Dear Editor,

We would like to thank the anonymous referees for their detailed and constructive comments on our manuscript, gmd-2016-111: "Optimal numerical solvers for transient simulations of ice flow using the Ice Sheet System Model (ISSM versions 4.2.5 and 4.11)." Kindly refer to our responses to the comments provided by the referees, attached below, which we greatly appreciate. Based on the comments and questions raised by both referees, we performed another series of tests (2652 simulations) using a different benchmark example that includes a nonlinear viscosity model for ice. Results from these new simulations both support and add additional insight to the initial results. Below our responses, we have attached an updated copy of the manuscript that includes these new results and addresses the additional comments raised by the reviewers. We believe that these modifications have substantially improved the manuscript.

Best regards,

Feras Habbal and co-authors

# **Response to RC1:**

In this work, the authors compare the performances of several different direct and iterative solvers, provided by MUMPS and PETSc libraries respectively, for solving the transient ice flow model using ISSM. Specifically, the authors target a well known transient benchmark problem (ISMIPHOM, test F), in the case of a frozen bed or sliding bed. The flow model is constituted by the ice velocity part (Blatter-Pattyn model with constant viscosity), a part for reconstructing vertical velocities, and the mass transport part. The authors highlight some of the solvers that perform better on different mesh resolutions, for both frozen or sliding bed.

The detailed comparison of the solvers available in ISSM is certainly useful for the several ISSM users.

However, I have a few reservations about the impact that this work can have on a broader community.

- The benchmark problem addressed in this work has several simplifications that makes it not very representative of real problems, most notably: 1. Geometry is very simple (in constrast with complex margins or bed roughness encountered in real ice sheets). 2. Viscosity is constant, making the model linear. In real problems viscosity strongly depends on velocity and temperature, which makes the problem much harder to be solved numerically. 3. A relatively high basal friction coefficient is considered, which is not representative of what can be found in ice streams and ice shelves.

Thank you for your comments and review. We chose to test a suite of solvers using a commonly used transient ice flow benchmark test (ISMIP-HOM experiment F), which makes the simplifications that you list, so that other researchers could reproduce the results as well as conduct their own tests using different, potentially customized, solvers or other ice sheet codes with a common and well-known model setup. In addition to updating the manuscript to highlight the limitations of our initial benchmark tests relative to real-world problems, we are including results from applying solvers to another benchmark test (ISMIP-HOM experiment A) in order to explore the impact of using a more realistic nonlinear viscosity model for solving the stress balance equations.

- The authors consider only off-the-shelf solvers that "naturally fit the ISSM framework", whereas several efforts (not mentioned by the authors) have been done in recent years in order to build efficient solvers/preconditioners tailored on the ice sheet problems. Some of these solvers have been demonstrated on large-scale simulations of Greenland or Antarctic ice sheets. See, for example, T. Isaac et al., SIAM J. Sci. Comput., 37(6), B804–B833; Tezaur et al., Procedia Computer Science, 51:2026-2035, ICCS, 2015, S. Cornford at al. J. Comput. Phys, 232(1):529-549, 2013; plus the one by Brown et al. already cited, but not discussed, by the authors. I recommend that the authors make it clear in the abstract that they are only considering the off-the-shelf solvers readily available in ISSM. I also recommend to consider more realistic problems and to mention relevant work in the literature.

We updated the text to include the recommended citations relevant to this work and specified that the focus of this work was to test readily available solvers in the abstract. As you mentioned, our results using PETSc solvers within ISSM are relevant to ISSM users. However, since many numerical models use PETSc, including the Parallel Ice Sheet Model (PISM) and the Community Ice Sheet Model (CISM), which has the ability to leverage PETSc solvers through the Trilinos package, we anticipate that our results should extend to other ice sheet models and benefit modelers beyond the ISSM community.

### **Minor comments:**

- At line 144 the authors mention that they apply single-point constraints on velocity and thickness equations. I'd like the author to expand on this, mentioning how/with what values they constrain in a single point the velocity and thickness. Typically, single-point constraining is used in presence of a singular problems (which should not happen here), and it is known to artificially modify the spectrum of the matrix, which in turn can deteriorate the convergence of iterative solvers.

The text referring to using single point constraints was misstated and is corrected in the updated manuscript to note that we impose Dirichlet boundary conditions. Removing these entries from the matrix does not adversely impact the condition number of the stiffness matrix.

- Line 150, how the vertical velocity is reconstructed? With an L2 projection?

We solve the incompressibility equation to recover the vertical velocity, which is constant per element. Subsequently, we use an L2 projection to evaluate the nodal velocity. We updated the manuscript to clarify this point.

- The time reported in the tables is solver time, or total time (including assembly, linear solvers and I/O)? The weak scaling results for the iterative solvers are not very good and it would be useful to understand what is causing this.

We updated the text in the manuscript to note that the timing results include solving the system of equations, assembling the stiffness matrix, load vector, and updating the input from the solution.

# **Response to RC2:**

This work aims to provide insight into different solver choices for a particular full-Stokes ice sheet model (ISSM) by testing a range of iterative solver choices from the widely available PETSc solver library on a specific test problem (ISMIP-HOM, experiment F) and contrasting with their native/default direct-solve approach (which uses MUMPS). They conclude that switching to the PETSc iterative solvers generally improves time to-solution and scaling as the problem size (number of elements in the finite-element mesh) increases, and are able to provide some suggestions as to which solvers appear to be better suited to their needs. In my opinion, this is a useful contribution to the literature, and I found it to be well-written and well-organized. I do have a few suggestions which I think would greatly increase the usefulness of this work.

My primary criticisms, if you can call them that, are regarding the choice of benchmark problem. While I think that the choice of ISMIP-HOM problem F is a reasonable choice for representing a fully- or mostly-grounded ice sheet (like the Greenland Ice Sheet), I wonder how extendable the results and conclusions are to systems with fast-flowing ice streams and large dynamic ice shelves as are found in Antarctica, represented, for example, by the MISMIP family of benchmarks. In our experience (admittedly not with a full-Stokes model), marine ice sheets are often much more challenging for the linear solvers due to the mathematical nature of the floating ice shelves.

My larger objection is that I strongly disagree with the choice of a linear (constant viscosity) rheology for these experiments. In our experience (again admittedly not with a full-Stokes model), one of the hardest things for many solvers to handle is the large range of viscosities produced by the normal nonlinear rheology. We've often had the case where solvers which perform perfectly well with constant viscosities perform poorly (or fail to converge) when the nonlinear rheology is turned on. I suspect you're getting an incomplete and possibly misleading view of solver performance for "real" ice sheet problems in this case. Is there a compelling reason not to use a "standard" nonlinear rheology for these tests?

Thank you for your review and comments. We used the ISMIP-HOM experiment F test since it involved a transient simulation and is a commonly used benchmark test. The intent of our study was to promote the use of iterative methods over linear solvers using a simplified model, which could then be refined in future work using a real-world simulation. As you mention, the specification of linear viscosity in this benchmark test is a limiting feature in relation to real-world problems. To address the impact of nonlinear rheology on solving the stress balance equations, we are including results from applying the same solvers on another benchmark test (ISMIP-HOM experiment A) that uses a nonlinear viscosity model for ice. We updated the manuscript to highlight the limitations of the transient benchmark test (experiment F) and will include the results from this new study.

#### Minor points -

1. line 95 – please cite some examples of the full-Stokes solver work that you're referring to

We added additional references to the manuscript.

2. line 102 - "well know" -> "well known"

# Fixed typo.

3. line 108 – FS isn't a requirement for active GL dynamics, e.g. MISMIP(1,3d,++). In fact, the authors of this work routinely use SSA for GL problems...

We updated the text to avoid implying that full Stokes is required for modeling grounding line dynamics.

4. line 123 - "suit" -> "suite"

Fixed typo.

5. line 145 – "period" -> "periodic"

Fixed typo.

6. line 171 – please elaborate on or clarify what you mean by "methods that naturally fit the ISSM framework"

We updated the manuscript to be clearer on the point that our intention was to use solvers that did not require customization or specialization of the solver routine within ISSM so that the conclusions based on our results could be used by other models as well.

7. line 172 – using only the default settings for the PETSc components is likely too limiting of a choice. I understand why you'd do that (putting yourself in the shoes of a model-user who doesn't want to fiddle with solver parameters or explore all of the options available). However, we've found that there are cases where minor changes in options result in major improvements in solver performance and robustness. I'd suggest that since the goal of this work is to be a reference for ISSM (and other ISM) users, you should make some effort (maybe by asking the PETSc developers or another linear solver expert for some advice) to make the solvers perform as well as possible. I think this work will have a much larger impact in that case. The other point, of course, is that "default" options can change. I'd suggest presenting two sets of results – one with the "default" settings, and one after some attempt has been made to tune the solver parameters. (it is, of course, possible that the default parameters \*do\* produce the best performance). Of course, then, you would also need to document the particular solver options you used.

As you summarized, our intention was to highlight strong performance gains that can be attained using iterative solvers in PETSc with limited intervention on the part of modelers (i.e. using default values). In this context, we avoided the large number of options that can be tuned for each combination of iterative scheme with a particular preconditioner and treated each solver with the same level of attention. Also, in light of the simplifications underlying the benchmark test there is no guarantee that speed-ups based on customization of the components would straight forwardly correlate to real-world models. Future work, aimed at refining the results presented in this work, will be based on more realistic models and address the impact of customizing individual components, as you suggested. We updated the manuscript to note that significant performance gains are attainable by customizing the options of the PETSc components for a preferred solver.

8. Conclusion – To give a bit of extra weight to your conclusions, it might be useful to embed your conclusion in the larger context of what many have found to be the case in other scientific computation fields – one suggestion would be to add a statement along the lines of "the conclusion that scalable iterative methods are better suited than direct methods for solving large linear systems echoes the experience of many other researchers across a wide range of scientific disciplines".

Indeed this was the main conclusion of this study. We adopted your suggestion and updated the manuscript to emphasize this conclusion.

9. line 301 – The acknowledgments end with a stray "(" after Jed's name. Perhaps they got cut off?

Fixed typo.

10. Figure 2 – I am impressed with Figures 2-4 – they do a good job of conveying a lot of information clearly. I'd suggest replacing "horizontal labels" and "vertical labels" with "horizontal rows" and "vertical columns" for clarity in the caption.

Thank you for your comments. We updated the figure caption for clarity as you suggested.

11. Figure 6 – It would be helpful to include an "ideal scaling" line in this plot for comparison. You mention the slopes in the text, but including it on the graph itself can make things easier for the reader.

As suggested, we updated the figures and captions to denote ideal scaling.

12. Figure 6 – More numbers than a single "10" on the horizontal axis would also be useful.

As suggested, we updated the axis bounds.

13. Figures 5 and 6 – If I read these plots correctly (not completely assured due to the lack of x-axis labeling in Figure 6), it appears that the number of elements per processor used for weak scaling in Figure 5 (~250) corresponds to the far-right data points (most processors/fewest elements per processor) in the strong-scaling plot in figure 6. In both of the examples, this is where it appears that you start to see a degradation in your solver scaling, which might imply that you're being a bit too aggressive when you generated figure 5 since you seem to have stepped out of your ideal scaling regime. In other words, it might be the case that if you took a look at weak scaling with more elements/processor (500, perhaps), your MUMPS weak scaling might look better.

While using 250 elements per processor provided the fastest results for iterative methods applied to all but the largest model, your assessment that the scaling deteriorates at larger model sizes, especially for the linear solver is correct. Also, figure 5 had an error in color scale, which misrepresented the results. We fixed this error in this figure and used 500 elements/CPU for presenting weak scaling, as you suggested.

14. Figure 6 – it would be nice to have one more data point for your strong scaling plots, since it appears that your scaling is just beginning to tail off for MUMPS at the largest number of processors. I also realize that it may be a point too far...

The number of points used for scaling was chosen to be consistent with the tests that were performed for all solvers and plotted in Figures 2-4.

# Optimal numerical solvers for transient simulations of ice flow using the Ice Sheet System Model (ISSM versions 4.2.5 and 4.11)

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#### Abstract.

Identifying fast and robust numerical solvers is a critical issue that needs to be addressed in order to improve projections of polar ice sheets evolving in a changing climate. This work evaluates the impact of using sophisticated advanced numerical solvers for transient ice flow simulations using the NASA-JPLice-flow simulations conducted with the JPL/UCI Ice Sheet System Model (ISSM). We identify optimal numerical solvers by testing them on a commonly used ice flow benchmark test, the a broad suite of readily available solvers, ranging from direct sparse solvers to preconditioned iterative methods, on the commonly used Ice Sheet Model Intercomparison Project for Higher-Order ice sheet Models (ISMIP-HOM) Experiment Fbenchmark tests. Three types of analyses are considered: mass transport, horizontal stress balance, and vertical stress balance. A broad suite of solvers is tested, ranging from direct sparse solvers to preconditioned iterative methods, incompressibility. The results of the fastest solvers for each analysis type are ranked based on their scalability across mesh size for each basal sliding conditionsspecified in Experiment Fand basal boundary conditions. We find that the fastest iterative solvers are  $\sim 1.5 - 100 - 100$  times faster than the default direct 15 solver used in ISSM, with speed-ups improving rapidly with increased mesh resolution. We provide a set of recommendations for users in search of efficient solvers to use for transient ice flow ice-flow simulations, enabling higher-resolution meshes and faster turnaround time. The end result will be improved transient simulations for short-term, highly resolved forward projections (10-100) 10-100 year time scale) and also improved long-term paleo-reconstructions using higher-order representation of stresses in the ice. This analysis will also enable a new generation of comprehensive uncertainty quantification assessments of forward sea-level rise projections, which rely heavily on ensemble or sampling approaches that are inherently expensive.

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#### 1 Introduction

Fast and efficient numerical simulations of ice flow are critical to understanding the role and impact of polar ice sheets (Greenland Ice Sheet, GIS, and Antarctica Ice Sheet, AIS) on sea-level rise in a changing climate. As reported in the Intergovernmental Panel on Climate Change AR5 Synthesis report (Pachauri et al., 2014), "The ability to simulate ocean thermal expansion, glaciers and ice sheets, and thus sea level, has improved since the AR4, but significant challenges remain in representing the dynamics of the Greenland and Antarctic ice sheets." One of these challenges is the fact that Ice Sheet Models (ISMs) need to resolve ice flow at high spatial resolution (500 m to 1 km) in order to capture mass transport through outlet glaciers. This is especially the case for the GIS, which has a significant number of outlet glaciers in the 5-10-5-10 km width range (Rignot et al., 2011; Morlighem et al., 2014; Moon et al., 2015). This leads to transient ice-flow simulations with highly resolved meshes, which in turn reduces the time step prescribed by the Courant-Friedrichs-Lewy (CFL) condition that is necessary for providing convergence and avoiding to maintain convergence and avoid developing numerical instabilities. This combination of high spatial and temporal resolution implies that ISMs are faced with challenges involving both scalability and speed.

The traditional approach to address this combined challenge is to solve a simplified set of equations for stress balance, relying on approximations to the stress tensor, which drastically reduce the number of degrees of freedom (dofs). These approximations have been extensively documented in the literature —(Hindmarsh, 2004) and will not be described in detail here. However, we provide a brief summary of the characteristics of these models in order to relate the implications of our results in terms of solver efficiencies. The most comprehensive system of equations for modeling stress balance in ice flow is the full-Stokes model (Stokes, 1845), which captures each component of the stress tensor, and is hence the most complete physical description of stress equilibrium. It comprises four dofs (i.e. three velocity components and pressure) that are solved on a 3D mesh.

The Blatter/Pattyn formulation Higher-Order formulation (HO, Blatter, 1995; Pattyn, 2003) uses the fewest assumptions to the stress tensor. This model neglects horizontal gradients of vertical velocities by assuming that these terms are negligible compared to vertical gradients of horizontal velocities. In addition, bridging effects are neglected. The resulting model comprises two dofs for horizontal velocity (with vertical velocity being recovered through the incompressibility equation) velocities that are solved on a 3D mesh. Subsequently, the vertical velocity is recovered using the incompressibility equation. The next simplified formulation, the Shallow-Shelf or Shelfy-Stream Approximation (SSA) (SSA, MacAyeal, 1989), arises from further assuming that vertical shear is negligible. This results in a set of two equations for the horizontal components of velocity (with vertical velocity also being that are collapsed onto a 2D mesh, where the vertical velocity is recovered through the incompressibility equation), collapsed onto a 2D mesh. This is one of the most efficient models used for fast-flowing ice streams and ice shelves, where motion is dominated by sliding (MacAyeal, 1989; Rommelaere, 1996; MacAyeal et al., 1998).

Finally, for the interior of the ice sheet, ISMs rely on the Shallow Ice Approximation (SIA) (SIA, Hutter, 1983). In this model, horizontal gradients of vertical velocity are neglected compared to the vertical gradients of horizontal velocities and only the deviatoric stress component components of vertical shear are included in the deviatoric stress (i.e.  $\sigma'_{xz}$  and  $\sigma'_{yz}$  are included). This reduces the stress balance equations to a simple analytical formula relating the surface slope, ice thickness, and basal friction at the ice/bedrock interface. It is computationally very efficient and has been relied upon for long paleo-reconstructions of ice from the Last Glacial Maximum (LGM) to present day (Payne and Baldwin, 2000; Ritz et al., 1996; Huybrechts, 2004).

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This list of model approximations is not exhaustive and does not include hybrid approaches such as the L1L2 formulation that mixes both SSA and SIA approximations. For readers that are interested in this topic, a comprehensive classification can be found in Hindmarsh (2004). Increasingly though, simple approximations such as the SIA have proven incapable of replicating observed velocity changes, such as the rapid acceleration of the West Antarctic Ice Sheet (Rignot, 2008) in the past two decades, or seasonal variations in surface velocities exhibited by GIS outlet glaciers (Moon et al., 2015). In addition, they are unable to capture ice-flow dynamics at resolutions compatible with most of the GIS outlet glaciers and fast ice streams of the AIS. In this context, the need for leveraging faster solvers within ISMs using accurate ice-flow formulations is critical for improving short-term projections of sea-level rise.

Our approach is to use a suite of solvers available within the Portable Extensible Toolkit for Scientific Computations (PETSc) to accelerate The Ice Sheet System Model (ISSM) simulations involving higher-order ice-flow formulations. Our goal is to identify the fastest and most scalable solvers that are stable across different basal sliding conditions. The ISSM framework relies on a massively parallelized thermo-mechanical finite element ice sheet model that was developed to simulate the evolution of Greenland and Antarctica in a changing climate (Larour et al., 2012). ISSM employs the full range of ice flow ice-flow approximations described above, and is therefore a good candidate for this studystudying the efficiency of different solvers on ice-flow models. By default, ISSM relies on a direct numerical solver called the MUltifrontal Massively Parallel sparse direct Solver (MUMPS) (MUMPS, Amestoy et al., 2001, 2006), to solve the system of algebraic equations resulting from the finite element discretization of the transient evolution of an ice sheet (i.e. solving the discrete mass transport, momentum balance, and thermal equations). However, ISSM can also use numerical methods provided by the extensive suite of PETSc solvers, in particular the iterative kind, along with preconditioners that are well suited for ice-flow simulations.

Relying on Using a direct parallel solver provides a robust and stable numerical scheme. However, this approach tends to be slow and memory intensive for larger large problems, where the number of dofs approaches 100,000 and more. Indeed, as or more. As noted by Larour et al. (2012), the CPU time consumed by the default solver (i.e. MUMPS) accounts for 95% of the total solution time. In addition, there are significant problems with scalability associated with the direct solver approach

Larour et al. (2012), which have not been explored to date, that preclude ISSM from efficiently running large-scale, high-resolution projections for the GIS and AIS. In addition to MUMPS, ISSM can also use numerical methods provided by the extensive suite of PETSc solvers, including iterative methods combined with preconditioning matrices that are well suited for ice-flow simulations. In addition to MUMPS, ISSM can also use numerical methods provided by the Portable Extensible Toolkit for Scientific Computations (PETSc, Balay et al., 1997), including iterative methods combined with preconditioning matrices that are well suited for ice-flow simulations. In order to reduce the impact of the numerical solver as the bottleneck on the ISSM solution time, this study evaluates the performance of using state-of-the-art numerical solvers for transient ice flow simulations. While there is a significant amount of research associated with solving the saddle point problem resulting from the finite element discretization of the full-Stokes model, the literature regarding optimal numerical solvers for simpler formulations is to our knowledge limited to .

This study assesses the convergence, speed, and scalability of preconditioned iterative numerical solvers applied to transient ice flow simulations. However, it does not provide a roadmap for identifying optimal solvers for the broad array of ice flow formulations available ice-flow simulations. Our approach is to modelers. Our approach is to carry out characterize the impact of using a suite of readily available PETSc solvers to accelerate ISSM simulations involving higher-order ice-flow formulations. Our goal is to identify fast and scalable solvers that are stable across different basal sliding conditions. Here, we conduct a comprehensive assessment of numerical solvers on a calibrated test case, the well-know using calibrated test cases from the well-known Ice Sheet Model Intercomparison Project for Higher-Order ice sheet Models (ISMIP-HOM) benchmark experiments (Pattyn et al., 2008). These benchmark tests provide a good platform for testing numerical solvers, particularly for Using these well-studied benchmark tests allows us to evaluate the performance of numerical solvers for ice-flow simulations employing the Blatter-Pattyn formulation. Our focus is specifically on this HO formulation in a repeatable manner.

This work specifically focuses on this widely used formulation, as it currently represents the most computationally demanding model (short of full-Stokes) capable of capturing vertical as well as horizontal shear stresses necessary to model an entire basin (Pattyn, 1996). For cases where active grounding line dynamics are considered, a high-resolution The finite element discretization of the full-Stokes model would be required .Howeverleads to a well-studied saddle point problem, which represents an active area research in geophysics (e.g. Benzi et al. (2005); Elman et al. (2014)). While recent work (e.g. Isaac et al. (2015)) has shown promising results, stable iterative full-Stokes solvers are not readily available , and and, in general, are significantly disruptive to integrate in terms of their code base, which is the reason we will not be considering them here. The Blatter/Pattyn in this study.

The HO model represents the next, most complete formulation and represents a significant computational bottleneck compared to its 2D and 1D counterparts, which are significantly less demanding

because of the drastic reduction in the number of dofs required for vertically collapsed 2D meshes (SSA) or local 1D analytical formulations (SIA). In light of the limited number of studies focused on efficient solvers for approximate flow models (i.e. Brown et al. (2013); Cornford et al. (2013); Tezaur et al. (2015)), this work surveys a broad range of solvers for the HO ice-flow model. While our analysis uses ISSM, our results are relevant to other ice-flow models and frameworks that use PETSc solvers.

The manuscript is structured as follows. In section 2, we describe the ISMIP-HOM Experiment F model and our approach for testing numerical methods on this benchmark testexperiments that we consider and the approach adopted for testing different numerical methods. In section 3, we summarize efficient baseline solvers to use for transient simulations that naturally fit using the ISSM framework. In section 4, we discuss the timing results from testing a wide range of solvers, which in addition to enabling large-scale simulations yields significant speed-ups in solution time. We then conclude on the scope of this study and summarize our findings.

## 2 Model and Setup

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In an effort order to identify optimal numerical solvers for a broad class of transient ice flow simulations ice-flow simulations, we test a suit suite of PETSc solvers on a synthetic ice flow experiment synthetic ice-flow experiments with varying basal sliding conditions. We consider the effectiveness of competing solvers (in terms of speed) using the ISMIP-HOM tests, since these experiments represent a suite of accepted benchmark tests that are commonly used in the community to validate proposed higher-order (3D) approximate ice flow models, approximations of the stress balance equations. We first use Experiment F of the ISMIP-HOM tests represents an ideal simulation for benchmarking to evaluate competing numerical solvers since it involves a transient ice flow simulation and two tests to compare entails a transient ice-flow simulation with two test cases involving distinct basal sliding regimes. This transient simulation allows us to independently test the solvers on each analysis component of (mass transport, horizontal stress balance, and incompressibility) underlying a transient simulation in ISSM and evaluate the performance of competing solvers across the specified for models using different basal sliding conditions. In addition, Experiment F is representative of the type of physics solved for in many scenarios of ice sheets retreating and advancing onto downward or upward-sloping bedrocks (provided the bedrock slope is adjusted, which is seamlessly done). It is therefore wide-ranging in terms of applicability and happens to be a commonly accepted benchmark experiment that is used by many ISMs. However, since Experiment F specifies a constant viscosity for ice, we also consider ISMIP-HOM Experiment A as it includes a nonlinear rheology for ice. While this is only a static test, Experiment A allows us to evaluate the performance of solvers applied to the horizontal stress balance equations for simulations using a more physically realistic model of ice rheology.

Specifically, Experiment F Experiment F consists of simulating the flow of a 3D slab of ice (10 km square, 1 km thick) over an inclined bedrock bed (3 degrees) with a superposed Gaussian-shaped bump (100 m in height) until the free surface geometry and velocities reach steady state. Here, we run our transient simulation for 1500 years, using 3-year time steps, in order to allow the free surface to relax and reach a steady-state steady-state configuration. The prescribed material law is a linear viscous rheology (resulting that results in a constant effective viscosity ) for ice. In order to test different friction parameterizations, Experiment F explores two test cases of boundary conditions at the bedrock/ice interface: 1) no-slip (frozen bed) and 2) viscous slip (sliding bed). For both scenariossingle-point constraints on the velocity and thickness are applied to the boundaries in order to constrain the system, we apply Dirichlet boundary conditions for the velocities along the boundary and set the values to zero. This is slightly different from the period using periodic boundary conditions suggested by the ISMIP-HOM benchmark test, but has more relevance to the boundary conditions typically tests; however, Dirichlet boundary conditions are more relevant to boundary conditions generally used by modelers. Fig. 1 displays the surface velocity and surface elevation results at the end of the transient simulation using ISSM. These results are in line consistent with typical steady state profiles for Experiment F, with slight differences near the boundaries affected by using different boundary conditions.

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In an effort to independently test the numerical methods on the underlying solution components of an ISSM transient simulation, a suite of preconditioners and iterative methods is independently tested. Experiment A simulates the flow of a 3D slab of ice (80 km square, 1 km thick) over an inclined bed (0.5 degrees) with sinusoidal bumps (500 m amplitude). This experiment assumes that the ice is frozen to the bed (i.e. no-slip boundary condition). While this test is prognostic in nature and does not consider the time-evolution of the ice configuration, it does include a nonlinear viscosity model for ice, which is more realistic than the constant viscosity specified in Experiment F. Similarly to Experiment F, we prescribe Dirichlet boundary conditions for the velocities along the boundary and set the value to zero.

Our approach for identifying efficient numerical methods for each analysis component of the transient simulation in ISSM is to independently test combinations of preconditioning matrices with iterative methods on the system of equations resulting from the finite element discretization of the stress balance and mass transport equations. Because Since we rely on the Blatter/Pattyn HO formulation, the stress balance is split into a only solves the horizontal stress balance (solving for the horizontal components of velocity) and and requires an additional step to recover vertical velocitiesusing solve for the vertical velocities. Here, we use the incompressibility equation —and an  $L_2$  projection to solve for the vertical velocities. We call these steps the horizontal velocity solution and vertical velocity incompressibility solution, respectively. In addition, running a transient simulation implies a mass transport module, which combined with the velocity analyses imply three

solution types for requires three systems of equations to be solved at each time step. For each solution type,

For each system of equations, we test a wide range of solvers is tested. This includes direct solvers as well as preconditioned iterative solvers including the default solver (MUMPS) and preconditioned iterative methods provided by PETSc. When referring to the solvers available through the PETSc interface, we rely on the abbreviations used in the PETSc libraries by labeling a preconditioning matrix as a PC and an iterative method as a KSP (Krylov subspace method). Here the a preconditioning matrix improves the spectral properties of the problem (i.e. the condition number) without altering the solution provided by the iterative method. Since the Jacobian of the system of equations resulting from the finite element discretization of the horizontal velocity solution stress balance is symmetric positive definite a wide range of iterative solvers and preconditioners are applicable and potentially efficient. For a complete review of potential solvers we point to Benzi et al. (2005) and Saad (2003). In the subsequent benchmark simulations, 10 PC matrices, and 20 KSP iterative methods are tested in unique solver combinations. Additionally, the effect of not applying a preconditioning matrix to the iterative method is tested for each KSP by using represented by PC=None in PETSenone. The solvers tested for all analysis types are indicated by the permutations of the KSP and PC methods listed in the headings of 4. In an attempt to use the PETSc solvers in ISSM with minimal invasiveness, we restrict the inclusion of KSPs and PCs from the PETSc suite by only testing methods that naturally fit the ISSM framework and rely on default settings for the specific PETSc components (i.e. without the need for customization or specialization of the solver routine). Anticipating that modelers may not tune the individual components in PETSc, we test each method using default values to evaluate baseline performance provided by each method natively.

The slab of ice in Experiment F is modeled using four levels of mesh refinement. The smallest, most coarse resolution coarsest-resolution model consists of 2000 elements resulting from a  $10 \times 10 \times 10$  (x,y,z) grid of triangular prismatic 3D elements. Three larger models are produced by refining each direction of the coarse smallest model by a factor of 2, leading to 16,000, 128,000, and 1,024,000 element models. Each model size is tested using four CPU cases: 250, 500, 1000, and 2000 elements per CPU. Only the fastest timing results for simulations where the solution passes three ISSM convergence tests (i.e. mechanical stress balance and convergence of the solution in both a relative and absolute sense) at each time step using default tolerances are included in the ranking results. All of the simulations are these simulations were performed on the NASA Advanced Supercomputing Pleiades cluster (Westmere nodes: 12.2 six-core Intel Xeon X5670 CPUs processors per node, 24 GB per node) using ISSM version 4.2.5 and PETSc version 3.3.

# 3 Results

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For each of the three ISSM solution types (horizontal velocity, vertical velocity, and mass transport) we run simulations with four mesh sizes (2000, 16,000, 128,000, and To study the impact of using a nonlinear viscosity model for ice on solver speed and convergence, we follow the same methodology applied to Experiment F (i.e. same solvers, discretization strategy, and CPU cases) and evaluate the performance of solvers applied to the stress balance equations for Experiment A. However, we omit testing the largest model size (i.e. 1,024,000 elements), four CPU cases (250, 500, 1000, and 2000 Elements per CPU), 10 PC matrices, and 20 KSP iterative methods due to the intense computational resources necessary for this model size and the limited information gained by this prognostic test relative to the more comprehensive transient model. Simulations of Experiment A were performed more recently on the Pleiades cluster using upgraded Broadwell nodes (2 fourteen-core Intel Xeon E5-2680v4 processors per node with 128 GB per node) with ISSM version 4.11 and PETSc version 3.7. Updates to the ISSM code from version 4.2.5 to version 4.11 have added new capabilities that are not used in this study. The solution methods and algorithms between these versions are the same, and the results from this study apply to all intermediate versions that users may be working with.

#### 3 Results

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Since our primary interest is identifying fast, stable solvers for transient ice-flow simulations, we first present the results from Experiment F. Our timing results, measured in seconds, consists of the CPU time associated with assembling the stiffness matrix, load vector, solving the system of equations, and updating the input from the solution. Only the fastest results for each model size, measured by CPU time (seconds), for solving the horizontal velocity analysis (fastest 10%), the vertical velocity incompressibility analysis (fastest 5%), and the mass transport analysis (fastest 5%) are shown in Figs. 2—4, respectively. These thresholds (i.e. 10%, 5%, and 5%) are chosen so as to exhibit clear trends in identifying the fastest and most robust solvers. Here, we associate the robustness of a solver (PC/KSP combination) in terms of efficiently solving a given analysis for across the wide range of tested model sizes and distinct basal sliding both basal boundary conditions. This classification is different from a solver that is the solvers that are optimal (i.e. fastest) for a specific scenario case, but it allows users to identify methods modelers to identify solvers that are fast across the largest set of conditions, be it mesh size, number of available CPUs, or basal sliding conditions. Users regime. Modelers interested in optimal performance for a specific simulation should consult Figs. 2-4 for each analysis component and use a solver corresponding to a color-filled symbol (i.e. fastest 1% result) closest to their model size, where the number of recommended CPUs is specified by the color of the symbol.

We For Experiment F, we highlight the most robust solvers (i.e. the fastest PC/KSP combinations across all model sizes and both basal sliding conditions) in Figs. 2—4 using red boxes. Thus, a red box highlights solver combinations a solver (PC/KSP combination) where all four symbols (i.e. all

tested mesh sizes) are present among the fastest methods for both basal sliding boundary conditions. Whereas the color-filled symbols only identify identify the solvers that are among the fastest timing results (top 1%) for the mesh size specified by the symbol type that mesh size and basal boundary condition. The highlighted solvers from Figs. 2-4 may be used as ISSM solver defaults for each analysis type underlying the transient solution of the transient simulation (i.e. horizontal velocity, vertical velocity incompressibility, and mass transport). For the horizontal velocity solution, the results in Fig. 2 show six highlighted solvers are robust (i.e. four symbols displayed for both sliding eases). Furthermore, these basal boundary conditions). These results indicate that using a block Jacobi preconditioner is well suited for this analysis type across both sliding cases for both sliding and frozen bed scenarios. For the vertical velocity incompressibility analysis, the highlighted solvers in Fig. 3 indicate that using a variant of the Jacobi preconditioner (block Jacobi, Jacobi or point block Jacobi), in conjunction with the corresponding KSPs yields the most robust results. For the mass transport analysis, the situation is more nuanced in terms of preconditioners, but both the bcgs and bcgsl KSP solvers tend to be robust across several preconditioners. Surprisingly, not using a preconditioner for the mass transport analysis seems to yield very fast and robust results when used in combination with the lsqr and bcgs solvers, which was not expected.

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FigFigs. 5 and Fig. 6 plot the weak and strong scalability associated with solving the ISMIP-HOM Experiment F test-Experiment F using the default ISSM solver (MUMPS) and iterative solvers selected from the highlighted solvers in Figs. 2-4 for each analysis component of type underlying the transient simulation. Here Specifically, we compare the default solver results to a combined strategy that uses a point block Jacobi (i.e. PC=pbjacobi) preconditioned preconditioner with a biconjugate gradient stabilized (i.e. KSP=begsl) iterative method to solve the mass transport analysis, a block Jacobi (i.e. (PC=bjacobi) preconditioned minimum residual (i.e. pbjacobi, KSP=minres)bcgsl), a block Jacobi preconditioner with a minimum residual iterative method to solve the horizontal velocity analysis (PC=bjacobi, KSP=minres), and a point block Jacobi (i.e. PC=pbjacobi) preconditioned conjugate gradient on preconditioner with a conjugate gradient iterative method applied to the normal equations (i.e. to solve the incompressibility analysis (PC=pbjacobi, KSP=cgne) iterative method to solve the vertical velocity analysis. One issue that arose while carrying out the weak scalability analysis was that simulations using MUMPS to solve the largest model (i.e. 1,024,000 elements) experienced memory and cluster issues for both sliding eases and frozen bed scenarios (e.g. computational nodes restarting and general memory issues). We-For these tests, we estimate the total time required to solve both sliding cases using MUMPS on the largest model with the MUMPS solver by linearly extrapolating the total time from the number of iterations completed during a two-hour and eight-hour run. These estimated timing results are displayed as the by diamond symbols in Fig. 5 for the direct solver only.

In considering the magnitude of the slopes representing the weak and strong scalability, we recall that our timing results include routines outside of the solver procedure (i.e. assembling the stiffness

matrix, load vector, and updating the input from the solution) that are not necessarily scalable. However, the relative scalability (i.e. differences in slope) between the preconditioned iterative methods and the direct solver illustrates the differences in performance between these approaches. Optimal weak scalability would imply a for a solver implies a horizontal slope in Fig. 5 and the ability to solve increasingly refined models with a fixed ratio of elements per CPU in constant time. Here, the slope slopes representing the weak scalability of the preconditioned iterative solver (i. e. 0.468) in Fig. 5 is much smaller than the slope of for the frozen bed and sliding bed configurations are 0.441 and 0.495, respectively. Whereas the slopes for the direct solver (i. e. 1.200), are much larger at 1.124 and 1.165 for the frozen and sliding bed configurations, respectively. For the largest model (i.e. 1,024,000 elements) the iterative solver is more than two orders of magnitude faster than the ISSM default solver:  $\sim$ 57 hours (estimated) compared to  $\sim$ 15 minutes. As Fig. 5 indicates, using a preconditioned iterative method over direct solvers the direct solver is increasingly beneficial for larger model sizes. For very small models (i.e. 2000 elements), using MUMPS is marginally slower  $(\sim 1.5 \text{ times})$  than the presented iterative methods (i. e.  $\sim 1.5 \text{ times faster}$ ). Optimal strong scalability would imply implies a slope equal to -1 in Fig. 6 and the ability to solve a model with a fixed number of elements faster by using more CPUs. The slope slopes in Fig. 6 for the direct solver (representing the strong scalability of the direct solver for the frozen and sliding bed configurations are -0.332 and -0.399, respectively. In comparison, the slopes for the combined iterative solvers applied to the frozen and sliding bed configurations are -0.897 and -0.911, respectively, clearly favoring these solvers over the direct solver.

To show the impact of nonlinear viscosity on the efficiency of the presented solvers, we plot the timing results for solving the stress balance equations in Experiment A (Fig. 7). Fig. 7 plots the fastest (top 15%) timing results for each mesh size, using the same symbols as the previous plots for Experiment F, where color-filled symbols represent the overall fastest results (i.e. -0.365) compared to the combined iterative solvers (top 1%) for each model size. In comparing our results to using the default ISSM solver (MUMPS), we plot the strong and weak scalability (Fig. 8) for the direct solver and one of the fastest solvers identified from Fig. 7 (KSP=cg, PC=bjacobi). Similar to the results for Experiment F, the slopes of the weak scalability (Fig. 8a) for the preconditioned iterative method (0.205) is also much smaller (i.e. -0.904) clearly favors the latter, closer to optimal scalability) than the direct solver (0.883). In comparing the strong scalability of these solvers (Fig. 8b), the slope of the preconditioned iterative method (-0.737) also indicates better performance than the slope of the direct solver (-0.270).

# 4 Discussion

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The results clearly show that Solving the horizontal velocity solution analysis dominates the CPU time needed to solve a transient simulation. This is not surprising given that the stiffness matrix

resulting from the discretization of the horizontal stress balance equations has the highest condition number of all analyses, and hence is the most difficult to efficiently preconditionsince this analysis involves more dofs and has a much higher condition number than the mass transport and incompressibility analyses. Our results, however, show that this bottleneck can be significantly reduced for moderate-sized models (i.e. 16,000 to 128,000 elements) by using any of the highlighted methods solvers, which leads to significant speed-up speed-ups relative to the default solver (i.e. ~7.5-37.26-37 times faster).

As Fig. 5 shows, using a direct solver such as MUMPS is not recommended for transient simulations of models using more than 128,000 elements. This is both due to the significant speed-ups (more than 10 times) achieved by applying iterative solvers to transient simulations of using iterative solvers for transient simulations involving large models (more than 20,000 elements) and to the inherent memory restrictions associated with using the direct solver that prevent massive transient simulations (more than 1,000,000 elements).

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Most of the limitations associated with using the default solver on large models arise from the LU Factorization phase in the MUMPS solver, which is not yet parallelized. This could be remedied by switching on the out-of-core computation capability for this decomposition, but this has not been successfully tested yet and would potentially shift the problem of memory limitations to disk space and read/write speeds (the size of the matrices being significant). Furthermore, Fig. 5 indicates that the highlighted solvers are not only capable of handling the largest model (1,024,000 elements), but the solution time is nearly equivalent to using the default MUMPS solver on a significantly smaller model size (i.e. ~20,000 elements).

In evaluating the effect of using a nonlinear viscosity model for ice on solver performance, we see that many of the methods which efficiently solve the horizontal velocity analysis for Experiment A (Fig. 7) are consistent with the solvers highlighted for Experiment F (Fig. 2), which includes a much simpler constant viscosity for ice. Specifically, we see that the block Jacobi preconditioner (PC=bjacobi) is effective across a number of iterative methods for both benchmark experiments. While this comparison only extends up to model sizes of 128,000 elements, we see from the plot of weak scalability (Fig. 8a) that using the iterative solver results in speed-ups ranging from ~1.2–19 times faster than using the default solver for model sizes increasing from 2,000–128,000 elements.

In practice, users may experience numerical convergence issues issues with numerical convergence when applying some of the iterative methods presented in Figs. 2—4 for their particular application. In these instances using the ISSM default solver (MUMPS) provides a stable solution strategy. Furthermore, since solving the horizontal velocity analysis is the most CPU-time intensive stage of the transient simulation process, using a direct solver for the other analysis types and relying on Fig. 2 to select an optimal solver for the horizontal velocity analysis may provide the best balance between stability and speed.

While the relative rankings of the numerical solvers, presented in Figs. 2-4, tested solvers presented in this work are specific to the ISMIP-HOM Experiment F test, testing the solvers with Experiments, applying these methods to simulations using realistic model parameterizations (e.g. nonlinear viscosity, anisotropic mesh, realistic data-driven boundary conditions, anisotropic meshes, and complex geometries) also results in significant speed-ups compared to the default solver, though these computations are not shown here. For those interested in further refining the findings of our analysis, we suggest testing. We acknowledge that in relation to using synthetic test cases, real-world model parameterizations may affect the convergence and relative performance of the iterative solvers tested in this work. However, since any of the highlighted solvers over a broad range of configurations of the ISMIP-HOM Experiment F benchmark test including varying the slope of the bed angle, the bed stickiness, the bedrock bump height, and using non-linear creep type rheologies for the ice viscosity. are significantly more efficient than using a linear solver, our results provide a useful starting point for modelers looking for efficient methods to use for specific ice-flow simulations.

We recommend that future refinement of these results include customization of the PETSc components, which can lead to significant performance gains over default values, and include more realistic geometries that include varying degrees of anisotropy. Finally, it should be noted that the presented optimal solvers do not require a supercomputer and may be used with fewer CPUs than the number indicated by the symbol color in Figs. 2—4. Indeed, the highlighted iterative methods may provide speed-ups (compared to using MUMPS) larger than we presented in Fig. 5 indicates when using computers with limited memory.

## 5 Conclusions

The results presented herein offer guidance for selecting fast and robust numerical solvers for transient ice-flow simulations across a broad range of model sizes and basal sliding boundary conditions. Here, the highlighted solvers offer significant speed-ups (~1.5-100-100 times faster) relative to the default ISSM-solver (MUMPS). Furthermore, the highlighted solvers enable large-scale, high-resolution transient simulations that were previously too large to run with the default solver in ISSM. While users of ISSM-These combined benefits are consistent with results across a broad range of computational disciplines, which also show that iterative solvers are significantly more efficient than direct solvers for solving sparse linear systems as the number of dofs becomes large. While modelers may prefer to use the default-a direct solver as a stable strategy, the performance gains afforded by significant performance gains attained using the preconditioned iterative methods identified highlighted in this study provide a compelling case worth considering consider. Here, taking the time to find an efficient solver is strongly recommended for computationally demanding simulations involving high-resolution meshes as well as uncertainty quantification studies or parameter studies entailing repeated simulations.

# 6 Code Availability

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The results from this work are reproducible using ISSM (versions 4.2.5–4.11) with the corresponding PETSc solvers used for each simulation. Hereanalysis type. Here, the current version of ISSM is available for download at . The model for simulating https://issm.jpl.nasa.gov, and previous versions are available from the svn repository. The models for simulating these ISMIP-HOM Experiment F is Experiments are documented on the website and is also included in the test directory of the download.

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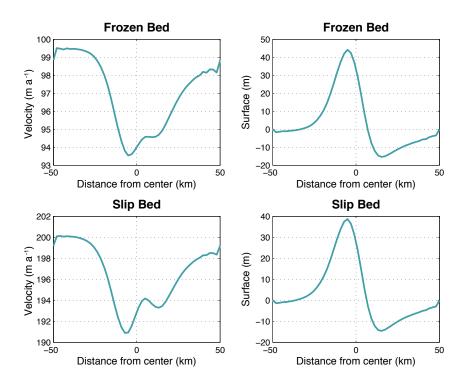
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**Figure 1.** ISSM results for the ISMIP-HOM benchmark Experiment F transient simulation after 1500 years. Surface velocity (m  $a^{-1}$ ) and steady state surface elevation profile (m) along the central flowline are shown for the frozen and sliding bed cases.

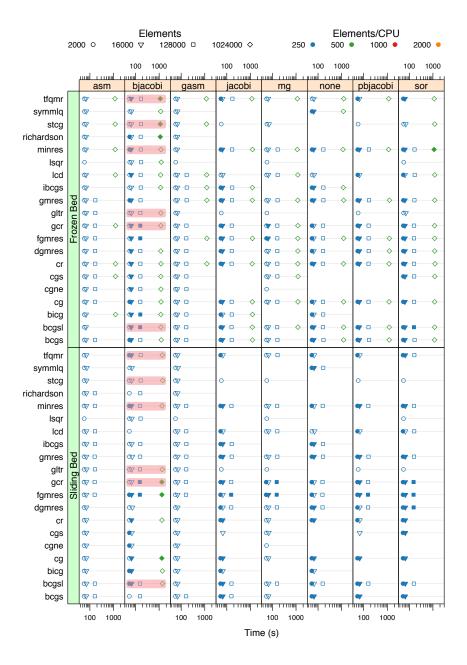
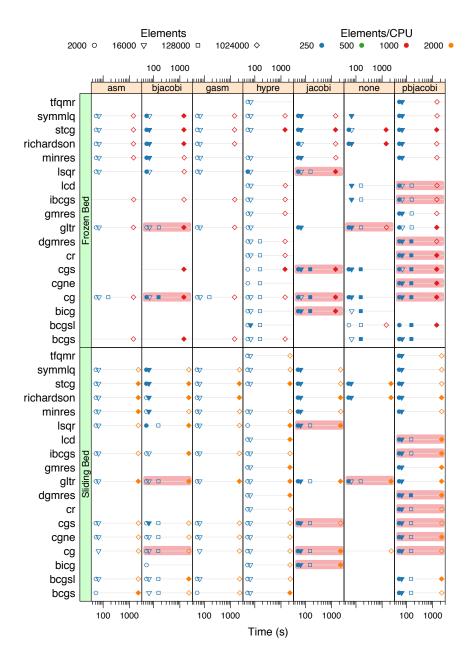
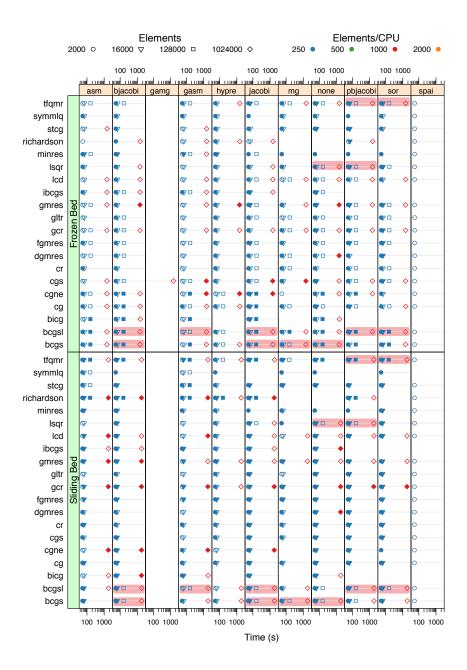


Figure 2. Horizontal velocity analysis: timing results for the fastest solvers (top 10%) tested on ISMIP-HOM Experiment F. The top (1%) timing results are distinguished using color-filled symbols. Both basal sliding boundary conditions for Experiment F are shown: frozen bed (upper half) and sliding bed (lower half). The Each solver is represented by the combination of a preconditioner (horizontal labelsrows) and a Krylov subspace method (vertical labelscolumns) using PETSc abbreviations. Simulations are performed using four mesh sizes (denoted by the symbols in the legend) and four CPU cases (denoted by the colors in the legend). Only the fastest CPU case (i.e. color) is displayed. Red boxes highlight solver combinations that rank among the fastest methods for all model sizes and both bed conditions (i.e. four symbols in the top and bottom frame).



**Figure 3.** Vertical velocity—Incompressibility analysis: timing results for the fastest solvers (top 5%) tested on ISMIP-HOM Experiment F. The top (1%) timing results are distinguished using color-filled symbols. Red boxes highlight solver combinations that rank among the fastest methods for all model sizes and both bed conditions (i.e. four symbols in the top and bottom frame). See Fig. 2 for more details.



**Figure 4.** Mass transport analysis: timing results for the fastest solvers (top 5%) tested on ISMIP-HOM Experiment F. The top (1%) timing results are distinguished using color-filled symbols. Red boxes highlight solver combinations that rank among the fastest methods for all model sizes and both bed conditions (i.e. four symbols in the top and bottom frame). See Fig. 2 for more details.

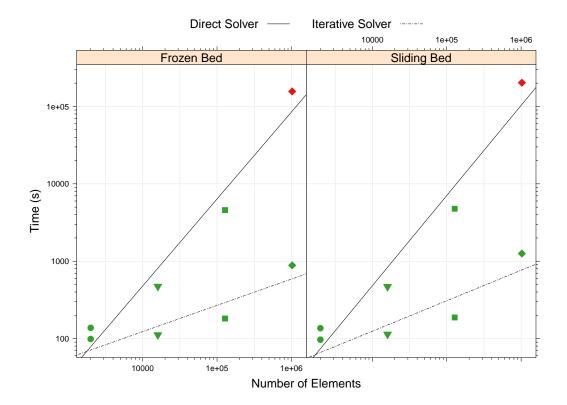
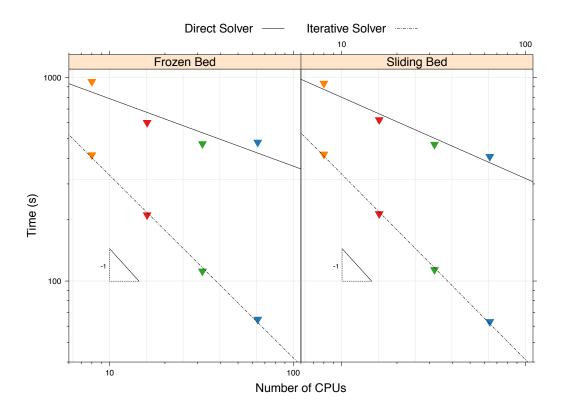
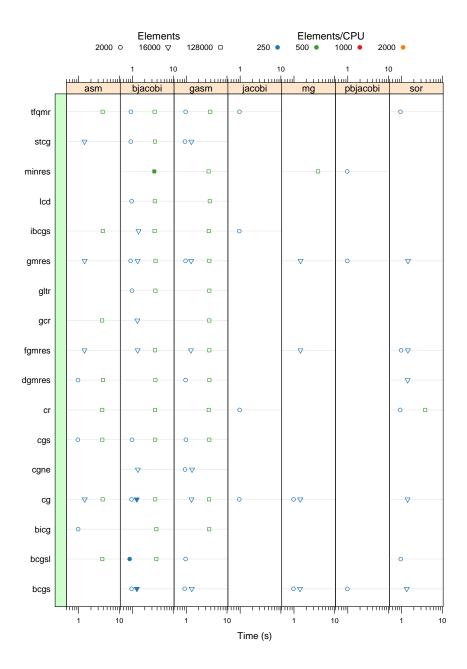


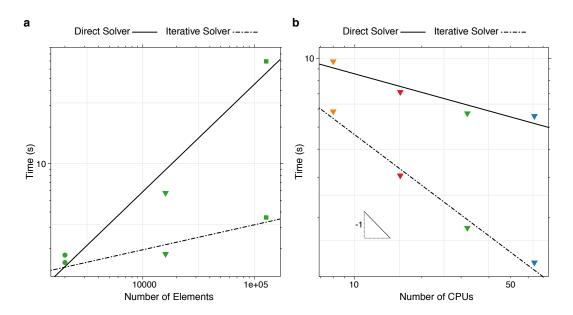
Figure 5. Weak scalability of for simulating ISMIP-HOM Experiment F using the default ISSM solver (MUMPS) compared with a combination of robust solvers (selected from the highlighted solvers in Figs. 2—4) for the components each analysis component of the transient ISSM-simulation ISMIP-HOM Experiment F. The simulations are carried out using a constant ratio of 250 elements per CPU and show the impact of increasing mesh size on simulation time (s). The This combination of iterative solvers is chosen according to the highlighted results presented in Fig. 4, 2 and 3. It consists of :1) a point block Jacobi (pbjacobi) preconditioned biconjugate gradient stabilized (bcgsl) iterative method for the mass transport analysis; 2), a block Jacobi (bjacobi) preconditioned minimum residual (minres) iterative method for the horizontal velocity analysis, and 3) a point block Jacobi (pbjacobi) preconditioned conjugate gradient on the normal equations (cgne) for the vertical velocity incompressibility analysis. These simulations are conducted using a constant ratio of 500 elements per CPU (except for the largest model with the direct solver) and show the impact of increasing mesh size on simulation time (seconds). Ideal weak scaling is consistent with a horizontal slope. Timing results include the CPU time associated with assembling the stiffness matrix, load vector, solving the system of equations, and updating the input from the solution.



**Figure 6.** Strong scalability of the default ISSM solver (MUMPS) compared with a combination of robust solvers (selected from the highlighted solvers in Figs. 2—4) for the components of the transient ISSM simulation of ISMIP-HOM Experiment F. See Fig. 5 for the specific solvers used specified for each analysis component. Strong scalability indicates represents the impact of increasing the number of CPUs while keeping the mesh size constant (16,000 elements). Color-filled symbols identify Ideal strong scalability is consistent with a slope equal to -1. Timing results include the number CPU time associated with assembling the stiffness matrix, load vector, solving the system of CPUs used to achieve equations, and updating the fastest result for each basal sliding caseinput from the solution.



**Figure 7.** Horizontal velocity analysis: timing results for the fastest solvers (top 15%) tested on ISMIP-HOM Experiment A. The top (1%) timing results are distinguished using color-filled symbols. See Fig. 2 for more details.



**Figure 8.** Scalability of the default ISSM solver (MUMPS) compared with a preconditioned iterative method (PC=bjacobi, KSP=cg) for ISMIP-HOM Experiment A. **a.** Weak scalability of solvers using a constant ratio of 500 elements per CPU; ideal weak scalability is represented by a horizontal slope. **b.** Strong scalability of solvers for a 16,000 element model; ideal strong scalability is represented by a slope equal to -1. Timing results include the CPU time associated with assembling the stiffness matrix, load vector, solving the system of equations, and updating the input from the solution.