## **Response to Referee 1**

There are some minor changes in the response based on further updates of the manuscript.

## **GENERAL COMMENTS**

The manuscript presents a sensitivity analysis of a Canadian one-dimensional land surface model, MESH to the thickness of modeled soil profile and the length of model initialization period. The main conclusions are that a soil profile of 20m or greater is necessary for this particular model to represent the energy dynamics of permafrost, and that an initialization period much longer than 100 years is necessary to condition the model properly. The same results have been reported by a number of previous researchers using different permafrost models, and the present study confirms well known facts. A new contribution of this study would have been to present a rigorous and systematic evaluation of the model sensitivity to soil profile thickness and initialization period. Unfortunately, the study falls short of delivering a new contribution due to a few important deficiencies in model boundary conditions as I explain below. I would suggest that the authors use appropriate boundary conditions and conduct new model sensitivity analyses that are scientifically defendable.

## **Response to General Comments**

We thank the referee for his/her insightful comments. While we certainly agree with the referee on the significance of geothermal flux, we would point out that the difference between the common implementation of the current generation of Land Surface Schemes (LSS), applied as the lower boundary condition for regional/general circulation models and hydrological applications, and that of permafrost models used to predict and evaluate the evolution of permafrost. In the former, the geothermal flux is commonly ignored in the literature and most of existing models do not have the parameterization to include it (the common assumption is no heat flux at the bottom of the soil layers), while in the latter, geothermal flux is considered an essential component of modelling. In response to the referee's comment, we have extended the analysis by including a new set of simulations with a constant geothermal flux (0.083 W/m2) at the bottom, based on available measurements at Norman Wells (Garland, G.D. and Lennox, D.H., Heat Flow in Western Canada. Geophys. J.R. Astron. Soc., 6,245-262, 1962).We have run the same set of 50 parameters with 17 different soil configuration combinations (850 simulations) for the average climate year (1945). Figure 1 shows the results obtained. Although some small differences are observed, the conclusions remain the same (e.g., 20 meters of soil depth are needed). The main difference is seen in some soil configurations having slightly warmer soil profile when "ggeo" flux is included. Figure 2 shows the cumulative distribution function of the difference of soil temperature at the non-oscillation depth with and without ggeo flux at the bottom. Approximately, in 60% of the simulation the difference is within +/-0.15°C. Upper boundary condition. We have corrected the description of the site location and clarified the assumptions made about the upper boundary condition. The land cover in the manuscript has been corrected to be a composition of moss lichen groundcover, ericaceous shrubs, black spruce and tamarack trees in an open canopy density (Smith et al., 2004). In this study, we perturbed the canopy parameters by a Monte Carlo analysis, not using a specific land cover type based on a look-up table. The range of variation selected in such a way that it covers most of the possible land covers present in the area. The purpose of that was to analyse the uncertainty in parameter values on the definition of the soil configuration and in land surface schemes that are typically run at a grid size ranging from  $\sim 10*10$  to  $\sim 250*250$  km2 (which can be different from an analysis performed to represent the processes at a point). We have

included two new sections to describe the boundary conditions used and to show the results obtained of the geothermal flux at the bottom. To better define the scope of our work we have restructured the introduction to better reflect the novelty of our contribution.

## SPECIFIC COMMENTS

1. P3, L13-15. This paragraph seems to be out of place. I suggest deletion.

Thank for your suggestion, we have removed the paragraph.

2. P4, L8. It is very unusual to have a 'grassland' ecosystem in a place like Normal Wells. I would suggest that the model be run with appropriate parameters to represent the vegetation typical of this environment.

We agree with the referee. The confusion here it is was derived from the Land Cover map used in this analysis, that came from a reclassification of a land cover map from a bigger area for the Mackenzie basin, where shrubs, grass and other cover were grouped together in a single unit unfortunately named grassland . In addition also the original pixels were upscaled and we only pick the dominant land cover type. However, in really, as the canopy parameters were perturbed by a Monte Carlo analysis, in fact, we have not used a specific land cover type based on a look-up table. The range of variation cover most of the possible land cover present in the area. The purpose to do not attach to a specific set of parameters representing a land cover was to show that regardless of their value you need to have a deeper soil configuration in cold regions. To avoid any kind misunderstanding we have corrected the land cover specific for the place adding a complete description of the site vegetation and canopy based on the site description reported in Smith et al., (2004). We removed any grass land cover reference from the text. As explained, we considerate that re-run the simulation are not necessary.

3. P5, L4. The data from this borehole (84-1) is critically important for the evaluation of model performance. The model should be set up with the top boundary condition representing the vegetation characteristic of the local site, because the model simulation is compared against local data. The borehole data and site characteristics (including photographs) are publicly available from a report published by Natural Resources Canada. It appears that this site is located in a wetland surrounded by black spruce forests, typical of the Normal Wells region. To present a rigorous analysis (P19, L8), the model should use a set of parameters for wetlands, not grasslands for the top boundary.

## Please see response to comment #2.

4. P6, L22. Again, grass land cover is inappropriate for this particular model simulation.

Please see response to comment #2.

5. P7, L1. The critical importance of geothermal heat flux applied to the bottom boundary is widely recognized by researchers in the permafrost modeling community, and is considered the standard practice. Geothermal heat flux data for the study region is readily available and used in previous studies (e.g. Zhang et al. 2008, cited by the authors). The absence of heat flux at the bottom boundary calls the scientific rigor of simulations in this study into question. I would strongly recommend that the authors re-run the simulations using a proper bottom boundary condition. If the model cannot handle geothermal flux, then it is not an appropriate modeling platform for permafrost environments.

We understand and also share your point. As we respond to the general comments, the focus of the present analysis was more to address the kind of Land Surface Schemes commonly used as lower boundary condition for regional/global circulation models and hydrological applications, rather than the kind of permafrost models used to predict and evaluate the evolution of permafrost presence. In this kind of application there is almost no inclusion of geothermal flux (model do not have the parameterization) and the common assumption is no heat flux. Class allow to include a constant geothermal flux at the bottom, we have included a sub set of simulation to compare the effect of geothermal flux as was described in the response to general comments.

6. P8, L6. Please report mean annual air temperature and total precipitation for these years, preferably in a table format.

## Added in Table 2.

 7. P9, L15. This statement is true with respect to annual temperature oscillation. However, the effects of lower-frequency temperature fluctuations (see Figure 6) can penetrate much deeper into the soil (see Figure 2). For a proper evaluation of model sensitivity, the non-oscillation depth should be defined using simulated temperature over multiple years.

Thanks for the comment. However, in the Experiment 1 we are running in a spinup mode recycling the same year over 2000 times. After that cycling we assume that a quasi-equilibrium between climate condition and the ground thermal state was reached for a year. One of the things that we are trying to show here is the effect on the selection of climate condition to stabilize a model, so only one year is used.

8. 8. P10, L9. It is not clear what is shown in Figure 5. The figure caption says it is annual average temperature, but it clearly is not. Please explain.

We apology for the confusion here, maybe the selection of words were not the best. The label: "... Trend comparison of annual average air temperature with subtracted mean for the whole period ..." have been modified to ". . .Trend comparison of residual of the difference between annual average air temperature and...".

9. P14, L7. As I mentioned above (P9, L15), the temperature invariance in annual time scale does not necessarily indicate the insensitivity of the model to soil profile depth when lower-frequency fluctuations in atmospheric forcing are considered.

Please see response to comment #7 P9 L15.

10. P16, L12-14. In addition to temperature, important variables in permafrost environments are the depth to the permafrost table (i.e. top of the permafrost) and the thickness of permafrost, as they exert strong influences on energy and water transfer processes. It is highly desirable to evaluate the model performance with respect to these key variables.

Thanks for the comment. However, as we responded to comment 5, the kind of model that we are addressing in the manuscript are more related to the common Land

Surface Model used in Regional/Global Circulation and hydrology models. It is out of the scope of the paper to have a complete and exhaustive permafrost simulation. Finally, we try to keep it simple, the analysis already have huge number of comparison, and we prefer to maintain the selected variables showed.

11. P19, L8. I cannot agree that this study presents a 'rigorous' analysis, as it suffers from fundamental problems concerning model boundary conditions. Please revise the boundary conditions and re-run the model simulations.

We appreciate your comment. Of course that word 'rigorous' has some implications, however, we have jointly cover many source of uncertainty not analyzed before, that could affect the definition of the depth of the soil configuration and how is initialized. Again, as we pointed out in response to comment #5 and #10 the scope of the paper is in other kind of models.



Figure 1 2d-Histogram of SCD and  $h_{T^{-}}$ non-oscillation depth. Counts are normalized by the number of simulation by SCD. The black line represents the limit to reach or not the  $h_{T^{-}}$ non-oscillation conditions. Bins to the left represent SCDs that never reach the  $h_{T^{-}}$  non-oscillation condition. a) No Geothermal flux, b) Constant Geothermal flux as lower boundary condition at the bottom of the soil layers.



*Figure 2. Cumulative distribution function (CDF) of the soil temperature difference at the hT-non-oscillation depth between simulations with and without geothermal flux.* 

## **Response to Referee 2**

There are some minor changes in the response based on further updates of the manuscript.

## **GENERAL COMMENTS**

The manuscript by Sapriza-Azuri and co-authors utilizes a well-established one dimensional land-surface model (the Canadian Land Surface Scheme within the MESH) to establish 'how deep does the soil need to be' to appropriately model ground surface temperatures with permafrost to depth, and 'how long do we need' to initialize the climate for the simulation The main results from this paper are not new, although there are certainly some unique aspects to this paper. First, the fact that one needs very deep soil representation to account for permafrost is well known and unsurprisingly confirmed here. The second contribution of long time-scales of simulation is also not particularly novel, however the authors have conducted the climate simulations in a relatively innovative manner by accounting for uncertainty and variability and providing robust estimates to this. The paper as it stands requires revision to make an important scientific contribution. While a lot of good work has gone into this paper, it's unique contributions need to be highlighted. Furthermore, there needs to be proper accounting for the site selection and parametrization. It appears that the authors picked the data out of some publicly available archive and ran the simulation with little understanding of realistic boundary conditions. The authors need to carefully consider the surface conditions (vegetation, near surface soils) for this to be an appropriate and meaningful contribution. Norman Wells is not a grassland.

## **Response to General Comments:**

We thank the referee by the constructive nature of his/her criticisms. To highlight the novelty of our contribution we have restructured the introduction and added more references. We have separated the literature review of previous works into three parts (1) the need for deep soil configuration, (2) the need for proper initialization, including the incorporation of uncertainty and the reconstruction of past climate time series, and (3) parameter uncertainty.

### We pointed out in the manuscript the following lines:

"...Despite significant advances, as briefly outlined above, the appropriate soil configuration depth (SCD) in land surface modelling of cold regions remains an open question. This question is further complicated by the fact that parameter uncertainty is typically ignored in LSMs, and parameter values are usually collected from look-up tables based on land cover and soil maps (Mendoza et al., 2015). Related to this, there have been some previous efforts for "sensitivity analysis" of model outputs to parameters (Razavi and Gupta, 2015) but these have been mainly limited to comparisons of different cover types (e.g., Paquin and Sushama, 2015; Yang et al., 1995) with some few exceptions (e.g., Bastidas et al., 2006).

In this paper, we focus on the three inter-related aspects of LSMs, namely soil depth, parameter uncertainty, and initializations, together to address the above question. Unlike the previous studies that focus on each aspect in isolation, this study looks at their joint and individual effects. We set up a series of systematic modelling experiments with the following three objectives to (1) identify the appropriate SCD for a given LSM and location in the presence of uncertainty in model parameter values and climate conditions, (2) assess the significance of including/excluding geothermal flux as the lower boundary condition in an LSM, (3) develop an

*initialization procedure for LSMs in cold regions based on paleo-reconstructions of climate variables and statistical bootstrapping. ..."* 

## The list of reference added:

- Yang, Z.-L., R. E. Dickinson, A. Henderson-Sellers, and A. J. Pitman. Preliminary study of spin-up processes in land surface models with the first stage data of Project for Intercomparison of Land Surface Parameterization Schemes Phase 1(a), J. Geophys. Res., 100(D8), 16553–16578, doi:10.1029/95JD01076, 1995.
- Rodell, M., P.R. Houser, A.A. Berg, and J.S. Famiglietti, Evaluation of 10 Methods for Initializing a Land Surface Model. J. Hydrometeor., 6, 146–155, https://doi.org/10.1175/JHM414.1, 2005. Shrestha, R., and P. Houser, A heterogeneous land surface model initialization study, J. Geophys. Res., 115, D19111, doi:10.1029/2009JD013252, 2010.
- Mendoza, P. A., M. P. Clark, M. Barlage, B. Rajagopalan, L. Samaniego, G. Abramowitz, and H. Gupta. Are we unnecessarily constraining the agility of complex process-based models?, Water Resour. Res., 51, 716–728, doi:10.1002/2014WR015820, 2015.
- Bastidas, L. A., T. S. Hogue, S. Sorooshian, H. V. Gupta, and W. J. Shuttleworth, Parameter sensitivity analysis for different complexity land surface models using multicriteria methods, J. Geophys. Res., 111, D20101, doi:10.1029/2005JD006377, 2006.
- Razavi, S., and H. V. Gupta, What do we mean by sensitivity analysis? The need for comprehensive characterization of "global" sensitivity in Earth and Environmental systems models, Water Resour. Res., 51, 3070–3092, doi:10.1002/2014WR016527, 2015.

## Regarding to surface conditions, please refer to response to specific comment #5.

## **Specific Comments**

1. P3 - line 13-15. This is out of place. Unsure as to why it is here.

Thank for your suggestion, we have removed the paragraph.

2. P3 - line 16-17 there is no doubt that deeper soil....' Yes, this is well established. The question then is why is this work being completed? Additional referencing could be provided as to this.

We appreciate your comment. We have removed those lines from the text and restructured the introduction and adding references. These change look for a better definition of the scope and to highlight the new contribution. Please refer to response to general comments to the reference added and main change in the introduction.

3. P3 - line 25 'the depth considered... generally arbitrary'. Can this statement be justified? I find it hard to believe that the work going in to establishment this depth is 'generally arbitrary'. Referencing would help.

We have removed that line from the text. Please refer to response to general comments to the reference added and main change in the introduction.

4. P3 - lines 30-34. I suggest the authors set up the paper less as a 'mystery' and with more direct language in how they are addressing the questions in the paper. I find the set up very colloquial.

Thanks for the suggestion. Those lines were removed from the texts and the introduction restructured. Please refer to response to general comments to the reference added and main change in the introduction.

5. P4 -line 8. The environment here is NOT characterized by grass. What is the influence of this on the simulation? Perhaps it is very little, but regardless, and appropriate upper boundary needs to be established here.

We agree with the referee and regret that the landcover was misrepresented in the original manuscript. Having a large-scale modelling approach in mind, the dominant landcover in a pixel of 10\*10 km2 was named grassland. The confusion here was due to the Land Cover map used in this analysis that came from a reclassification of a land cover map from a bigger area for the Mackenzie basin, where shrubs, grass and other types of land covers were grouped together in a single unit, unfortunately named grassland. In addition, the original pixels were upscaled and only the dominant land cover type was picked. We fixed this problem in the writing of the revised manuscript. We have corrected the land cover type of this specific location and added a complete description of its vegetation and canopy based on the site description reported in Smith et al., (2004). The analyses and results didn't need to be changed; the reason is as the canopy parameters were perturbed by a Monte Carlo analysis, we have not used a specific land cover type based on a look-up table. The range of variation covered most of possible land cover types present in the area. As an aside, we mention that our analyses showed that regardless of parameter values, a deep soil configuration would be needed in large-scale modelling of cold regions.

6. P5, line 2 - The paragraph starts a bit awkwardly and there is no real justification as to WHY this site was chosen. There is historical data here, but there is elsewhere as well.

We have changed the start of the paragraph as follow: "Annual soil temperature profiles are available based on the maximum and minimum daily average of soil temperature at several borehole locations in the Mackenzie Valley, administrated by the Geological Survey of Canada (Smith et al., 2004). . . ." The selection was made on the availability of data and, of course other places could be selected. As future work the plan is to generalize to other locations as was pointed out in the conclusion.

7. the "Back to the past" language is again colloquial. I am not sure that this type of phrasing will be adopted in the scientific community and I would suggest the authors adjust their language to be one that is more technical.

*Thanks for the suggestion. We have changed 'Back to the past" to "Paleo-Reconstruction".* 

8. Figure 4 is nicely set up and I am wondering if Table 1 can be described in a more technical way or in a figure format as it is repetitive and as a reader not particularly helpful. There is an obvious sequence here than can simply be described.

We have changed Table 1 to a figure format. The Figure 5 has the model discretization.

9. I am unsure as to how the parameters in Table 2 were given their upper or lower bounds.

Yes, there was a Monte Carlo sampling with a uniform distribution, but LAI, minimum LAI, albedo, etc., to me seem as if they are incorrect for the environment. Please more carefully consider the rationale for this parametrization scheme and provide the reader with an understanding as to which one of these parameters is the most important for the setup and simulation. The rational here was to have more flexibility in the parameter range so, the result could be more robust about of what does matter in norther places (climate, soils depth or parameters). The parameter range cover mainly most of the land cover presence in that area from. To clarify this point we have added the following lines. . . ". . . The range of the canopy parameters values represent different vegetation cover that are present in the area based on the look-up table from CLASS user manual (Versegey, 2009). ..."

10. P10, line 3. Please provide a reference to the end of the first sentence

We have added the following reference: Yang, Z.-L., R. E. Dickinson, A. Henderson-Sellers, and A. J. Pitman (1995), Preliminary study of spin-up processes in land surface models with the first stage data of Project for Intercomparison of Land Surface Parameterization Schemes Phase 1(a), J. Geophys. Res., 100(D8), 16553–16578, doi:10.1029/95JD01076.

11. I have no real issue with the presentation of the results. As mentioned, a lot of thought and time went into the setup here and certainly a lot of computational resources were applied. I do, however, encourage the authors to highlight their scientific contribution here. The result of deeper soil configurations has been well defined for over a decade (or longer?) now. I believe that there is more value in exploring (appropriate) parameter sensitivity and the generation of relevant climate conditions. There were a lot of realizations here, but I am not sure that the authors have detailed the importance of these runs. What clear guidance can the authors provide other groups working in cold environments.

We appreciate your comment. We have restructured the introduction in a way to better highlight the main contribution of this work. Please see response to general comments. We have added to the Discussion and conclusion section the following lines in relation to reconstruction of past climate time series: ". . . An important remark here is that the effect of stochasticity in the reconstructed time series is minimal, so what is important is to reproduce historical (low frequency) trends. ... " The recommendation are detailed in the Discussion and Conclusion section and they are: (a) Minimum soil depth of 20 m (b) Initialization in two stages: i. First stage spin-up using a single average year to reach quasiequilibrium condition on fluxes and state variables. ii. Reconstruction of past climate time series, to allow the model evolve over time on the time period preceding the period of records as to be able to simulate current conditions. iii. Recognize the parameter uncertainty.

# List of main change in the manuscript:

- Last paragraphs of the Introduction to better reflex the objective and the novelty of the paper.
- Correction of the description of the land cover
- Table 1 represented as Figure 5
- Table 1 added that describe the temp and precip for each climate year
- New section describing the lower boundary conditions
- We include in the analysis the incorporation of ggeo flux as lower boundary condition at bottom of the soil layers
- New result section that describes the effect of include or not ggeo flux. Two new figures that show those results.
- Figures from result section -Initialization by Paleo-Reconstructions that compare SCD and RMS were grouped in one figure (Figure 15a,b)
- Update in conclusion including new results.

# On the Appropriate Definition of Soil Profile Configuration and Initial Conditions for Land Surface-Hydrology Models in Cold Regions

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**Abstract.** Arctic and sub-arctic regions are amongst the most susceptible regions on Earth to global warming and climate change. Understanding and predicting the impact of climate change in these regions require a proper process representation of the interactions between climate, the carbon cycle, and hydrology in Earth system models. This study focuses on Land Surface Models (LSMs) that represent the lower boundary condition of General Circulation Models (GCMs) and Regional

- 15 Climate Models (RCMs), which simulate climate change evolution at the global and regional scales, respectively. LSMs typically utilize a standard soil configuration with a depth of no more than 4 meters, whereas for cold, permafrost regions, field experiments show that attention to deep soil profiles is needed to understand and close the water and energy balances, which are tightly coupled through the phase change. To address this gap, we design and run a series of model experiments with a one-dimensional LSM, called CLASS (Canadian Land Surface Scheme), as embedded in the MESH (Modélisation
- 20 Environmentale Communautaire Surface and Hydrology) modelling system, to (1) characterize the effect of soil profile depth under different climate conditions and in the presence of parameter uncertainty, (2) assess the effect of including or excluding the geothermal flux in the LSM at the bottom of the soil column, and (3 and (2) develop a methodology for temperature profile initialization in permafrost regions, where the system has an extended memory, by the use of paleo-records and bootstrapping. Our study area is in Norman Wells, Northwest Territories of Canada, where measurements of soil temperature profiles and
- 25 historical reconstructed climate data are available. Our results demonstrate <u>a dominant rolethat the adequate depth of soil</u> profile in an LSM varies for <u>parameter warmer and colder conditions and is sensitive to model parameters and the uncertainty</u>. that is often neglected in LSMs. Considering such high sensitivity to parameter values and dependency on the climate condition around them. In general, however, we show that a minimum <u>depth</u> of 20 meters of <u>soil</u> profile is essential to adequately represent the temperature dynamics. We further show that our proposed <u>Our results also indicate the significance of model</u>
- 30 initialization procedure is effective and robust to uncertainty in paleo-climate reconstructions and that in permafrost regions and our proposed spin-up method requires running the LSM over more than 300 years of reconstructed climate time series are needed for proper model initialization.

#### **1** Introduction

Arctic and subarctic regions are amongst the most susceptible on Earth to climate change (IPCC 2013; Hinzman et al., 2005).

- 5 For example, shrub expansion into the tundra regions (Sturm et al., 2001), permafrost thaw (Connon et al., 2014; Rowland et al., 2010), and glacier retreat (Marshall 2014) are some of the current manifestations of climate change. All these changes are triggered by the interaction of climate, the carbon cycle and hydrology in response to global warming (Schuur et al., 2015). These effects are expected to be exacerbated due to global warming trends in the coming years (IPCC 2013; Slater and Lawrence 2013; Lawrence and Slater 2005). Therefore, being able to evaluate and assess the impact of climate change in cold
- 10 regions is a primary concern for the scientific community, stakeholders and First Nations communities in northern regions. The significance of this problem in Canada has led to the creation of the Changing Cold Regions Network (DeBeer et al., 2015; www.ccrnetwork.ca), which aims to provide improved science and modelling to address these concerns. Earth system models are essential tools for evaluating the impacts of climate change. At global and regional scales, General Circulation Models (GCMs) and Regional Climate Models (RCMs) are used to simulate climate change evolution. Land
- 15 Surface Models (LSMs) are used with GCMs and RCMs (coupled or offline) to represent the hydrological processes associated with the lower boundary condition of the atmosphere. These models typically represent the coupled energy and water balance in the soil, based on numerical solution of the Richards' equation and using a relatively coarse vertical discretization. In general, a standard soil configuration with a depth of no more than 4 meters is used in all LSMs that are commonly
- 20 configuration depth in LSMs implemented in some GCMs). The typical boundary conditions to solve the energy and water balance in the soil column are: (1) the exchanges with atmosphere at the top, (2) no lateral exchange of water or energy with the surrounding grids (only vertical fluxes), and (3) no heat flux at the bottom of the soil. For moderate climate conditions and at the spatial <u>scales</u>seale on which these models are commonly applied, the above depth

implemented in GCMs and RCMs (see for example the comparison made by Slater and Lawrence (2013) for the soil

and boundary conditions are <u>commonly deemed to be</u> sufficient to capture the intra-annual variability in the energy and water

- 25 balance. However, for cold regions, where the energy balance is closely related to the water balance through the phase change (Woo 2012), deeper soil configurations and more representative boundary conditions are needed. A deeper soil profile in a model can result in a more accurate process representation as it allows the heat signal to propagate through the soil-to deeper soil layers and hence avoids erroneous near-surface states and fluxes, such as overheating or over-freezing during summer and winter, respectively (e.g., Lawrence et al., 2008; Stevens et al., 2007). Deeper soil/rock configurations, however, have longer
- 30 system memories, and as such, particular care should be taken to define the initial conditions for the subsurface system. An alternative to modelling a deeper soil profile is the incorporation of a <u>rigorousgeothermal heat flux as the</u> lower boundary condition <u>that adaptively changes with time and includes a geothermal heat flux to the soil</u> (Hayashi et al., 2007). <u>Developing</u>

and incorporating a dynamic lower boundary condition is, however, impracticalHowever, in most case due to lack of adequate data; in additionpractice, the geothermal heat flux is usually ignored in LSMs, as its effects on temperature dynamics within the upper 20-30 meters of soil are considered negligible on century time scales (Nicolsky et al., 2007). not included in models due to lack of data.

- 5 The aforementioned challenges and shortcomings have been recognized by the climate, permafrost, and hydrology community. For climate models, Slater and Lawrence (2013), Alexeev et al. (2007), Nicolsky et al. (2007) and Stevens et al. (2007), have disputed the validity of GCM future projections due to the shallow soil profile depth in LSMs for the reasons stated above. There <u>have been studiesare however examples</u> of how the spatial distribution of permafrost is improved by including deeper soil configurations in <u>ana</u> LSM. For example, Paquin and Sushama (2015) <u>considered</u>, <u>applied the Canadian RCM</u>, <u>which</u>
- 10 uses Canadian Land Surface Scheme (CLASS) (Verseghy, 1991) as the LSM, for the arctic region, and by considering a 65<u>meter-m</u> deep soil configuration for the arctic region with a spin-up period of 200 years through recycling the 1970-1999 period in the Canadian RCM, which uses Canadian Land Surface Scheme (CLASS) (Verseghy, 1991) as the LSM, and showed an<del>,</del> they improved spatial distribution of permafrost-in cold regions. Zhang et al. (2003, 2006, and 2008) used a thermal soil model that includes soil water balance and showed the importance of considering deep soil configurations. Ednie et al. (2008)
- 15 illustrated the necessity of a suitable model initialization to properly simulate soil thermal profiles in permafrost regions. In the context of LSMs, Troy et al. (2012), simulated river basins in northern Eurasia using a 50 <u>-</u>meter-deep soil configuration with a spin-up of 500 years by recycling the 1901-2001 period 5 times. Decharme et al. (2013), who applied the ISBA model to the whole of France, concluded that an 18<u>-meter-m</u> depth was <u>neededenough</u> to properly simulate the energy and-the water balance.
- 20 <u>In addition, At a plot scale, Quinton et al., (2009, 2011) showed the importance of permafrost thaw in the hydrological model</u> response. Hayashi et al., (2007) also showed the importance of incorporating adequate lower boundary conditions to simulate the propagation of heat coupled with water flow in soils.

In light of the above, there is no doubt that deeper soil/rock configurations possess extended in LSMs must be considered for simulating the land surface hydrology in cold regions. In addition, an increase in the soil configuration depth (SCD) results

- 25 in a modelling system memories, and as such, particular care should be taken to properly define the initial conditions for the subsurface system with longer memory, requiring longer spin up periods for initialization. The presence of significant non-stationarity in climate and hydrology (Razavi et al. 2015) further complicateschallenges the process of model initialization, as it leads and necessitates the availability of long historical records in order to significant changes to the statistical properties include past non-stationarity that may affect the present state and envelope of variability of forcings (Razavi et al.
- 30 <u>2015).flux variables.</u> Due to <u>suchthis</u> non-stationarity, it may be inadvisable to initialize a model by recycling the <u>(typically short)</u> historical records (i.e., repeating the simulation over the same period multiple times and using the final model state of one run as the initial state of the next run), as implemented in Troy et al., (2012) or Paquin and Sushama, (2015); such practice, in particular, may result in serious misrepresentation of soil processes, because the significant warming trend in the historical records of cold regions leads to unrealistically warmer soil states after each cycle. Together, these reasons highlight the pressing

need for multi-century-long hydroclimatic records to include past non-stationarity that may affect the present state and flux variables. Proxy records such as tree rings can provide a vehicle to reconstruct long hydroclimatic time series, typically at annual to multi-year time scales (Razavi et al. 2016).), since there is a warming trend in temperature which results in warmer and warmer soil states after each cycle.

- 5 The sensitivity of LSMs to initial conditions and the initialization methods has been the focus of several studies (e.g., Yang et al. 1995; Rodell et al. 2005; *Shrestha and Houser 2010*). However, most of these works have focused on relatively shallow soil profiles located in areas other than cold regions. An exception is the work of Ednie et al. (2008) that illustrated the need for a suitable model initialization procedure to properly simulate soil thermal profiles in permafrost regions and applied a simplified thermal model of soil by using reconstructed past climate variables.
- 10 Despite significant advances, as briefly outlined above, the appropriate soil configuration depth (SCD) in land surface modelling of cold regions remains an open question. This question is further complicated by the fact that *parameter uncertainty* is typically ignored in LSMs, and parameter values are usually collected from look-up tables based on land cover and soil maps (Mendoza et al., 2015). Related to this, there have been some previous efforts for "sensitivity analysis" of model outputs to parameters (Razavi and Gupta, 2015) but these have been mainly limited to comparisons of different cover types (e.g.,
- 15 Paquin and Sushama, 2015; Yang et al., 1995) with some few exceptions (e.g., Bastidas et al., 2006). In this paper, we focus on the three inter-related aspects of LSMs, namely soil depth, parameter uncertainty, and initializations, together to address the above question. Unlike the previous studies that focus on each aspect in isolation, this study looks at their joint and individual effects. We set up a series of systematic modelling experiments with the following three objectives to (1) identify the appropriate SCD for a given LSM and location in the presence of uncertainty in model parameter values and
- 20 climate conditions, (2) assess the significance of including/excluding geothermal flux as the lower boundary condition in an LSM, (3) develop an initialization procedure for LSMs in cold regions based on paleo-reconstructions of climate variables and statistical bootstrapping.

Notwithstanding these facts, the depth considered and the way that initialization is set up in the literature are in general arbitrary. Moreover, the effect of model parameter uncertainty has not been considered in previous work, and only soil types

- 25 from "look up tables" and peat soils were compared (Paquin and Sushama 2015). The effect of the climate conditions used to spin up has also not been analysed. The modeller often faces challenging questions, such as: (1) Do we have to set soil depth to 20 m, 30 m or 60 m? (2) If we use 30 meters, do we need to spin up over 150, 500, or 1000 years? Do we have to use a sequence of years with different hydroclimatic conditions or one year with a particular condition? Or to go further, do we have to simulate longer historical periods by generating synthetic climatic time series based on proxy records such as tree ring
- 30 widths? What are the effects of model parameters and the uncertainty around them in the definition of the model configuration? This study is an attempt to address these questions.

## 2 Methods

To advance our understanding and modelling capability of soil moisture and energy dynamics in permafrost regions, we developed two <u>series of</u> numerical experiments for a study area located in the Northwest Territories, Canada, where observations of soil temperature at several depths and historical reconstructed climate data are available.

## 5 2.1 Study Area and Data

The experimental test case is located at Norman Wells, in the Mackenzie Valley, Northwest Territories, Canada (Figure 1). Based on the Permafrost Map of Canada (Geological Survey of Canada, 2000), the area is located in a zone of extensive discontinuous permafrost. The main-land cover is characterized by moss lichen groundcover, ericaceous shrubs, grass and black spruce and tamarack trees (Smith et al., 2004). the subsurface is formed by ice-rich silt clays. The climate of the region is subarctic, according to the Köppen climate classification (Pell et al., 2007), with an average annual mean daily temperature of -5 °C and average annual precipitation of 295 mm/year.



Figure 1: Permafrost Map of Canada and location of the area of study. Temperature soil profiles are available at the borehole P84-15 (yellow dot).

This area is selected due to the availability of both soil temperature at several depths down to 20 meters (Smith et al., 2004) and dendroclimatic reconstructions of summer air temperature (Szeicz and MacDonald, 1995). These data will be used to test the proposed methodology to define the SCD and the initialization approach.

#### 5 2.1.1 Soil Temperature Profiles

Administrated by the Geological Survey of Canada (Smith et al., 2004), annual soil temperature profiles are available based on the maximum and minimum daily average of soil temperature at several borehole locations in the Mackenzie Valley, administrated by the Geological Survey of Canada (Smith et al., 2004).- Figure 2 shows the temperature profiles for the borehole 84-1-T5 selected for our analysis. The soil temperatures were measured at the following depths (in meters) {1.0, 2.0,

10 3.0, 4.0, 6.0, 8.0, 10.0, 12.0, 15.0, 18.0, 19.6} for period 1985-2001. The active layer thickness, defined as the soil depth that encapsulates the seasonal freeze-and-thaw cycle (Woo, 2012), was also reported and varied from 1.5 m at the beginning of the period of records (1985) up to 3.0 m to the end of the period (2000), showing an increasing trend in the active layer thickness over time.



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Figure 2: Permafrost Annual maximum and minimum soil temperature profiles for the borehole 84-1-T5 located in Normal Wells. Each colour represent an individual year (1985-2000).

#### 2.1.2 Reconstructed Summer Air Temperature

Szeicz and MacDonald (1995) generated proxy climate records of average summer (June-July) air temperature based on tree rings for period 1638-1988 in north-western Canada near to Norman Wells (Figure 3). These proxy data have been previously used by other authors (Edine et al. 2008; Esper et al., 2002). For example, Edine et al. (2008) showed that the linear trend of proxy summer air temperature can be used as an approximation of the linear trend of the mean annual air temperature for the region. Following this approach, we generate a stochastic climate time series (Section 23.5.1) that follows the historical

reconstructions of mean annual air temperature based on the proxy data of Szeicz and MacDonald (1995).



10 Figure 3: Reconstructed summer (June-July) air temperature from <u>based on age-dependent</u> tree <u>ringsring modelling</u> for period 1638-1988 <u>along</u> with <u>itsa</u> 15 year moving average.

## 2.2 Design of Experiments

The methodology and experiments were designed to be carried out in two stages. In the first stage, we focus on the characterization of the adequate soil profile depth for land surface-hydrologic modelling in the permafrost regions, in relation to climate condition and model parameterization. For this purpose, we run a 1D model under a variety of soil profile, parameter,

and-climate configurations, and lower boundary conditions. This stage is referred to as "Experiment 1" in this paper.
In the second stage, "Experiment 2" we propose a method to handle the presence of non-stationarity in climate and hydrology, in order to include effects of past non-stationarity on the present state and flux variables. This method utilizes paleo-climate reconstructions to generate long, synthetic time series of climate variables for model initialization. We call this stage "Back to the present".

20 the past".

5

#### 2.3 The 1D-Model

The core of the experiments is a 1D model implemented in MESH, Environment and Climate Change Canada's community model (Pietronero et al., 2007). This integrates the CLASS LSM (Verseghy et al., 1993; Verseghy 1991), which solves coupled

energy and water balance equations for vegetation, snow and soil and their exchange of heat and moisture with the atmosphere, and WATROF (Soulis et al., 2000) or PDMROF (Mekonnen et al., 2014) to solve the horizontal flow processes for basin-scale integration. MESH discretizes the spatial domain based on regular grid cells and each individual cell is then subdivided in Grouped Response Units (GRUs) based on land cover and/or soil types. <u>MESH has been commonly used to simulate land</u>

- 5 surface-hydrology processes in many cold regions (e.g., Yassin et al. 2017; Haghnegahdar et al. 2017). The 1D CLASS model is implemented here at one grid cella point, and a unique GRU based on grass land cover was used. The upper boundary condition of the model is formed by atmospheric forcings. <u>AtNo heat flux is assumed as</u> the lower boundary condition, <u>in</u> terms of heat, we include two cases: no heat flux and geothermal flux (only in Experiment 1), and in terms of mass, we assume the water flux that reaches the bottom of <u>the soil</u> profile drains to generate base flow.
- 10 The climate forcings needed are temperature, precipitation, shortwave radiation, longwave radiation, specific humidity, wind velocity and atmospheric pressure.

#### 2.4 Experiment 1

A schematic representation of the <u>modellingmodel</u> experiment is illustrated in Figure 4. Several 1D model set-ups were implemented by a combination of (1) various <u>SCDs</u>-soil depth configuration, (2) several climate conditions selected to spin-up

15 the model, -and (3) different values for the parameters that control hydrological processes (water and energy balance), and (4) the inclusion or exclusion of the geothermal flux as the lower boundary condition.).



Figure 4: Schematic representation of the model experiment for Experiment 1. The model set-ups are defined as combinations of 5 different climate conditions, 50 randomly selected sets of parameter values within their uncertainty ranges, condition, 50 sampling
 parameters and 17 different soil configurations. Each model is then run in a spin-up mode for 2000 cycles. The last year of spin-up is taken to compute the daily annual max and min soil temperature profilesprofile and their difference is computed. At the depth at which this where such difference becomes less than 0.1 is referred to as "non-oscillation-we define the depth" or as the h<sub>T</sub>-non-oscillation condition.

2.4.1 Variable Soil Depth Configuration

10 For thisthe experiment, a series of 1D models with an-incremental <u>numbers</u> of soil layers (<u>corresponding to</u> different total soil depths) are defined. The soil configurations of the 1D models are <u>illustratedspecified</u> in <u>Figure 5Table 1</u>, and range from the standard CLASS configuration of 3 layers with a 4.1 <u>-</u>meter depth<u>-up</u> to 20 layers corresponding to a depth of 71.59 <u>meters</u>. The <u>thickness</u> width of each layer is increased exponentially for deeper soil layers.<sup>2</sup> A total of 17 different soil configurations are tested.





Fi	gure	5:
	-	_

Soil Config	№ Soil Layers	Depth of each layer [m]	
1	3	0.1, 0.25, 3.75	4.1
2	5	0.1, 0.25, 0.51, 0.91, 1.32	3.09
3	6	<b>0.1, 0.25, 0.51, 0.91,</b> 1.32, 1.72	4.81
4	7	<b>0.1, 0.25, 0.51, 0.91,</b> 1.32, 1.72, 2.13	6.94
5	8	<b>0.1, 0.25, 0.51, 0.91,</b> 1.32, 1.72, 2.13, <b>2.54</b>	9.48
6	9	0.1, 0.25, 0.51, 0.91, 1.32, 1.72, 2.13, 2.54, 2.94	12.42
7	10	0.1, 0.25, 0.51, 0.91, 1.32, 1.72, 2.13, 2.54, 2.94, 3.35	15.77
8	11	<b>0.1, 0.25, 0.51, 0.91,</b> 1.32, 1.72, 2.13, <b>2.54, 2.94, 3.35, 3.75</b>	19.52
9	12	0.1, 0.25, 0.51, 0.91, 1.32, 1.72, 2.13, 2.54, 2.94, 3.35, 3.75, 4.16	23.68
10	13	0.1, 0.25, 0.51, 0.91, 1.32, 1.72, 2.13, 2.54, 2.94, 3.35, 3.75, 4.16, 4.57	28.25
11	14	0.1, 0.25, 0.51, 0.91, 1.32, 1.72, 2.13, 2.54, 2.94, 3.35, 3.75, 4.16, 4.57, 4.97	33.22
12	15	0.1, 0.25, 0.51, 0.91, 1.32, 1.72, 2.13, 2.54, 2.94, 3.35, 3.75, 4.16, 4.57, 4.97, 5.38	38.60
13	16	0.1, 0.25, 0.51, 0.91, 1.32, 1.72, 2.13, 2.54, 2.94, 3.35, 3.75, 4.16, 4.57, 4.97, 5.38, 5.79	44.39
14	17	0.1, 0.25, 0.51, 0.91, 1.32, 1.72, 2.13, 2.54, 2.94, 3.35, 3.75, 4.16, 4.57, 4.97, 5.38, 5.79, 6.19	50.58
15	18	0.1, 0.25, 0.51, 0.91, 1.32, 1.72, 2.13, 2.54, 2.94, 3.35, 3.75, 4.16, 4.57, 4.97, 5.38, 5.79, 6.19, 6.60	57.18
16	19	0.1, 0.25, 0.51, 0.91, 1.32, 1.72, 2.13, 2.54, 2.94, 3.35, 3.75, 4.16, 4.57, 4.97, 5.38, 5.79, 6.19, 6.60, 7.00	64.18
17	20	0.1, 0.25, 0.51, 0.91, 1.32, 1.72, 2.13, 2.54, 2.94, 3.35, 3.75, 4.16, 4.57, 4.97, 5.38, 5.79, 6.19, 6.60, 7.00, 7.41	71.59

Table 1: The variable soil configuration profiles defined for the 1D model: number of soil layers, depth of each layer and total depth. Each colour <u>represents a group of in column 3 represent grouped</u> layers that areand assigned the same <u>parameter values</u>. <u>Panel (A)</u> shows all the configurations and panel (B) shows a zoom-in window-to the parameters of the previous panellayers in each group except for the first few layers. The first soil configuration (3 layers) represents and the standard CLASS first two layer for all the soil model configuration.eonfigurations (black colour).

#### 2.4.2 Climate Conditions

To account for the effect of climate conditions, years 1998 (warm), 1983 (dry), 1974 (cold), 1962 (wet), and 1945 (average) (<u>Table 1</u>) are used with <u>everyeach</u> model configuration. Each model was run <del>over</del>-five <u>times (for the five years) over</u> 2000year-long sequences, each of which comprised 2000 back-to-back repetitions of one of the above years. These five climate

10 conditions are defined based on temperature and precipitation obtained from the WATCH FD (WCH-FD) gridded data base of climate forcing (Weedon et al., 2011) for the period 1901-2001 at the location of our study area. We do not use the historical sequence of years 1901-2001 to avoid overheating effects that could be introduced due to the warming trend of the last past century.

Year	Precipitation [mm/year]	Temperature [°C]	Climate Condition
1945	396	-6.5	Average
1962	667	-5.6	Wet
1974	534	-8.3	Cold
1983	252	-7.1	Dry
1998	363	-3.6	Warm

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Table 1: Climate conditions of the five representative years used in this study.

#### 2.4.3 Parameter UncertaintyParameters

Three groups of parameters representing canopy, soil and drainage processes are perturbed within their ranges of uncertainty to analyze their influence on SCD. Table 2 describes all the parameters considered along with their lower and upper

- 20 <u>boundsintervals</u> of variation. Monte \_Carlo sampling with a uniform distribution is applied to generate a collection of 50 samples for each parameter. The range of the canopy parameter values used represents different vegetation covers that are present in the area based on the look-up table from the CLASS user manual (Versegey, 2009). To set a consistent parametrization scheme for the soil texture across the models with different numbers of layers, we grouped layers and assigned the same values to the parameters of the layers in each group. These groups are represented with different colors in Figure
- 25 <u>5.Table 1, column 3 (Depth of each layer)</u>.

Id	Name	Units	Lower Bound	Upper Bound	Description
1	LAMX	[-]	2.0	4.0	Annual Max leaf-ar ea index
2	LAMN	[-]	2.0	4.0	Annual Min leaf-area index
3	ALVC	[-]	0.03	0.06	Avg visible albedo of the vegetation when fully-leafed
4	ALIC	[-]	0.2	0.34	Avg near-infrared albedo of the vegetation when fully-leafed
5	ROOT	[m]	0.2	1.55	Root depth
6	SDEP	[m]	2.0	Max Depth	Permeable Depth
7	GRKF	[-]	0.001	1.0	Fraction of the saturated surface soil conductivity moving in the horizonal direction
8	KSAT	[m s-1]	0.0001	5.5	Saturated surface soil hydraulic conductivity
9	SAND*	[%]	0.0	100	% sand textur e
10	CLAY *	[%]	0.0	100	% clay textur e
11	ORG *	[%]	0.0	100	% material organic texture
12	ZSNL	[m]	0.05	0.5	Minimum depth to consider 100% cover of snow on the ground surface
13	ZPLS	[m]	0.05	0.5	Maximum depth of liquid water allowed to be stored on the ground surface for snow-covered areas
14	ZPLG	[m]	0.05	0.5	Maximum depth of liquid water allowed to be stored on the ground surface for snow-free areas

 Table 2: List, Parameters list description, with the upper and ranges of model parameters perturbed in this study. The values of soil lower bound interval used. For the texture parameters (\*) SAND, CLAY, and ORG (denoted by \*) sampled such that

 5
 they the sampling is made to sum to 100%.

2.3.4.4 Lower boundary conditions: The Geothermal Flux

To assess the effect of the lower boundary condition on the energy balance and soil temperature profile, an analysis was made to compare two scenarios: (1) no heat flow at the bottom of the lowest soil layer, and (2) a constant geothermal flow (called ggeo flux in CLASS). The comparative analysis was carried out for the average climatic condition (year 1945). All the 17

10 different soil configurations and 50 sets of parameter values were tested, resulting in a total of 850 model configurations to be run for scenario 2 above. For this scenario, the geothermal heat flow was set to be 0.083 W/m<sup>2</sup>, based on measurements made in a borehole in Norman Wells (Garland and Lennox, 1962).

### 2.4.5 Non-Oscillation Depth

In Experiment 1, we ran a total of  $\{(17 \text{ SCD})^*(5 \text{ climates})^*(50 \text{ parameters}) + 850 \text{ (with geothermal flux})\} = 5100\} + 4250$ 

15 model combinations. In each of these model set-ups, a 2000-year model run was performed. All the models were set with the same initial conditions and constant temperature and liquid/ice saturation soil profiles. The soil thermal profile was defined at -3.0 °C and all the soil water was defined as ice content. We assume that after the spin-up a quasi-equilibrium between the climate conditions and the ground thermal state was reached. The last cycle, a complete <u>one</u>+ year simulation, was used to

compute the annual soil temperature profiles based on the maximum (maxTsp) and minimum (minTsp) daily average of soil temperature (Figure 4). Next, we <u>computed</u> the difference between maxTsp and minTsp and <u>defined</u> define a depth (h) <u>at whichwhere</u> this difference was less than 0.1 °C. We <u>named</u> this depth h as the "non-oscillation depth" of annual soil temperature. Therefore, h, which is a function of climate condition, parameter values, and simulated soil depth, represents the

5 depth at which the soil thermal response remains invariant over <u>seasons</u>a <u>season</u>. In other words, the non-oscillation depth indicates the depth at which the SCD has not longer a significant effect on the energy balance computed by the model.

#### 2.5 Experiment 2: Back to the past

To be able to simulate the hydrology using LSMs in cold regions in the last century (period of records) and in the future, it is necessary to correctly set the initial conditions of the models. When the SCD of the model is considered to be shallow (no

10 more than 4 meters), the initialization can be easily carried out with a relatively short spin-up period (Yang et al., 1995).-However, with deeper SCDs, the memory of the system is longer, and it remembers the past climate regimes and trends. Therefore, it is necessary to run the model over an extended period of time to diminish the effect of uncertainty in initial conditions on model predictions. This is a major challenge, however, as the typical length of periods of records (say ~100 years) is not sufficient.

#### 15 2.5.1 Methodology of Reconstruction

To overcome <u>the above</u>this challenge, we stochastically generated past climate variables, back to year 1678 based on proxy data of reconstructed summer air temperature described in section 2.1.2. To this end, we applied a block bootstrapping technique (Razavi et al., 2015; Politis and Romano 1994).

The stochastic time series of climate variables were generated as follows:

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(1)

First, we assumed that the reconstructed summer air temperature by Szeicz and MacDonald (1995) can be used as proxy data to derive the past trends in air temperature. The historical temperature trend back to 1678 ( $T_{Htrend}$ ) was estimated by first computing the moving average with a window of 15 years and then subtracting the moving average from the annual time series. Figure <u>65</u> compares both temperature trends (15-year moving average) obtained from WCH-FD data and tree <u>ringsring</u> for the same period, showing <u>a reasonablegood</u> agreement, with a Pearson correlation coefficient of 0.66. The existing discrepancy may be in part due to a lack of consideration of longer-term variability (longer than annual) in the reconstruction of the time series, an issue explained in Razavi et al.<sub>27</sub> (2016).



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Figure 6: Trend comparison of <u>the</u> annual average air temperature <u>data (15-year moving average) based on</u><del>with subtracted mean</del> for the whole period for WCH-FD and tree <u>-</u>ring<u>-based reconstructions</u>-data.

- (2) Then, we decomposed the WCH-FD temperature time series (6<u>-hourly-hour</u> time resolution) for the period 1901-2001 into its trend (based on the 15-year moving average) and its seasonality component ( $T_{seas}$ ).
  - (3) Next, we applied the block bootstrapping technique with a block size of 5 years to  $T_{seas}$ . We sampled 45 blocks of 5 years so as to generate a time series long enough to cover the 1678-1901 period.
  - (4) To finish the reconstruction reconstructions of the 6-hourly time resolution of temperature data, we added  $T_{seas}$  to the  $T_{Htrend}$  from step (1).
    - (5) The other six climate variables needed by MESH to run were precipitation, shortwave and longwave radiation, specific humidity, wind, and atmospheric pressure. They were generated by applying the block bootstrapping with the same time indexes of the temperature blocks (step 3). In this way, we maintained the interdependence between all the climate variables.
- 15 (6) Finally, we generated 100 realizations of the climate variables for period 1678-1901. The complete climate time series of 1678-2000 was finally obtained by combining the generated ones and the WCH-FD data for 1901-2000. Figure <u>76</u> shows the mean annual temperature <u>of these 6-hourly time series</u> generated with the methodology presented.



Figure 7: Combined air Temperature time series generated using the block bootstrapping technique and WCH-FD. The time series is divided in two periods. From 1678-1900 the temperature and the other 6 climate variables wereare generated using the block bootstrapping with a block of 5 years assembled on tree-ring-based reconstructions. The. In the figure are shown 100 realizations (grey lines), the 5-95 % confidence-5 % confident interval (red lines), and the average of the ensemble (black line) are shown. In). The second period (1901-2000) the climate variables variable are used directly from the WCH-FD database.

#### 2.5.24 Evaluation procedure

We used the 100 realizations of the climate variables of section 2.5 to run the models with the <u>50100</u> parameter sets and 17
SCDs used before. For the initial conditions, we used the stabilized model outputs obtained from the 2000 cycles for the-year 1945 (average with respect to temperature and precipitation). Finally, the simulated soil temperature profiles obtained were compared with the observed <u>data (see section 23.1.1)</u> by computing the root mean <u>squaredsquare</u> error (RMSE).) to evaluate if it is possible to reproduce the soil thermal behaviour. The RMSE was computed by calculating, for each individual simulation of the annual soil temperature profile, the annual minimum and maximum daily soil temperature at the same location as that at which the observed soil temperature was measured (section 3.1.1). To have a more general view of the model performance in reproducing the observations (1985-2000), individual maximum and minimum soil temperature profile of simulated and observed <u>data</u> were used to compute a-RMSE for each individual year. Then all the values of RMSE obtained.

#### **3** Results

#### 20 **3.1 Soil Configuration Depth**

Using the experiments proposed in Experiment 1, we explored the combined and individual effects of climate, parameters and SCD on the non-oscillation depth of in the annual soil temperature profile. Figures 7, 8, 9 and 109 summarize these analyses

one (maximum and minimum) for each year, were averaged to obtain the overalla unique RMSE of corresponding simulation.

as 2D histograms: (SCD,  $h_T$ -non-oscillation) (Figure  $\underline{87}$ ); (years,  $h_T$ -non-oscillation) (Figure  $\underline{98}$ ); and (parameter sample group,  $h_T$ -non-oscillation) (Figure  $\underline{109}$ ). Notably, Figure  $\underline{87}$  shows that for SCDs less than 15 m, there is a high probability that the  $h_T$ -non-oscillation condition is never reached, <u>regardless</u> independently of the parameter <u>valuesvalue selection</u> and the climate conditions (year). For SCDs of greater than 20 m, the  $h_T$ -non-oscillation condition is always reached, with a higher





Figure 8: <u>The</u> 2d-Histogram of SCD and  $h_T$ -non-oscillation depth. Counts are normalized by the number of <u>simulations per</u> <u>eachsimulation by</u> SCD. The <u>thick</u> black line <u>separatesrepresents</u> the <u>frequencies of reaching/limit to reach or not reaching</u> the  $h_T$ -10 non-oscillation conditions: Bins to the left <u>of this line are for simulationsrepresent SCDs</u> that never <u>reachedreach</u> the  $h_T$ -nonoscillation condition.

The variability observed in  $h_T$ -non-oscillation depth for each SCD is, in general, mainly explained by the <u>variation in</u> parameter valuesparameters rather than the year selected (i.e., climate condition) for spinning up the modelspin up (Figure <u>98</u> and <u>109</u>).



Figure 9: The 2d-Histogram of climate condition (years) and h<sub>T</sub>-non-oscillation depth. Counts are normalized by the number of simulations per each simulation by year. The <u>thick</u> black line <u>separates the frequencies of reaching/represent limit to reach or not</u> reaching the  $h_{T}$ -non-oscillation conditions; Bins to the <u>left of this line are for simulations</u> lefts represent 1d model that never

5 <u>reached</u> reach the  $h_T$ -non-oscillation condition.



Figure 10: The 2d-Histogram of parameter and h<sub>T</sub>-non-oscillation depth. Counts are normalized by the number of 10 simulations by parameter sample. The thick black line separates the frequencies of reaching/represent limit to reach or

not <u>reaching</u> the  $h_T$ -non-oscillation conditions: Bins to the <u>left of this line are for simulations</u> that never <u>reached</u> reached the  $h_T$ -non-oscillation condition.

From the previous results, it seems clear that we need at least an SCD of greater than 20 metersm to adequately represent the temperature dynamics of permafrost. This conclusion is supported by the fact that the soil temperature at which  $h_T$ -non-

5 *oscillation* condition is reached remains invariant throughout the annual cycle. The distribution of this "non-oscillating temperature" is shown using 2d-histograms in Figure <u>1140</u> and <u>1244</u> with respect to the SCD and the climate conditions (years), respectively.

Figure <u>1140</u> shows that for shallow <u>SCDsSCD</u>, from 3.1 m up to 16 <u>metersm</u>, there is a tendency to obtain a warmer soil temperature such that the permafrost is thawed. In the SCDs with the depth of 16 <u>metersm</u> and deeper, there is much more

10 variability in the soil temperature (between -6 °C to 0 °C), but with a high probability that the soil temperature at *h<sub>T</sub>-non-oscillation* condition is between -3 °C to -2.5 °C. In Figure <u>12</u>44 the effect of the climate condition can be appreciated. The main <u>behaviouralbehaviour</u> difference is for the warmest year (1998) when, as expected, the warmest soil temperatures at the *h<sub>T</sub>-non-oscillation* condition occur. As for the other climate conditions, the behaviours are quite similar and in general have a range of variation between -7°C to 0.5 °C. As before (Figure <u>1140</u>), the probability distribution for each climate condition is





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Figure 11: <u>The</u> 2d-Histogram of SCD and temperature at  $h_{T}$ -non-oscillation depth. Only <u>SCDs</u>SCD that have reached the  $h_{T}$ -non-oscillation condition are included. The black line represent the 0 °C temperature.



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Figure 12: <u>The</u> 2d-Histogram of climate condition (years) and temperature at  $h_T$ -non-oscillation depth. Only <u>SCDsSCD</u> that have reached the  $h_T$ -non-oscillation condition are included. The black line represent the 0 °C temperature.

#### 3.2 Lower boundary conditions

Figure 13 shows the 2D histograms (SCD, h<sub>T</sub>-non-oscillation) for simulations where the geothermal flux is not included
(Figure 13a) and with the geothermal flux (Figure 13b) in the lower boundary condition. On both experiment same number of models are run ({(17 SCD)\*(1 climate year)\*(50 parameters)}=850). The visual comparison indicates that the histogram differences are negligible in most cases. Some marginal differences suggest, as expected, that the models with a constant geothermal flux result in slightly warmer soil profiles and slightly deeper non-oscillation depth compared with no-heat flow counterparts. These differences are small, and the results confirm that more than 20 meters of soil depth are needed to

15 adequately represent the temperature dynamics. To further compare the two scenarios, Figure 14 shows the cumulative distribution function of the differences in soil temperature at the non-oscillation depth of the two simulation scenarios (with and without geothermal flux at the bottom). As shown, the temperature difference of the two scenarios is small in most simulations, and is within +/-0.15°C in approximately 60% of simulations.



Figure 13: 2d-Histogram of SCD and h<sub>T</sub>-non-oscillation depth. Counts are normalized by the number of simulation by SCD. The black line represents the limit to reach or not the h<sub>T</sub>-non-oscillation conditions. Bins to the left represent SCDs that never reach the h<u>T</u>-non-oscillation condition. a) No Geothermal flux, b) Constant Geothermal flux as lower boundary condition at the bottom of the soil layers.





### 3.3 Initialization by Paleo-Reconstructions going Back to the Past

- 5 The previous <u>sections havesection has</u> shown evidence that regardless of the climate conditions, <u>parameter uncertainty</u>, and <u>lower boundary conditions and model parameters</u>, we need to have an SCD that is deeper than 20 <u>metersm</u>. However, such depths make the model initialization problem more challenging. Here, we show the results <u>offrom driving</u> our 1D <u>models with different SCDs and parameter values when driven by model (varying SCD and parameters) applying</u> a set of 100 <u>tree-ring</u>, <u>bootstrap-based</u> reconstructed climate forcing realizations <u>for period by going back to the past (1678-2001.)</u>.
- 10 Figure 15a shows A general overview of the model's ability to reproduce (or not) the observed soil thermal behaviour between years the year 1985 to 2000, by plotting the is presented in Figure 12. We plot a 2d histogram of that compares the SCD and against the RMSE. The colours represent the probability of a RMSE value for a specific SCD represent the frequency distribution of RMSE values; the variability in this distribution that includes the effects effect of different parameter values and climate forcing realizations. The RMSE was calculated as described in section 2.5.2+. In general, for the shallower SCDs (say
- 15 less than 15 meters). SCD, the RMSE tends to be larger with a higher variability (1.5 °C to 9.0 °C). The frequency distributions for As deeper SCDs become, however, the behaviour becomes quite similar regardless of the depthuniform for all SCDs, with an RMSE range of RMSE between 1 °C to 5 °C with a high density and a higher probability that the RMSE is around 1.5 °C to 3.0 °C.

20	(a)	<u>(b)</u>	
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Figure 15: 2d-<u>histograms</u>histogram of SCD and RMSE for period 1985-2000 when initialized by. All the <u>bootstrap-based paleo-</u> reconstructions. In plot (a) all the simulationsSCD are included, but in plot (b) only the simulations that regardless if the SCD have reachered the *h*<sub>T</sub>-non-oscillation condition are -

In the previous comparison (Figure 12), all the SCDs were included.

In the histogram of Figure 15a, we included all the simulations, even if in a simulation from Experiment 1, the soil temperature at the  $h_{P}$ -non-oscillation conditions hadeondition has not been reached. -for an individual SCD. In-Figure 15b, however, presents 13 we compare only the simulations SCDs that have reached the  $h_{P}$ -non-oscillation condition with the RMSE, in a 2d-

10 histogram. For the SCDs that have reached the non-oscillation condition. As can be seen, the histograms of Figures 15a and 15 b become the same for SCDs are deeper than 16 meters .0 m, the behavior is quite similar. to those obtained in Figure 12. This is explained by the fact that almost all the simulations with SCDs that are sufficiently deep (>16.0 m) reach the *h<sub>T</sub>*-*non-oscillation* condition.

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#### Figure 16 shows a series of histograms of RMSE values generated by

## Figure 13: 2d-histogram of SCD and RMSE. Only the SCD that reached the *h<sub>T</sub>-non-oscillation* condition are included.

To identify the relative effect of the different realizations of the reconstructed past climate series, each of which for a different set of parameter values. This figure is designed to assess the relative effects of the variation in the different reconstructed climate time series (a manifestation of data uncertainty) and variation in model parameters (a manifestation of parameter

20 <u>uncertainty</u>) on the variability of RMSE. obtained in RMSE, we plot a 2d histogram comparing RMSE and parameter sample (Figure 14). Here, we are only taketaking into account the simulations SCDs that have reached the *hr*-non-oscillation condition.

<u>As can be seen, the range of variation Results in RMSE Figure 14 show that for each set of parameter valuesset the RMSE is quite narrow compared to the union of all the ranges across the different sets of parameter values.</u> Therefore, two points can be made here: (1) the variability observed obtained in RMSE in RMSE can be Figure 13 is mainly attributed mainly to the parameter variations, indicating the significant role of parameter uncertainty-variability, and (2) the effect of stochasticity in

5 the reconstructed time series for the period preceding the period of records is minimal on the model performance in the evaluation periodis minimal. This result reinforces the importance of adequately reproducing the long term trends in data used for model initialization.



# 10 Figure <u>16:</u>14: 2d-Histogram of parameter sample and RMSE. Only the <u>simulations</u> that reached the *h<sub>T</sub>-non-oscillation* condition are included.

#### 4 Discussion and conclusions

This study concludes that for permafrost regions, deeper soil configurations in LSMs are needed than commonly adopted, to be able to correctly simulate the coupled energy and water balance in the subsurface. This conclusion can be extended to all
earth system models that incorporate <u>ane LSM withand</u> permafrost representation. While this conclusion has <u>also</u> been pointed out by other authors, this work <u>investigated incorporates a rigorous analysis of the individual and jointSCD</u>, which evaluates the effects of parameter uncertainty, total soil depth, <u>lower boundary conditions (geothermal flux)</u>, and climate conditions.

Further, this work addresses the uncertainty in the reconstructions of past climate for model initialization and also the question of and how the initialization should be carried out.

Our analysis shows that the minimum total soil depth should be around 20 m. This value is independent of the <u>reliable depth</u> <u>considering uncertainty and variability in model parametersparameter selection</u> and climate <u>conditions</u> used to

5 initialize the model, and whether or not the geothermal flux is included as lower boundary condition. The metric defined to assess this depth was based on a depth at which the annual maximum and minimum of daily soil temperature are equal, referred to as *h<sub>T</sub>*-*non-oscillation* condition in this paper. This depth represents a <u>thermallythermal</u> stable condition and ensures that the lower boundary condition is deep enough to accommodate a no-heat-flux <u>or constant-heat-flux</u> boundary condition at the bottom of the soil configuration. An alternative, not explored here, is to consider a variable heat flux at the bottom boundary

#### 10 and reduce the total SCD.

The variability observed in the <u>value</u>values of  $h_{T}$ -non-oscillation across the many simulations we conducted was mainly explained by <u>parameter perturbations</u> the parameters rather than the climate conditions. This <u>assessment was the case</u> result is valid for the both <u>sets of analyses in Experiments</u>: Experiment 1 and <u>2</u>-Back to the Past,' the long term simulation using stochastic reconstructed climate time series. This emphasizes the importance of recognizing and addressing parameter

- 15 uncertainty and raises serious issues with the common practice in using LSMs with GCMs, where model capabilities are constrained by using hard coded parameters determined based on look-up tables (Mendoza et al., 2015). We argued that model spin-ups that are based on recycling of the 20th century data should be avoided, as simulations on back-to-back repetitions of any, or a sequence of years with a warming trend will result in an unrealistically warm soil temperature profile.should be avoided. Instead, we recommend a two-stage procedure to setto define the initial conditionseondition of the
- 20 model: in stage 1 (as conducted in , we recommend to proceed in two stages: Experiment 1), we spin-up the model on an "average" year, and then in stage 2, we further run the model on a multi-century long bootstrap-based paleo-reconstructions can be used to the beginningexplore sensitivity of the period of record. soil depth and parameterisation and then "back to the past" to generate the relevant initial conditions. This should always be the case when deeper SCDs are going to be implemented in a LSM in cold regions. The first phase has a stabilizing effect and stabilization assures that coherent state variables and
- 25 fluxes are set before subsequent initialization of the model. This is an important step, as the majority of the LSMs have <u>a large number of statemultiple</u> variables and fluxes to initialize (e.g., CLASS has 17). For the first step, we recommend selecting an average year in term of air temperature and precipitation, and recycle that year <u>in simulation untilup</u> to the point that stabilization in-soil temperature profile is <u>stabilizedreached</u>. Then, in the second step, we recommend <u>usinggenerating</u> multicentury long time series of climate variables generated records based on the procedure proposed in this study. The proposed
- 30 procedure reconstructspaleo reconstructions, and running the model of step 1 on that. This will let the model evolve over time on the time seriesperiod preceding the period of temperature records as to be able to simulate current conditions. Here, we reconstructed past climate using proxy recordsdata of summer temperatures derived from tree rings and generates the concurrent time series of other climate variables such as precipitation by, applying block -bootstrapping on historical records. We were able to reproduce quite well the past trends of summer temperature and we included the effect of uncertainty in the

climate time series by generating 100 realizations. An important remark here is that the effect of short-time scale (e.g., annual) fluctuations in the reconstructed time series used for initialization was minimal, while low frequency trends were important. The length of reconstructions required for proper initialization is longer for deeper SCDs. The number of years that are necessary to go back to the past will be a function of how deep is the SCD chosen. Deeper SCDs retain more memory of past

5 climate and require longer spin-up periods.

Finally, we envision our future work being directed to generalize the results obtained here by extending the analyses to other <u>locationsplaces</u> where observations (of <u>past elimate and soil profile temperature and past elimate</u>)-are available. Furthermore, implementing a variable <u>SCD</u>, increasing the number of parameters sampled to better explore the parameter space, and comparing several model parametrizations, including the effect of heat flux as a lower boundary condition at the bottom of the

- 10 soil. For application in regional and global models may, the SCD can be investigated, variable as also was proposed by Brunke et al. (2016) for in the Community Land Model version 4.5. However, the overall, computational burden is a bottleneck for large-scale simulations. To address the computational issues, surrogate modelling strategies that develop cheaper-to-run statistical or mechanistic surrogates of the original models may be explored (Razavi et al. 2012), and also an endeavour may be made by the cryosphere community to generate a unified gridded data set for the last millennium or so (1000 years back to
- 15 the past) (Jungclaus et al., 2016; Landrum et al., 2013; Schmidt et al., 2011) that approximates soil temperature profiles with adequate soil depth, considering and the effect of parameter uncertainty via generating by considering different ensembles of approximations.

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