain decomposition is not well 462 suited for the use of classical Lagrangian coarse spaces, which would require the con-463 struction of a coarse triangulation of the geometry. However, this is not required for 464GDSW type coarse spaces which can be constructed without an additional coarse tri-465 466 angulation. Hence they can easily be constructed for the considered land ice problems. 467

4.5. Reuse strategies for nonlinear problems. The model problems in section 2 are highly nonlinear; as can be seen in section 6, the coupled problem requires a particularly high number of nonlinear iterations. Therefore, we will investigate several strategies to reuse information from the first iteration in later Newton iterations, such that the total time to solution can be improved. Note that other approaches where the information is updated in certain multiple Newton iterations, e.g. in every *n*th iteration, are also possible but out of the scope of this paper.

The different reuse strategies, which are listed in Table 1, are used in different 475476 numerical experiments in section 6. Since neither the topology nor the domain decomposition of our problem changes during the nonlinear iteration, it is a safe assumption 477 that the index sets of the overlapping subdomains and the interface components stay 478 the same. This saves mostly communication, which dominates the time for identify-479 ing the index sets; see section 5. If the sparsity pattern of the system matrix is also 480constant during the nonlinear iteration, the symbolic factorizations for A_i and A_0 can 481 be easily reused as well. 482

In GDSW type preconditioners, the coarse basis functions Φ change with the tangent matrix, which is used to compute the extensions (4.6) in each nonlinear iteration. However, in practice, the coarse basis computed with the tangent matrix in the first Newton iteration can also be used in later iterations. In some cases, the complete coarse matrix A_0 and its factorization can even be reused. **5. Software framework.** The land ice problems are implemented in Albany Land Ice (formerly referred to as Albany FELIX) [47, 45], a C++ finite element library that relies on the Trilinos packages [49] for MPI+X parallelism (Tpetra, Kokkos), linear (Belos/AztecOO) and nonlinear (NOX) solvers, preconditioners (Ifpack2, Muelu, ShyLU, FROSch [20, 28, 27, 26]), discretization tools (STK, Intrepid2, Phalanx) and automatic differentiation (Sacado). Albany Land Ice is part of the land ice code MALI [33].

The GDSW type preconditioners described in section 4 are implemented in the 495FROSch framework [27, 26], which is part of Trilinos [49]. FROSch can use both 496distributed-memory parallelism using the Tpetra package of Trilinos and shared-497memory parallelism while using the direct solvers interfaced through Amesos2 package 498 499 of Trilinos [2]. With respect to shared-memory parallelism, in this paper, we restrict ourselves to using CPU threads. Specifically, we use the Pardiso solver provided with 500 the Intel MKL software, which can also make use of shared-memory parallelism using 501 OpenMP threads. FROSch is called from Albany Land Ice using the unified Trili-502nos solver interface Stratimikos and directly uses the Tpetra matrices and vectors 503 which have been assembled in. Moreover, FROSch makes use of the index set of the 504 505nonoverlapping domain decomposition and the null space basis provided by Albany Land Ice in form of Tpetra map and multivector objects; cf. the discussion in [21]. 506

6. Numerical results. In this section, we will present numerical results for the 507flow (subsection 2.1), temperature (subsection 2.2), and coupled (subsection 2.3) prob-508 lems. For the flow problem, we will use the uniform meshes for Antarctica, whereas we 509 will use the non-uniform Greenland meshes for the two other model problems; cf. Fig-510ures 3 and 4. The experiments were performed using the Haswell compute nodes (2 511sockets with a 16-core Intel Xeon Processor E5-2698 v3 with 2.3 GHz each) of the Cori 512supercomputer at NERSC (National Energy Research Scientific Computing Center); 513we always employed one processor core per thread. The code was compiled using 514Intel 19.0.3.199 compilers and Intel MKL. The subdomain problems and the coarse 515problem are solved on one MPI rank using used Pardiso from the Intel MKL with 516 OpenMP parallelization if more than one OpenMP thread is used. 517

The nonlinear problems are solved using the inexact Newton method with back-518 tracking implemented in the Trilinos package NOX up to a relative reduction of the 519residual of 10^{-5} . As the linear solver we employ the GMRES (generalized minimal 520residual) method [44] from Trilinos AztecOO preconditioned by two-level overlapping 521 Schwarz domain decomposition preconditioners from Trilinos FROSch (part of the 522 package ShyLU) as described in section 4; cf. [28, 27, 22, 23, 26]. We iterate the 523GMRES method up to a relative reduction of the residual of 10^{-7} for the flow and 524temperature problems or 10^{-9} for the coupled problem. Since the number of nonlin-525 ear iterations is not influenced by our preconditioners, we always report the number 526 527 of linear iterations averaged over the number of Newton iterations.

With respect to the Schwarz preconditioners, if not stated otherwise, we will always use one layer of overlap as determined from the sparsity pattern of the matrix. On the first level, we apply scaled prolongation operators; cf. subsection 4.2. As already discussed in [28], we will use two communication steps in order to transfer information from the first to the second level (scatter and gather); only during the discussion in subsection 6.1.3, we will also present results using only one or three communication steps.

6.1. Flow problem for Antarctica. In this section, we will present an extensive numerical study of GDSW type preconditioners for the land ice flow problem

	Wi	thout rotatio	nal coarse	e basis func	tions (2 ri	gid body me	odes)	
	GDS	\mathbf{W} (IS & SF	1 & SF2 &	& CB)	RGD	SW (IS & S	F1 & SF2	& CB)
MPI		avg. its	avg.	avg.		avg. its	avg.	avg.
ranks	$\dim V_0$	(nl its)	setup	solve	$\dim V_0$	(nl its)	setup	solve
512	4 598	40.8 (11)	$15.36\mathrm{s}$	$12.38\mathrm{s}$	1834	42.6(11)	$14.99\mathrm{s}$	$12.50\mathrm{s}$
1024	9 306	43.3 (11)	$5.80\mathrm{s}$	$6.27\mathrm{s}$	3740	44.5(11)	$5.65\mathrm{s}$	$6.08\mathrm{s}$
2048	18634	41.7 (11)	$3.27\mathrm{s}$	$2.91\mathrm{s}$	7586	42.7(11)	$3.11\mathrm{s}$	$2.79\mathrm{s}$
4096	37 184	41.4 (11)	$2.59\mathrm{s}$	$2.07\mathrm{s}$	15324	42.5(11)	$1.07\mathrm{s}$	$1.54\mathrm{s}$
8 1 9 2	72964	39.5 (11)	$1.51\mathrm{s}$	$1.84\mathrm{s}$	30620	42.0(11)	$1.20\mathrm{s}$	$1.16\mathrm{s}$
	W	Vith rotation	al coarse l	oasis functi	ons $(3 rigi$	id body mod	les)	
	GDS	\mathbf{W} (IS & SF	1 & SF2 &	& CB)	RGDSW (IS & SF1 & SF2 & CB)			
MPI		avg. its	avg.	avg.		avg. its	avg.	avg.
ranks	$\dim V_0$	(nl its)	setup	solve	$\dim V_0$	(nl its)	setup	solve
512	6 897	35.5 (11)	$15.77\mathrm{s}$	$11.21\mathrm{s}$	2751	40.7(11)	$15.23\mathrm{s}$	$12.22\mathrm{s}$
1024	13959	35.6 (11)	$6.16\mathrm{s}$	$5.78\mathrm{s}$	5610	42.9(11)	$5.65\mathrm{s}$	$6.04\mathrm{s}$
2048	27951	33.5 (11)	$3.78\mathrm{s}$	$3.45\mathrm{s}$	11379	42.2(11)	$3.17\mathrm{s}$	$2.81\mathrm{s}$
4096	55776	31.8 (11)	$2.21\mathrm{s}$	$3.80\mathrm{s}$	22986	44.3(11)	$1.95\mathrm{s}$	$2.70\mathrm{s}$
8 1 9 2	109 446	29.3 (11)	$2.49\mathrm{s}$	$5.33\mathrm{s}$	45930	40.8(11)	$1.19\mathrm{s}$	$3.13\mathrm{s}$
				TADLE 2				

ABLE Z

Comparison of different coarse spaces for the flow problem on the Antarctica mesh with 4 km horizontal resolution and 20 layers of elements in vertical direction and a total of 35.3 m degrees of freedom. The linear iteration counts (avg. its), setup times (avg. setup), and solve times (avg. solve) are averaged over the number of Newton iterations (nl its). Lowest average iterations counts, setup times, and solve times in each row are marked in **bold**.

# subdomains	512	1024	2048	4096	8 1 9 2				
GDSW	2299	4653	9317	18592	36482				
RGDSW	917	1870	3793	7662	15310				
TABLE 3									

Number of coarse components Γ_i for the Antarctica mesh with 4km horizontal resolution. The dimension of the coarse space is the number of coarse components multiplied by the dimension of the null space.

for Antarctica. Most of the simulations are performed on a medium size mesh with 537 4 km horizontal resolution and 20 layers of elements in vertical direction. We compare 538one level Schwarz methods and different GDSW type coarse spaces (subsection 6.1.1) 539 and investigate several reuse strategies (subsection 6.1.2) as well as certain paral-540lelization aspects (subsection 6.1.3). Moreover, we investigate the robustness with 541respect to an increasing number of mesh layers of elements in vertical direction (sub-542section 6.1.4), and compare our results using FROSch against the algebraic multigrid 543 package MueLu [4, 3] (subsection 6.1.6). 544

Finally, we provide weak scaling results ranging from the coarsest mesh with horizontal resolution to the finest mesh with 1 km horizontal resolution. The largest computation in this weak scaling study was performed on 32 768 processor cores using 8192 MPI ranks and 4 OpenMP threads per MPI rank solving a problem with more than 566 m degrees of freedom.

6.1.1. Comparison of different Schwarz preconditioners. First, we compare the classical GDSW and the reduced dimension GDSW (RGDSW) coarse spaces in a strong scaling study using both the full three-dimensional null space and a twodimensional null space where the rotation has been omitted; cf. the discussion in subsection 4.1. In this study, we reuse the index sets (IS), the symbolic factorizations (SF1 & SF2), and the coarse basis (CB) from the first nonlinear iteration. As can be seen in Table 2, all preconditioners scale numerically, but the iteration counts are

	One-level Schwarz											
	one layer o	of algebraic	overlap	two layers o	f algebrai	c overlap						
MPI	avg. its	avg.	avg.	avg. its	avg.	avg.						
ranks	(nl its)	setup	solve	(nl its)	setup	solve						
512	67.7(11)	$13.80\mathrm{s}$	$19.55\mathrm{s}$	56.2 (11)	$17.95\mathrm{s}$	$18.40\mathrm{s}$						
1 0 2 4	79.1(11)	$5.00\mathrm{s}$	$10.60\mathrm{s}$	66.5 (11)	$6.74\mathrm{s}$	$10.56\mathrm{s}$						
2 0 4 8	96.1(11)	$1.74\mathrm{s}$	$6.09\mathrm{s}$	80.8 (11)	$2.58\mathrm{s}$	$6.31\mathrm{s}$						
4096	113.3(11)	$0.81\mathrm{s}$	$3.59\mathrm{s}$	94.8 (11)	$1.21\mathrm{s}$	$3.99\mathrm{s}$						
8 1 9 2	132.0(11)	$0.47\mathrm{s}$	$2.15\mathrm{s}$	109.5 (11)	$0.65\mathrm{s}$	$2.35\mathrm{s}$						
	RG	DSW (IS &	z SF1 & SF	F2 & CB & CI	M)							
	one layer o	of algebraic	overlap	two layers of algebraic overlap								
MPI	avg. its	avg.	avg.	avg. its	avg.	avg.						
ranks	(nl its)	setup	solve	(nl its)	setup	solve						
512	46.7(11)	$14.94\mathrm{s}$	$13.81\mathrm{s}$	42.1 (11)	$18.89\mathrm{s}$	$14.13\mathrm{s}$						
1 0 2 4	49.2(11)	$5.75\mathrm{s}$	$6.78\mathrm{s}$	44.3 (11)	$6.95\mathrm{s}$	$7.21\mathrm{s}$						
2 0 4 8	47.7 (11)	$2.92\mathrm{s}$	$3.10\mathrm{s}$	44.3 (11)	$2.66\mathrm{s}$	$3.56\mathrm{s}$						
4 0 9 6	48.9(11)	$0.95\mathrm{s}$	$1.75\mathrm{s}$	45.5 (11)	$1.28\mathrm{s}$	$2.15\mathrm{s}$						
8 192	50.1(11)	$0.63\mathrm{s}$	$1.35\mathrm{s}$	46.0 (11)	$0.76\mathrm{s}$	$1.66\mathrm{s}$						
			TADLE 4									

Comparison of one-level and RGDSW Schwarz preconditioners for the flow problem on the Antarctica mesh with 4 km horizontal resolution and 20 layers of elements in vertical direction and a total of 35.3 m degrees of freedom. The linear iteration counts (avg. its), setup times (avg. setup), and solve times (avg. solve) are averaged over the number of Newton iterations (nl its). Lowest average iterations counts, setup times, and solve times in each row are marked in **bold**.

better for the classical GDSW coarse spaces compared to the respective RGDSW 557coarse spaces. In particular, the best iteration counts are obtained using the classical 558GDSW coarse space with the full null space. However, the parallel performance is 559 clearly better when reducing the dimension of the coarse space by either omitting the 560rotational rigid body mode or by using the RGDSW coarse space; see also Table 3 for 561562 the number coarse components used in the GDSW and the RGDSW coarse spaces, which, together with the dimension of the employed subspace of the null space, deter-563 mines the size of the coarse space. In total, the variant with the smallest coarse space, 564 i.e., RGDSW without rotation, yields both the highest iteration counts but the best 565 566 parallel performance. Hence, we will concentrate on this coarse space in the following experiments. 567

Moreover, we compare one-level and two-level Schwarz methods in Table 4. We observe that the one-level methods do not scale numerically. However, due to the geometry of the ice sheet, the increase in the iteration count of the one-level preconditioners is lower compared to usual fully three-dimensional domain decompositions. Due to the reuse strategies for the two-level methods used in this comparison, the setup cost for the one-level preconditioners is only slightly lower; even the coarse matrix is reused. However, due to numerical scalability, the two level methods perform clearly better in the solve phase.

6.1.2. Reuse strategies. In Table 5, we investigate the performance improvements due to the use of reuse strategies on the coarse level. As the baseline, we consider reusing the index sets (IS) and the symbolic factorization for the first level (SF1). We then consider reusing only the symbolic factorization of the coarse matrix (SF2) and coarse basis functions (CB) as well as also reusing the coarse matrix itself (CM). As can be observed, the iteration counts increase and, at the same time, the setup cost reduces if parts of the second level are reused. In particular, for lower numbers of MPI ranks and large subdomain problems, the setup cost is significantly

	I	S & SF1		IS & SI	F1 & SF2	& CB	IS & SF1 & SF2 & CB & CM		
MPI	avg. its	avg.	avg.	avg. its	avg.	avg. its	avg. its	avg.	avg.
ranks	(nl its)	setup	solve	(nl its)	setup	solve	(nl its)	setup	solve
512	41.9 (11)	$25.10\mathrm{s}$	$12.29\mathrm{s}$	42.6 (11)	$14.99\mathrm{s}$	$12.50\mathrm{s}$	46.7(11)	$14.94\mathrm{s}$	$13.81\mathrm{s}$
1 0 2 4	43.3 (11)	$9.18\mathrm{s}$	$5.85\mathrm{s}$	44.5 (11)	$5.65\mathrm{s}$	$6.08\mathrm{s}$	49.2(11)	$5.75\mathrm{s}$	$6.78\mathrm{s}$
2 0 4 8	41.4 (11)	$4.15\mathrm{s}$	$2.63\mathrm{s}$	42.7 (11)	$3.11\mathrm{s}$	$2.79\mathrm{s}$	47.7(11)	$2.92\mathrm{s}$	$3.10\mathrm{s}$
4 0 9 6	41.2 (11)	$1.66\mathrm{s}$	$1.49\mathrm{s}$	42.5 (11)	$1.07\mathrm{s}$	$1.54\mathrm{s}$	48.9(11)	$0.95\mathrm{s}$	$1.75\mathrm{s}$
8 1 9 2	40.2 (11)	$1.26\mathrm{s}$	$1.06\mathrm{s}$	42.0 (11)	$1.20\mathrm{s}$	$1.16\mathrm{s}$	50.1(11)	$0.63\mathrm{s}$	$1.35\mathrm{s}$

TABLE 5

Comparison of different reuse strategies for the two-level RGDSW Schwarz preconditioner for the flow problem on the Antarctica mesh with 4 km horizontal resolution and 20 layers of elements in vertical direction and a total of 35.3 m degrees of freedom. The linear iteration counts (avg. its), setup times (avg. setup), and solve times (avg. solve) are averaged over the number of Newton iterations (nl its). Lowest average iterations counts, setup times, and solve times in each row are marked in **bold**.

	1 comr	n. step	2 comr	n. step	3 comm. step	
MPI	avg.	avg.	avg.	avg.	avg.	avg.
ranks	setup	solve	setup	solve	setup	solve
512	$15.38\mathrm{s}$	$13.8\mathrm{s}$	$14.99\mathrm{s}$	$12.50\mathrm{s}$	$15.75\mathrm{s}$	$13.85\mathrm{s}$
1 0 2 4	$5.68\mathrm{s}$	$6.25\mathrm{s}$	$5.65\mathrm{s}$	$6.08\mathrm{s}$	$5.63\mathrm{s}$	$6.10\mathrm{s}$
2 0 4 8	$2.91\mathrm{s}$	$3.27\mathrm{s}$	$2.94\mathrm{s}$	$2.78\mathrm{s}$	$3.40\mathrm{s}$	$2.75\mathrm{s}$
4 0 9 6	$1.35\mathrm{s}$	$3.77\mathrm{s}$	$1.07\mathrm{s}$	$1.54\mathrm{s}$	$1.15\mathrm{s}$	$1.56\mathrm{s}$
8 1 9 2	$2.5{ m s}$	$12.22\mathrm{s}$	$1.29\mathrm{s}$	$1.13\mathrm{s}$	$1.29\mathrm{s}$	$1.17\mathrm{s}$
			TADIE			

Variation of the number of communication steps for the scatter and gather operations on the coarse level for the RGDSW Schwarz preconditioner for the flow problem on the Antarctica mesh with 4 km horizontal resolution and 20 layers of elements in vertical direction and a total of 35.3 m degrees of freedom. The linear iteration counts (avg. its), setup times (avg. setup), and solve times (avg. solve) are averaged over the number of Newton iterations (nl its). Lowest average iterations counts, setup times, and solve times in each row are marked in **bold**.

reduced. Due to the better overall performance, we will only consider results using IS & SF1 & SF2 & CB or IS & SF1 & SF2 & CB & CM for the following results using two-level preconditioners for the flow problem.

6.1.3. Parallelization aspects. Here, we discuss two parallelization aspects. 587 First, we discuss the communication between all MPI ranks and the single MPI 588rank which computes the coarse problem, the *coarse rank*. In particular, both all-to-589one and one-to-all communication patterns are necessary in our implementation: In 590 the setup phase, the coarse matrix, which is computed by an RAP product on all MPI ranks, has to be communicated to the coarse rank. Then, in each linear iteration of the 592solve phase, the right hand side of the coarse problem has to be communicated from all ranks to the coarse rank and the corresponding solution has to be communicated 594595 back. As already discussed in [28, section 4.7], this type of communication does not perform well for large numbers of MPI ranks using the Trilinos import and export 596objects. In [28, section 4.7] Epetra import and export objects were employed, whereas 597their Tpetra counterparts are considered here. Therefore, we introduce nested sets 598 of MPI ranks, beginning with all MPI ranks and ending with the single coarse rank, 599600 and perform the all-to-one and one-to-all communication using multiple steps; cf. [28, section 4.7] for a more detailed discussion. 601

In Table 6, we present corresponding results, varying the number of communication steps between one to three. As can be observed, using two or three communication steps, we obtain good the parallel scalability. However, if only a singe import/export

	OpenMP	parallelizatio	n (512 MP	'I ranks)	MPI parallelization				
	OpenMP	avg. its	avg.	avg.	MPI	avg. its	avg.	avg. its	
cores	threads	(nl its)	setup	solve	ranks	(nl its)	setup	solve	
512	1	42.6 (11)	$14.99\mathrm{s}$	$12.50\mathrm{s}$	512	42.6 (11)	$14.99\mathrm{s}$	$12.50\mathrm{s}$	
1024	2	42.6 (11)	$9.43\mathrm{s}$	$6.80\mathrm{s}$	1 0 2 4	44.5 (11)	$5.65\mathrm{s}$	$6.08\mathrm{s}$	
2048	4	42.6 (11)	$5.50\mathrm{s}$	$4.02\mathrm{s}$	2 0 4 8	42.7 (11)	$3.11\mathrm{s}$	$2.79\mathrm{s}$	
4096	8	42.6 (11)	$3.65\mathrm{s}$	$2.71\mathrm{s}$	4 0 9 6	42.5 (11)	$1.07\mathrm{s}$	$1.54\mathrm{s}$	
8 1 9 2	16	42.6 (11)	$2.56\mathrm{s}$	$2.32\mathrm{s}$	8 192	42.0 (11)	$1.20\mathrm{s}$	$1.16\mathrm{s}$	
				TABLE 7					

Comparison of increasing the numbers of OpenMP threads or MPI ranks for the RGDSW Schwarz preconditioner for the flow problem on the Antarctica mesh with 4 km horizontal resolution and 20 layers of elements in vertical direction and a total of 35.3 m degrees of freedom. The linear iteration counts (avg. its), setup times (avg. setup), and solve times (avg. solve) are averaged over the number of Newton iterations (nl its). Lowest average iterations counts, setup times, and solve times in each row are marked in **bold**.

		Con	Constant number of MPI ranks				128 MPI ranks per 5 layers			
#	#	MPI	avg. its	avg.	avg.	MPI	avg. its	avg.	avg.	
layers	dofs	ranks	(nl its)	setup	solve	ranks	(nl its)	setup	solve	
5	10.1 m		39.2(11)	$0.42\mathrm{s}$	$0.58\mathrm{s}$	128	38.8(12)	$5.47\mathrm{s}$	$7.79\mathrm{s}$	
10	$18.5\mathrm{m}$		41.0(11)	$0.79\mathrm{s}$	$1.15\mathrm{s}$	256	37.8(11)	$8.46\mathrm{s}$	$8.57\mathrm{s}$	
20	$35.3\mathrm{m}$	2 0 4 8	42.7(11)	$2.94\mathrm{s}$	$2.78\mathrm{s}$	512	42.6(11)	$14.99\mathrm{s}$	$12.50\mathrm{s}$	
40	69.0 m		45.6(12)	$5.77\mathrm{s}$	$6.67\mathrm{s}$	1024	47.8 (12)	$19.00\mathrm{s}$	$15.72\mathrm{s}$	
80	136.3 m		45.3(15)	$14.41\mathrm{s}$	$14.53\mathrm{s}$	2048	45.3(15)	$14.41\mathrm{s}$	$14.53\mathrm{s}$	

TABLE	8
LADLL	0

Performance of the RGDSW Schwarz preconditioner for an increasing number of layers for the flow problem on the Antarctica mesh with 4 km horizontal resolution and 20 layers of elements in vertical direction. Left: constant number of MPI ranks and subdomains. Right: increasing the number of MPI ranks and subdomains proportial to the number of layers. The linear iteration counts (avg. its), setup times (avg. setup), and solve times (avg. solve) are averaged over the number of Newton iterations (nl its).

call from Tpetra is performed in each scatter/gather operation, the parallel scalability deteriorates due to a significant communication overhead. In particular, the solve time, where one scatter and one gather operation is performed in each linear iteration, is increased significantly. Hence, in all other experiments, we use two communication steps.

In Table 7, we compare OpenMP parallelization and MPI parallelization. Starting 610 with 512 MPI ranks, we increase the number of processor cores up to 8192 using 611 either OpenMP threads or a higher number of MPI ranks. As can be observed, MPI 612 parallelization is clearly superior in this comparison even though the size of the coarse 613 problem increases with an increasing number of MPI ranks and subdomains, whereas 614it stays constant for OpenMP parallelization. Only for large numbers of MPI ranks 615 and subdomains, it may be reasonable to additionally use OpenMP parallelization 616 617 since it does not further increase the coarse problem size. Alternatively, more levels could be added to the the GDSW type preconditioners; cf. [29, 30]. Hence, we will 618 restrict ourselves to using MPI parallelization; only in the largest weak scalability 619 study in subsection 6.1.5, we also show results using OpenMP parallelization in 620 addition to MPI parallelization. 621

622 **6.1.4. Increasing the number of layers of elements in vertical direction.** 623 In most of our numerical simulations, we use 20 layers of elements in vertical direction; 624 this corresponds to a rather fine resolution in vertical direction, which would also be 625 used in production runs of the land ice simulations. However, we are also interested in

1 OpenMP thread											
		IS & SI	F1 & SF2 &	k CB	IS & SF1 &	z SF2 & Cl	B & CM				
mesh	#	avg. its	avg.	avg.	avg. its	avg.	avg.				
	dofs	(nl its)	setup	solve	(nl its)	setup	solve				
$16\mathrm{km}$	2.2 m	24.1(11)	$11.97\mathrm{s}$	$9.47\mathrm{s}$	24.0 (11)	$11.18\mathrm{s}$	$9.45\mathrm{s}$				
$8\mathrm{km}$	8.8 m	32.0 (10)	$14.08\mathrm{s}$	$8.71\mathrm{s}$	32.6(10)	$14.06\mathrm{s}$	$8.93\mathrm{s}$				
$4\mathrm{km}$	$35.3\mathrm{m}$	42.6 (11)	$14.99\mathrm{s}$	$12.50\mathrm{s}$	42.6 (11)	$16.14\mathrm{s}$	$14.19\mathrm{s}$				
$2\mathrm{km}$	$141.5\mathrm{m}$	61.0 (11)	$22.83\mathrm{s}$	$19.76\mathrm{s}$	67.1(11)	$22.65\mathrm{s}$	$21.69\mathrm{s}$				
$1\mathrm{km}$	$566.1\mathrm{m}$	67.1 (14)	$17.36\mathrm{s}$	$22.91\mathrm{s}$	73.0(14)	$16.80\mathrm{s}$	$28.48\mathrm{s}$				
		4 C	penMP th	reads							
		IS & SI	F1 & SF2 &	k CB	IS & SF1 &	z SF2 & Cl	B & CM				
mesh	#	avg. its	avg.	avg.	avg. its	avg.	avg.				
	dofs	(nl its)	setup	solve	(nl its)	setup	solve				
$16\mathrm{km}$	2.2 m	23.5 (11)	$4.15\mathrm{s}$	$3.25\mathrm{s}$	23.8(11)	$3.93\mathrm{s}$	$3.28\mathrm{s}$				
$8\mathrm{km}$	8.8 m	32.0 (10)	$4.97\mathrm{s}$	$2.85\mathrm{s}$	32.6(10)	$4.62\mathrm{s}$	$2.82\mathrm{s}$				
$4\mathrm{km}$	$35.3\mathrm{m}$	42.6 (11)	$5.50\mathrm{s}$	$4.02\mathrm{s}$	46.7(11)	$5.27\mathrm{s}$	$4.45\mathrm{s}$				
$2\mathrm{km}$	$141.5\mathrm{m}$	61.0 (11)	$7.36\mathrm{s}$	$6.55\mathrm{s}$	67.1(11)	$7.15\mathrm{s}$	$7.34\mathrm{s}$				
$1\mathrm{km}$	$566.1\mathrm{m}$	67.1 (14)	$6.20\mathrm{s}$	$7.39\mathrm{s}$	73.0(14)	$5.75\mathrm{s}$	$7.92\mathrm{s}$				
	mesh 16 km 8 km 2 km 1 km mesh 16 km 8 km 4 km 2 km 1 km	$\begin{array}{c c} \text{mesh} & \# \\ \text{dofs} \\ \hline \text{dofs} \\ \hline 16 \text{ km} & 2.2 \text{ m} \\ 8 \text{ km} & 8.8 \text{ m} \\ 4 \text{ km} & 35.3 \text{ m} \\ 2 \text{ km} & 141.5 \text{ m} \\ 1 \text{ km} & 566.1 \text{ m} \\ \hline \hline \\ \hline \\ \text{mesh} & \# \\ \text{dofs} \\ \hline 16 \text{ km} & 2.2 \text{ m} \\ 8 \text{ km} & 8.8 \text{ m} \\ 4 \text{ km} & 35.3 \text{ m} \\ 2 \text{ km} & 141.5 \text{ m} \\ 1 \text{ km} & 566.1 \text{ m} \\ \hline \end{array}$	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c c c c c c c c c c c c c c c c c c c $				

Table 9

Weak scalability studies for the RGDSW Schwarz preconditioner for the flow problem on the Antarctica mesh with 4 km horizontal resolution and 20 layers of elements in vertical direction. We consider the cases of 1 OpenMP thread (top) and 4 OpenMP threads (bottom) per MPI rank as well as IS & SF1 & SF2 & CB (left) and IS & SF1 & SF2 & CB & CM (right) reuse strategies. The linear iteration counts (avg. its), setup times (avg. setup), and solve times (avg. solve) are averaged over the number of Newton iterations (nl its). Lowest average iterations counts, setup times, and solve times in each row are marked in **bold**.

investigating the influence of an increasing number of layers on the performance of our 626 preconditioners. In Table 8, we employ the RGDSW preconditioner and fix the top 627 surface mesh while increasing the number of vertical layers of elements from 5 up to 80. 628 For both cases, keeping the number of MPI ranks fixed and increasing it proportional 629 to the number of layers, the iterations counts are very robust. However, the number of 630 631 nonlinear iterations increases slightly from 11 to 15. Note that we use 2048 MPI ranks for all problems in this experiment when we keep constant number of MPI ranks. This 632 also allows comparing scalability of the solver for different problems to 2048 ranks. 633 For example, even the 5 layer problem achieves 13.4x speedup in average solve going 634 from 128 MPI ranks to 2048 MPI ranks demonstrating good parallel scalability. 635

636 **6.1.5. Weak scaling.** In Table 9, we provide four weak scalability studies, where 637 we increase the number of MPI ranks proportional to the resolution of the top surface 638 mesh; the number of vertical layers is again fixed to 20. In particular, we consider 1 639 or 4 OpenMP threads per MPI rank combined with the IS & SF1 & SF2 & CB and 640 IS & SF1 & SF2 & CB & CM reuse strategies; cf. subsections 4.5 and 6.1.2.

We observe good weak scalability from 32 to 8192 (1 OpenMP thread per MPI 641 642 rank) and from 128 to 32768 (4 OpenMP threads per MPI rank) processor cores. However, there is a moderate increase in the number of iterations, which is most 643 likely caused by the unstructured domain decomposition, where subdomains with 644 645 irregular shape and bad aspect ratio may occur in certain cases, in particular, at the boundary of the top surface mesh; cf. Figure 3. For all configurations, the setup time 646 647 scales very well, whereas the increase in the solve time is more pronouced; however, except for the case of 1 OpenMP rank and IS & SF1 & SF2 & CB & CM reuse, the 648 solve times does increase clearly less than the number of iterations. 649

Generally, we observe a speedup by a factor of approximately 3 when using 4 threads instead of 1 OpenMP thread. However, the former uses 4 times the number

FROSCH PRECONDITIONERS FOR LAND ICE SIMULATIONS

		FROSch							
	IS & SF1			IS & SF1 & SF2 & CB & CM			Vertical Semi-Coarsening		
MPI	avg. its	avg.	avg.	avg. its	avg.	avg.	avg. its	avg.	avg.
ranks	(nl its)	setup	solve	(nl its)	setup	solve	(nl its)	setup	solve
512	41.9(11)	$25.10\mathrm{s}$	$12.29\mathrm{s}$	46.7(11)	$14.94\mathrm{s}$	$13.81\mathrm{s}$	31.0 (11)	$0.35\mathrm{s}$	$3.00\mathrm{s}$
1024	43.3(11)	$9.18\mathrm{s}$	$5.85\mathrm{s}$	49.2(11)	$5.75\mathrm{s}$	$6.78 { m s.}$	30.7 (11)	$0.32\mathrm{s}$	$1.66\mathrm{s}$
2048	41.4(11)	$4.15\mathrm{s}$	$2.63\mathrm{s}$	47.7 (11)	$2.92\mathrm{s}$	$3.10\mathrm{s}$	31.0 (11)	$0.36\mathrm{s}$	$1.02\mathrm{s}$
4 0 9 6	41.2(11)	$1.66\mathrm{s}$	$1.49\mathrm{s}$	48.9(11)	$0.95\mathrm{s}$	$1.75\mathrm{s}$	30.9 (11)	$0.80\mathrm{s}$	$1.69\mathrm{s}$
8 1 9 2	40.2 (11)	$1.26\mathrm{s}$	$1.06\mathrm{s}$	50.1(11)	$0.63\mathrm{s}$	$1.35\mathrm{s}$	48.5(11)	$1.05\mathrm{s}$	$2.55\mathrm{s}$

TABLE 10

Comparison of the RGDSW Schwarz preconditioner with two different reuse strategies against MueLu algebraic multigrid for the flow problem on the Antarctica mesh with 4 km horizontal resolution and 20 layers of elements in vertical direction and a total of 35.3 m degrees of freedom. The linear iteration counts (avg. its), setup times (avg. setup), and solve times (avg. solve) are averaged over the number of Newton iterations (nl its). Lowest average iterations counts, setup times, and solve times in each row are marked in **bold**.

of cores compared to the latter. Hence, OpenMP parallelization has to be carefully considered with respect to the size of the problems and the available parallelism.

654 **6.1.6.** Comparison against multigrid. As a final result for the velocity problem for Antarctica, we compare the strong scalability for the RGDSW preconditioner 655 in the FROSch package to an algebraic multigrid preconditioner described in [50] and 656 using MueLu. The method uses a vertical semi-coarsening approach designed for the 657 ice sheet problems. As can be observed in Table 10, for small numbers of MPI ranks 658 659 and subdomains, the total time is clearly higher for FROSch compared to MueLu. This is caused by the superlinear complexity of the direct solvers which are used 660 to solve the problems on the overlapping subdomains. However, when increasing the 661 number of subdomains and therefore reducing the size of the overlapping subdomains, 662 we observe a better speedup compared to MueLu. We note that MueLu settings were 663 not fine-tuned for this particular problem. However, it is fair to say that FROSch 664665 is competitive for large number of sub-domains especially considering the fact that FROSch is used almost as a black box. 666

6.2. Temperature problem for Greenland. As a second problem for land 667 ice simulations, we consider the temperature problem described in subsection 2.2 for 668 Greenland; see also Figure 4. In Table 11, we compare one-level Schwarz precondi-669 670 tioners and RGDSW preconditioner using one and two layers of algebraic overlap. As can be observed, already the one-level methods scale well since all subdomains are ad-671 672 jacent to the Dirichlet boundary, which is the whole upper surface; cf. subsection 2.2. Due to the lower setup and application cost of the one-level method, both the setup 673 and the solve times are also lower. Therefore, one-level Schwarz methods are very 674 675 well suited for solving the temperature problem, and hence, it is not necessary to add a second level. Note that the standalone steady-state temperature problem is not 676 677 physically meaningful because the temperature equilibration is on time scales that are much larger than the velocity ones. For this reason, we focus our attention on the 678 coupled problem. 679

680 **6.3.** Coupled problem for Greenland. Finally, we consider the coupled prob-681 lem for the non-uniform Greenland meshes and present, for the first time, results for 682 scalable monolithic two-level preconditioners for this problem. Note that the nonlin-683 ear iteration is very sensitive for the coupled problem. In particular, even though a 684 very strict stopping tolerance of 10^{-9} is used for the GMRES iteration, changing the

One-level Schwarz										
	one laver o	of algebrai	c overlap	two lavers	of algebrai	c overlap				
MPI	avg.	avg.	avg.	avg.	avg.	avg.				
ranks	its	setup	solve	its	setup	solve				
512	18.1 (11)	0.42 s	$0.35\mathrm{s}$	17.1 (11)	0.51 s	$0.40\mathrm{s}$				
1024	23.7 (11)	$0.25\mathrm{s}$	$0.25\mathrm{s}$	22.1 (11)	$0.27\mathrm{s}$	$0.27\mathrm{s}$				
2048	29.6 (11)	$0.16\mathrm{s}$	$0.17\mathrm{s}$	27.6 (11)	$0.23\mathrm{s}$	$0.20\mathrm{s}$				
4096	39.8 (11)	$0.15\mathrm{s}$	$0.15\mathrm{s}$	35.6 (11)	$0.17\mathrm{s}$	$0.17\mathrm{s}$				
	RGDSW (IS & SF1 & SF2 & CB)									
	one layer o	of algebrai	c overlap	two layers	of algebrai	c overlap				
MPI	avg.	avg.	avg.	avg.	avg.	avg.				
ranks	avg. its	setup	solve	avg. its	setup	solve				
512	19.5(11)	$0.44\mathrm{s}$	$0.41\mathrm{s}$	18.7 (11)	$0.55\mathrm{s}$	$0.46\mathrm{s}$				
1 0 2 4	25.2(11)	$0.28\mathrm{s}$	$0.29\mathrm{s}$	23.9 (11)	$0.35\mathrm{s}$	$0.33\mathrm{s}$				
2048	31.5(11)	$0.26\mathrm{s}$	$0.24\mathrm{s}$	29.5 (11)	$0.25\mathrm{s}$	$0.27\mathrm{s}$				
4096	42.2 (11)	$0.25\mathrm{s}$	$0.27\mathrm{s}$	38.2 (11)	$0.25\mathrm{s}$	$0.29\mathrm{s}$				
			TABLE 1	1						

Comparison of one-level and RGDSW Schwarz preconditioners for the temperature problem on the Greenland mesh with $1-10 \,\mathrm{km}$ horizontal resolution (fine mesh) and 20 layers of elements in vertical direction and a total of $1.9 \,\mathrm{m}$ degrees of freedom. The linear iteration counts (avg. its), setup times (avg. setup), and solve times (avg. solve) are averaged over the number of Newton iterations (nl its). Lowest average iterations counts, setup times, and solve times in each row are marked in **bold**.

fully coupled extensions									
			NR		IS & CB				
MPI		avg. its	avg.	avg.	avg. its	avg.	avg.		
ranks	$\dim V_0$	(nl its)	setup	solve	(nl its)	setup	solve		
256	1 400	100.1(27)	$4.10\mathrm{s}$	$6.40\mathrm{s}$	18.5 (70)	$2.28\mathrm{s}$	$1.07\mathrm{s}$		
512	2852	129.1(28)	$1.88\mathrm{s}$	$4.20\mathrm{s}$	24.6 (38)	$1.04\mathrm{s}$	$0.70\mathrm{s}$		
1 0 2 4	6 0 3 6	191.2(65)	$1.21\mathrm{s}$	$4.76\mathrm{s}$	34.2 (32)	$0.66\mathrm{s}$	$0.70\mathrm{s}$		
2 0 4 8	12368	237.4(30)	$0.96\mathrm{s}$	$4.06\mathrm{s}$	37.3 (30)	$0.60\mathrm{s}$	$0.58\mathrm{s}$		
decoupled extensions									
			NR		IS & CB				
MPI		avg. its	avg.	avg.	avg. its	avg.	avg.		
ranks	$\dim V_0$	(nl its)	setup	solve	(nl its)	setup	solve		
256	1 400	23.6(29)	$3.90\mathrm{s}$	$1.32\mathrm{s}$	21.5 (34)	$2.23\mathrm{s}$	$1.18\mathrm{s}$		
512	2852	27.5(30)	$1.83\mathrm{s}$	$0.78\mathrm{s}$	26.4 (33)	$1.13\mathrm{s}$	$0.78\mathrm{s}$		
1 0 2 4	6036	30.1(29)	$1.19\mathrm{s}$	$0.60\mathrm{s}$	28.6 (43)	$0.66\mathrm{s}$	$0.61\mathrm{s}$		
2 0 4 8	12368	36.4(30)	$0.69\mathrm{s}$	$0.56\mathrm{s}$	31.2 (50)	$0.57\mathrm{s}$	$0.55\mathrm{s}$		
TABLE 12									

Comparison of monolithic RGDSW Schwarz preconditioners with different coarse spaces **ne**glecting rotational coarse basis functions for the velocity degrees of freedom for the coupled problem on the Greenland mesh with 3-30 km horizontal resolution (coarse mesh) and 20 layers of elements in vertical direction and a total of 7.5 m degrees of freedom. The linear iteration counts (avg. its), setup times (avg. setup), and solve times (avg. solve) are averaged over the number of Newton iterations (nl its). Lowest average iterations counts, setup times, and solve times in each row are marked in **bold**.

preconditioner may result in significant variations in the number of nonlinear iterations; cf. Tables 12, 13, 15, and 16. Note again that, in this work, we report linear iteration counts averaged over the total number of Newton iterations, so that our results are not influenced much by the sensitivity of the nonlinear solver.

First, we compare different monolithic coarse spaces for a coarse Greenland mesh with 3-30 km horizontal resolution, 20 layers of elements in vertical direction, and a total of more than 7.5 m degrees of freedom. In order to focus only on the coarse basis,

⁶⁹² we only consider two following reuse strategies. On the one hand, we do not reuse any

fully coupled extensions									
			NR		IS & CB				
MPI		avg. its	avg.	avg.	avg. its	avg.	avg.		
ranks	$\dim V_0$	(nl its)	setup	solve	(nl its)	setup	solve		
256	1 750	99.3(27)	$4.20\mathrm{s}$	$6.35\mathrm{s}$	21.9 (30)	$2.35\mathrm{s}$	$1.22\mathrm{s}$		
512	3565	131.4(28)	$1.95\mathrm{s}$	$4.40\mathrm{s}$	22.8 (50)	$1.09\mathrm{s}$	$0.66\mathrm{s}$		
1 0 2 4	7545	261.7(31)	$1.22\mathrm{s}$	$5.47\mathrm{s}$	31.3 (29)	$0.73\mathrm{s}$	$0.61\mathrm{s}$		
2 0 4 8	15460	325.7(27)	$1.08\mathrm{s}$	$8.53\mathrm{s}$	41.7 (25)	$0.74\mathrm{s}$	$1.16\mathrm{s}$		
		de	ecoupled	extension	is				
			NR		I	S & CB			
MPI		avg. its	avg.	avg.	avg. its	avg.	avg.		
ranks	$\dim V_0$	(nl its)	setup	solve	(nl its)	setup	solve		
256	1 750	22.0 (28)	$3.98\mathrm{s}$	$1.23\mathrm{s}$	22.8 (27)	$2.23\mathrm{s}$	$1.28\mathrm{s}$		
512	3565	24.7 (32)	$1.92\mathrm{s}$	$0.72\mathrm{s}$	23.8 (39)	$1.11\mathrm{s}$	$0.69\mathrm{s}$		
1 0 2 4	7545	31.9 (27)	$1.23\mathrm{s}$	$0.62\mathrm{s}$	33.1(27)	$0.74\mathrm{s}$	$0.76\mathrm{s}$		
2 0 4 8	15460	31.2 (38)	$0.99\mathrm{s}$	$0.77\mathrm{s}$	34.7(34)	$0.69\mathrm{s}$	$1.05\mathrm{s}$		
TABLE 13									

Comparison of monolithic RGDSW Schwarz preconditioners with different coarse spaces including rotational coarse basis functions for the velocity degrees of freedom for the coupled problem on the Greenland mesh with 3-30 km horizontal resolution (coarse mesh) and 20 layers of elements in vertical direction and a total of 7.5 m degrees of freedom. The linear iteration counts (avg. its), setup times (avg. setup), and solve times (avg. solve) are averaged over the number of Newton iterations (nl its). Lowest average iterations counts, setup times, and solve times in each row are marked in **bold**.

# subdom	256	512	1024	2048	4096			
RGDSW	3-30 km	350	713	1509	3092	6245		
	1-10 km	-	721	1536	3230	6615		
TABLE 14								

Number of coarse components Γ_i for the two non-uniform Greenland meshes with 3-30 km and 1-10 km horizontal resolution. The dimension of the coarse space is the number of coarse components multiplied by the dimension of the null space.

information from the first Newton iteration (NR), on the other hand, we only reuse 693 index sets and the coarse basis (IS & CB); in both cases, we do not reuse symbolic 694 factorizations because of variations in the sparsity pattern of the system matrix. In 695 combination with these two reuse strategies, we consider monolithic RGDSW precon-696 ditioners (see subsection 4.3) with fully coupled extensions using (4.10) and decoupled 697 extensions using (4.12), respectively. As in subsection 6.1.1, we consider neglecting the 698 rotational coarse basis functions and including the rotational coarse basis functions 699 for the velocity part in Table 12 and Table 13, respectively. We clearly observe that 700 using the standard monolithic coarse space (without reuse of the coarse basis func-701 702 tions) does not yield a scalable two-level method. Adding the rotational coarse basis function even yields higher iterations counts compared to neglecting rotational coarse 703 704 basis functions. However, using the decoupled extensions described in subsection 4.3 instead, we obtain a scalable monolithic RGDSW preconditioner. Moreover, it seems 705 that the coupling terms in the first Newton iteration do not deteriorate the scalability. 706 707 Hence, reusing the coarse basis from the first Newton iteration even yields a scalable preconditioner for both cases, the fully coupled and the decoupled extensions. 708

Moreover, as for the velocity problem (see subsection 6.1.1), the time to solution is lower when neglecting the rotational coarse basis functions due to the lower coarse space dimension; see also Table 14 for the numbers of interface components. Consequently, we will only consider the case of neglecting rotational coarse basis functions for the monolithic RGDSW coarse spaces in the following experiments. A. HEINLEIN, M. PEREGO, AND S. RAJAMANICKAM

	decoupled (NR)			fully coupled (IS & CB)			decoupled (IS & SF1 & CB)		
MPI	avg.	avg.	avg.	avg.	avg.	avg.	avg.	avg.	avg.
ranks	(nl its)	setup	solve	(nl its)	setup	solve	(nl its)	setup	solve
512	41.3 (36)	$18.78\mathrm{s}$	$4.99\mathrm{s}$	45.3(32)	$11.84\mathrm{s}$	$5.35\mathrm{s}$	45.0(35)	$10.53\mathrm{s}$	$5.36\mathrm{s}$
1 0 2 4	53.0(29)	$8.68\mathrm{s}$	$4.22\mathrm{s}$	47.8 (37)	$5.36\mathrm{s}$	$3.82\mathrm{s}$	54.3(32)	$4.59\mathrm{s}$	$4.31\mathrm{s}$
2 0 4 8	62.2(86)	$4.47\mathrm{s}$	$4.23\mathrm{s}$	66.7(38)	$2.81\mathrm{s}$	$4.53\mathrm{s}$	59.1 (38)	$2.32\mathrm{s}$	$3.99\mathrm{s}$
4 0 9 6	68.9 (40)	$2.52\mathrm{s}$	$2.86\mathrm{s}$	79.1(36)	$1.61\mathrm{s}$	$3.30\mathrm{s}$	78.7(38)	$1.37\mathrm{s}$	$3.30\mathrm{s}$

TABLE 15

Comparison of monolithic RGDSW Schwarz preconditioners with different reuse strategies for the coupled problem on the Greenland mesh with $1-10 \,\mathrm{km}$ horizontal resolution (fine mesh) and 20 layers of elements in vertical direction and a total of 68.6 m degrees of freedom. The linear iteration counts (avg. its), setup times (avg. setup), and solve times (avg. solve) are averaged over the number of Newton iterations (nl its). Lowest average iterations counts, setup times, and solve times in each row are marked in **bold**.

One-level Schwarz (NR)									
	Ċ	$\delta = 1h$		$\delta = 2h$					
MPI	avg. its avg. avg.		avg. its	avg.	avg.				
ranks	(nl its)	(nl its) setup solve		(nl its)	setup	solve			
512	48.7(35)	$11.3\mathrm{s}$	42.6 (33)	$15.2\mathrm{s}$	$5.80\mathrm{s}$				
1024	61.9(40)	$5.29\mathrm{s}$	$4.75\mathrm{s}$	58.8 (30)	$6.92\mathrm{s}$	$5.48\mathrm{s}$			
2048	89.9(30)	$2.52\mathrm{s}$	73.5 (34)	$3.83\mathrm{s}$	$6.24\mathrm{s}$				
4096	116.1(31)	$1.17\mathrm{s}$	$3.68\mathrm{s}$	103.1 (33)	$1.86\mathrm{s}$	$4.87\mathrm{s}$			
One-level Schwarz (NR & SF1)									
	Ċ	$\delta = 1h$		$\delta = 2h$					
MPI	avg. its	avg.	avg.	avg. its	avg.	avg.			
ranks	(nl its)	setup	solve	(nl its)	setup	solve			
512	52.2(32)	$10.16\mathrm{s}$	$5.88\mathrm{s}$	42.6 (39)	$13.80\mathrm{s}$	$5.77\mathrm{s}$			
1024	66.2(35)	$4.32\mathrm{s}$	$4.91\mathrm{s}$	35.7 (72)	$5.98\mathrm{s}$	$3.19\mathrm{s}$			
2048	82.0(37)	$2.07\mathrm{s}$	$5.27\mathrm{s}$	68.5 (39)	$3.20\mathrm{s}$	$5.81\mathrm{s}$			
4096	120.39(31)	$0.92\mathrm{s}$	$3.83\mathrm{s}$	95.5 (32)	$1.48\mathrm{s}$	$4.53\mathrm{s}$			
TABLE 16									

Strong scaling study for monolithic one-level Schwarz preconditioners with one or two layers of algebraic overlap for the coupled problem on the Greenland mesh with 1-10 km horizontal resolution (fine mesh) and 20 layers of elements in vertical direction and a total of 68.6 m degrees of freedom. The linear iteration counts (avg. its), setup times (avg. setup), and solve times (avg. solve) are averaged over the number of Newton iterations (nl its). Lowest average iterations counts, setup times, and solve times in each row are marked in **bold**.

Next, we investigate different reuse strategies in Table 15 for a fine Greenland mesh with 1-10 km horizontal resolution, 20 layers of elements in vertical direction, and a total of more than 68 m degrees of freedom. As can be observed, the best parallel performance can be obtained when reusing the index sets (IS) as well as the symbolic factorization on the first level (SF1) and the coarse basis (CB) from the first Newton iteration. Note that reusing the symbolic factorization on the second level, the iteration counts always deteriorated in our experiments.

Finally, we also provide results for monolithic one-level Schwarz preconditioners in 721 comparison to the two-level monolithic RGDSW preconditioner. As can be observed 722 723 in Table 16, the iteration counts for the one-level preconditioners with one level of overlap are clearly higher compared to the RGDSW preconditioner with one layer of 724 725 overlap in Table 15. Therefore, the solve time is reduced by adding an appropriate second level. On the other hand, the setup cost for the two-level methods is again 726 higher; in particular, the additional coarse problem is also a fully coupled multi-727 physics problem in this case. The computing time for an overlap of two layers was 728 729 higher for both the one-level and the two-level method.

Note that we observed that the matrix structure of the coupled problem is not well-suited for OpenMP parallelization of the node-level solver Pardiso. In particular, the speedup was always lower than a factor of 2 when using 4 OpenMP threads and one processor core per OpenMP thread. For the case of 4 096 MPI ranks, the speedup was even reduced to a factor of less than 1.2.

7. Conclusions. We have presented a flexible preconditioning framework based 735 on the GDSW method, which yields scalable and robust preconditioners for all con-736 sidered land ice problems. In particular, the implementation of this framework in 737 738 FROSch can be applied out-of-the-box; between the different problems, only minor 739 changes of the input parameters are necessary. Moreover, to the best of our knowledge, we have presented the first scalable two-level method for the coupled problem 740 741 for land ice simulations. Compared to the single physics problems, the extension operators have to be decoupled, which can easily be done be done by changing one 742 parameter in FROSch. Otherwise, the coarse basis from the first Newton iteration 743 also resulted in a scalable method. 744

The parallel results of several strong and weak scaling studies, involving different coarse space variants and reuse strategies as well as OpenMP parallelization and MPI communication aspects, prove both the robustness and numerical scalability of the methods as well as the parallel scalability of the implementation in FROSch.

Furthermore, we have observed that the direct solvers in our two-level method are the main bottleneck. On one hand, the direct solvers on the first level determine the computing time for a small number of MPI ranks and large subdomain problems. On the other hand, the direct solver on the coarse level may become the scaling bottleneck for very large numbers of MPI ranks and subdomains. The improvement of the subdomain and coarse solvers for these complex problems will be subject of future research.

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762 **Disclaimer.** This paper describes objective technical results and analysis. Any 763 subjective views or opinions that might be expressed in the paper do not necessarily 764 represent the views of the U.S. Department of Energy or the United States Govern-765 ment.

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