Dear Anonymous Referee #2,

Thank you very much for your review and your constructive comments. The entire text of your comment is shown (RC) together with our authors' responses (AR).

Kind regards, Niccolò Tubini – on behalf of all authors

Remarks

1. **RC**: In the abstract, the authors state that "the nonlinear behaviour of enthalpy as function of temperature can prevent thermal models of snow, ice and frozen soil from converging to the correct solution" but do not provide a description or citation for this claim. Reading further into the paper, this claim is based on a survey of experts, cited as personal communications. I appreciate the point that the authors are trying to make and it is indeed an important advance of the NCZ method, but the phrasing could be improved throughout for clarity.

   AR: The description and citation is contained in the introduction and in lines 115-128 of the discussion manuscript. Later, in lines 126-148 we discuss the three forms of the governing equation and the numerical drawbacks that arise when they are solved.

2. **RC**: The main advance that this paper reports is the implementation of a novel algorithm for solving phase change problems. However, the pseudocode included in the paper is not very useful as opposed to a well-documented version of the code that is easy to run. While the code is released publicly, the github documentation is unclear, written in java (for good reason), and not approachable. I was hopeful that I could run the code but that did not seem feasible.

   AR: The pseudocode has been rewritten in a clearer way. We also increased the documentation of the code which is provided on Github in the Jupyter_Notebook directory, 00_FreezeThaw.ipynb. Our code must be run inside the OMS3 Console (David et al. 2012) or using the Dockerized version. OMS3 was chosen because it allows to use ancillary components for radiation, calibration and other components. For setting up the environment there are a certain number of steps to be performed which are described on the first Github page.

   The code is written in a clear Java where classes have an extensive name which refers to what the classes do, but we are aware that it could not be so easy to understand the runtime combination in which the classes are used.

   The executable of the version used in the paper are available under Zenodo. For executing them once installed OMS3 please follow the instructions contained in the Jupyter_Notebook /_README.ipynb and Jupyter_Notebook /00_FreezeThaw1D.ipynb for all the details about the simulation input and parameters.

   We added these details also in the revised manuscript in Section Code availability

3. **RC**: This paper neglects to cite or engage with Schoof and Hewitt (2016), who derive a general enthalpy model for phase change. Schoof and Hewitt (2016) follows on from Aschwanden and Blatter (2009) and Aschwanden et al. (2012), where only the first paper is referenced in the manuscript. Beyond the numerical implementation of the NCZ method, it is not clear what this paper adds beyond Schoof and Hewitt (2016) in terms of physical understanding and the role of enthalpy in phase change.

AR: We inserted citations to the above papers and also Hewitt and Schoof 2017, where the authors present the numerics of their algorithm for the first time. The mathematical description of glaciers using enthalpy has enthalpy in common with our permafrost model, but the other aspects of the physical problem differ. For example, heating is generated by internal friction of the flowing ice. We have only external forcing driving our physics and, at present, no fluid flow. What we improved with respect to the shared challenge of enthalpy is the treatment of its nonlinear dependencies on temperature. Specifically, the derivative of enthalpy is non monotonic and cannot be integrated by a traditional Newton algorithm and a globally convergent Newton method has to be used instead. Many of these methods were implemented in the past by using “tricks” (Paniconi et al., 1994, Dall’Amico et al. 2011,) because a safely convergent method was unavailable. The more evident result is that we do not need to track where the front between ice and water (cold and temperate ice) is. With NCZ, we do not need a section like the Section 3 in Schoof and Hewitt 2016, which is required to preserve properly the mass in absence of an appropriately convergent algorithm, and we do not need to use an algorithm to solve the energy equation like that one presented in Appendix A.

Specific comments

1. **RC**: I suggest replacing the title with: “An undated numerical method for solving the heat equation with phase change".

   AR: We thank the reviewer, but we prefer to stick with our original title. It is long but, in our opinion, clearer in conveying the usefulness of out method.

2. **RC**: line 105: is theta_s defined anywhere?

   AR: We have added the definition of theta_s

3. **RC**: line 115: the kink in the sfcc only matters if the authors take the derivative, which is not required! I am not sure about the value of this `straw-man' argument about the three 'identical yet different' representations of the heat equation. First off, the language is unclear, so it is opaque as to what method the authors will actually use.

   AR: To solve a nonlinear system it is necessary to use the derivative to linearize the function, as required by Newton type algorithms. This is a general comment meant to say that the treatment of this nonlinear relationship between temperature and enthalpy is challenging independently of the numerical scheme (finite differences, finite volumes or finite element) one would adopt. The equation form we are going to solve is stated at lines 69-73 of the submitted manuscript.

4. **RC**: line 163: semi-implicit is not required, implicit is required. semi-implicit is a convenient method of mixing explicit and implicit methods to decrease time step restrictions.

   AR: The thermal conductivity is a function of the solution and therefore, by using a full implicit discretization one obtains a fully nonlinear system of equation. To solve it, it is possible to use a

Picard iteration (Casulli and Zanolli, 2010). In this case we adopted only one Picard iteration obtaining a semi-implicit discretization, but yes, this is just a legitimate option and we added in the Appendix C of the revised manuscript.

5. RC: line 169: ok, let me get this straight: the authors asked their colleagues if there is guaranteed convergence for nonlinear problems using the `currently used algorithms' and they said no? Tell me more. Tell me why convergence is not guaranteed and how NCZ guarantees it - don't refer me to their paper. That is not the point. All the authors need to say is that NCZ offers advantages. Instead the authors generate an entire table showing that all of the methods they can think of have drawbacks, based on the word of their colleagues? The articulation of this argument needs substantial bolstering.

   AR: The convergence, assured by the NCZ algorithm, is only fully realized with a numerical scheme formulated to be conservative. Given the number of established models representing temperature and phase change, and how central the issue is for cryosphere research, some readers may be left with the impression that there must be a model that is conservative and guaranteed to converge. Appendix A and its summary in Table 1 shows that this is not the case based on: (1) the form of the initial equations and (2), when available, statements by the authors of the algorithms. Actually, we cannot determine here where the theoretical limitations might translate into relevant practical consequences, and, besides we show that the problem we solve is shared across differing fields of cryospheric modelling.

   In order to be clearer, we have updated the table adding the references to papers and added a reference to Appendix A in the caption. For clarity, we will also change line 148 (discussion manuscript) to "A summary of relevant models is given in Table 1 and more details in Appendix A".

   As we discuss more deeply in the revised manuscript, the rational of (1) is discussed in Casulli and Zanolli, 2010; Nicolski et al., 2007; Voller, 1990. Moreover, the work by Roe states that the only way to preserve the chain rule at the discrete level is to respect Eq. 9 (of our manuscript) that leads to solve the so-called enthalpy form of the equation. Richards' equation presents the same numerical issues, convergence problems arise when solving the so-called psi-based equation, i.e., the form in which the time derivative is expressed in the form of

$$\frac{\partial\,\theta}{\partial\,t} = \frac{\partial\,\theta}{\partial\,\psi}\frac{\partial\,\psi}{\partial\,t}$$

   This shortcoming it is not only stated in Casulli and Zanolli 2010, but also in D'Amboise et al. 2017 where they solve the Richards equation to simulate water flow in the snowpack.

   About the DECP approach, Nicolsky et al. 2007, Section 2.3 "One of the consequences of this two-step procedure is that the region where the phase change occurs can be artificially stretched, leading to inaccuracies in the simulation of active layer depth".

6. **RC**: line 195: it looks like it comes down to the fact that the enthalpy is, for some reason, not monotonic with temperature, but isn't that the reason to use the enthalpy: because it is monotonic?

I agree that at the melting temperature there is a jump in enthalpy governed by the latent heat, but does that mean that it is not monotonic?

AR: The enthalpy function is monotonic sure, but what we need is that its derivative be monotonic within any neighbourhood of the root for any Newton type algorithm to converge. This in principle is not a problem if the initial guess is carefully chosen to be sufficiently close the solution and, in an interval where the derivative is monotonic. However, the drawback of an unhappy choice of the initial guess is shown in Figure G1: the algorithm enters in a loop without reaching the convergence. Therefore, the so-called globally convergent Newton methods rely on a trick that consists in reducing with a damping factor the increment to calculate the new approximation, but this search is not guaranteed to succeed in advance and in the favorable situations implies many trial and search. The advantage on the NCZ algorithm is that it guarantees convergence of the solution for any choice of the initial guess. Figure G2 shows the numerical solution obtained with the Newton algorithm, the Newton algorithm with a dampening factor and the NCZ. Figure G3 shows that the choice of the dampening factor affects the numerical solution, and it is a source of uncertainty.

We tried to make it clear in the text as we added at the beginning of section 3.2 "Difficulties in solving the nonlinear system of Eq. (16) arise from the non-monotonic behaviour of the derivative of the enthalpy, h(T), with respect to temperature, and because for some parametrizations used for substances - like water - the derivative of the enthalpy is not correctly defined."

7. **RC**: line 202: I must be very confused, why don't you just solve for the enthalpy and use the jump conditions to determine the temperature (Schoof and Hewitt, 2016, SH2016)?

   AR: When following the approach of SH2016, we need to capture the moving boundary separating the two domains (liquid water and ice), an operation that is computationally expensive and difficult to implement, as stated in lines 44-69 of our submitted manuscript. Another reason is that in the SH2016 algorithm: (a) temperature cannot be larger than T_m. This is not acceptable in models where soil and soil moisture can experience temperatures larger than T_m. This means that Eq. (19) cannot be used since in case of $h^{n-1} \geq \rho c(T_m - T_{ref})$, T cannot be assigned a priori. (b) T is defined accordingly to the value of h at the previous time step (Hewitt and Schoof, 2017, HS2017 Eq. 19)

   Moreover, in HS2017 Eq. 19 Section 3 "All the terms in $\nabla \cdot Q$ are discretized explicitly", a procedure which causes restriction in choosing the time step which must be controlled.

   Furthermore, we like to point out that in SH2016 and HS2017, the numerical test is performed for a steady state problem, where the time derivative is 0. Our cases are non-stationary and the NCZ algorithm is used because of the nonlinear behaviour of the terms that comes from the discretization of the time derivative. These terms in a steady state problem do not exist.

8. **RC**: section 4: I have no idea what the Neumann and Lunardini solutions are: describe the problems physically? I can certainly look in the appendix (and did) to find the mathematics, but until I saw Figure 2, I was totally confused at what problem you were trying to solve.

   AR: We added a description of the problem in the text for both the problems.

9. **RC**: line 288: SUTRA uses an ε in the enthalpy function as well?

   AR: As reported in Kurylyk, et al., 2014, Section 3

   "*Hence, SUTRA and other cold region thermohydraulic models generally utilize some form of a soil freezing curve that considers freezing over a range of temperatures less than 0°C. However, the previously detailed analytical solutions employ the crude assumption that the soil freezing curve is represented as a step function. It is difficult to employ a step function soil freezing curve in a numerical model because the apparent heat capacity in the zone of freezing or thawing is dependent on the slope of the soil freezing curve[4,5], which would be infinite for a step function. A very steep piecewise linear soil freezing curve was employed in SUTRA to approximate a saturated step function soil freezing curve.*"

10. **RC**: table 2: there does not seem to be monotonic convergence. given that this paper is claiming guaranteed convergence, I would have liked to see a convergence plot showing that the solution does converge at the power of the discretization, both in space and time. Also, it is worth mentioning the error order for both, especially since the method is first-order in time! predictor-corrector methods (or Heun's method) could be used instead of Crank-Nicholson to increase the resolution without the same time step restrictions.

    AR: Actually, Table 2 is not referring to the convergence of the algorithm. Instead, the convergence rate is for the errors in the NCZ algorithm. Moreover, the solution of the zero-isotherm is obtained by interpolation of the numerical solution. To make it clearer, we added to the text: "For the numerical solution the position of the thawing front has been reconstructed from the linear interpolation of the temperature profile. Table 2 reports the deviations of the reconstructed position of the zero-isotherm from the analytical solution."

11. **RC**: figure 4: if the point is to show that the left and right panels are the same, then I suggest, plotting them on one panel and using the other panel to show the difference.

    AR: In the resubmitted manuscript we now show the difference between the numerical and analytical solutions.

12. **RC**: section 4.2: what defines the mushy zone in the Lunardini analytical solution? and how is this different than Katz (2008)?

    AR: Oeterling and Watts (2004, in Katz, 2008) discuss the mushy region referring to the development of the ice sheet. The mushy zone is characterized by an increase of solutes concentration, primarily salt but also anthropogenic pollutants, with a consequent variation of the density. This gradient density '*provide the potential energy to drive convection within the interstices of the ice matrix and the water below the ice'*.

    Referring to the Lunardini analytical solution, the mushy zone is used to indicate the transition zone between where ice and liquid water coexist in varying proportions in the soil. In the Lunardini problem neither the water flow nor solutes concentration are considered. Thus, the variation of water density due to the expulsion of solutes, and the consequent convection flow is not considered. To avoid possible misunderstanding, we changed ‘mushy zone’ to ‘partially frozen zone’.

13. **RC**: line 329: is this a paragraph fragment?

    AR: We have corrected it.

14. **RC**: Most figures: the axis labels as well as figure text are missing letters and difficult to read.

    AR: Sorry for this inconvenient. We have corrected the Figures.

15. **RC**: line 510: why ε is required? It seems that the value of the enthalpy is that there is a smooth transition across the phase change - adding ε negates the authors' claim that they are `guaranteeing energy conservation', because they have added a fictious mushy zone.

    AR: There is no way to avoid the introduction of ε since the enthalpy function needs to be continuously differentiable and enthalpy function with a step change at the melting temperature is not. See assumption C1 on the apparent heat capacity function, lines 204-206 of the submitted manuscript.

    However, the temperature range ε can be chosen sufficiently small in order to make this approximation negligible when compared to the physical behaviour of water, considering that: (a) The melting of water in temperate ice is known to actually occur progressively below 0ºC along grain boundaries (Langham 1974; Nye and Frank 1973). (b) Freezing often occurs below the melting point. (c) In porous media such as soil, ice melts across a range of temperatures due to the Gibbs-Thompson effect in pores and surface affects at the interfaces between ice and particles (Rempel et al., 2004; Watanabe and Mizoguchi 2002).

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