

# An intermediate-scale model for thermal hydrology in low-relief permafrost-affected landscapes

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## Abstract

Integrated surface/subsurface models for simulating the thermal hydrology of permafrost-affected regions in a warming climate have recently become available, but computational demands of those new process-rich simulation tools have thus far limited their applications to one-dimensional or small two-dimensional simulations. We present a mixed-dimensional model structure for efficiently simulating surface/subsurface thermal hydrology in low-relief permafrost regions at watershed scales. The approach ~~simplifies the~~replaces ~~a~~ full three-dimensional system ~~to~~with a two-dimensional overland thermal hydrology system ~~with~~and a family of one-dimensional vertical columns, where each column represents a fully coupled surface/subsurface thermal hydrology system without lateral flow. The ~~overland thermal hydrology~~ system is then operator split, ~~incrementally updating lateral surface fluxes with no sources to redistribute mass and energy horizontally, followed and update including sources and sinks to couple to the columns~~sequentially

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updating the overland flow system without sources and the one-dimensional columns without lateral flows. We show that the approach is highly scalable, supports subcyclng of different processes, and compares well with the corresponding fully three-dimensional representation at significantly less computational cost. ~~These advances enable state-of-the-art~~ Those advances enable recently developed representations of freezing soil physics to be coupled with thermal overland flow and surface energy balance at scales of 100s of meters. Although developed and demonstrated for permafrost thermal hydrology, the mixed-dimensional model structure is applicable to integrated surface/subsurface thermal hydrology in general.

*Keywords:* ~~Mixed-dimensional model~~ Multiscale models, Permafrost thermal hydrology, Integrated surface/subsurface flow modeling, Arctic

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## 1. Introduction

Approximately 23% of the land surface in the Northern Hemisphere is underlain by continuous permafrost (91-100% frozen area), and another 17% is occupied by discontinuous permafrost (50-90% frozen area) [1, 2]. A  
5 massive amount of organic carbon is stored in those regions [3, 4], which are warming at a rate considerably faster than the rest of the planet [5, 6, 7]. As the soils in that region warm, they have the potential to transform from a net sink to a net source of carbon to the atmosphere, which could increase the concentration of carbon in the atmosphere and in turn lead  
10 to further increase in the temperature (e.g. [8]). Further, thawing and the resulting degradation of permafrost can cause significant changes in the surface and subsurface thermal hydrology and eventually can substantially alter the Arctic tundra ecosystems [9, 10, 11, 12, 13].

Those potential impacts and feedbacks in the terrestrial Arctic have motivated the development of increasingly sophisticated tools for simulating permafrost dynamics in a warming climate. Such simulations can help to better understand the consequences of soil warming and responses of tundra ecosystems to warming trends, and further expose the effects of permafrost degradation on surface and subsurface thermal hydrology. However, simulating permafrost dynamics in a complex and coupled surface/subsurface thermal hydrological environment is a challenging task, especially at larger spatiotemporal scales [14]. A comprehensive review of the modeling efforts of the surface and subsurface can be found in [15]. Early research efforts focused on one-dimensional simulations for fundamental understanding of infiltration in cold climates; see, for example, [16, 17, 18]. Similar one-dimensional approximations have been adopted as coarse-scale models in global land surface models [19, 20, 21, 13]. Two-dimensional simulations with simplified physics (i.e. saturated conditions, subsurface only) have been used for understanding evolution of field-scale groundwater systems [22, 23], but do not represent key unsaturated zone processes that are needed to understand active layer dynamics and decomposition of soil organic matter. It is worth pointing out that mathematical models with limited complexity, reduced dimensionality, and relatively coarse spatial resolutions provide some insight into permafrost dynamics but fail to represent important processes such as cryosuction, lateral surface and subsurface flows, and advective heat transfers. Simulations with more mechanistic representations of surface and vadose zone process in three-dimensions are essential to accurately capture the potential impacts of permafrost thawing on the surface and subsurface thermal hydrology and the resulting effects on the carbon cycle.

Two- and three-dimensional models with explicit physics-based repre-

presentations of ice/liquid/gas partitioning in the vadose zone ~~[24]~~ have only  
 recently started to appear. ~~Painter 2011~~ ~~[24]~~. ~~Painter~~ [25] developed the  
 three-phase, two-component model MarsFlo which has been used in Mars  
 [26] and Earth permafrost studies [27]. Karra et al. ~~2014~~ [28] simplified that  
 45 subsurface freezing-soil thermal hydrology representation by ignoring gas  
 advection and implemented that Richards-like approximation in the highly  
 parallel PFLOTRAN [29] code. Kumar et al. ~~2016~~ [30] used that implemen-  
 tation in three-dimensional microtopography-resolving thermal hydrology  
 simulations of polygonal tundra. Those computer codes are all subsurface-  
 50 only models; that is, they do not represent surface flows and surface energy  
 balance. Painter et al. ~~2016~~ [31] recently introduced the Arctic Terrestrial  
 Simulator, which uses a sophisticated multiphysics management framework  
~~[?]~~ [32] to couple the three-dimensional subsurface representation of [28]  
 with a two-dimensional non-isothermal surface flow model, surface energy  
 55 balance with and without snow, and a simple snow distribution model.

Despite the significant progress in developing integrated surface/subsurface  
 permafrost thermal hydrology models, significant challenges remain in mov-  
 ing to climate-relevant spatiotemporal scales. One of the challenges is that  
 the integrated system is numerically stiff because of the highly dynamic sur-  
 60 face system [31] and the ice-liquid phase transition [33], which often results  
 in relatively small time steps to achieve convergence. Small time steps are  
 not problematic in one-dimensional simulations because a well-designed sim-  
 ulation tool will recover the time step quickly after a convergence failure.  
 However, a small time step becomes problematic in large three-dimensional  
 65 runs because it becomes increasingly likely that, at any given time, at least  
 one computational cell will be experiencing a phase change and thus a small  
 time step. The other major challenge is tracking thaw-induced subsidence.

Traditional hydrological simulators are mainly designed to conduct three-dimensional simulations, however, deformations in a three-dimensional simulation are not easy to track due to mesh tangling and can be computationally expensive; further, poor mesh quality may raise questions about the accuracy of the results.

To address the aforementioned challenges, we present a mixed-dimensional modeling strategy for process-rich simulations of integrated surface and subsurface thermal hydrology in tundra systems with low topographic gradients. The approach is intended for spatial scales intermediate between microtopography-resolving fine-scale simulations and the scale of an Earth system model grid cell. We demonstrate with simulations of polygonal tundra, large and carbon-rich regions of northern Siberia, Alaska, and Canada where soil cracking has led to the formation of subsurface ice wedges that honeycomb the subsurface and ~~tessellate~~tessellate the land surface into polygonal patterns. Rather than solve a fully three-dimensional subsurface system tightly coupled to surface processes as in [31], we take advantage of physical insights gained from fine-scale simulations and approximate the integrated surface/subsurface dynamics with mutually independent 1-D columns, each associated with an ice wedge polygon. The columns are then sequentially coupled to a surface thermal flow system, solving the surface problem in an operator-split manner. This mixed-dimensional modeling approach is motivated by fine-scale simulations at the ice-wedge polygon scale that showed that differences in the thermal conditions among centers, rims and troughs of ice-wedge polygons are largely equilibrated by lateral heat transport during summer such that the system behaves similarly to a one-dimensional system on seasonal time scales. Mixed-dimensional model structures have been used previously in simulations of variably saturated

95 flow at watershed scales, in particular to couple multiple 1-D unsaturated  
(vadose) zone representations to a two- or three-dimensional saturated zone;  
for example see [34, 35, 36]. Here we apply the mixed-dimensional model  
structure to an integrated surface/subsurface flow system including surface  
and subsurface thermal processes and evaluate the accuracy and computa-  
100 tional advantages of the approximation.

The paper is organized as follows: Section 2 highlights the Advanced/Arctic  
Terrestrial Simulator (ATS) and the Arcos multiphysics management frame-  
work, within which we implemented our approach. Section 3 presents some  
fine-scale simulation results and analysis that motivated the approach. In  
105 Section 4 we introduce our mixed-dimensional modeling approach, loosely  
coupled scheme and the ATS refactoring strategy. To illustrate the perfor-  
mance and efficiency of our modeling strategy, in Section 5 we compare our  
numerical results with the three-dimensional simulations based on strong  
coupling, and present speedup and scalability of the new technique. Con-  
110 cluding remarks and future research are offered in Section 6.

## 2. The ATS Software

We implemented our mixed-dimensional modeling strategy in open-source  
parallel software known as Amanzi-ATS [37] (or simply ATS). Amanzi-  
ATS is the result of extending the flow and reactive transport simulator  
115 Amanzi [38] by adding an advanced multiphysics management system known  
as Arcos [32]. Arcos is key to managing the complex spatial structures  
used here. It was originally built to manage couplings among process models  
(denoted process kernels and abbreviated as PKs), which may be selected at  
runtime. A PK encapsulates the mathematical representation of a particu-

lar physical process or coupled set of processes; PKs are coupled together through Multiprocess Coordinators MPCs. An MPC is regarded as a PK by MPCs at higher levels in the tree, thus allowing complex hierarchical model structures to be built dynamically at runtime. In this work, we used Arcos to coordinate not only process kernels but also subdomains of the larger spatial domain.

Amanzi, and by extension ATS, uses the Trilinos [39] framework for parallel infrastructure. An unstructured mesh framework [40] is included for interacting with the computational mesh. General polyhedral meshes are supported. Discretization accuracy is maintained on the potentially distorted grids through the use of the mimetic finite difference (MFD) method [41, 42]. The backward Euler method is used for time stepping with a Non-linear Krylov Acceleration (NKA) method [43, 44] to solve the resulting discretized residual equations.

The initialism ATS may refer to either the Advanced Terrestrial Simulator, which is the general capability, or the Arctic Terrestrial Simulator, which is one particular configuration [31], depending on context. The Arctic Terrestrial Simulator configuration solves strongly coupled surface energy balance, and surface and subsurface thermal hydrology with freeze/thaw dynamics. This work extends the ATS to work with a multicolumn spatial structure.

### 3. Motivation: Results from Fine-scale Simulations

This mixed-dimensional approach is motivated by the results of fine-scale, two-dimensional simulations on vertical cross-sections across ice-wedge polygons at the Barrow Environmental Observatory. The simulations cou-

145 pled a surface energy balance model potentially including snow, snow dis-  
tribution models, models for thermal overland flow including phase change,  
and a recently developed three-phase subsurface thermal hydrology model.  
The soil properties were calibrated against borehole temperature data in a  
previous study [45]. The simulations were forced with meteorological data  
150 for the site. Those simulations used an unstructured mesh that conforms  
to surface topography derived from lidar measurements. Horizontal mesh  
resolution is approximately 0.25 m. Vertical resolution is 0.02 cm at the  
surface and gradually increases with depth. Details on boundary conditions  
and the spinup process can be found in [31].

155        Snapshots of ice and liquid saturation indices in cross-section across two  
ice-wedge polygons are shown in Fig. 1. These snapshots are for October  
15, 2013, which is during the fall freeze-up. During this period, the rims of  
the ice-wedge polygons are significantly colder than the centers and troughs  
because the thermally insulating snowpack is smaller on the rims. Previous  
160 one-dimensional simulations [46] have shown that thermal differences caused  
by differences in snow depth lead to differences in active layer thickness, the  
depth of the annual thaw. However, in the two-dimensional simulations  
shown here, the active layer thickness shows little variation across the poly-  
gon (Fig. 2). Although transient differences in subsurface temperature occur  
165 due to differences in snow depth, soil moisture content, and albedo, lateral  
heat transport is sufficient to equilibrate those differences by the time of  
maximum thaw. Thus, the active layer thickness, which is a primary con-  
trol on the annual carbon decomposition rates, is not directly affected by  
microtopographic position within an ice-wedge polygon in cases where or-  
170 ganic matter is relatively uniform. This lack of sensitivity suggests a model  
structure where the ice-wedge polygon becomes the unit computational cell



on the surface.

#### 4. An Intermediate-scale Model

Recognizing the lack of sensitivity to lateral, subsurface flow described  
175 above, we ~~derive~~propose an intermediate-scale model to leverage this simpli-  
fication. This model has two components: a spatial structure that combines  
one-dimensional and two-dimensional domains, and an operator splitting  
scheme that decouples the columns by solving lateral flow on the surface  
system independently of the sources and sinks of mass and energy which  
180 couple the surface and subsurface systems. We describe those aspects in  
this section, followed by a discussion of the refactoring strategy used to  
implement this model within the ATS.

##### 4.1. Mixed-Dimensional Modeling Approach

To build an intermediate scale model, we first tessellate the land sur-  
185 face into  $N$  surface cells, where each cell in the surface mesh corresponds  
to an ice-wedge polygon. Custom mesh generation tools are then used  
to construct a 3D mesh by extruding each of the surface polygons verti-  
cally into the subsurface, ~~introducing soil layering, etc~~honoring soil layering  
structure. This 3D mesh represents the entire domain of interest and is  
190 referred to as the primary mesh. For the purpose of this model, each  
~~tessellated~~tessellated ice-wedge polygon, along with the volume of soil di-  
rectly below it, is extracted as a single, one-dimensional (in the z-direction)  
~~, column of soil~~column. On each column, vertical flow of mass and transport  
of energy are solved, ~~and allowing for ponding of water and accumulation~~  
195 of associated energy on each column's surface, ~~a (local)~~. A surface bal-  
ance is ~~performed also performed on each column's surface~~ to determine

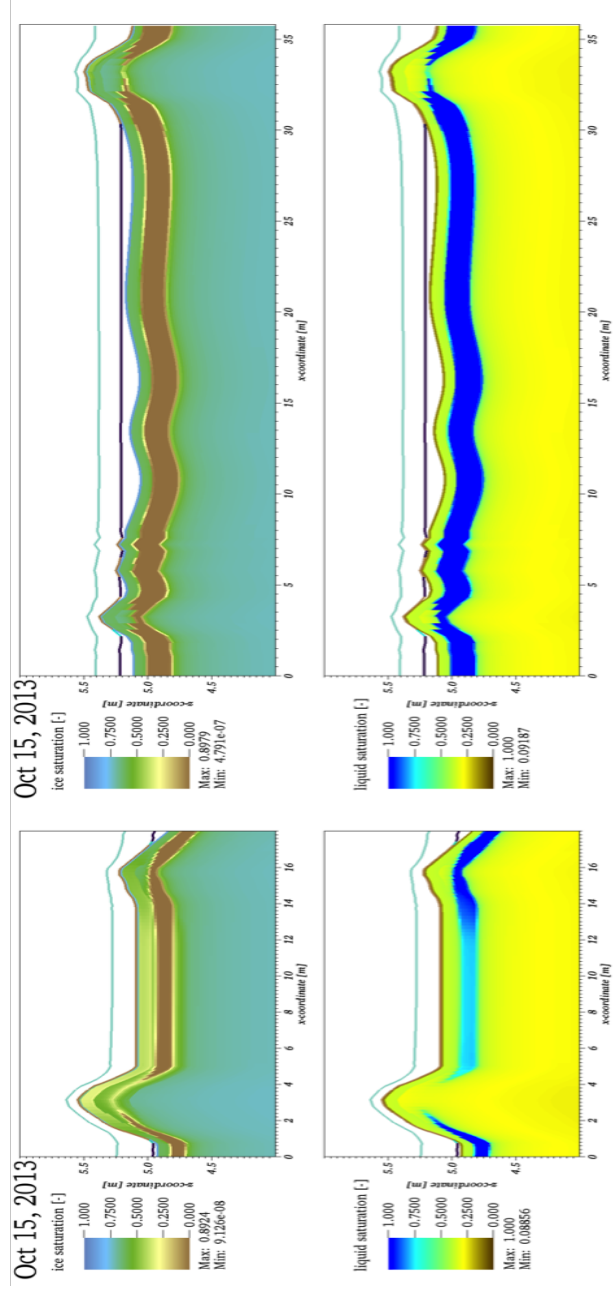


Figure 1: Results from two-dimensional fine-scale modeling. Shown are snapshots of ice saturation index and liquid saturation index in cross-sections across two ice-wedge polygons.

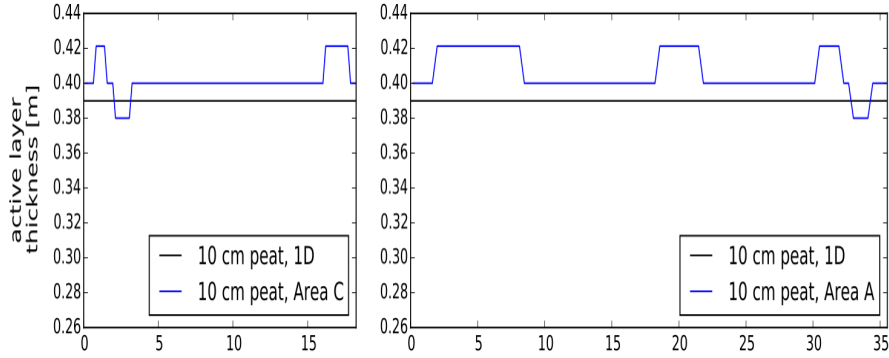


Figure 2: Active layer thickness from fine-scale modeling. Note that the mesh resolution here is  $2\text{cm}$ , and the discontinuities reflect jumps between cells of the mesh.

the net source of mass and energy into the system. ~~These columns are then coupled through lateral surface flow, which quickly moves water and energy throughout the domain.~~ We note that strong (globally implicit) coupling of the ~~surface-to-subsurface fluxes~~ surface, subsurface, and surface energy balance are critically important for ~~mass and energy conservation and accuracy~~ accuracy and stability of the system ~~through strong nonlinearities.~~ in the presence of strong nonlinearities; this is imposed by solving each column as an integrated system that includes a surface cell in addition to the soil below. The columns are then coupled through lateral surface flow, which quickly moves water and energy throughout the domain.

#### 4.2. Operator Splitting Scheme

Due to ~~this needed the need for~~ strong coupling between the surface and subsurface, the above mixed-dimensional strategy ~~alone still results in a computational~~ would, by itself, still result in a computationally expensive system of equations. ~~The tight coupling results in the need to solve that solves~~ all the columns and the surface flow equations simultaneously.

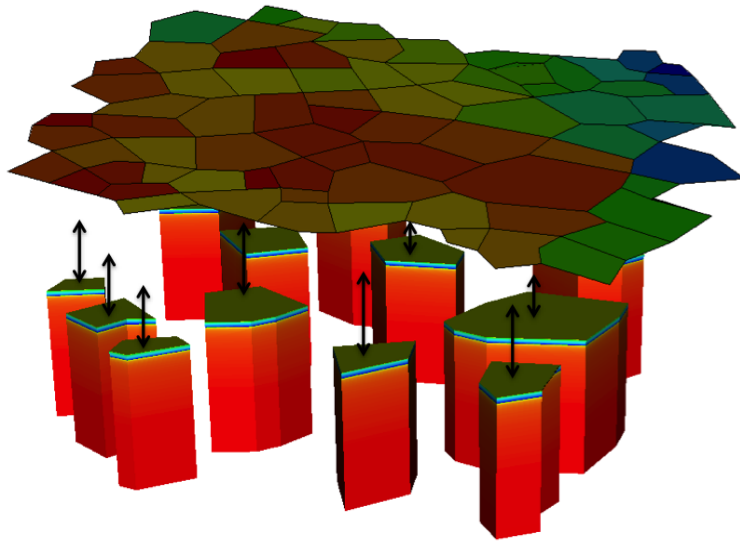


Figure 3: An illustration of the independent 1D **subsurface** columns coupled to the over-land system. Although shown here as a subsurface system only, each column also includes a single surface cell with the soil column, and is coupled to a surface energy balance calculation.

To ~~break this system, we develop~~ reduce that computational burden, we developed a two-stage operator-split strategy for the surface flow and energy equations. Under this strategy, we split the lateral fluxes from the coupling fluxes, ~~incrementally~~ first advancing one and then the other. In the first stage of the splitting, lateral fluxes are allowed to redistribute water and energy across the surface domain with no sources or sinks. This stage is hereafter called the “overland system.” Then, in a second update, the coupling fluxes and columnar subsurface ~~may be~~ are solved implicitly, but independently of every other column. Each column consists then of the subsurface thermal hydrology, surface energy balance, and surface ponding and energy exchange fluxes with no lateral flow. This stage is hereafter called the “~~column-surface~~ column system.” This splitting is shown schematically in Fig. 4. For the sake of clarity, we will refer to the pressure and temperature fields after the first stage as “overland-flow” pressure and temperature, while those after the second step will be called “subsurface” and “column-surface” pressures and temperatures. The splitting scheme conserves mass and energy but introduces splitting error, which is quantified through numerical experiments below.

#### 4.3. Model Implementation with ATS and Arcos

This implementation of this strategy requires significant software infrastructure and refactoring support. First, and not trivially, physics and simulation data must be entirely modular and encapsulated, so that multiple instances of each physics process can be instantiated, allowing ~~seperate~~ separate solution on multiple domains. Next, coupling these many processes on many domains requires a flexible, hierarchical coupling framework. Much of this was supported by Amanzi-ATS’s multiphysics library, Arcos[?]–.

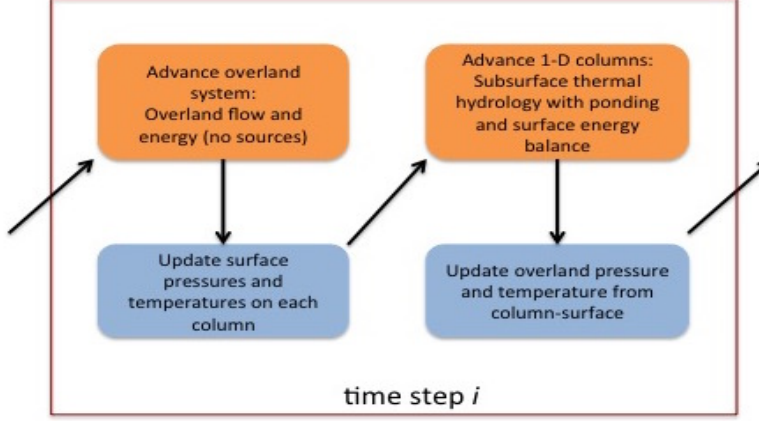


Figure 4: Schematic of the operator splitting scheme for our mixed-dimensional model.

A brief overview of the Arcos framework is provided in section 2, for more  
 240 details see [32]. Arcos represents physics on these domains as a hierarchical  
~~PK~~ Process Kernel (PK) tree which shows how the processes are coupled on  
 and across these domains, as illustrated in Fig. 5. The PK tree consists of  
 individual conservation equations (for example, the diffusion wave equation  
 for overland flow), strong (globally implicit) couplers, and weak (sequen-  
 245 tial) couplers highlighted in blue, light cyan, and orange colors, respectively.  
 In our approach, the operator splitting between the overland and column-  
 surface systems happens at the top level weak MPC. As discussed earlier, an  
 MPC is a Multiprocess Coordinator which manages coupling among PKs.  
 The strong MPC (on the left at the second level) is the overland system;  
 250 the weak MPC at the second level iterates over all the column subdomains.  
 The PK-I,  $I = 1, 2, 3, \dots, N$  denote an integrated system composed of sur-  
 face energy balance, column-surface (a single cell for coupling fluxes) and  
 subsurface (1D column) system. The tree attached to the black octagon

shape is replicated across all PK-I,  $I = 1, 2, 3, \dots, N$ .

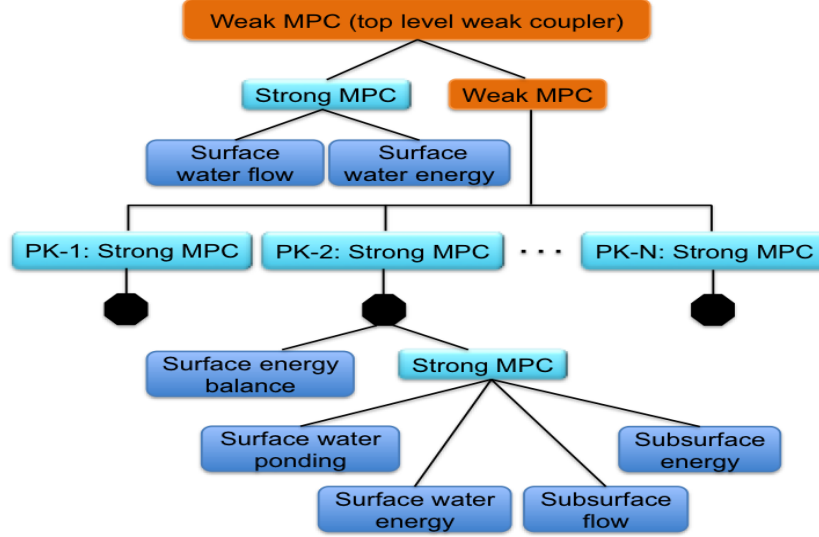


Figure 5: A customized hierarchical structure of the process kernels. Blue blocks highlights independent process ~~models~~kernels; Light blue blocks strongly coupled independent process kernels; Orange blocks represent weak couplers. Multiprocess Coordinator (MPC) highlighted by the light blue blocks couple the lower level PKs. A Process Kernel in the lower levels represents a single partial differential equation.

255 Refactoring of both ATS and its use of Arcos were needed to implement this strategy. To manage data encapsulation and replication, Arcos’s state object stores a dynamic, runtime-determined set of simulation data. Each data is identified by a unique key, e.g. “ponded\_depth”, and a set of meta-  
 260 data including domain of applicability, mesh entity, number of degrees of freedom, etc. In order for each PK to be instantiated multiple times, that PK’s data was altered to enforce uniqueness of its keys by prefixing a domain identifier such as “column\_0\_surface-ponded\_depth”. This refactoring allows multiple instances of any given PK, each attached to a different mesh

representing a subdomain of the primary mesh.

265 Furthermore, Amanzi-ATS relies on a meshing infrastructure, MSTK,  
[40] which can generate meshes as subdomains or subsets of existing meshes.  
This framework was extended to allow column meshes to be generated from  
an existing three-dimensional mesh. In this workflow, a surface mesh consist-  
ing of the surface polygons are extruded vertically, following pre-determined  
270 soil horizon structure, to create a 3D mesh. By insisting that the extrusion  
process works only in the vertical, well-defined columns then exist in the  
the three-dimensional mesh. At run-time, columns can then be identified,  
and extracted to form a one-dimensional mesh. This mesh is altered to  
ensure it is a one-dimensional submanifold of three-dimensional space, i.e.  
275 each cell has two faces, and all face-normals are  $\pm\hat{z}$ . Once this is done,  
Amanzi-ATS's existing operators can work on this mesh without changes.  
Furthermore, this mesh follows polygonal ground, and therefore consists of  
stacked polygonal-prisms. Few mesh and visualization libraries or utilities  
support this fully-unstructured mesh type; a Silo[47] capability was added  
280 to to Amanzi-ATS's existing output options to enable visualization of the  
resulting solution.

Each of these refactors was accomplished in reasonable time thanks to  
a close ~~adherence~~adherence to computational software best practices. A  
series of unit and regression tests were added for each new capability, and  
285 the existing regression tests were updated with the domain prefixes. Version  
control enabled close collaboration on this process across multiple develop-  
ers, and project-management Kanban tools were used to ensure each devel-  
oper in the workflow knew the needs of the client code component. These  
best practices, along with the use of libraries such as Silo, MSTK, and Ar-  
290 cos, greatly improved the efficiency of what otherwise would have been a



difficult development effort.

## 5. Results and Discussions

In this section, we present numerical results that ~~highlights~~highlight the accuracy and efficiency of our modeling technique. At the development stage, several numerical experiments were performed to verify the physical behavior of the refactored modules (PKs) of the ATS, code verification details are presented in Appendix A. The spinup process (i.e., model’s initialization) has been described in detail in [31].

### 5.1. Numerical Results – A Comparative Study

To demonstrate the accuracy of our modeling technique, we compare numerical results of the mixed-dimensional model against a fully coupled three-dimensional simulations that act as a benchmark for our simulations. The domain under consideration has surface elevation varying between 4.14-4.62 m, is 40 m deep, and enclosed by a rectangle in the horizontal plane  $173 \times 160 \text{ m}^2$ ; see Fig. 6. This domain is a part of the low-gradient polygonal tundra in Barrow, Alaska and consist of 75 ice wedge polygons. As highlighted in Fig. 6, we select five spots (based on different elevations) to perform a location-based comparison of the numerical results of the two schemes.

In addition to evaluating the quality of our mixed-dimensional approach for the Barrow tundra, we also want to understand when it will give inaccurate results. Because our modeling strategy is based on a loosely coupled scheme and neglects subsurface lateral flow between ice wedge polygons, it should eventually become inaccurate if the topographic relief is sufficiently large. To identify the range of applicability, we consider three variants of

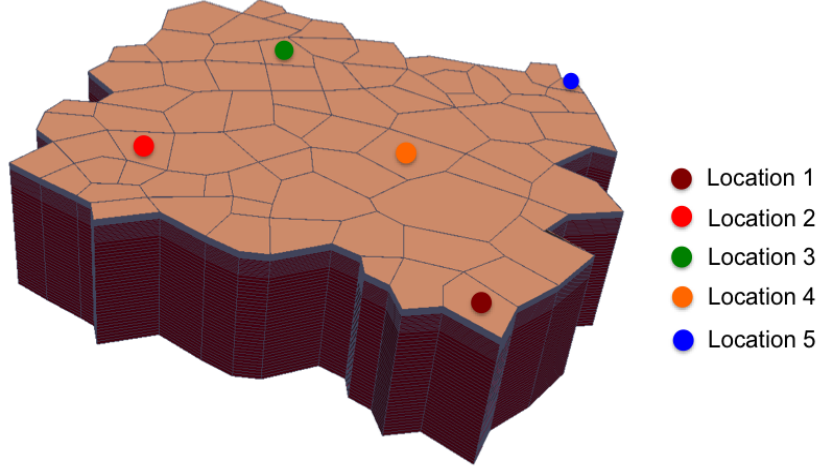


Figure 6: An illustration of the five spatial locations on 75 polygons cluster for location-based comparison of the two schemes. Location 1: Outlet. Location 2: High elevated spot. Location 3-4: Intermediate elevation spots. Location 5: Low elevation spot.

the surface topography. We use the following equation to exaggerate the surface topography,

$$\bar{Z} = \alpha(Z - \mu) + \mu. \quad (1)$$

Here  $\bar{Z}$  is the exaggerated elevation,  $Z$  is the original elevation with mean  $\mu$ , and  $\alpha$  is the exaggeration parameter. Equation (1) preserves the mean while the standard deviation depends on the value of  $\alpha$  and is given in meters by  $0.14\alpha$ . The coefficient in front of  $\alpha$  is the standard deviation of the original elevation  $Z$  – in our case  $Z$  correspond to the domain shown in Fig. 6. Our three variants correspond to  $\alpha = 1, 3$ , and  $5$ . The value  $\alpha = 1$  corresponds to the original topography with ~~percentage~~ slope (between the highest and lowest elevation spots) of ~~0.37~~~~%. The percentage %.~~ 0.37%. The slope increases from 0.37% to 1.1% and 1.85% for  $\alpha = 3$ , and  $5$ , respectively. We expect the model to give promising results for simulating low-gradient polygonal tundra, and

320 believe that the values of  $\alpha$  we choose provide sufficient variation across a domain of 100s of meter.

Our numerical experiments confirm a high agreement between the results of the mixed-dimensional model and the 3D model at all selected location for all three  $\alpha$  values. Figs. 7 and 8 compare the subsurface water saturations and temperatures, respectively, at locations 1 and 5 and for  $\alpha = 1$ . The 325 accuracy of our results for the Barrow topography ( $\alpha = 1$ ) is evident. The surface ponded depths and temperatures obtained with the two models are depicted in Fig. 9 and 10, respectively. As ~~expect~~expected, our results fit the 3D model's results very well. We see the same level of agreement at the 330 other locations as well, but we are not showing them here. In Fig. 11 we plot the mean annual thaw depth at five locations for the three variants,  $\alpha = 1, 3$ , and 5. We use the annual mean of the thaw depth rather than the maximum thaw depth (i.e. the active layer thickness) because the mean annual thaw depth depends on both the duration of thaw and maximum 335 thaw depth. Thus it is a direct measure of soil available for decomposition, averaged over the year. Not surprisingly, as the value of  $\alpha$  increases the mean annual thaw depth deviates from the results of the 3D model to some extent, but we still see the results of the mixed-dimensional model agree well with the corresponding benchmark solution. The annual thaw depth is mainly determined by heat input to the subsurface during the summer season with a very limited memory effect from the previous year. Thus, we do not expect errors in the annual thaw depth to accumulate year to year.

The consistency of our numerical results with the fully coupled 3D simulations confirm the appropriateness of ~~this approximated scheme. the~~ 345 approximate scheme. As with any splitting scheme, accuracy and numerical performance will depend on the time step size. Results shown here were

obtained with an adaptive time step determined by the minimum preferred time step for surface and subsurface PKs.

Lastly, for demonstration purpose only, the surface ponded depth and temperature during the snowmelt in 2012 are presented in Fig. 13 for the 468 polygon domain. Fully coupled 3D simulations at such a scale are computationally very expensive.

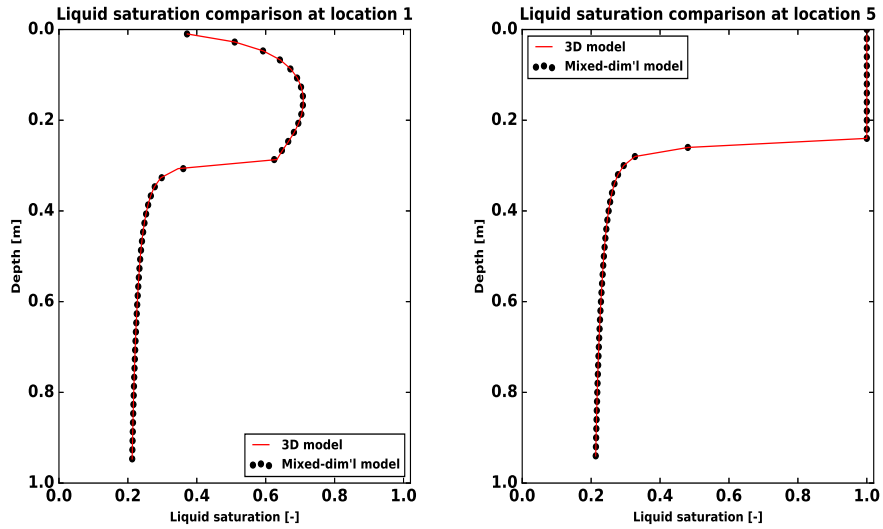


Figure 7: Comparison of the subsurface water-liquid saturation at locations 1 and 5 during the summer. Results correspond to  $\alpha = 1$ .

## 5.2. Speedup Study

We discuss speedup and parallel efficiency for two spatial domains, one with 75 polygons as depicted in (see Fig. 6) and a larger one consisting of 468 ice-wedge polygons, as shown in polygons (see Fig 12). The surface ponded depth and temperature during the snowmelt in 2012 are presented in Fig. 13 for the 468 polygon domain. Fully coupled 3D simulations at such

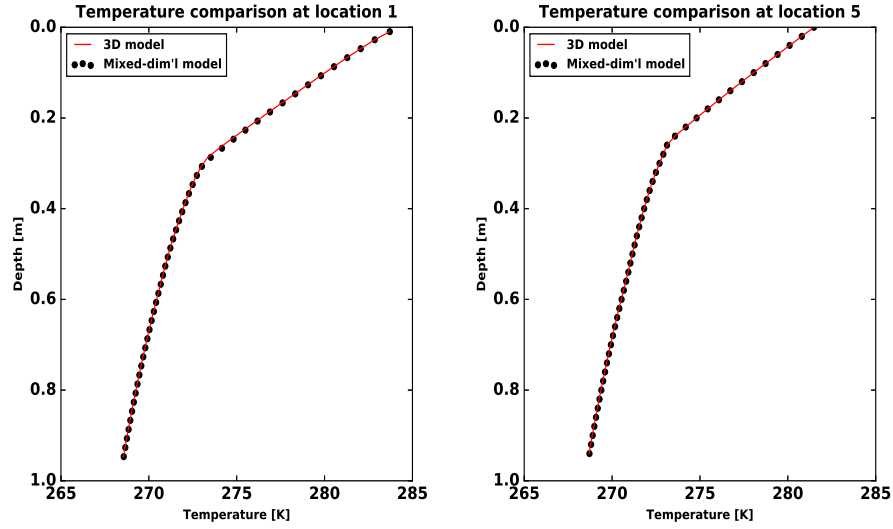


Figure 8: Comparison of subsurface temperature at locations 1 and 5 during the summer.

Results correspond to  $\alpha = 1$ .

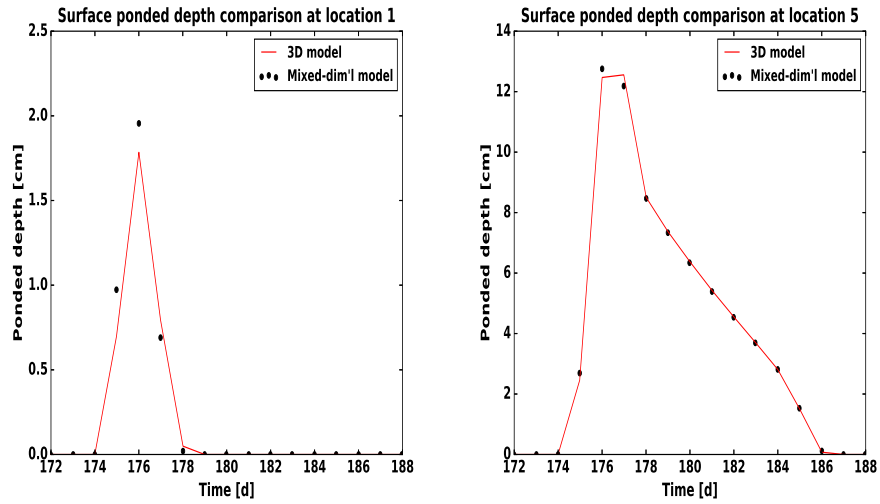


Figure 9: An illustration of the surface ponded depths of the two schemes at locations 1 and 5 when during the snow-melt starts summer. Results correspond to  $\alpha = 1$ .

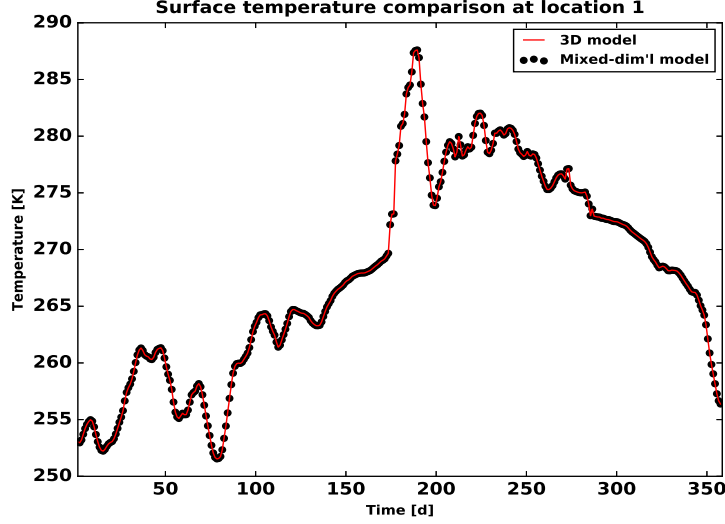


Figure 10: An illustration of the surface temperature of the two schemes at location 1 for the entire year. Results correspond to  $\alpha = 1$ .

~~a-scale are computationally very expensive.~~

360     ). We highlight two aspects of the efficiency of this modeling approach:  
 (i) how the simulation time decreases in comparison with three-dimensional simulations, and (ii) how efficiently it scales with number of processes.

Fig. 14 compares the computational time of the multidimensional strategy versus the three-dimensional solution for the domain consisting of 75  
 365 columns. It can be seen that for a fixed number of processors, the computational time decreases by a factor of about four with the multidimensional technique. This is a huge computational advantage without sacrificing numerical accuracy.

We show parallel strong scaling for the ~~aforementioned domains~~ 468  
 370 polygons domain in Fig. 15. Speedup of the ~~smaller domain~~ 75-polygon  
domain (not shown) is significantly less than the linear ideal; this is caused

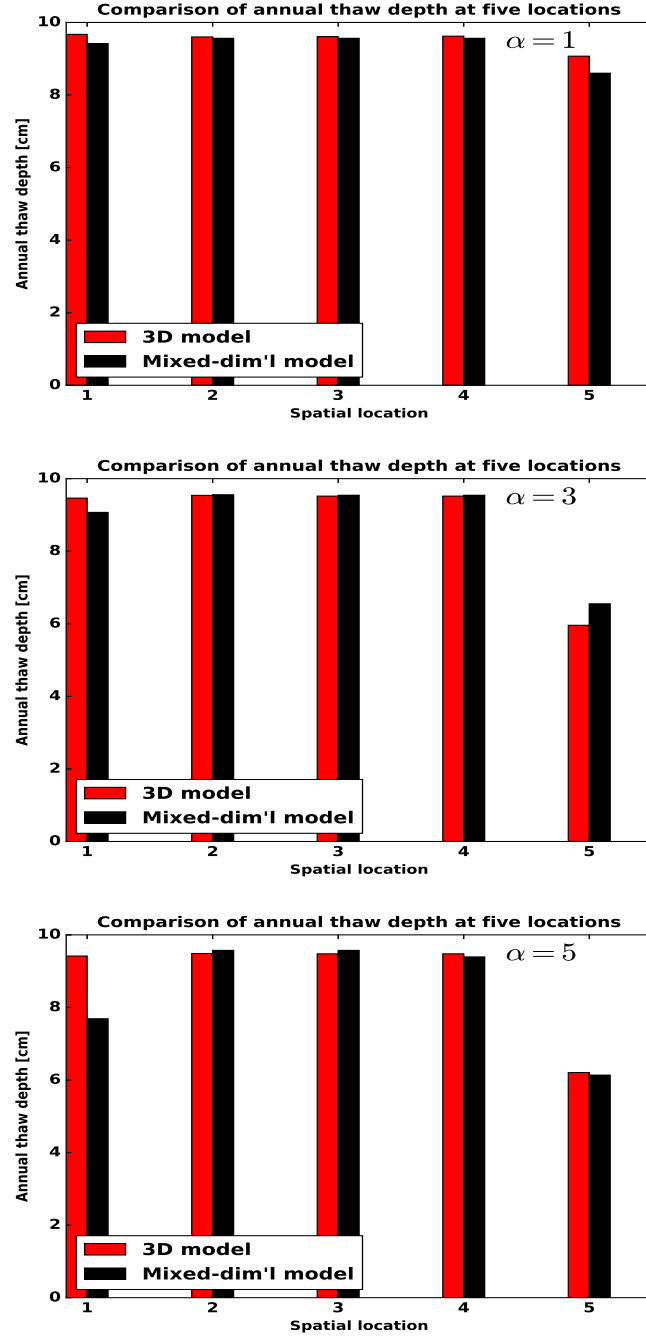


Figure 11: A comparison of the annual thaw depth at the selected locations of the three studies. [Results correspond to  \$\alpha = 1\$ .](#)

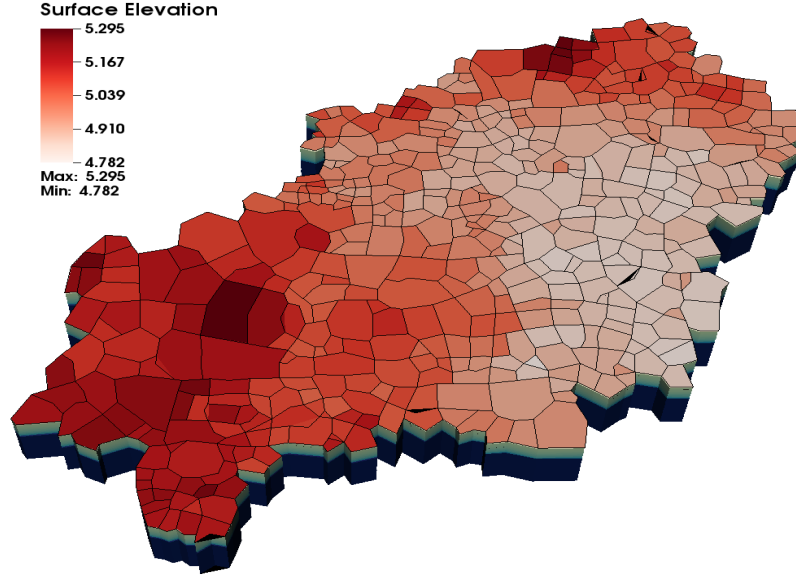


Figure 12: A watershed at Barrow, Alaska.

by communication overhead in the overland-flow system. Without consid-  
 eration of the overland-flow system, the problem is perfectly parallel. To  
 minimize communication between the overland-flow system and the column  
 systems, the overland-flow mesh is partitioned so that a column and the co-  
 375 incident mesh cells on the overland-flow system reside on the same processor.  
 If there are too few columns per processor, the interprocessor communica-  
 tion for the overland-flow system becomes the limiting factor despite the  
 lower computational burden for the overland-flow system compared with  
 380 the columns. As expected, the scaling is better for a larger domain. Scal-  
 ing is close to linear up to about 16 cores, which corresponds to about 30  
 columns per core.



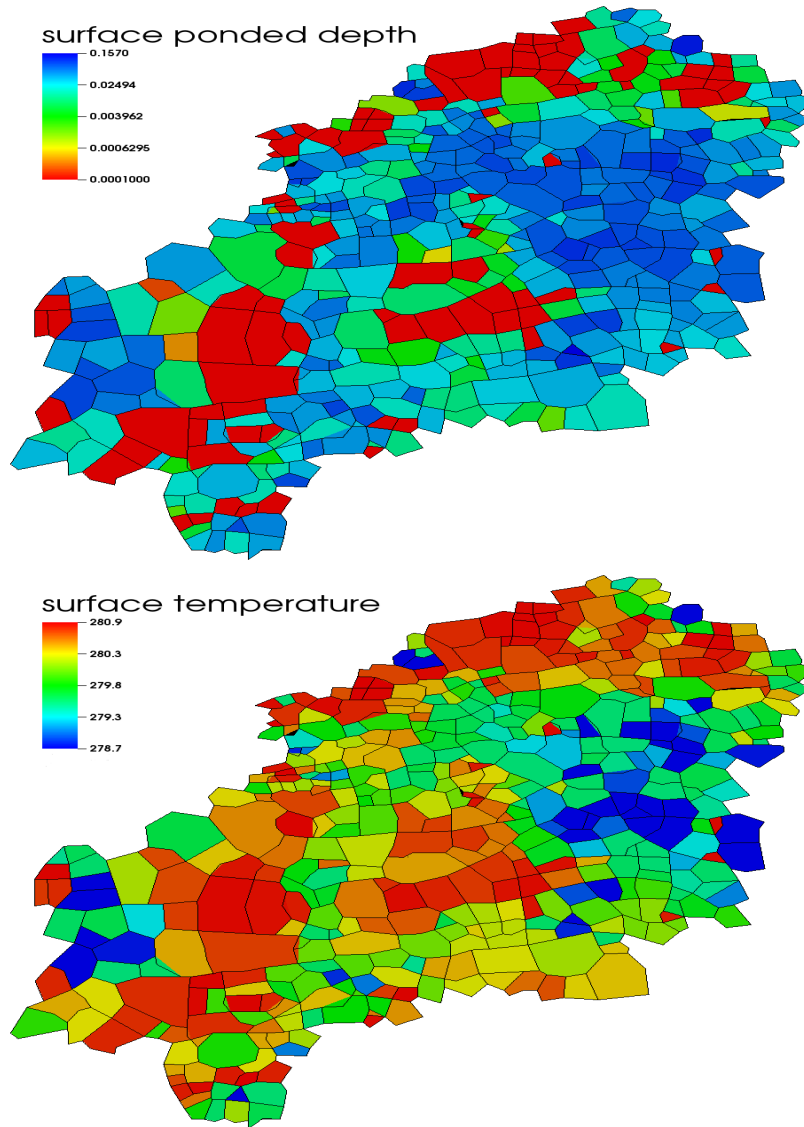


Figure 13: Simulation results ~~of the~~ from our mixed-dimensional model. ~~Showing~~ Shown are the surface ponded depth and temperature during the snowmelt of 2012. For clarity, the subsurface variables are not shown.

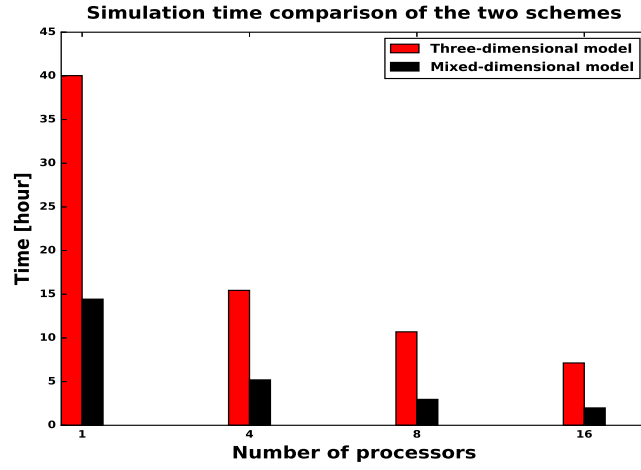


Figure 14: A comparison of the computational time taken by the mixed-dimensional and 3D models.

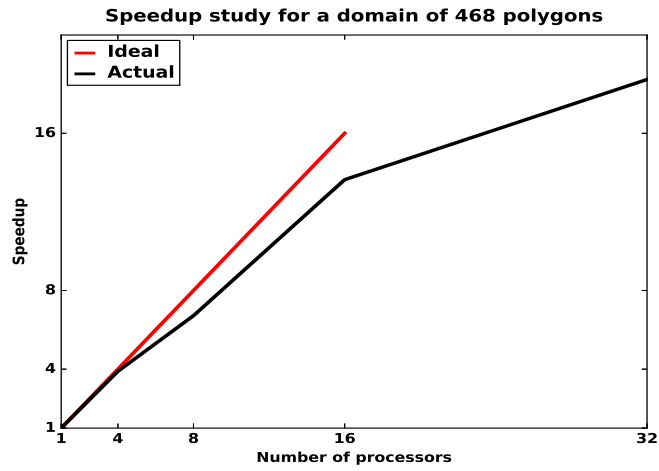


Figure 15: An illustration of the speedup study of a simulation with ~~75-polygon-cluster~~ (top) and 468 polygons ~~barrow-watershed~~(bottom).

### 5.3. Subcycling Process Kernels

One advantage of sequentially coupling different PKs, as opposed to a fully coupled approach, is that sequential coupling makes subcycling possible. With subcycling, individual PKs take their own time step rather than a global time step. The independently evolving PKs are then synchronized on a larger time step. The idea is to assign a suitable local time-step to each subdomain rather than one single global time-step. It is a very convenient approach for simulating permafrost type regions because a relatively small time step may be required when a cell is going through a phase change. Without subcycling, a timestep failure or small timestep caused by phase change in a single cell results in a small global time step. With subcycling, the effects of that phase transition are limited to a single column. Our mixed-dimensional modeling approach efficiently allows subcycling PKs because we discretize subsurface as independent columns/subdomains. Thus, the subdomains can advance in time with their preferred time-steps until they hit the synchronized time. Fig. 16 displays percentage reduction in the simulation time for the domains consisting of 21, 75, and 468 polygons. With the increase in the number of subsurface columns the computational time decreases, and we see up to 40% reduction in the computational time in comparison with simulations without subcycling. The choice of the synchronization time is crucial, and requires further optimization, which will be studied in future work.

## 6. Conclusions and Future Work

~~Out~~ Our intermediate-scale model for integrated surface/subsurface thermal hydrology of low-relief permafrost-affected regions is constructed from

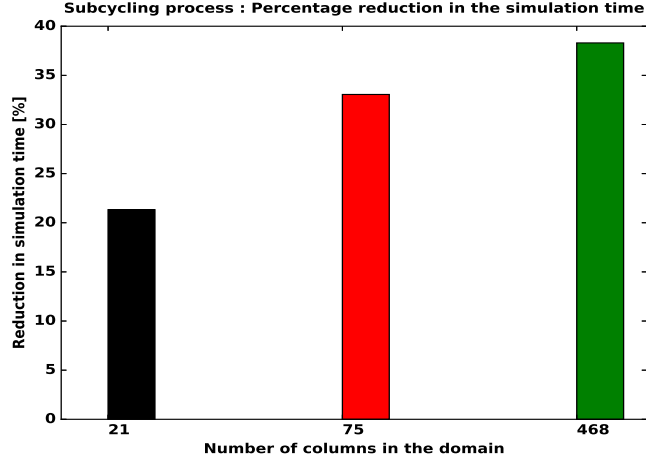


Figure 16: (Subcycling PKs) Percentage reduction in the computational time for the domains consisting of 21, 75 and 468 polygons.

two components: a mixed-dimensional spatial structure that is based on discretizing the subsurface as independent columns that are indirectly coupled  
 410 through a two-dimensional surface system, and an operator splitting scheme for coupling the column domains to the surface system. The spatial structure was motivated by fine-scale simulations of permafrost regions. This is the first demonstration of advanced representations of freezing soil physics coupled to overland thermal flow and surface energy balance at scales of  
 415 100s of meters.

An operator splitting algorithm is used to advance our mixed-dimensional model. First, we solve a two-dimensional surface thermal hydrology system that spatially distributes mass and energy, and initializes the system of the second step. The second step solves a family of independent one-dimensional  
 420 columns, where each represents an integrated system of the subsurface, surface ponding and surface energy balance. That step updates the 2D surface

system of the first step for the next iteration.

We compared our numerical results to the conventional scheme of a fully 3D subsurface that is strongly coupled to a surface system to demonstrate the efficiency and accuracy of our modeling approach. The fully coupled results act as a benchmark for our scheme. Numerical results show our scheme closely approximates the fully coupled system but is significantly more efficient. The scheme also allows for subcycling of individual subdomains, which further improves the numerical efficiency. With subcycling we see about an order of magnitude improvement in execution time compared to the fully 3D configuration on a 75-polygon mesh. However, we expect the computational advantages to improve with the system size. Indeed, we were not able to run the 468-polygon domain in fully 3D mode due to computational limitations, but were readily able to do it with the mixed-dimensional approximation.

This work is part of a larger effort to provide process-rich, watershed-scale simulations capability for permafrost regions. ~~A next step would be~~ Given the good scaling properties of our approach, we anticipate that simulations resolving individual ice-wedge polygons are now feasible for domains corresponding to those of a next-generation Earth system model grid cell ( $\approx 10$  km). in addition, the spatial structure used here is applicable at continental scales if a coarser discretization is used, wherein each surface grid cell corresponds to a sub-watershed in a ESM grid cell.

From the model development perspective, an important next step is to incorporate a subgrid model to represent the effects of variations of topography below our discretization unit of the ice wedge polygon. Another future direction is to represent thaw-induced subsidence. Thawing of permafrost and melting of massive subsurface ice can cause differential subsidence, leading to dynamic microtopography (low-centered polygons can transform to

high-centered polygons) [48, 49], substantial changes in hydrology and soil  
 450 moisture, and altered drainage networks, thus potentially transforming a ~~dry~~  
~~region to a wetland ecosystem~~ wetland ecosystem to a dry region [50, 51].  
 This modeling strategy is designed to tractably represent thaw-induced sub-  
 sidence. Representing subsidence in one dimension is significantly easier  
 than a fully three-dimensional representation because mesh tangling and  
 455 other mesh quality issues arise in a fully three-dimensional dynamic mesh  
 but are avoided in one dimension. Indeed, simulations of thaw-induced sub-  
 sidence on a single one-dimensional integrated surface/subsurface system  
 has already been demonstrated [14]; the work described here will allow the  
 same techniques to be used at scale with many columns coupled to an over-  
 460 land flow system. ~~Lastly, refactoring ATS not only supports subdomain~~  
~~modeling techniques but is also potentially useful future extensions. We can~~  
~~efficiently implement and independently test many process representations~~  
~~(physical, chemical, biological and geological processes) as PKs and let them~~  
~~interact through MPCs.~~

465 Although we mainly focus on simulating the thermal hydrology of de-  
 grading permafrost, elements of the work presented here have greater appli-  
 cability. A hybrid spatial structure mixing one-dimensional representations  
 of the vadose zone with two-dimensional representations of the saturated  
 zone and overland flow system are important approximations in watershed  
 470 modeling. This operator-split scheme of Fig. 4 is broadly applicable to  
 those systems and to integrated surface/subsurface simulations, in general.  
 This mixed-dimensional representation may be used as an alternative to a  
 fully coupled system or as a way of accelerating the time-consuming task  
 of spinup. In addition, this work demonstrates the advantages of Arcos or  
 475 other multiphysics management frameworks in greatly simplifies the process

of building models with hybrid spatial structure.

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## 485 Appendix A. Numerical Experiments – Code Verification

We have performed a series of tests at the development stage for code verification, and compared our results against numerical solution of three-dimensional model. The 3D results serve as a benchmark for our scheme. In 3D models the surface and subsurface systems are strongly coupled and  
490 solved implicitly. Since our model required major refactoring of the ATS, so individual pieces of the code were deeply tested before integration – they are listed below:

- Problem Test 1 (Subsurface Flow): We consider multiple subsurface columns with flat top surface – each column is an independent domain.  
495 Put water table below the surface, infiltrates and fills the subsurface columns.
- Problem Test 2 (Surface and Subsurface Flow only): This is an extension of the Test 1. We put water table below the surface. Water infiltrates and fill subsurface columns prior to surface ponding.

- 500 • Problem Test 3 (Subsurface Thermal Hydrology): We add energy equation to Test 1. Initially, establish water table close to the surface, and start freezing from below. The frozen subsurface columns are thawed from the top.
- 505 • Problem Test 4 (Surface and Subsurface Thermal Hydrology): In this test, we incorporate surface thermal hydrology into Test 3. A warm rain precipitation thaws the subsurface columns, saturate them and afterwards water ponds on the surface.
- 510 • Problem Test 5 (Surface Energy Balance, Surface and Subsurface Thermal Hydrology): A fully integrated surface and subsurface processes test. We introduce an energy balance equation to Test 4. An initially established ice table below the surface has been thawed by warm rain, incoming-short radiation and air temperature.

Due to symmetry in the domains of above numerical tests, that is, the subsurface columns are copies of each other and surface is flat, we get identical results and compare very well with its corresponding three-dimensional simulation results. Passing all the above tests conclude refactoring of the ATS a success. In the preceding discussion, we consider general polyhedra due to the polygonal structure of the Arctic landscape.

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