

A mixed-dimensional model for the simulation of soil thermal hydrology in polygonal tundra

Abstract

Permafrost soils harbor massive amount of frozen organic carbon and are warming at a rate significantly larger than the rest of the planet. Modeling and simulation techniques are essential tools for studying the complex hydrological environment of the Arctic regions. These tools help to determine the responses of the Arctic ecosystems to changing climate.

We present a novel mixed-dimensional model, motivated by fine-scale simulations, to simulate soil thermal hydrology in degrading permafrost regions and make these process-rich simulations tractable at watershed scales. The approach indirectly couples one-dimensional subsurface columns with a two-dimensional surface system, and has two fundamental steps. Step 1 solves overland thermal hydrology system with no sources, mainly act as a spatial distributor of the mass and energy, and updates the subsurface system before it advances in time. Step 2 implicitly solves the subsurface system with surface ponding but no surface lateral flow, and use the output of that half-step to update the pressure and temperature of Step 1 for the next iteration.

This is a first attempt to couple state-of-the-art representation of freezing soil physics with overland flow and surface energy balance at scales of 100s of meters. We demonstrate the accuracy and efficiency of our scheme. Our scheme is highly scalable, supports subcyclong of different processes, and compares well with fully 3D representation, but is computationally less expensive. Further, it allows for efficient tracking of thaw-induced subsidence and avoids any mesh tangling that can result from representing dynamic topography in a 3D simulation. Although we focus on permafrost thermal hydrology, the model structure is ap-

plicable to many integrated surface and subsurface thermal hydrology problems at field-scale.

Keywords: Mixed-dimensional model, Permafrost dynamics, Process-rich simulations, Arctic

1. Introduction

Permafrost soils, perennially frozen ground, are large carbon pools and reservoirs. Approximately 23% of the land surface in the Northern Hemisphere is covered by continuous permafrost (91-100% frozen area), and another 17% is occupied by discontinuous permafrost (50-90% frozen area) [1, 2]. A massive amount of organic carbon (approximately 1672 Pg) is stored in the Northern Hemisphere and these high-latitude regions are warming at a rate considerably faster than most of the world [3, 4, 5, 6]. In a warming climate, permafrost regions are under potential risk of carbon release to the atmosphere and can transform from a carbon sink to a carbon source – that could increase the concentration of carbon in the atmosphere, which in turn would lead to further increase in the temperature. Thawing of permafrost and thereby its considerable degradation can cause significant changes in the surface and subsurface thermal hydrology and eventually can bring substantial changes to the Arctic tundra ecosystems [7, 8, 9, 10, 11]. Therefore, due to increasing computing power, modeling and simulations turned to be useful and reliable tools that should be used to gain more insight into the role of permafrost degradation in temperature-sensitive Arctic ecosystems and to accurately project the consequent changes at larger spatial and temporal scales.

There has been a great interest in studying permafrost dynamics in warming climate through modeling and simulation techniques. Though such techniques help to better understand the role of soil warming, responses of these sensitive ecosystems to warming trends, its consequences on the degradation of permafrost and the associated changes in the surface and subsurface thermal hydrology. However, simulating permafrost dynamics in a complex and

coupled surface/subsurface thermal hydrological environment is a hard and an important challenge, particularly, at larger spatial and temporal scales; see [12]. Pertinent to literature, early research efforts mostly focused on one-dimensional simulations of subsurface thermal hydrology, for example, [13, 14, 15]. In previous decade, some studies were directed to demonstrate coarse-scale surface modeling techniques [16, 17, 18]. More recently a few studies demonstrated two- and three-dimensional simulations of permafrost dynamics with simplified (or subsurface only) models; see [19, 20, 11, 21]. A comprehensive review of the published modeling efforts of the surface and subsurface can be found in [22].

It is worth to point out that mathematical models with limited complexity, relatively coarse resolutions etc. provide some insight into permafrost dynamics but are not accurate representation the Arctic ecosystems – process-rich simulations are essential to capture the potential impact of permafrost thawing on the surface and subsurface thermal hydrology and the consequent changes.

We need sophisticated hydrological computer codes to simulate fully integrated surface and subsurface system and process-rich complex models over long temporal and spatial domains. However, as said earlier, simulating soil thermal hydrology in degrading permafrost regions is challenging due to strong coupling among thermal and hydrologic processes on the surface and in the subsurface, thaw-induced subsidence, complex microtopographic features (i.e., topography at the scale of polygons) etc. One of the challenges is a small time-step issue during phase transition. Frozen subsurface are less permeable and blocks infiltration, as ice begins to melt (phase change occurs), the soil hydraulic conductivity increases, consequently, the time-step of numerical methods decreases [23]. To ensure a long-term projection, a small time-step is not practical, because a huge amount of computational time is spent in recovering the time-step, which may not recover in a reasonable amount of time. The other major challenge is tracking thaw-induced subsidence. Most of the existing 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 could cost huge computational burden, further, a poor mesh

quality may question accuracy of the results. In addition, lack of flexibility and extensibility of the simulators also limit and discourage future extensions.

To address the aforementioned challenges, we present a multipurpose novel
60 mixed-dimensional modeling technique for process-rich simulations of integrated surface and subsurface permafrost thermal hydrology. It has also some additional exciting capabilities, for example, easy and efficient subcycling of a particular region of the computational domain. The approach indirectly couples individual (one-dimensional) ice-wedge polygons that discretize the horizontal
65 landscape to two-dimensional surface system. The implementation of a mixed-dimensional model requires a coupling scheme that provides interaction at the interface between different dimensions. In this work, we loosely couple the two-dimensional surface system with subsurface polyhedra that are treated as one-dimensional columns. These type of mixed-dimensional model approximations
70 are typically found in hydrology simulations at watershed-scale. The unsaturated (vadose) zone is horizontally divided into sub-regions and each of which are considered as 1D columns, and then coupled to vertically discretized saturated zone; for example see [24, 25]. Our approach to simulate process-rich soil thermal hydrology has broader scope.

75 This mixed-dimensional modeling approach is motivated by some fine-scale simulations of the permafrost regions. Fine-scale simulations showed significant differences in the thermal conditions among centers, rims and troughs of ice-wedge polygons, largely equilibrated by the lateral heat transport during summer, thereby an intermediate-scale representation is more practical and appropriate at larger scales; more details are presented later in the paper. Though
80 this modeling capability has broader scope but here we mainly focus on simulating permafrost thermal hydrology in polygonal tundra near Barrow, Alaska.

We have implemented our mixed-dimensional modeling strategy in an open-source state-of-the-art software known as Advanced Terrestrial Simulator (ATS)
85 [26, 27]. Particularly related to this work, ATS solves strongly coupled surface energy balance, and surface and subsurface thermal hydrology in a highly parallel 3D environment. We present details about the ATS in later sections, but it is

mainly a collection of PKs and MPCs. A PK (Process-Kernel) refers to a mathematical model, and MPC stands for Multiprocess Coordinator that couples
90 different PKs, that is, it facilitates communication among individual PKs.

The paper is organized as follows: Section 2 presents some fine-scale simulations’ results and analysis that motivated the approach. Section 3 highlights the Arctic Terrestrial Simulator (ATS) and the Arcos framework for the implementation of the model. In Section 4 we introduce our mixed-dimensional
95 modeling approach, loosely coupled scheme and the ATS refactoring strategy. To illustrate the performance 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. Concluding remarks and future research are offered in Section 6, followed
100 by references.

2. Motivation: Fine-scale Simulation Study

Our 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 coupled a
105 surface energy balance model with and without snow, snow distribution 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 [?]. The simulations were forced with meteorological data for the site. Those simulations
110 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 [27].

Snapshots of ice and liquid saturation indices in cross-section across two ice-wedge polygons are shown in Figure X. These snapshots are for October 15,
115 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 one-dimensional simulations [?] 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 polygon (Figure Y). Although transient differences in subsurface temperature occur 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 control on the annual carbon decomposition rates, is not directly affected by microtopographic position within an ice-wedge polygon. This lack of sensitivity suggests a model structure where the ice-wedge polygon becomes the unit computational cell on the surface.

3. Arcos Framework

As stated earlier, studying permafrost dynamics at large-scale is an important challenge, and requires simulators to be capable of handling many surface and subsurface processes, and the mutual interactions among them. Most existing hydrological computer codes, in the context of implicit-based coupling among processes, and the implementation architecture, don't efficiently allow and encourage modelers to study permafrost evolution at larger spatial and temporal scales. These simulators lack the flexibility of future development for extensions, that is, incorporating more processes and/or increasing the complexity of existing models for accurate representation of reality (e.g., changes in the Arctic ecosystem and predictability of carbon emissions and its content to the atmosphere in warming climate) is not a trivial task.

The Arcos framework enhances modeling capabilities more efficiently than existing simulators, and offers flexible process-rich simulations' environment to address challenging problems such as permafrost degradation. The Arcos framework manages the process kernels (a mathematical model) in a hierarchical way

(i.e., process tree form). In other words, the Arcos framework provides an architecture that manages multiphysics models and allow them to interact through a Multiprocess Coordinator (MPC). This hierarchical structure keeps the implementation of each mathematical model isolated that can be coupled with many
150 other models through an MPC. Due to this flexibility and significant extensibility, the Arcos framework-based simulators provide ideal modeling environment, tackle the complexities efficiently, and encourage future extensions. In this study, we use publicly available state-of-the-art computer code the Advanced Terrestrial Simulator (ATS). The ATS is inherited from Amanzi – Amanzi is a
155 flow and reactive transport simulator mainly build on the Arcos framework [28]. In subsequent sections, we describe how we refactored the ATS for our modeling technique. More details about the ATS and Amanzi are available in [26, 28, 27].

4. Modeling Approach, Coupling Scheme, and ATS Refactoring Strategy

160 In this section, we first describe the mixed-dimensional modeling approach then present the weakly coupled scheme followed by the refactoring strategy of the ATS.

4.1. Mixed-Dimensional Modeling Approach

Technically, our modeling strategy splits a 3D domain into $2N + 1$ subdomains, where N is the total number of surface elements. The total $2N + 1$
165 subdomains include N subdomains for 1D subsurface columns, one subdomain for the 2D overland system, and there are also N 1D surface cells placed upon each 1D subsurface column for water ponding and forcing data (e.g., rain precipitation, air temperature, wind speed etc.) To avoid confusion, hereafter the
170 2D overland system is referred to as surface-star system, and the 1D surface cells will collectively be called surface system. The 1D columns and surface-star system is highlighted in Fig. 1. The $2N + 1$ subdomains form a complex PK tree with $2N + 1$ processes as illustrated in Fig. 2. The PK tree consists of independent, strongly and weakly coupled PKs highlighted in light blue, light cyan,

175 and orange colors, respectively. In our approach, the interaction at the interface
 between the surface-star and 1D columns happens at the top level weak MPC.
 The strong MPC (on the left at the second level) is the surface-star system.
 The weak MPC at the second level iterates over all the surface and subsurface
 subdomains. The PK-I, $I = 1, 2, 3, \dots, N$ denote integrated surface (a cell) and
 180 subsurface (1D column) system. The tree attached to the black octagon shape
 is replicated across all PK-I, $I = 1, 2, 3, \dots, N$.

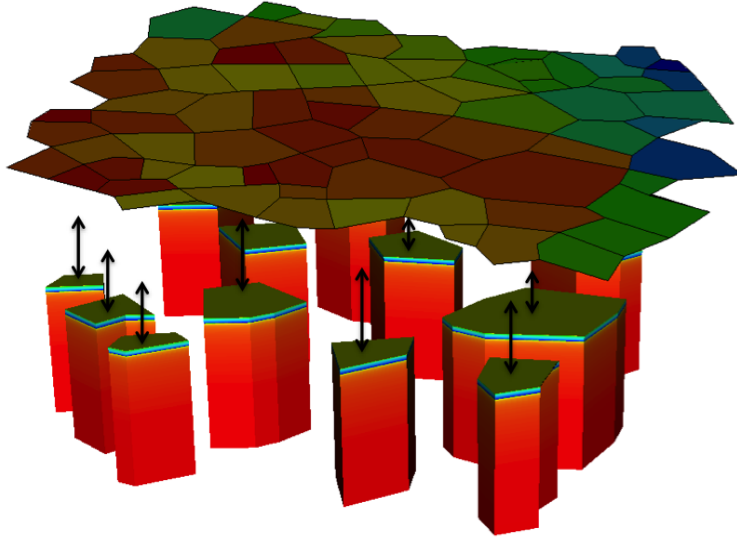


Figure 1: An illustration of the independent 1D subsurface columns coupled to the surface-
 star system. The surface system (1D cells lying on the top of corresponding columns) are not
 shown.

4.2. Weakly Coupled Scheme

The weakly coupled scheme for analyzing our mixed-dimensional model in-
 volves two fundamental steps. Step 1 solves surface-star thermal hydrology
 system without any external and exchanged sources. Step 2 solves subsurface
 185 system with surface ponding but no lateral surface flow. The first step mainly
 acts as a spatial distributor of the mass and energy, that is, distribute the pres-
 sures and temperature values across 2D overland system, and its solution serves

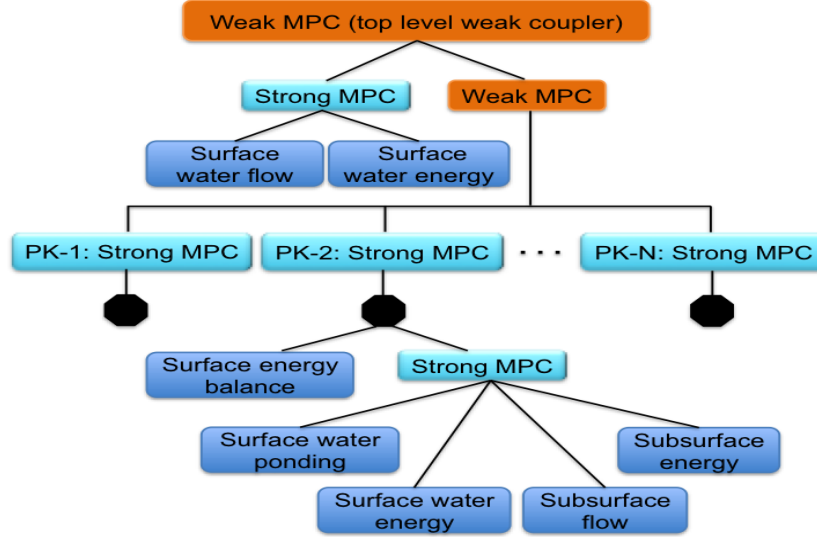


Figure 2: A customized hierarchical structure of the process kernels. Blue blocks highlights independent process models; Light blue blocks strongly coupled independent process kernels; Orange blocks represent weak couplers.

as initial condition for Step 2. That is, the surface-star system updates the
 190 subsurface system (one-dimensional columns) before the subsurface system ad-
 vances in time. After the update from Step 1, we implicitly solve subsurface
 system with surface ponding but no surface lateral flow, and use the output
 of that half-step to update surface-star pressure and temperature for the next
 iteration in the algorithm. As depicted in Fig. 3, the top and bottom blue spots
 195 represent 2D surface-star system and 1D subsurface columns, respectively, and
 the cyan colors (in the middle) are intermediate steps for updating surface-star
 and surface/subsurface systems. For the sake of clarity, we will refer to the
 pressure and temperature fields of step 1 as surface-star pressure and tempera-
 200 ture, while that of Step 2 will be called as subsurface and surface pressures and
 temperatures.

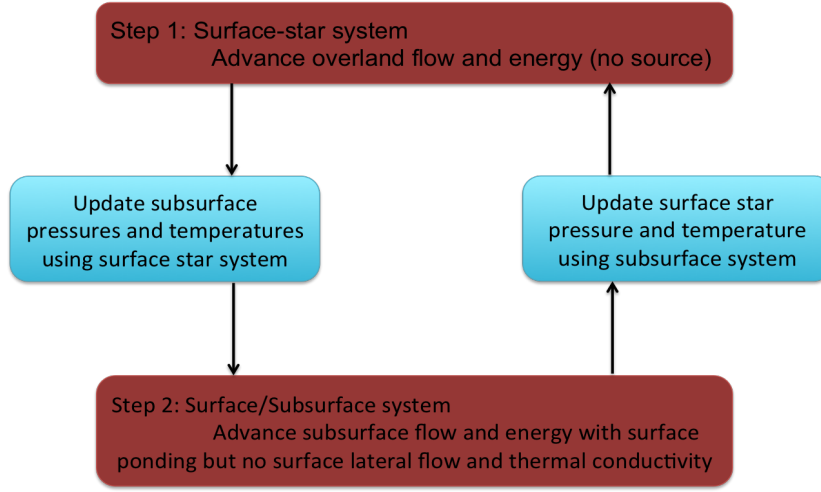


Figure 3: Schematic of the loosely coupled scheme for our mixed-dimensional model. Brown represents advancement of PKs in time; Cyan shows intermediate steps for initialization of PKs within a single iteration.

4.3. ATS Refactoring Strategy

The ATS was significantly refactored to accommodate the above customized weak MPC. The refactoring allows PKs to be replicated across multiple subdomains (meshes), that is, each PK is state independent. This stateless structure permits each surface and subsurface subdomain to have its own domain name, say `column_n`, `surface_column_n`, $n = 1, 2, 3, \dots, N$. In fact, the refactoring strategy prefixes the variables (primary, secondary, and independent) with their corresponding subdomain names (e.g., `column_n-pressure`, `column_n-temperature`, $n = 1, 2, 3, \dots, N$) – that yields each PK in its most general form. These generic PKs now allow to construct any type of customize MPC for mixed-dimensional modeling technique.

Complexity of the multiphysics PK tree in our modeling strategy could not have been achieved without the Arcos framework. Though the complexity in the PK tree is evident but additional complications are intended as we include more processes (physical, chemical, biological and geological processes) and their mutual interactions. All these processes are equally important for an accurate

and reliable long-term projections of permafrost regions. That said, the refactored ATS is more effective in addressing important challenges in the permafrost thawing in warming climate.

220 5. Results and Discussions

In this section, we present numerical results that highlights 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
 225 A. The spinup process (i.e., model’s initialization) has been described in detail in [27].

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-
 230 dimensional simulations that act as a benchmark for our simulations. The domain under consideration has surface elevation varying between 4.14-4.62 m, enclosed by a horizontal plane $173 \times 160 \text{ m}^2$, and 40 m deep; see Fig. 4. This domain is a part of the low-gradient polygonal tundra in Barrow, Alaska and consist of 75 general polyhedra. As highlighted in Fig. 4, we select five spots
 235 (based on different elevations) to perform a location-based comparison of the numerical results of the two schemes. We demonstrate three set of studies based on the variations introduced in the surface elevation. 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 μ ,
 240 and α is the exaggeration parameter. Equation (1) preserves the mean while the standard deviation depends on the value of α and is given by 0.14α . The coefficient in front of α is the standard deviation of the original elevation Z – in

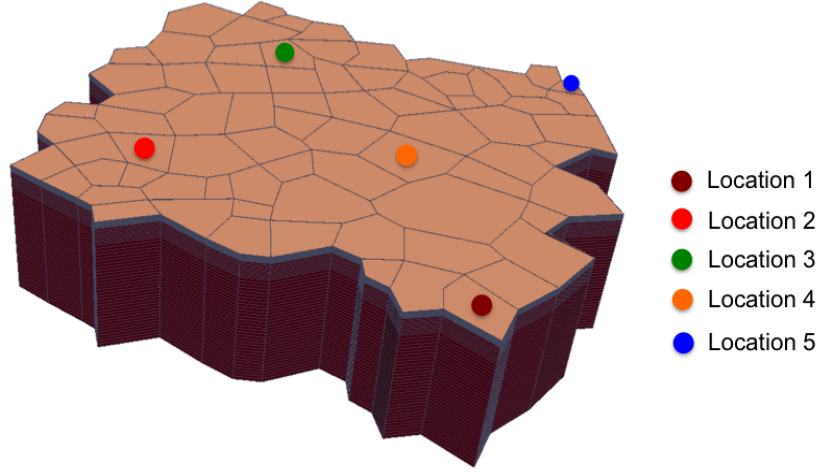


Figure 4: An illustration of the five spatial locations on 75 polygons cluster for location-based comparison of the two schemes. Location 1: Outlet. Location 2: High elevated spot. Location 3-4: Intermediate elevation spots. Location 5: Lowest elevation spot.

our case Z correspond to the domain shown in Fig. 4. Our three set of studies correspond to $\alpha = 1, 3$, and 5. These studies aim to determine (in an approximate sense) the failure of the mixed-dimensional model. In other words, since
245 our modeling strategy is mainly based on a loosely coupled scheme thereby it should eventually results in breakdown due to significant heterogeneity in the surface elevations. We expect the model to give promising results for simulating low-gradient polygonal tundra, and believe that the values of α we choose
250 provide reasonably enough variations for a domain of 100s of meter. For the sake of clarity, hereafter, we refer to the cases of $\alpha = 1, 3$ and 5 as Study-I, II and III, respectively.

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
255 studies. We present the results of study I in more detail, and it serves as a representative of the other two studies. Also, most of the presented plots correspond to the early summer. Fig. 5 and 6 compares the subsurface water saturations and temperatures at locations 1 and 5, respectively. The accuracy of our results

is evident. The surface ponded depths of the two models are depicted in Fig. 7.

260 We compare the surface temperatures obtained with the two-schemes in Fig. 8 at locations 1 and 5. Fig. 8 also displays the difference in the surface temperatures at the two locations highlighting spatial variability in the temperatures. As expect, our results fit the 3D model's results very well. We see the same level of agreement at the other locations as well, but we are not showing them here.

265 The root mean square difference in the subsurface water saturations of the two models of study-I, II, and III are shown in Fig. 9. Not surprisingly, as the value of α increases the error grows to some extent, but we still see the results of the mixed-dimensional model converge to the corresponding benchmark solution. The consistency of our numerical results with the fully coupled 3D simulations

270 validate the accuracy of our scheme.

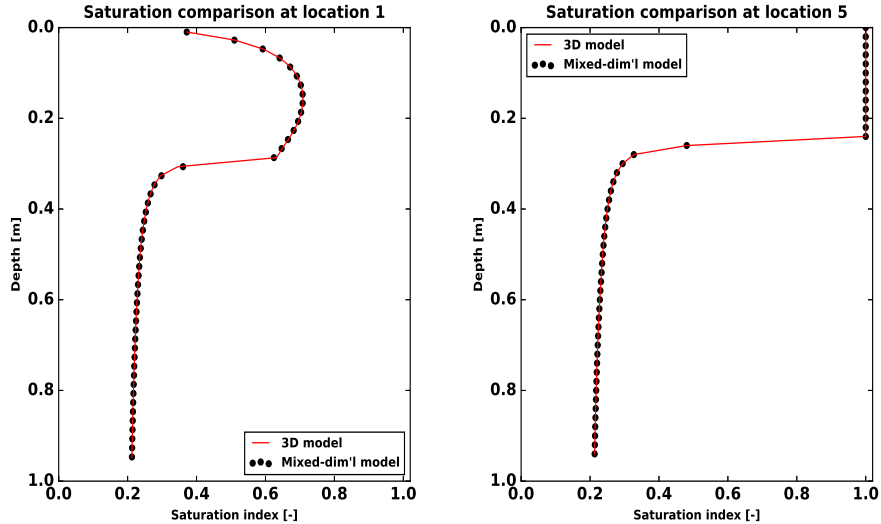


Figure 5: Comparison of the subsurface water saturation at locations 1 and 5 during the summer.

5.2. Speedup Study

We discuss speedup study for two spatial domains – one with 75 polygons as depicted in Fig. 4 and the other one (not shown here) consists of 468 general

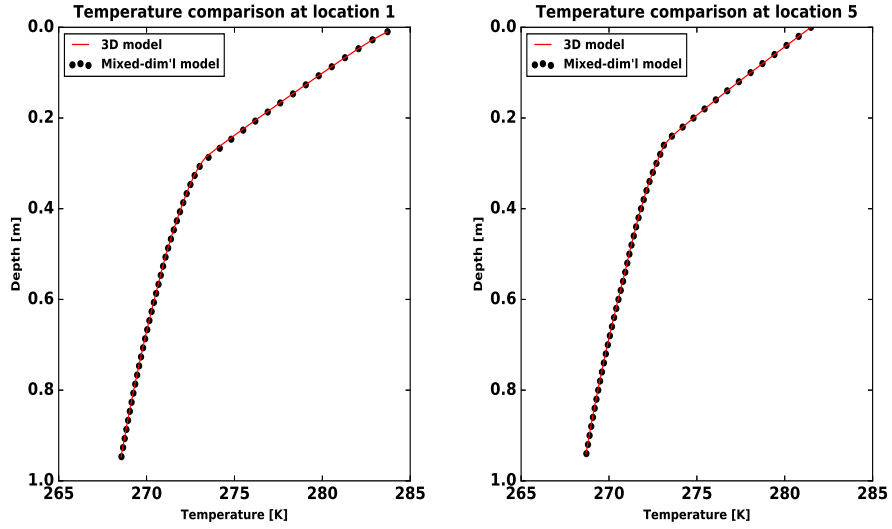


Figure 6: Comparison of subsurface temperatures at locations 1 and 5 during the summer.

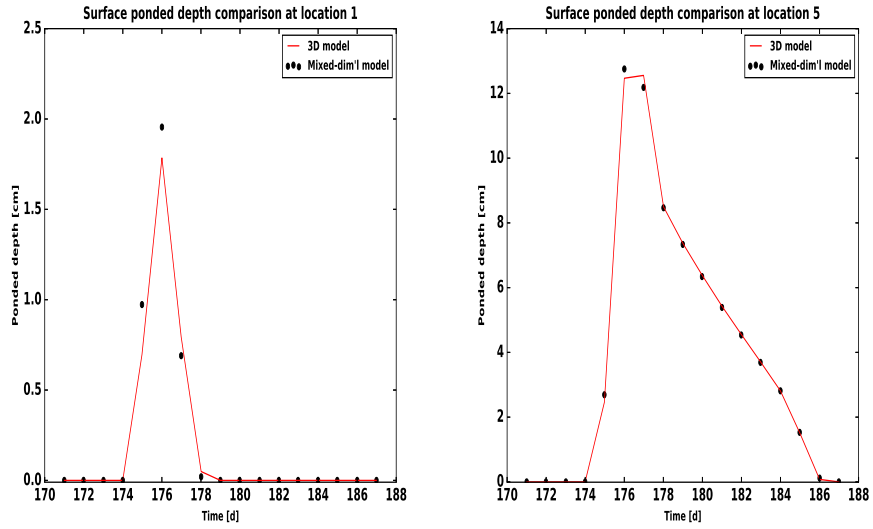


Figure 7: An illustration of the surface ponded depths of the two schemes at locations 1 and 5 when the snow melt starts.

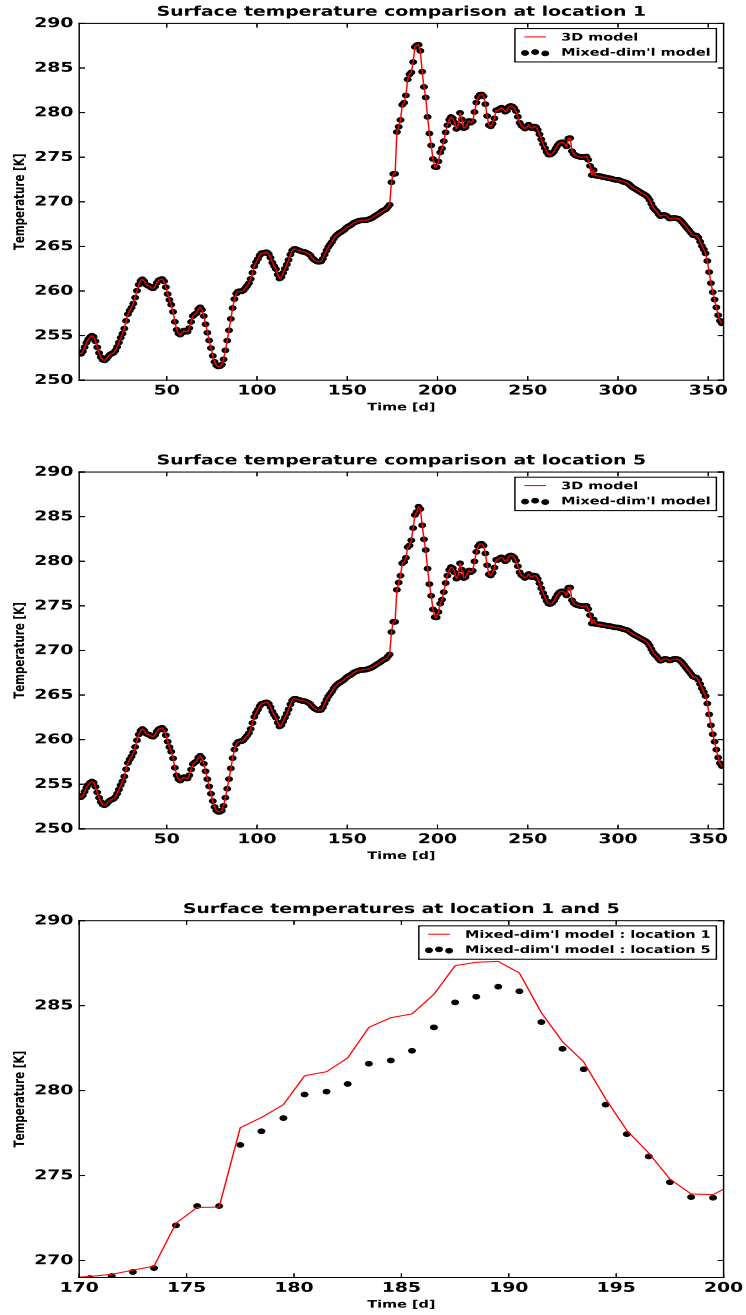


Figure 8: An illustration of the surface temperatures of the two schemes at locations 1 and 5 for the entire year. The bottom plot highlights the difference between the temperatures at location 1 and 5, though they appear quite similar in the top two plots.

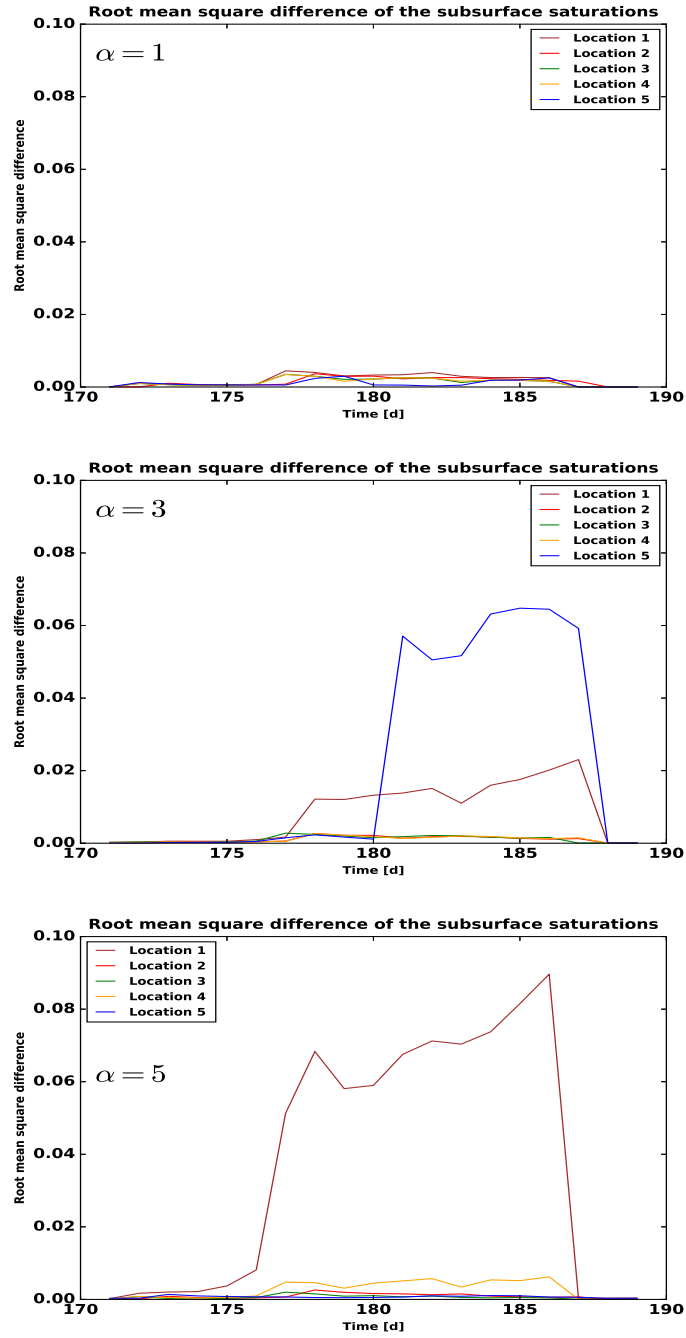


Figure 9: The root mean square difference of the subsurface water saturations at the selected locations of the three studies.

polyhedra that is about 6-7 times larger than the first one. We highlight two
 275 aspects of the efficiency of our modeling approach: (i) how the simulation time
 decreases in comparison with three-dimensional simulations; (ii) how efficiently
 it scales? Figs. 10 compare the computational time of the two modeling ap-
 proaches for the domain consisting 75 polyhedra. It can be seen that for a fixed
 number of processors, the computational time decreases by a factor of about 4
 280 with our modeling technique. This is a huge computational advantage without
 sacrificing the numerical accuracy. We show the speedup study for the afore-
 mentioned domains in Fig. 11. We see that the framework scales up better for
 larger domain. A considerable improvement pertaining to computational time
 and resources is expected with increasing size of the spatial domain. Ideally,
 285 one would want to employ the same number of processor as that of the sub-
 surface columns to achieve the maximum efficiency, however, with increasing
 number of processors, the cost of interprocessor communication in the overhead
 2D domain (i.e., the surface-star system) also increases and hence supersedes
 the performance. Overall, our novel modeling approach significantly reduces
 290 computational time without degrading numerical accuracy.

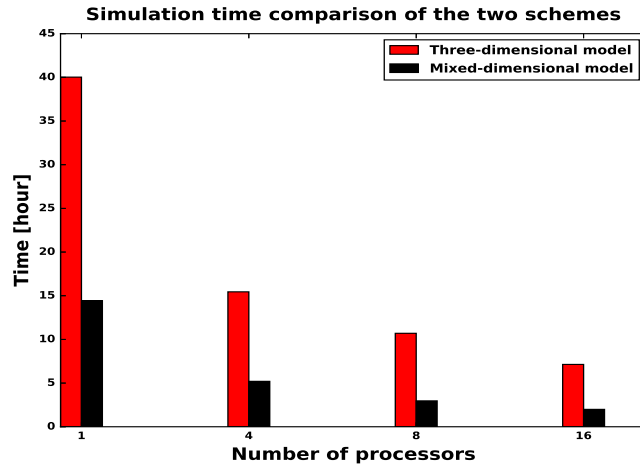


Figure 10: A comparison of the computational time taken by the mixed-dimensional and 3D models.

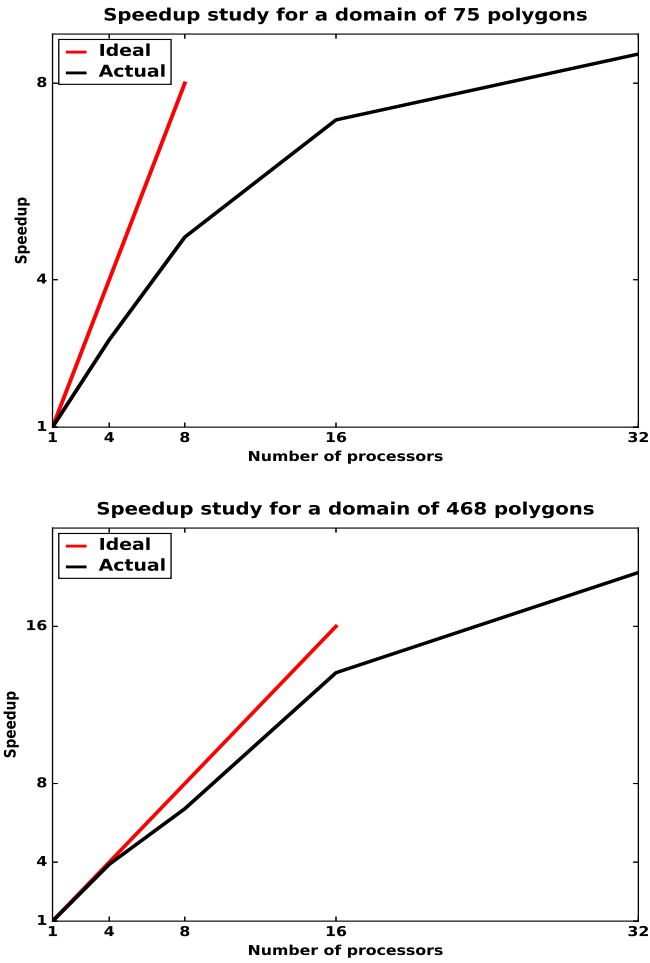


Figure 11: An illustration of the speedup study of a simulation with 75-polygon cluster (top) and 468 polygons barrow watershed (bottom).

5.3. Subcycling Process Kernels

Subcycling is a multi time stepping approach in simulations. The idea is to assign a suitable local time-step to each subdomain rather than one single global time-step. The subcycling is a very convenient approach for simulating permafrost type regions because during the time of snowmelt and snow accumulation, the time-step of the numerical methods is relatively smaller, and a reasonable amount of computational time is spent during these periods. Further, in permafrost simulations, due to the spatial variations in the thermal and hydrological conditions the phase change is mainly local, but its affects are global pertaining to the time-step.

Our mixed-dimensional modeling approach efficiently allows subcycling PKs because we discretize subsurface as independent columns/subdomains. Thereby the subdomains can advance in time with their preferred time-steps until they hit the synchronized time. We see a 15-20% decrease in the computational time as compared to no subcycling simulations. We intend to explore this topic and a report a detailed study in near future as we believe the subcycling approach should significantly reduce computational time.

6. Conclusions and Future Work

6.1. Closing Remarks

We present a novel mixed-dimensional modeling approach that is mainly based on discretizing subsurface as independent columns and then indirectly coupled to a two-dimensional surface system. This approach has motivated by fine-scale simulations of permafrost regions that explored spatial variations in the thermal conditions among centers, rims, and troughs of ice-wedge polygons during the summer, and mainly equilibrated by lateral heat transport.

Simulating a fully integrated surface and subsurface thermal hydrology in permafrost-affected regions is both important and challenging. The importance lies in the fact that permafrost stores massive amount of organic carbon and the degree of warming in these regions is a few times greater than the global mean.

320 That said, these regions may become a major contributor of carbon release to the atmosphere in warming climate. The strong coupling among thermal and hydrologic processes on the surface and in the subsurface, permafrost degradation, numerical issues, and large-scale projections make these simulations significantly challenging.

325 This is a very first attempt to couple state-of-the-art representation of freezing soil physics with overland flow and surface energy balance at scales of 10s of meters. Our novel mixed-dimensional modeling approach is implemented in state-of-the-art Arctic Terrestrial Simulator (ATS). The ATS is an open-source simulator, leverages Amanzi (a flow and transport simulator) and uses Arcos
330 framework. The Arcos framework manages the process kernels (a mathematical model) in a hierarchical structure, and couples many independent processes through a Multiprocess Coordinator (MPC). It allows the flexibility of extending existing modeling capabilities, and provides highly suitable environment for managing complexity in the process-rich simulations.

335 The coupling algorithm for analyzing our mixed-dimensional model has two fundamental steps. The first step solves a two-dimensional surface thermal hydrology system, that spatially distributes mass and energy, and initializes subsurface system at each time-step. The second step solves an integrated subsurface and surface ponding system, and at the end it updates surface system
340 for next time-step.

We compare our numerical results with a fully coupled surface and subsurface scheme to demonstrate the efficiency and accuracy of our modeling approach. The fully coupled scheme acts as a benchmark for our scheme. Numerical results show our scheme is computationally more efficient and as accurate as a fully
345 coupled scheme.

Our modeling approach has many advantages over existing hydrological simulators. Many available simulators are designed to work with a single spatial domain, don't support subdomains modeling techniques, large-scale deformations, flexible future extensions. Our modeling technique does not pose such
350 limitations on simulating process-rich permafrost dynamics. We can effectively

incorporate many processes (physical, chemical, biological and geological processes) and let them interact through MPCs. The scheme is computationally more efficient, accurate and scalable. In addition, it can efficiently track thaw-induced subsidence, allows subcycling individual subdomains, and avoids any
 355 mesh tangling and poor mesh quality that can result from representing dynamic topography in a three-dimensional simulation.

6.2. Future Directions

This is a first attempt to provide process-rich simulations capability of the permafrost regions at watershed-scale. However, the work is not yet complete,
 360 we intend to extend this capability to address more challenging problems in the near future. A very first task would be to incorporate a subgrid model for dynamic microtopography. Thawing of permafrost can cause ice-wedge polygons to deform, mold and change the landscape (low-centered polygons can transform to high-centered polygons) [29, 30]. Further, it can bring substantial changes in
 365 hydrology and soil moisture, can alter the drainage network, and transform a dry region to a wetland ecosystem [31, 32]. Our modeling strategy is designed in a way that can easily allow to track thaw-induced subsidence in simulating permafrost dynamics, because we are mainly working with one-dimensional columns (i.e., the discretization is based on independent 1D columns).

370 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 solved implicitly.
 375 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. Put water table below the surface, infiltrates and fills the subsurface columns.

- 380 • 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.
- Problem Test 3 (Subsurface Thermal Hydrology): We add energy equation
to Test 1. Initially, establish water table close to the surface, and start
385 freezing from below. The frozen subsurface columns are thawed from the
top.
- 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
390 water ponds on the surface.
- 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
395 radiation and air temperature.

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

References

- [1] J. Brown, O. Ferrians Jr, J. Heginbottom, E. Melnikov, Circum-Arctic map
of permafrost and ground-ice conditions, 45, 1997.
- 405 [2] M. T. Jorgenson, C. H. Racine, J. C. Walters, T. E. Osterkamp, Permafrost
degradation and ecological changes associated with a warmingclimate in
central alaska, Climatic change 48 (2001) 551–579.

- [3] C. Tarnocai, J. Canadell, E. Schuur, P. Kuhry, G. Mazhitova, S. Zimov, Soil organic carbon pools in the northern circumpolar permafrost region, Global biogeochemical cycles 23 (2009).
410
- [4] J. Turner, J. E. Overland, J. E. Walsh, An arctic and antarctic perspective on recent climate change, International Journal of Climatology 27 (2007) 277–293.
- [5] J. Hansen, R. Ruedy, J. Glascoe, M. Sato, Giss analysis of surface temperature change, Journal of Geophysical Research: Atmospheres 104 (1999) 30997–31022.
415
- [6] A. C. I. Assessment, Impacts of a warming arctic-arctic climate impact assessment, Impacts of a Warming Arctic-Arctic Climate Impact Assessment, by Arctic Climate Impact Assessment, pp. 144. ISBN 0521617782. Cambridge, UK: Cambridge University Press, December 2004. 1 (2004).
420
- [7] T. Osterkamp, Response of alaskan permafrost to climate, in: Fourth International Conference on Permafrost, Fairbanks, Alaska, 1983, pp. 17–22.
- [8] M. A. Walvoord, R. G. Striegl, Increased groundwater to stream discharge from permafrost thawing in the yukon river basin: Potential impacts on lateral export of carbon and nitrogen, Geophysical Research Letters 34 (2007).
425
- [9] S. Lyon, G. Destouni, R. Giesler, C. Humborg, C.-M. Mörtz, J. Seibert, J. Karlsson, P. Troch, Estimation of permafrost thawing rates in a sub-arctic catchment using recession flow analysis, Hydrology and Earth System Sciences 13 (2009) 595–604.
430
- [10] R. K. Pachauri, M. Allen, V. Barros, J. Broome, W. Cramer, R. Christ, J. Church, L. Clarke, Q. Dahe, P. Dasgupta, et al., Climate change 2014: Synthesis report. contribution of working groups i, ii and iii to the fifth assessment report of the intergovernmental panel on climate change (2014).
435

- [11] C. D. Koven, W. J. Riley, A. Stern, Analysis of permafrost thermal dynamics and response to climate change in the CMIP5 earth system models, *Journal of Climate* 26 (2013) 1877–1900.
- [12] S. Painter, J. Moulton, C. Wilson, Modeling challenges for predicting hydrologic response to degrading permafrost, *Hydrogeology Journal* (2013) 1–4.
- [13] R. Harlan, Analysis of coupled heat-fluid transport in partially frozen soil, *Water Resources Research* 9 (1973) 1314–1323.
- [14] G. L. Guymon, J. N. Luthin, A coupled heat and moisture transport model for arctic soils, *Water Resources Research* 10 (1974) 995–1001.
- [15] G. S. Taylor, J. N. Luthin, A model for coupled heat and moisture transfer during soil freezing, *Canadian Geotechnical Journal* 15 (1978) 548–555.
- [16] K. Takata, S. Emori, T. Watanabe, Development of the minimal advanced treatments of surface interaction and runoff, *Global and planetary Change* 38 (2003) 209–222.
- [17] D. Nicolsky, V. Romanovsky, V. Alexeev, D. Lawrence, Improved modeling of permafrost dynamics in a gcm land-surface scheme, *Geophysical research letters* 34 (2007).
- [18] J. M. McKenzie, C. I. Voss, D. I. Siegel, Groundwater flow with energy transport and water–ice phase change: numerical simulations, benchmarks, and application to freezing in peat bogs, *Advances in water resources* 30 (2007) 966–983.
- [19] V. Bense, G. Ferguson, H. Kooi, Evolution of shallow groundwater flow systems in areas of degrading permafrost, *Geophysical Research Letters* 36 (2009).
- [20] D. M. Lawrence, A. G. Slater, S. C. Swenson, Simulation of present-day and future permafrost and seasonally frozen ground conditions in ccsm4, *Journal of Climate* 25 (2012) 2207–2225.

- [21] S. Karra, S. Painter, P. Lichtner, Three-phase numerical model for subsurface hydrology in permafrost-affected regions, *Cryosphere Discuss* 8 (2014) 149–185.
- [22] B. L. Kurylyk, K. T. MacQuarrie, J. M. McKenzie, Climate change impacts on groundwater and soil temperatures in cold and temperate regions: Implications, mathematical theory, and emerging simulation tools, *Earth Science Reviews* 138 (2014) 313–334.
- [23] M. Dall’Amico, S. Endrizzi, S. Gruber, R. Rigon, A robust and energy-conserving model of freezing variably-saturated soil, *The Cryosphere* 5 (2011) 469–484.
- [24] M. F. Pikul, R. L. Street, I. Remson, A numerical model based on coupled one-dimensional richards and boussinesq equations, *Water Resources Research* 10 (1974) 295–302.
- [25] Y. Zhu, Y. Zha, J. Tong, J. Yang, Method of coupling 1-d unsaturated flow with 3-d saturated flow on large scale, *Water Science and Engineering* 4 (2011) 357–373.
- [26] E. T. Coon, J. D. Moulton, S. L. Painter, Managing complexity in simulations of land surface and near-surface processes, *Environmental Modelling & Software* 78 (2016) 134–149.
- [27] S. L. Painter, E. T. Coon, A. Atchley, B. Markus, G. Rao, J. D. Moulton, S. Daniil, Integrated surface/subsurface permafrost thermal hydrology: Model formulation and proof-of-concept simulations, *Environmental Modelling & Software* (submitted) (2016).
- [28] J. D. Moulton, M. Berndt, R. Garimella, L. Prichett-Sheats, G. Hammond, M. Day, J. Meza, High-level design of amanzi, the multi-process high performance computing simulator, office of environmental management, united states department of energy, washington dc (2012).

- [29] M. T. Jorgenson, Y. L. Shur, E. R. Pullman, Abrupt increase in permafrost degradation in arctic alaska, *Geophysical Research Letters* 33 (2006).
- [30] A. Liljedahl, L. Hinzman, J. Schulla, Ice-wedge polygon type controls low-gradient watershed-scale hydrology, in: *Proceedings of the Tenth International Conference on Permafrost*, volume 1, 2012, pp. 231–236.
- [31] L. D. Hinzman, N. D. Bettez, W. R. Bolton, F. S. Chapin, M. B. Dyurgerov, C. L. Fastie, B. Griffith, R. D. Hollister, A. Hope, H. P. Huntington, et al., Evidence and implications of recent climate change in northern alaska and other arctic regions, *Climatic Change* 72 (2005) 251–298.
- [32] J. C. Rowland, C. E. Jones, G. Altmann, R. Bryan, B. T. Crosby, L. D. Hinzman, D. L. Kane, D. M. Lawrence, A. Mancino, P. Marsh, J. P. McNamara, V. E. Romanovsky, H. Toniolo, B. J. Travis, E. Trochim, C. J. Wilson, G. L. Geernaert, Arctic landscapes in transition: Responses to thawing permafrost, *Eos, Transactions American Geophysical Union* 91 (2010) 229–230.