

Robust reconstruction of historical climate change from permafrost boreholes

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Key Points:

- We propose a new method to estimate historical ground surface temperatures from boreholes in permafrost using Bayesian inverse modeling.
- We evaluate our method on both synthetic test cases for cold and warm conditions as well as real data from a 100 m deep borehole in Siberia.
- We find that seasonal freezing and thawing of the active layer has a significant impact on the reconstructed ground surface temperatures.

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19 Abstract

20 Reconstructing historical climate change from deep ground temperature measure-
 21 ments in cold regions is often complicated by the presence of permafrost. Existing meth-
 22 ods are typically unable to account for latent heat effects due to the freezing and thaw-
 23 ing of the active layer. In this work, we propose a novel method for reconstructing his-
 24 torical ground surface temperatures (GST) from borehole temperature measurements
 25 that accounts for seasonal thawing and refreezing of the active layer. Our method cou-
 26 ples a recently developed fast numerical modeling scheme for two-phase heat transport
 27 in permafrost soils with an ensemble-based method for approximate Bayesian inference.
 28 We evaluate our method on two synthetic test cases covering both cold and warm per-
 29 mafrost conditions as well as using real data from a 100 m deep borehole on Sardakh Is-
 30 land in northeastern Siberia. Our analysis of the Sardakh Island borehole data confirms
 31 previous findings that ground surface temperatures in the region have likely risen by 5
 32 to 9 °C between the pre-industrial period of 1750–1855 and 2012. We also show that la-
 33 tent heat effects due to seasonal freeze-thaw have a substantial impact on the resulting
 34 reconstructed surface temperatures. We find that neglecting the thermal dynamics of
 35 the active layer can result in biases of roughly -1 to -1.5 °C in cold conditions (i.e. mean
 36 annual ground temperature below -5 °C) and as much as -2 to -3 °C in warmer con-
 37 ditions where substantial active layer thickening (> 200 cm) has occurred. Our results
 38 highlight the importance of considering seasonal freeze-thaw in GST reconstructions from
 39 permafrost boreholes.

40 Plain Language Summary

41 Long-term changes in the temperature of the atmosphere are recorded in the solid
 42 Earth due to the insulating properties of soil and rock. As a result, it is possible to es-
 43 timate past changes in temperature at the interface between the ground and the atmo-
 44 sphere by measuring ground temperatures deep below Earth’s surface. In cold regions,
 45 the presence of permafrost, i.e. ground that remains frozen throughout the year, com-
 46 plicates such analyses due to the effects of water freezing and thawing in the soil. In this
 47 work, we present a new method for reconstructing past changes in ground surface tem-
 48 perature from boreholes situated in permafrost using a computational model of heat flow
 49 that accounts for these effects. We evaluate our method on both synthetic test cases as
 50 well as real data from a 100 m deep borehole in northeastern Siberia. Our results demon-
 51 strate that annual freezing and thawing of water near the surface has a substantial im-
 52 pact on the reconstructed ground surface temperatures, especially in regions where per-
 53 mafrost is thawing. The proposed method is the first to be widely applicable to ground
 54 temperatures measured in permafrost and thus constitutes a valuable new tool for un-
 55 derstanding past and present climate change in cold regions.

56 1 Introduction

57 Reconstructing historical climate change is crucial to provide context for the re-
 58 cent warming trends observed in the late 20th and early 21st centuries. Global instru-
 59 mental surface-air temperature records date back only to the mid-19th century (Benestad
 60 et al., 2019), and such long-term records are even more limited in Arctic regions (Gilichin-
 61 sky et al., 1998) where much of the surface is underlain by permafrost, i.e. ground that
 62 remains perennially frozen. Recent studies have established from ground temperature
 63 records that permafrost is warming globally over the last two decades (Biskaborn et al.,
 64 2019). Long-term historical simulations of land surface heat exchange (Langer et al., 2024)
 65 as well as ice core reconstructions (Opel et al., 2013) suggest that this warming trend
 66 likely dates back to the conclusion of the Little Ice Age in the early- to mid-19th cen-
 67 tury. However, paleoclimate reconstructions from proxy data carry with them significant

68 uncertainties (Hernández et al., 2020) and thus may not always be representative for ter-
69 restrial permafrost regions.

70 Temperature measurements from deep boreholes provide a valuable source of in-
71 sight into how the thermal state of the Earth has evolved over time scales ranging from
72 decades to millennia. This is possible due to the fact that temperature fluctuations at
73 the surface diffuse relatively slowly through rock and soil (Huang et al., 2000). The solid
74 Earth thereby acts as a low-pass filter that smooths the temperature signal over long time
75 frames, with the length-scale of the smoothing kernel increasing with depth. As a result,
76 it is possible to detect past changes in ground surface temperature (GST) from deep bore-
77 hole temperature measurements (Lachenbruch & Marshall, 1986). Since its original con-
78 ception by Beck & Judge (1969), this problem has been extensively studied (Vasseur et
79 al., 1983; Shen & Beck, 1991; Huang et al., 1996; Dahl-Jensen et al., 1998; Pollack et al.,
80 1998; Mann et al., 2003). One of the most commonly applied solutions uses singular value
81 decomposition to solve the linear inverse problem posed by an analytical forward model
82 of heat transport (Mareschal & Beltrami, 1992). This approach was recently augmented
83 by Cuesta-Valero et al. (2022) to account for uncertainty through a bootstrap sampling
84 approach. Such methods are, however, limited to simple forward models of conductive
85 heat transport to which linear inversions are applicable. Furthermore, they do not eas-
86 ily permit the inclusion of a priori information about surface temperatures or other un-
87 knowns. In contrast, Bayesian approaches to GST reconstruction have the advantage of
88 fully accounting for uncertainty in the ill-posed inverse problem and allowing for the di-
89 rect incorporation of external information through prior distributions (Wang, 1992; Wood-
90 bury & Ferguson, 2006). Hopcroft & Gallagher (2023) recently applied one such method
91 (Hopcroft et al., 2007) to the International Heat Flow Commission database (Huang &
92 Pollack, 1998) of 1012 temperature profiles, reaffirming that 20th century warming is anoma-
93 lous in comparison to the 500-year period prior to industrialization. This database, how-
94 ever, features relatively few profiles in Arctic and subarctic regions, where permafrost
95 is often a key feature of the landscape.

96 In cold regions where permafrost is present, effective thermal diffusivity in the so-
97 called “active layer”, i.e. the top layer of ground subjected to annual freezing and thaw-
98 ing (Harris et al., 1988), can drop to $0.1 \text{ m}^2 \text{ yr}^{-1}$ ($3.17 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$) or lower during
99 the thawing and refreezing seasons due to the effects of latent heat (D. Riseborough, 1990).
100 This has two important implications for geothermal reconstructions of GST where per-
101 mafrost exists: Firstly, when surface temperatures are reconstructed as annual or multi-
102 annual averages, i.e. neglecting seasonal freezing and thawing, the reconstructed upper
103 boundary represents the long-term average temperature at the top of the permafrost (TTOP)
104 rather than that of the land surface (Lachenbruch & Marshall, 1986). Consequently, such
105 reconstructions necessarily assume that the depth of the permafrost table does not change
106 over the full reconstruction period since the spatial domain of the model is typically treated
107 as constant. Secondly, in regions with warmer permafrost, here defined as those with mean
108 annual top of permafrost temperatures $\geq -5 \text{ }^\circ\text{C}$ (Nitzbon et al., 2023), and finer grained
109 soils with moderate to high silt or clay content, latent heat effects may be present even
110 well below the top of the permafrost (Romanovsky & Osterkamp, 2000; Nicolsky & Ro-
111 manovsky, 2018). This is due to the presence of unfrozen water in soil pores at subzero
112 temperatures as a result of capillary action (Koopmans & Miller, 1966). The presence
113 of such effects generally precludes the application of most existing GST reconstruction
114 techniques, which typically ignore non-conductive heat transport, to borehole temper-
115 ature measurements in permafrost soils (Beltrami, 1996; Mann & Schmidt, 2003; Mot-
116 taghy & Rath, 2006). As a result, most studies which have applied such methods to bore-
117 holes in cold regions have either neglected seasonal freezing and thawing (Kneier et al.,
118 2018), selected boreholes in low porosity material such as bedrock (Isaksen et al., 2000;
119 Guglielmin et al., 2018), or omitted permafrost boreholes altogether from the analysis
120 (Pollack et al., 2003). There is, therefore, a general need for GST reconstruction meth-
121 ods that can account for latent heat effects in frozen ground.

122 In this work, we propose a new method for inverting GST from permafrost bore-
 123 holes where latent heat effects play a dominant role due to both seasonal and long-term
 124 thawing of ground ice. Our method builds upon the thermal modeling scheme of *Cryo-*
 125 *GridLite* (Langer et al., 2024), which allows for efficient, high-fidelity simulation of two-
 126 phase heat conduction over large time scales. Similar to Hopcroft et al. (2007), we em-
 127 ploy a Bayesian formulation of the inverse problem that provides a probabilistic inter-
 128 pretation of uncertainty in the reconstructed GST histories and permits the inclusion
 129 of prior information where available. We adapt the Bayesian inverse modeling workflow
 130 of Groenke et al. (2023) to GST reconstruction in order to efficiently obtain an approx-
 131 imate posterior distribution over plausible GST histories. We first evaluate the method
 132 on synthetic datasets where the “true” surface temperature history is known and com-
 133 pare GST parameterizations with and without latent heat effects included. We then fur-
 134 ther apply our method to a real-world temperature profile from a 100 m deep borehole
 135 on Sardakh Island in northeastern Siberia and reconstruct historical ground surface tem-
 136 peratures over the time period of 1750–2012.

137 2 Methods

138 2.1 Forward model of two-phase heat transport

139 In order to recover past changes in GST from measured temperature profiles, a for-
 140 ward model of subsurface heat transport is required to map changes in temperature at
 141 the surface to the resulting ground temperature profiles. Vertical conductive heat trans-
 142 port in the Earth’s subsurface can be represented according to the standard form of the
 143 heat equation, with the upper boundary set according to surface temperature and the
 144 lower boundary set to an appropriate geothermal heat flux (Lachenbruch & Marshall,
 145 1986; Jaeger, 1965). The resulting temperature field can then be represented as devia-
 146 tions from the quasi-linear steady state solution:

$$147 \quad T(z, t) = T_0 + \frac{Q_{\text{geo}}}{k(z)}z + \Delta T(z, t) \quad (1)$$

148 where $T = T(z, t)$ is the temperature field (K) over depth z (m) and time t (s), T_0 is
 149 the mean annual GST (K), Q_{geo} is the geothermal heat flux (W m^{-2}), and $k(z)$ is the
 150 thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$) which may vary with depth. In regions where per-
 151 mafrost exists, latent heat effects due to the freezing and thawing of groundwater play
 152 a significant role in the thermal dynamics. Phase change can be accounted for by rewrit-
 153 ing the heat equation in terms of enthalpy (Jury & Horton, 2004) as

$$154 \quad \frac{\partial}{\partial z} \left[k \frac{\partial T}{\partial z} \right] - \frac{\partial h(T)}{\partial t} - S = 0, \quad (2)$$

155 where $k = k(T)$ is the temperature-dependent bulk thermal conductivity of the ma-
 156 terial, and $S = S(z, t)$ is a potential external heat source or sink (W m^{-3}). The volu-
 157 metric enthalpy (J m^{-3}) of the soil volume is then defined as

$$158 \quad h(T) = \overbrace{c(T)(T - T_{\text{ref}})}^{\text{Sensible}} + \overbrace{L\theta_w(T)}^{\text{Latent}}, \quad (3)$$

159 where $\theta_w(T)$ is the volumetric unfrozen water content ($\text{m}^3 \text{m}^{-3}$), L is the volumetric la-
 160 tent heat of fusion of water (J m^{-3}), $c(T)$ is the temperature-dependent bulk material
 161 heat capacity ($\text{J K}^{-1} \text{m}^{-3}$), and $T_{\text{ref}} = 0^\circ\text{C}$ is the reference temperature set to the freez-
 162 ing point of water at standard conditions. The two additive terms on the right hand side
 163 are respectively referred to as sensible and latent energy. We parameterize the bulk ther-
 164 mal properties $k(T)$ and $c(T)$ of the soil volume as simple mixtures of four constituent
 165 materials, such that

$$1 \quad 1 = \theta_w + \theta_i + \theta_o + \theta_m, \quad (4)$$

166 where $\theta_i = \theta_{\text{tot}} - \theta_w$ is volumetric ice content ($\text{m}^3 \text{m}^{-3}$), $\theta_o = (1 - \theta_{\text{tot}})\omega$ is volumetric
 167 organic content, and $\theta_m = (1 - \theta_{\text{tot}})(1 - \omega)$ is volumetric mineral content. Here $\theta_{\text{tot}} =$
 168 $\theta_w + \theta_i$ is the total water content, and ω represents the scaled organic fraction of the
 169 solid material. Throughout this study, we assume saturated conditions, so θ_{tot} is taken
 170 to be equal to the natural porosity of the soil volume. For further details on the param-
 171 eterizations of the thermal properties, see Groenke et al. (2023); Langer et al. (2024).
 172 Note also that equations (1) to (3) assume strictly conductive heat transport without
 173 any internal heat sources or sinks other than those due to the phase change of water. This
 174 model therefore neglects both lateral heat transport as well as advection of heat due to
 175 groundwater flow. Boreholes which are known to be significantly affected by such pro-
 176 cesses are thus not suitable for inversion with this approach.

177 The constitutive relation $\theta_w(T)$ represents the unfrozen water content as a mono-
 178 tonic function of temperature. For fine-grained soils with high silt or clay content, this
 179 function can be highly nonlinear due to the effects of capillary action on the effective freez-
 180 ing point of water in the soil (Koopmans & Miller, 1966). As a result of this nonlinearity,
 181 obtaining forward solutions to Eq. (2) is generally nontrivial and requires numer-
 182 ical integration with time steps typically ranging from seconds to minutes for high res-
 183 olution discretizations of the soil volume (≤ 10 cm). To mitigate this, we follow Langer
 184 et al. (2024) in using the numerical scheme of Swaminathan & Voller (1992) to efficiently
 185 simulate two-phase heat conduction over multiple centuries. We configure the spatial do-
 186 main of the model to correspond to a 1000 m vertical column extending below the sur-
 187 face of the Earth. The spatial discretization has a grid cell spacing of 10 cm in the up-
 188 per 2.5 m of the ground, where the freeze-thaw dynamics play the largest role, which is
 189 then increased non-uniformly to 10 m in the bottom 900 m of the domain. We augment
 190 the numerical scheme of Langer et al. (2024) to allow for more realistic forms of $\theta_w(T)$
 191 that can represent the freezing characteristics of common soils when seasonal freezing
 192 and thawing is considered. More details on the modified numerical scheme are given in
 193 Appendix A.

194 We represent the GST in our forward model as the sum of three independent com-
 195 ponents as

$$196 \quad T(0, t) = T_0 - A \sin\left(\frac{2\pi}{P}(t - t_0)\right) + \sum_{i=1}^N \psi_i(t) \left[\tau_i + \frac{\tau_{i+1} - \tau_i}{t_{i+1} - t_i}(t - t_i) \right], \quad (5)$$

197 where $T_0 = T(0, t_0)$ is the initial ground surface temperature ($^{\circ}\text{C}$) at the beginning of
 198 the simulation period, A is the annual amplitude ($^{\circ}\text{C}$) at the surface, and $P = 1$ yr is
 199 the period of the seasonal cycle. In cases where the annual cycle is neglected $A = 0$.
 200 Deviations in the GST history from the initial surface temperature T_0 are represented
 201 as a continuous piecewise linear function with knots τ_i covering N time segments, where
 202 $\psi_i(t)$ correspond to boxcar functions that are zero everywhere outside of the interval $[t_i, t_{i+1})$.
 203 We follow Kneier et al. (2018) in setting the endpoints of each segment such that each
 204 interval spans a range of $\pm \frac{1}{3}t'$, where t' is the time before the borehole measurement.
 205 This loosely reflects the expected loss of temporal resolution that is characteristic of dif-
 206 fusive heat transport (Demezhko & Shchapov, 2001). We set the minimum value of t'
 207 to one year since we are only interested in reconstructing GSTs beyond this time hori-
 208 zon.

209 2.2 Borehole temperature data

210 Temperature profiles $\mathbf{T} = [T(z_1, t), T(z_2, t), \dots, T(z_N, t)]$ typically consist of a se-
 211 quence of N temperature measurements along a vertical profile perpendicular to the Earth's
 212 surface. Such measurements are typically made by inserting thermistor chains into deep
 213 holes drilled into the Earth, often referred to as boreholes. Temperatures can then be
 214 measured from boreholes either as point measurements, i.e. where the temperature sen-
 215 sors are covered and then left to equilibrate with the subsurface temperature at the time

216 of measurement, or as temporal averages computed from a series of measurements made
 217 at regular (sub-daily) intervals over a longer time period, typically at least one annual
 218 cycle.

219 In the latter case, stochastic measurement noise can generally be presumed to be
 220 dominated by model error, and seasonal fluctuations in the temperature signal are averaged
 221 out over the full profile. In the more common case where \mathbf{T} is a point measurement,
 222 temperatures measured at depths above the depth of zero annual amplitude (ZAA)
 223 should generally be discarded for the purposes of GST reconstructions since they are affected
 224 by seasonal variations that are typically below the time scale considered in the
 225 inversion. Furthermore, measurement error due to the accuracy and resolution limits of
 226 the temperature sensor also need to be considered in such cases since fluctuations below
 227 these limits should not be allowed to affect the reconstruction. This can be accounted
 228 for by setting the error term equal to the sensor resolution (see section 2.3).

229 In this work, we consider only the former case of temperature profiles which are
 230 computed as temporal averages over at least one full annual cycle. This is the case for
 231 both the synthetic experiments, where daily temperature profiles produced by the forward
 232 model are averaged over the final simulation year, as well as the experiment using
 233 data from an instrumented borehole on Sardakh Island where hourly measurements are
 234 available. Note, however, that our method is also readily applicable to point measurements,
 235 so long as the aforementioned considerations are taken into account.

236 **2.3 Bayesian inversion of ground temperatures**

237 Bayesian inference provides a natural framework for constraining uncertainty about
 238 unknown model parameters using data observed from the system under investigation (Berliner,
 239 2003). For GST reconstruction, we seek to obtain the posterior distribution over the unknown
 240 parameters $\phi \in \Phi$ for a particular forward model $\mathcal{M} : \Phi \mapsto T(\mathbf{z}, t_n)$ given
 241 some observed temperature profile \mathbf{T} over depths \mathbf{z} at time t_n

$$p(\phi|\mathbf{T}, \mathcal{M}) \propto p(\mathbf{T}|\phi, \mathcal{M})p(\phi|\mathcal{M}) \quad (6)$$

242 where $p(\phi|\mathcal{M})$ represents the prior distribution over model parameters ϕ for a given forward
 243 model \mathcal{M} , and $p(\mathbf{T}|\phi, \mathcal{M}) = \mathcal{N}(\mathcal{M}(\phi), \Sigma_T)$. The model parameters ϕ consist of
 244 both the unknowns in Eq. (5) (i.e. T_0 , A , and τ) as well as a subset of the unknown parameters
 245 required for the heat conduction model such as the soil porosity, solid material thermal conductivity,
 246 and the geothermal heat flux at the lower boundary, Q_{geo} . It is important to note that, while we do not
 247 generally expect to be able to uniquely determine both the material thermal properties and the GST
 248 history simultaneously from a single temperature profile, including them in the posterior distribution
 249 still allows us to account for their associated uncertainties in the reconstructed GST histories (Wang,
 250 1992; Shen et al., 1995).

252 Computing the GST history from Eq. (5) over samples from the posterior distribution characterizes
 253 the most plausible surface temperature reconstructions after considering the observed temperature profile.
 254 One common problem in ground surface temperature reconstruction is enforcing smoothness in the
 255 reconstructed temperature history (Hartmann & Rath, 2005). As noted by Hopcroft et al. (2007), the
 256 Bayesian approach of computing averages or quantiles over the posterior distribution naturally produces
 257 a smoother reconstruction without additional regularization or constraints. However, we observed
 258 that neglecting temporal correlation in the prior artificially inflates the spread of the posterior
 259 due to the presence of unrealistically large oscillations in independently sampled temperature histories.
 260 To mitigate this, we place a multivariate normal prior with Töplitz covariance structure over the
 261 temperature offsets. This corresponds to the covariance of a first order autoregressive process where
 262 each GST offset is assumed
 263

264 to be correlated with the offset from the previous segment:

$$265 \quad \tau_{i+1} = \rho\tau_i + \epsilon, \quad (7)$$

266 where $\epsilon \sim \mathcal{N}(0, \sigma^2)$. Since we model the temperature within each segment as a linear
 267 ramp between τ_i and τ_{i+1} , it is natural to choose $\rho = \frac{1}{2}$ based on the observation that
 268 the average GST within each segment is always $\frac{\tau_{i+1} + \tau_i}{2}$. In all of our experiments, we
 269 set $\sigma = 2^\circ\text{C}$ which translates into a prior on temperature deviations with 95% cov-
 270 erage over the interval -4 to 4°C . Note that this does not preclude inference of values
 271 outside of this range but naturally requires very strong evidence to override the prior.
 272 The initial surface temperature T_0 is assigned a Gaussian prior with mean based on his-
 273 torical air temperatures and variance identical to that of the τ_i parameters.

274 For the soil parameters (i.e. porosity, mineral thermal conductivity, and organic
 275 content in the top layer), we use logit-normal priors centered on the values in the ini-
 276 tial stratigraphy with $\sigma = 0.5$; this translates into a prior uncertainty of roughly 5 to 10%
 277 in the constrained parameter space, although the exact deviation depends on the loca-
 278 tion of the parameter due to the nonlinearity introduced by the logit transform. The log-
 279 amplitude, $\log(A)$, is similarly assigned a Gaussian prior with $\sigma = 0.1$ which translates
 280 into a variance of roughly $\pm 4^\circ\text{C}$ in the positive constrained space. The mean of the log-
 281 amplitude prior can be set for any given site based on the earliest available estimates of
 282 air temperature, though it's worth noting that the true GST amplitude will generally
 283 be smaller than that of air temperature in cold regions due to the insulating effect of snow
 284 cover in the winter (Park et al., 2015). Note that the aforementioned standard devia-
 285 tions are defined in the transformed parameter space and are thus dimensionless.

286 The posterior distribution in Eq. (6) typically has no analytical form for arbitrary
 287 priors $p(\phi)$ and nonlinear forward models \mathcal{M} . As a result, numerical sampling methods
 288 are required in order to obtain approximate samples from the posterior. Markov Chain
 289 Monte Carlo (MCMC) algorithms are generally considered the gold standard of numer-
 290 ical sampling algorithms due to their asymptotic convergence guarantees (Gelman et al.,
 291 2013). The method employed by Hopcroft et al. (2007), for example, uses a “reversible
 292 jump” variant of MCMC that permits the sampler to vary not only the parameter val-
 293 ues but also the number of parameters (i.e. the number the of time points in the recon-
 294 struction). Such methods are tractable when the forward model has a low computational
 295 cost. Accurately resolving freeze-thaw dynamics in the forward model used in this work,
 296 however, makes this impractical at multi-century time scales due to the nonlinearities
 297 induced by freezing and thawing.

298 To circumvent this issue, we use the Ensemble Kalman Sampling (EKS) algorithm
 299 of Garbuno-Inigo et al. (2020) as previously outlined by Groenke et al. (2023). EKS is
 300 a gradient-free method for approximate Bayesian inference that evolves an initial param-
 301 eter ensemble as an interactive particle system governed by Langevin dynamics. The al-
 302 gorithm is formulated such that the steady state distribution of the ensemble members
 303 corresponds to the posterior distribution in the limit of infinite iterations of the algorithm.
 304 Like other ensemble or particle-based sampling algorithms, EKS has the advantage of
 305 allowing parallel execution of the model ensemble at each iteration, thus greatly improv-
 306 ing efficiency over sequential sampling and optimization methods. To limit the overall
 307 computational cost of each experiment, we run EKS for a maximum of 20 iterations with
 308 ensembles of size $N_{\text{ens}} = 256$. We specify the residual noise covariance as $\Sigma_T = 4\delta^2 I$
 309 where I is the identity matrix. We found empirically that setting δ to the minimum ab-
 310 solute temperature change in the observed profile generally produced good results and
 311 prevented overfitting for both the synthetic and measured temperature profiles.

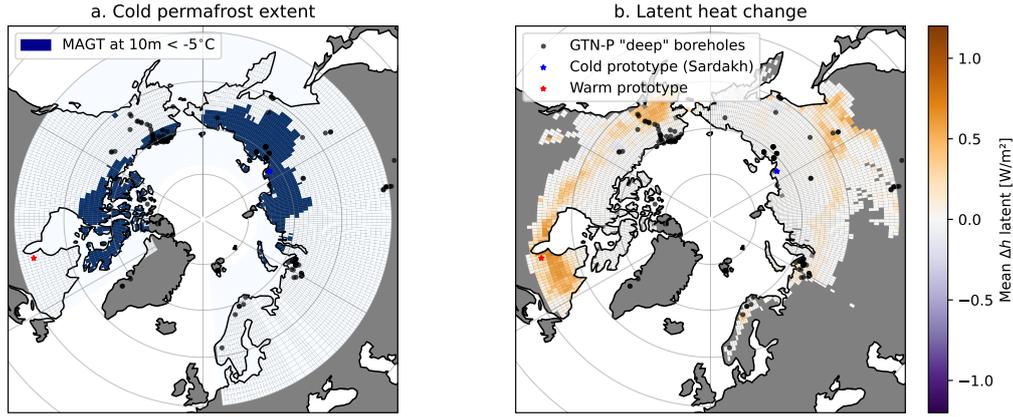


Figure 1. Maps showing the prototype warm and cold locations used by the synthetic experiments in this study, as well as GTN-P boreholes deeper than 50 m, overlain on a map of “cold” permafrost extent (a), here defined as areas where simulated mean annual ground temperatures (MAGT) are below -5°C at 10 m depth. We calculate the spatial extent of cold permafrost, by this definition, to be approximately 34.1 % of the total area considered here.. The second panel (b) shows total latent heat change as estimated by Nitzbon et al. (2023) for the time period 1980-2018. Higher latent heat change generally indicates more thaw.

3 Synthetic test cases

3.1 Experiment setup

We first evaluate our GST inversion method on synthetic test cases where the “true” GST history is known. In order to generate a synthetic temperature profile, we run our forward model over the time period 500-2010 CE forced by air temperatures at the upper boundary taken from the paleoclimate reconstruction of Phipps et al. (2013) for the years 500-1979 and ERA-interim (ERA-I) reanalysis (Dee et al., 2011) for the more recent period of 1979-2010. The paleoclimate reconstruction is based on simulations from the climate system model Mk3Lv1.2. Further details regarding the forcing data are given by Langer et al. (2024). It is important to note that, for the purposes of this experiment, the historical accuracy of the air temperature forcing is not particularly important, as we only aim to produce a semi-realistic temperature profile and GST record that we can use to evaluate the inversion method.

We consider two different synthetic test cases: one based on cold conditions (section 3.2) and one based on warm conditions (section 3.3). This is motivated by recent findings that the thermal response of cold vs. warm permafrost to climate change often differ substantially (Nicolosky & Romanovsky, 2018; Groenke et al., 2023) as well as by the hypothesis that latent heat effects will likely be more dominant in regions where permafrost has temperatures closer to 0°C . We select the Lena River Delta in northeastern Siberia as the prototype for cold conditions since it lies well within the region characterized by our working definition of cold permafrost (Figure 1a). For the warm prototype, we select a region east of the James Bay in western Quebec where previous studies indicate that significant permafrost thaw has likely occurred (Figure 1b). By this definition, roughly two-thirds of permafrost in the northern hemisphere can be considered “warm” which underscores the importance of correctly representing such regions in geothermal climate reconstructions.

338 For each synthetic test case, we apply constant freezing and thawing degree-day
 339 factors (Lunardini, 1978; Groenke et al., 2023) to the air temperatures in order to roughly
 340 approximate the thermal offset between near-surface air temperature and GST due to
 341 snow, vegetation, and other factors. We initialize the forward model with a steady state
 342 temperature profile corresponding to a fixed initial surface temperature T_0 and geother-
 343 mal heat flux $Q_{\text{geo}} = 53 \text{ mW m}^{-2}$. We select 1700-2010 CE as the inversion period with
 344 the first 1200 year period (500-1700 CE) of the forward run discarded as spin-up. The
 345 “observed” temperature profile datasets are then produced by taking the mean annual
 346 ground temperature profile at ten depths ranging from 1 to 100 m over the final simu-
 347 lation year.

348 We use a simple, three-layer soil stratigraphy (Table 1) in the forward model which
 349 consists of a 1 m thick organic rich layer (A Horizon) followed by a 19 m thick medium
 350 porosity subsoil layer (B Horizon) and low-porosity layer representing a combined sub-
 351 stratum and bedrock layer (C + R Horizon) thereafter (Jahn et al., 2006). In order to
 352 investigate the impact of freeze-thaw dynamics on the reconstruction, we use a freezing
 353 characteristic curve where 27.5% of the pore water remains unfrozen at -10°C . This
 354 is a typical freezing characteristic for soils with high silt or clay content (D. W. Risebor-
 355 ough, 2002; Ren & Vanapalli, 2019). While such soils are not necessarily representative
 356 of all the soil types actually found in the study regions considered here, they represent
 357 the end-member case in which we would expect freeze-thaw dynamics to be most likely
 358 to affect the observed temperature profiles even at temperatures well below the nomi-
 359 nal freezing point of water.

360 For each dataset, we compare four different parameterizations of the forward model
 361 used in the inversion:

- 362 1. *Homogeneous soil without seasonal thaw* (FW1L). The soil stratigraphy is misspec-
 363 ified as a homogeneous medium with all material and thermal properties invari-
 364 ant with depth. No seasonal cycle is applied to the upper boundary (i.e. $A = 0$)
 365 thereby excluding the active layer. The idealized “free water” freezing character-
 366 istic (see Appendix A) is used in place of a soil freezing characteristic. As a re-
 367 sult, freezing and thawing at the surface will not occur unless the mean annual
 368 GST exceeds the melting point $T_m = 0^\circ\text{C}$.
- 369 2. *Three-layer soil without seasonal thaw* (FW3L). This configuration is the same as
 370 the FW1L but using the “true” three-layer soil stratigraphy given in Table 1.
- 371 3. *Three-layer sandy soil with seasonal thaw* (SS3L). Three-layer soil stratigraphy
 372 with seasonal temperature variation applied to the GST. The van Genuchten pa-
 373 rameters (van Genuchten, 1980) governing the shape of the soil freezing charac-
 374 teristic curve are intentionally misspecified using typical values for a sandy soil.
 375 In sandy soils, freezing occurs much earlier when temperatures fall below 0°C .
- 376 4. *Three-layer clay soil with seasonal thaw* (CS3L). This configuration corresponds
 377 to the ground truth forward model with a simplified upper boundary following Eq.
 378 5. Note, however, that the soil parameters in each layer are still varied, so each
 379 sampled model realization is generally not identical to the ground truth forward
 380 model.

381 Comparing configurations 1 (FW1L) and 2 (FW3L) allows us to quantify the impact of
 382 neglecting spatial heterogeneity in the soil properties while comparing configurations 3
 383 (SS3L) and 4 (CS3L) allows us to assess the impact of misspecifying the soil freezing char-
 384 acteristic. We can additionally compare configurations 2 (FW3L) and 3 (SS3L) in or-
 385 der to quantify the impact of excluding seasonal freeze-thaw effects.

386 In each experiment, the set of model parameters considered in the inversion includes
 387 the initial GST T_0 , the geothermal heat flux Q_{geo} , and the 10 GST offsets at geomet-
 388 rically spaced intervals between 1500 and 2010 (see section 2.1). For the cases where sea-

Table 1. Three-layer soil stratigraphy used for the synthetic forward runs. Soil properties are treated as homogeneous within each layer. Here θ_{tot} refers to the total water/ice content, presumed equal to porosity ($\text{m}^3 \text{m}^{-3}$), ω to the organic solid fraction ($\text{m}^3 \text{m}^{-3}$), and k_m to the thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$) of the mineral constituent. Uncertainties refer to the (approximate) standard deviations of the prior.

Layer	Depth	$\theta_{\text{tot}} \times 100$	$\omega \times 100$	k_m
1	0.0	65 ± 10	30 ± 10	2.8 ± 0.5
2	1.0	35 ± 10	1	3.1 ± 0.5
3	20.0	5 ± 5	0	3.5 ± 0.5

389 sonal thaw is considered, the annual amplitude is also included as a parameter. In the
 390 homogeneous soil configuration, the porosity and mineral thermal conductivity are varied
 391 as parameters, and in the three-layer soil stratigraphy, these parameters are varied
 392 independently within each of the layers for a total of six additional parameters. Since
 393 the primary goal of these experiments is to evaluate differences in the reconstructed GST
 394 histories rather than recover the soil parameters, we center the parameter priors for the
 395 three-layer model configurations on the true values used in the forward model (Table 1)
 396 to avoid introducing a priori biases into the inversion.

397 3.2 Cold conditions

398 For the first experiment, we use a dataset generated by the forward model forced
 399 by air temperatures from a region in northeastern Siberia (E 127° N 72°) at the edge
 400 of the Laptev Sea. We use freezing and thawing degree day factors of 0.7 (fairly cold,
 401 low to moderate snow cover) and 0.9 (minimal insulation from vegetation) respectively.
 402 The region lies within the continuous permafrost zone and is characterized by histori-
 403 cally low mean annual air temperatures (-16°C for the pre-industrial period 1500-1850
 404 CE). As a result, mean annual ground temperatures can reach -10°C or lower even at
 405 depths well below the active layer (Romanovsky et al., 2007). We can therefore reason-
 406 ably expect the presence of unfrozen water in the deeper permafrost layers, despite the
 407 relatively significant depression of the freezing point due to the assumed freezing char-
 408 acteristics of the soil. The average GST in the ground truth simulation increased by 2.4°C
 409 over the study period (1700-2010 CE) with active layer thickness (ALT) increasing from
 410 roughly 40 cm to 60 cm over the same time frame.

411 All four model configurations are able to produce temperature profiles which fit well
 412 to the synthetic temperature profile (Figure 2b) with the mean absolute error and full
 413 90% highest density interval $< 0.05^\circ \text{C}$ in all cases (Table 2). We note that the poste-
 414 rior predicted ground temperatures from all three of the model configurations which use
 415 the “true” three-layer soil stratigraphy are nearly identical, whereas the homogeneous
 416 soil variant has larger uncertainty below 30 m depth. This can be attributed to the model’s
 417 inability to account for heterogeneity in the soil thermal properties, thereby producing
 418 biases in the predicted temperature profiles. The median predicted temperature profile
 419 nevertheless shows good agreement. This seems to indicate that the temporal variations
 420 in the inverted GSTs can compensate for such biases arising from misspecification of the
 421 soil thermal properties. This is consistent with the findings of Shen et al. (1995) who as-
 422 sessed the impact of heterogeneous thermal properties on the reconstructions.

423 The reconstructed GST histories for each model configuration (Figure 2a) are largely
 424 consistent in terms of relative warming with the exception of the second model config-
 425 uration (FW3L). This model infers a cooling event of roughly 0.5°C for the first two postin-
 426 dustrial periods of 1855-1933 CE and 1933-1971 CE. This appears to be a result of the

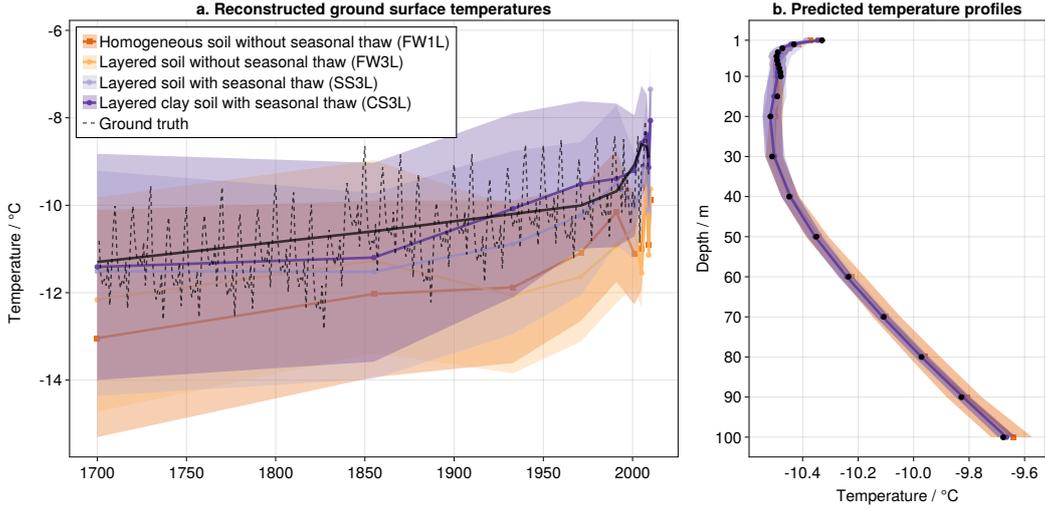


Figure 2. Reconstructed ground surface temperatures for synthetic borehole data in cold conditions (a) along with the corresponding predicted temperature profiles (b). The dotted black line shows the “true” mean annual ground surface temperature history produced by running the forward model with air temperature forcing from northeastern Siberia (E 127° N 72°) while the solid black line is its corresponding long-time average over the reconstruction intervals. The solid colored lines correspond to the median and the shaded regions to the 90% highest density interval over the posterior ensemble.

427 inversion algorithm reducing the mineral conductivity of the second stratigraphy layer
 428 to $2.0 \pm 0.3 \text{ W m}^{-1} \text{ K}^{-1}$ in order to compensate for the positive bias in bulk thermal con-
 429 ductivity due to the pore ice remaining frozen.

430 The posterior median GSTs for the third and fourth model configurations (SS3L
 431 vs. CS3L) are both able to accurately recover the total warming ($\approx 2.4 \pm 0.1 \text{ }^\circ\text{C}$) since
 432 the pre-industrial period (1750-1855 CE). The largest deviation between the two recon-
 433 structions is in the mid-to-late 20th century (1933–1977 CE) where the GSTs from the
 434 sandy soil model are roughly $1 \text{ }^\circ\text{C}$ cooler than with the clay soil. This is similarly due
 435 to higher average thermal conductivity as a result of higher pore ice content, which thereby
 436 requires lower average GSTs to compensate.

437 The first model variant (FW1L), which excludes seasonal thaw, infers a cooling pat-
 438 tern over the 1991-2001 CE reconstruction period. There is some evidence of such an event
 439 in the ground truth surface temperature which shows a slight cooling in 1998 ($0.8 \text{ }^\circ\text{C}$)
 440 and 1999 CE ($1.1 \text{ }^\circ\text{C}$) over the previous two year average. This could be a result of the
 441 1997–1999 CE El Niño/La Niña event which is known to have teleconnections to cen-
 442 tral and northern Siberian air temperatures (Vicente-Serrano et al., 2006). However, this
 443 event does not appear to have had a significant impact on the long-term average at the
 444 time scale of the reconstruction (see the solid black line in Figure 2a); thus the SS3L and
 445 CS3L reconstructions are still arguably more faithful to the true long-term average GST.

446 Both of the models which exclude seasonal thaw, thereby neglecting latent heat ef-
 447 fects, produce GSTs with a cold bias of $-1.3 \pm 0.2 \text{ }^\circ\text{C}$ compared to biases of $-0.5 \pm 0.2 \text{ }^\circ\text{C}$
 448 and $0.1 \pm 0.4 \text{ }^\circ\text{C}$ in the sand and clay models, respectively (Table 2). This can be at least
 449 partially explained by the thermal offset in mean annual ground temperatures typically
 450 observed in the active layer. We note again that, when the active layer is neglected in

Table 2. Summary statistics for evaluating the inversion produced by each model configuration under cold vs. warm conditions: ground surface temperature reconstruction bias, mean absolute error in the predicted temperature profiles, and Pearson correlation with the true (averaged) ground surface temperature history. Uncertainties correspond to the standard deviation over the posterior ensemble ($N = 256$).

Model	Cold			Warm		
	Rec. bias ($^{\circ}\text{C}$)	Pred. MAE ($^{\circ}\text{C}$)	Corr.	Rec. bias ($^{\circ}\text{C}$)	Pred. MAE ($^{\circ}\text{C}$)	Corr.
FW1L	-1.34 ± 0.18	0.02 ± 0.01	0.79 ± 0.17	-2.59 ± 0.26	0.04 ± 0.01	0.71 ± 0.15
FW3L	-1.26 ± 0.15	0.01 ± 0.0	0.72 ± 0.23	-2.27 ± 0.23	0.06 ± 0.01	0.67 ± 0.14
SS3L	-0.24 ± 0.28	0.02 ± 0.03	0.83 ± 0.14	-0.93 ± 0.52	0.04 ± 0.02	0.84 ± 0.1
CS3L	0.22 ± 0.43	0.02 ± 0.01	0.85 ± 0.11	-0.34 ± 0.5	0.05 ± 0.02	0.94 ± 0.05

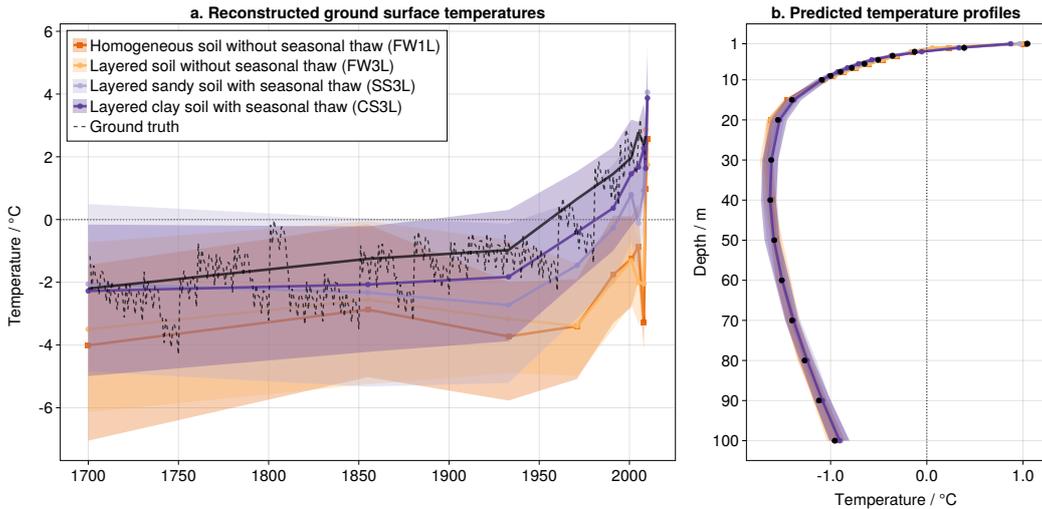


Figure 3. Reconstructed ground surface temperatures for synthetic borehole data in warm conditions (a) along with the corresponding predicted temperature profiles (b). The dotted black line shows the “true” mean annual ground surface temperature history produced by running the forward model with air temperature forcing from western Quebec, east of the James Bay ($W 77^{\circ} N 53^{\circ}$). The solid colored lines correspond to the median and the shaded regions to the 90% highest density interval over the posterior ensemble.

451 the model, its thermal offset is not present, and the reconstructed GSTs effectively represent the temperature at the top of the permafrost (Lachenbruch & Marshall, 1986).
452

453 3.3 Warm conditions

454 For this experiment, we use air temperatures from western Quebec, east of the James
455 Bay ($W 77^{\circ} N 53^{\circ}$) to force the forward model. The region lies outside of the contin-
456 uous permafrost zone and is characterized by historical mean annual air temperatures
457 of -6°C for the pre-industrial time period of 1500-1850. The average GST in the ground
458 truth simulation increased by 4.9°C over the study period (1700-2010 CE) with ALT
459 increasing substantially from 80 cm to 350 cm over the same time frame.

460 We find that the inversion method is again able to produce temperature profiles
461 that are in good agreement with the simulated observations (Figure 3b) with the mean
462 absolute prediction error $< 0.1^{\circ}\text{C}$ for all four model configurations (Table 2). We note,

463 however, that unlike in the cold experiment, the two soil models which incorporate sea-
 464 sonal freeze-thaw have a larger spread in the predicted temperature profiles. This is likely
 465 due to the sensitivity of two-phase heat transport to uncertainty in soil parameters such
 466 as porosity, which directly determines the amount of water/ice which undergoes freez-
 467 ing and thawing. This is the case for all subzero temperatures, but the effects are stronger
 468 at temperatures closer to the freezing point of water, where the constitutive relation be-
 469 tween temperature and unfrozen water content becomes increasingly nonlinear.

470 Like in the cold experiment, the reconstructed GSTs for both model configurations
 471 which neglect phase change (FW1L and FW3L) have significant cold biases ($-2.6\pm 0.2^\circ\text{C}$
 472 and $-2.3\pm 0.2^\circ\text{C}$ respectively) when averaged over the study period (Figure 3a and Ta-
 473 ble 2). Since we use the same ground truth stratigraphy setup in both experiments, we
 474 can infer that the larger magnitude of the bias in this case can only be explained by the
 475 deeper active layer, which naturally results in a larger offset between the ground surface
 476 and the top of the permafrost. As permafrost thaws and the active layer deepens, this
 477 offset becomes larger, which may explain the minimal change in the early 20th century
 478 GSTs from both of these model configurations (Figure 3). In contrast, the inversion for
 479 the clay soil model (CS3L) accurately recovers the warming trend over both the 19th and
 480 20th centuries, though there is still a slight cold bias of $-0.3\pm 0.5^\circ\text{C}$ which may be due
 481 to short-term warming events in the forcing data that are below the time scale resolv-
 482 able by the GST parameterization.

483 All four models consistently reproduce the warming trend of the late 20th century,
 484 though the models excluding seasonal thaw (FW1L and FW3L) tend to slightly over-
 485 estimate the rate of warming. Both of these models also infer a large jump ($> 3^\circ\text{C}$) in
 486 the GST for the most recent two time periods in order to fit the uppermost depths in
 487 the temperature profile at 1 m and 2 m. This is because the mean annual ground tem-
 488 peratures at these depths are significantly higher due to being in the active layer at the
 489 end of the study period. Since both of these model configurations do not include sea-
 490 sonal thaw, they are not able to represent the active layer, and thus the only way to fit
 491 these points is by dramatically increasing the GST in the most recent years. This effect
 492 could be mitigated by simply removing these points from the inversion and setting the
 493 upper boundary of the soil domain to a depth that is assumed to be well below the ac-
 494 tive layer throughout the study period. However, this requires ALT for the site or re-
 495 gion to be known a priori and precludes direct comparison with other GST records from
 496 observations or land surface models that are able to represent freezing and thawing of
 497 the active layer.

498 **4 Inversion of borehole data from Sardakh Island**

499 We additionally evaluate our method on real-world borehole data from a 100 m bore-
 500 hole on Sardakh Island which was drilled in 2009 (Kneier et al., 2018). Sardakh Island
 501 lies in the southern part of the Lena River Delta in northeastern Siberia and is charac-
 502 terized by very long and cold winters with temperatures reaching -45°C and below. The
 503 site lies within the region covered by the forcing data described in section 3.2 and thus
 504 can be assumed to have likely experienced similar pre-industrial mean annual air tem-
 505 peratures of roughly -16°C . Recent analyses of air temperatures at the nearby Samoylov
 506 Island station (Boike et al., 2019), which lies roughly 50 km southwest of Sardakh, show
 507 significant warming of at least 0.1 K yr^{-1} over the last two decades with recent mean an-
 508 nual air temperatures ranging from -12 to -8°C (Groenke et al., 2023).

509 We use the same underlying dataset and stratigraphy information for the site as
 510 published previously by Kneier et al. (2018). We select, however, the slightly more re-
 511 cent time frame of 2011–2012 instead of 2010–2011 due to the data record having fewer
 512 gaps after cleaning and quality control. We discard temperature measurements above
 513 1 m depth since these are likely to be affected by land surface processes that our model

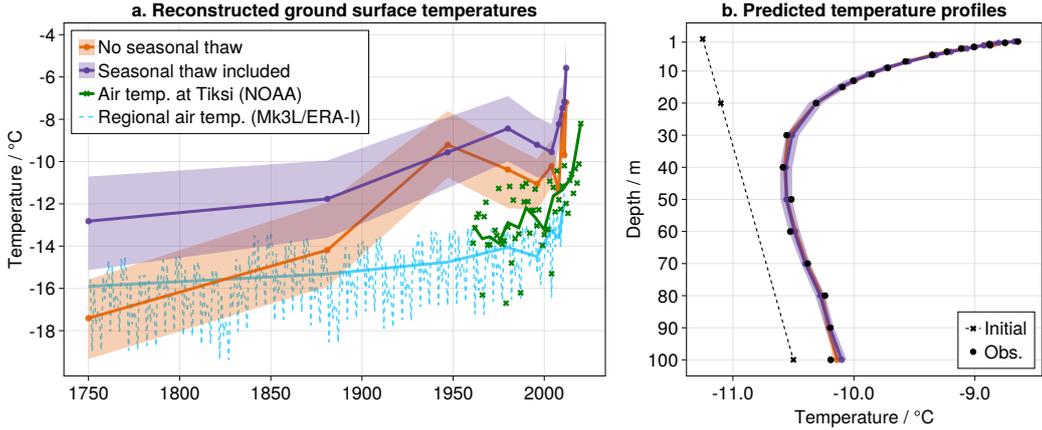


Figure 4. Reconstructed ground surface temperatures from the 100 m borehole on Sardakh Island (a) along with the corresponding predicted temperature profiles (b) both including and excluding seasonal temperature variations at the surface. The dashed blue line in panel (a) represents the air temperature forcing of Langer et al. (2024) for the region (see section 3.2) over the full study period; the corresponding solid blue line shows the same data averaged over the reconstruction intervals. The green crosses show annual average air temperatures measured from the nearby NOAA meteorological station at Tiksi with the solid line showing half-decadal averages. The black dots in panel (b) are mean annual ground temperatures at each depth for the period 2011-10-1 to 2012-10-1. The dashed line shows the upper part of the temperature profile used to initialize the forward model in the year 1600 CE.

514 cannot resolve. We also use a condensed, eight-layer version of the soil stratigraphy (Ta-
 515 ble B1) that includes a half meter thick organic layer at the top of the soil profile. Like
 516 in the synthetic experiments, we allow the porosity and mineral thermal conductivity
 517 to vary as parameters in each of these layers.

518 The reconstructed GST histories and predicted temperature profiles, both includ-
 519 ing (purple) and excluding (orange) seasonal freezing and thawing, are shown in Figure
 520 4. The inversions from both model configurations indicate substantial warming of 5 to
 521 9 °C over the last two centuries. Furthermore, consistent with the results shown in sec-
 522 tions 3.2 and 3.3, the model variant excluding freezing and thawing at the upper bound-
 523 ary generally underestimates GSTs due to the thermal offset of the active layer. In this
 524 case, this offset does not appear to be entirely constant over the 160 year time period.
 525 This may be in part due, however, to the deepest temperature measurement at 100 m
 526 depth which appears unusually cold in comparison to the geothermal gradient. This is
 527 discussed further in Appendix B.

528 Both variants also indicate a cooling period during the latter half of the 20th cen-
 529 tury though they disagree about the timing and magnitude of this cooling. The first re-
 530 construction excluding seasonal thaw (Figure 4a) suggests that GSTs initially peaked around
 531 1950 before cooling by roughly 1.5 °C by the end of century. The second reconstruction
 532 that includes seasonal thaw indicates the onset of cooling to have started in the mid-1970s.
 533 Observed air temperatures from the nearby NOAA station at Tiksi appear to suggest
 534 that this cooling may have started even later (early to mid 1980s), though there are two
 535 unusually cold years (below $-16\text{ }^{\circ}\text{C}$) in the two decades prior (1966 and 1979). This dis-
 536 crepancy could be due to the fact that the reconstructions are limited in their capacity
 537 to resolve the timing of past changes by the fixed time intervals. The half-decadal av-

538 eraged air temperatures at Tiksi show a decrease of roughly 1°C from 1986 to 1995 which
 539 is consistent with the reconstruction that includes seasonal thaw. This timing is also roughly
 540 consistent with previous reconstructions from the same borehole (Kneier et al., 2018).
 541 Ice core reconstructions from the Russian high Arctic have also indicated similar 20th
 542 century cooling, though the timing varies across samples (Fritzsche et al., 2005; Opel et
 543 al., 2013).

544 The reanalysis air temperature record for the region shown by the blue line in Fig-
 545 ure 2a (Langer et al., 2024) also largely agrees with the timing of the cooling indicated
 546 in the second reconstruction, although the long-term average (solid line) suggests a smaller
 547 magnitude of roughly 0.2°C . The model variant excluding seasonal thaw is able to re-
 548 solve the short-term temperature fluctuation during the mid 2000s seen in the reanal-
 549 ysis air temperature record, while the model variant including seasonal thaw does not.
 550 This may be due to the freezing and thawing of the active layer effectively damping out
 551 this fluctuation in the forward model, reducing the apparent effect size of these GSTs
 552 in the inversion. This hypothesis is further supported by the observation that the first
 553 model variant without seasonal thaw accurately predicts the ground temperature at 30 m
 554 depth while the second model variant with seasonal thaw has a warm bias of roughly 0.05°C
 555 which may be due to this cooling event not being resolved.

556 5 Discussion

557 Both our synthetic and real-world test cases demonstrate that latent heat effects
 558 have a significant impact on the inverted GSTs due to the impacts of freezing and thaw-
 559 ing on the thermal dynamics of the soil. This is especially the case in warmer regions
 560 where permafrost temperatures are higher than -5°C and ALT varies significantly over
 561 time. However, our results also indicate that, under cold conditions where ALT remains
 562 relatively stable, the impact of seasonal freeze-thaw on GST reconstructions is limited
 563 primarily to a quasi-constant shift due to the thermal offset of the active layer. Long-
 564 term warming at the surface may also be underestimated when neglecting the active layer
 565 since energy being consumed as latent heat is not accounted for. Under such conditions,
 566 classical inversion methods that neglect latent heat effects could still be used so long as
 567 the inverted upper boundary temperatures are carefully interpreted as TTOP and are
 568 not directly compared to measured or simulated ground temperatures within or above
 569 the active layer. Latent heat effects can also generally be ignored in boreholes where the
 570 porosity of the solid material is lower than 5% (Mottaghy & Rath, 2006). However, in
 571 the more common high porosity permafrost soils where the active layer is likely to play
 572 a significant role, existing methods that ignore seasonal thawing of the active layer should
 573 not be used, as they will produce physically incoherent inversions due to the non-stationary
 574 position of the upper boundary (i.e. the permafrost table). Our method provides a vi-
 575 able solution to this problem by directly accounting for the seasonal freezing and thaw-
 576 ing of the active layer in the forward model and representation of the GST, thus mak-
 577 ing it more suitable for boreholes in frozen soils. We note also that our approach has the
 578 advantage of being broadly applicable to arbitrarily complex forward models of heat (and
 579 potentially water) flow, so long as the numerical scheme allows for large enough time steps
 580 to make simulations on time scales of centuries to millennia feasible within a given com-
 581 putational budget.

582 Despite the advantages of our proposed method, there are some important caveats
 583 to consider. Firstly, the EKS algorithm that we use for inference is still relatively costly,
 584 requiring a total of 5120 forward model evaluations over the full inversion period (310
 585 years for the synthetic experiment); i.e. 20 iterations of an ensemble of size $N_{\text{ens}} = 256$.
 586 Even with the (relatively) efficient forward model which required 5-10 minutes of wall-
 587 clock execution time per forward model evaluation, this translated into each iteration
 588 taking roughly 20-30 minutes on a compute cluster with a 64-core AMD EPYC 7742 pro-
 589 cessor (256 vCPUs) and 1 TB of memory. Thus, reconstructions spanning multiple mil-

lennia may be prohibitively expensive depending on available compute resources. Future work might therefore consider alternative inference algorithms that employ emulators or reduced-order models to reduce this cost, e.g. the “calibrate, emulate, sample” method of Cleary et al. (2021).

Secondly, our formulation of the GST currently assumes the annual amplitude to remain fixed over the full inversion period. This is a significant source of potential uncertainty since there is ample reason to believe that winter warming has been stronger than summer warming in many Arctic regions (Meyer et al., 2015; Rantanen et al., 2022). While it is theoretically possible within our framework to parameterize the GST amplitude as a time-varying function in addition to the long-term mean, this would greatly increase both the size and the complexity of the resulting inverse problem. As such, we consider the constant amplitude assumption to be a reasonable first order approximation.

Thirdly, our approach uses a fixed length parameterization of the GST function; i.e. we do not consider the impacts of varying the size and number of time segments in the reconstruction. This constitutes a significant source of unquantified uncertainty since the timing of each change point has a substantial impact on the observed temperature profile. One possible improvement could be to combine our forward thermal model of permafrost with the reversible-jump Markov Chain Monte Carlo (RJ-MCMC) approach of Hopcroft et al. (2007). There are significant computational challenges in doing so, however, since such algorithms tend to require tens of thousands of (sequential) iterations to converge, which is prohibitively difficult given the much higher resolution of our forward model.

Another natural continuation of this work would be to apply our method to a circumpolar or global dataset such as the GTN-P (Biskaborn et al., 2015) or the Xibalbá database (Cuesta-Valero et al., 2022). This would enable larger scale GST reconstructions across the cryosphere. However, deep boreholes, here defined as those that extend to depths of at least 50 m below the surface, are relatively rare in Arctic and subarctic regions. This is especially the case in many of the warmer areas where permafrost is likely to be rapidly thawing (see Figure 1b). Boreholes with accessible temperature records spanning both the active and deeper permafrost layers, as well as metadata describing the soil properties, are unfortunately even rarer. Furthermore, despite the development of borehole metadata networks such as GTN-P, ground temperature data from existing boreholes are generally not readily accessible at a global scale.

There is, therefore, an urgent need for a global campaign to install additional deep boreholes in regions where limited historical climate data are available as well as for an improved global database of temperature profiles from permafrost boreholes. Novel reconstruction methods such as ours significantly increase the value of such efforts since, in addition to providing information about the present and future thermal state of permafrost, these data can also provide valuable information about historical climate change predating available observational records. For the time being, however, significant challenges remain in conducting a robust, global scale reconstruction of historical GSTs in permafrost regions from borehole temperature measurements.

6 Conclusions

In this work, we presented a novel method for reconstructing historical ground surface temperatures (GST) from permafrost boreholes using Bayesian inversion of a fast numerical model of two-phase heat transport in permafrost soils. There are two key innovations in our work: Firstly, this is the first study to systematically analyze the impact of seasonal freezing and thawing on GST reconstructions in both cold and warm permafrost environments. Secondly, our proposed method is, to the best of our knowl-

640 edge, the first method for geothermal climate reconstruction that is widely applicable
 641 to boreholes in regions underlain by permafrost. We demonstrated through experiments
 642 with both synthetic and real-world data that latent heat effects due to seasonal thaw-
 643 ing and refreezing of the active layer can have a substantial impact on the reconstructed
 644 GST histories, especially in warmer regions where permafrost is most likely to be thaw-
 645 ing. This implies that such effects should not be ignored in studies which aim to recon-
 646 struct surface temperatures from boreholes in regions where permafrost currently is or
 647 previously was present. Our work highlights the need for further collection and aggre-
 648 gation of borehole data in cold regions in order to facilitate such reconstructions and im-
 649 prove our understanding of the past, present, and future evolution of permafrost.

650 Appendix A Numerical details of the forward model

651 The permafrost thermal modeling approach of Langer et al. (2024) is based on the
 652 numerical scheme of Swaminathan & Voller (1992). This approach solves the discretized
 653 partial differential equation using a first-order, backwards Euler time stepping scheme
 654 where the energy state at each time step is solved iteratively:

$$655 \quad h_i^{j+1} = h_i^j + \frac{\partial h}{\partial T_i^j} \left[T_i^{j+1} - h^{-1}(h_i^j) \right] \quad (\text{A1})$$

656 where j and i refer to the iteration and discretized grid cell indices respectively. The ini-
 657 tial iteration h_i^0 is set to the energy state from the previous time step. The temperature
 658 field at each iteration is solved by linearizing the diffusion equation (2) at the next time
 659 point t and solving the linear system for \mathbf{T}^{j+1} :

$$660 \quad A\mathbf{T}^{j+1} - \frac{\partial h}{\partial \mathbf{T}^j} \frac{\mathbf{T}^{j+1} - \mathbf{T}^j}{\Delta t} - \frac{h(\mathbf{T}^j) - \mathbf{h}^0}{\Delta t} - \mathbf{b} = 0 \quad (\text{A2})$$

661 where \mathbf{T}^j is the discretized temperature state vector at iteration j , A is the tridiagonal
 662 diffusion matrix, \mathbf{h}^0 is the previous energy state, $\Delta t = 24$ hr is the time step size, and
 663 \mathbf{b} is a forcing term appropriately augmented with the corresponding Dirichlet or Neu-
 664 mann boundary conditions at the current time step.

665 Key to this approach is the invertible enthalpy-temperature relation, $h(T_i)$, which
 666 corresponds to the general enthalpy function given by Eq. (3). For simplicity, Langer
 667 et al. (2024) use the so-called “free water” freezing characteristic which defines the un-
 668 frozen water content θ_w in terms of enthalpy:

$$669 \quad \theta_w(h_i) = \begin{cases} \theta_i^{\text{tot}} & h_i > L\theta_i^{\text{tot}} \\ \frac{h_i}{L} & 0 \leq h_i \leq L\theta_i^{\text{tot}} \\ 0 & h_i < 0 \end{cases} \quad (\text{A3})$$

670 where θ_i^{tot} is the total volumetric water and ice content of the i 'th soil volume, typically
 671 equal to the porosity under saturated conditions. Temperature is then correspondingly
 672 determined according to the inverse enthalpy relation:

$$673 \quad h^{-1}(h_i) = \begin{cases} \frac{(h_i - L\theta_i^{\text{tot}})}{C_i} & h_i > L\theta_i^{\text{tot}} \\ 0 & 0 \leq h_i \leq L\theta_i^{\text{tot}} \\ \frac{h_i}{C_i} & h_i < 0 \end{cases} \quad (\text{A4})$$

674 where $C_i = C(\theta_i)$ is the volumetric heat capacity at grid cell i , and here $\theta_i = \theta_w(h_i)$
 675 as defined above. The free water freezing characteristic corresponds to the idealized case
 676 of phase change in pure water. We also use this formulation in the model variants which
 677 exclude seasonal thaw.

Table B1. Soil stratigraphy used for the Sardakh Island borehole inversion. Soil parameters are assumed to be homogeneous within each layer. Here θ_{tot} refers to the total water/ice content, presumed equal to porosity ($\text{m}^3 \text{m}^{-3}$), ω to the organic solid fraction, and k_m to the thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$) of the mineral constituent. Uncertainties refer to the (approximate) standard deviations of the prior.

Layer	Depth [m]	$\theta_{\text{tot}} \times 100$	$\omega \times 100$	k_m
1	0.0	80 ± 10	25 ± 10	2.5 ± 0.5
2	0.5	50 ± 10	1	2.5 ± 0.5
3	9.0	20 ± 10	0	2.5 ± 0.5
4	13.0	10 ± 5	0	3.0 ± 0.5
5	18.0	20 ± 10	0	2.5 ± 0.5
6	30.0	5 ± 5	0	2.5 ± 0.5
7	50.0	5 ± 5	0	1.0 ± 0.5
8	80.0	10 ± 5	0	2.5 ± 0.5

678 As discussed in section 2.1, realistic representations of the freezing and thawing of
679 water in porous media such as soils are complicated by the presence of capillary action
680 which effectively lowers the freezing point of water in the soil pores. In order to account
681 for these effects in the implicit integration scheme described above, it is necessary to de-
682 fine an inverse function for Eq. (3). While no analytical inverse function is generally avail-
683 able, temperature can be recovered by solving a nonlinear system for T_i in the i 'th grid
684 cell:

$$\frac{h_i - L\theta_w(T_i)}{C_i} - T_i = 0 \quad (\text{A5})$$

685 where $C_i = C(T_i)$ is the temperature dependent volumetric heat capacity. For com-
686 putational efficiency, we pre-calculate this inverse function over a large temperature range
687 (-50 to 0°C) within each stratigraphy layer using an adaptive linear interpolation scheme
688 with an error tolerance of 10^{-4} or 0.01%. In order to ensure good convergence of the
689 iterative scheme (A1), we found it necessary to reduce the integration time step Δt to
690 12 hr.

691 Our scheme is generally agnostic to the choice of freezing characteristic, $\theta_w(T)$, so
692 long as the resulting enthalpy-temperature relation is monotonic and has a unique so-
693 lution for any given energy state. For the synthetic experiments, we use the freezing char-
694 acteristic described by Painter & Karra (2014) with van Genuchten (van Genuchten, 1980)
695 parameters $\alpha = 1$ and $n = 2$ for the prototypical sandy soil case and $\alpha = 0.02$ and
696 $n = 1.4$ for the clay soil case. For the Sardakh Island borehole, in order to be consis-
697 tent with the previous analysis of Kneier et al. (2018), we use instead the empirical func-
698 tion derived by Langer et al. (2011) for a nearby site on Samoylov Island.

699 Appendix B Additional details for Sardakh Island inversion

700 The soil stratigraphy used for the Sardakh Island borehole inversion is given in Ta-
701 ble B1. We derived this stratigraphy manually based on the details provided in the sup-
702 plement of Kneier et al. (2018) regarding the Sardakh Island borehole. The eight lay-
703 ers correspond roughly to the lithology of the region, and the specific values for the soil
704 parameters in each layer are taken from the inversion results published in the same work.

705 The posterior densities of the porosity and thermal conductivity parameters in each
706 layer are shown in Figure B1. There is relatively minimal deviation from the priors ex-
707 cept in the porosity of the top organic layer which is poorly constrained given that we
708 do not include temperature measurements above 1 m. There are some slight deviations

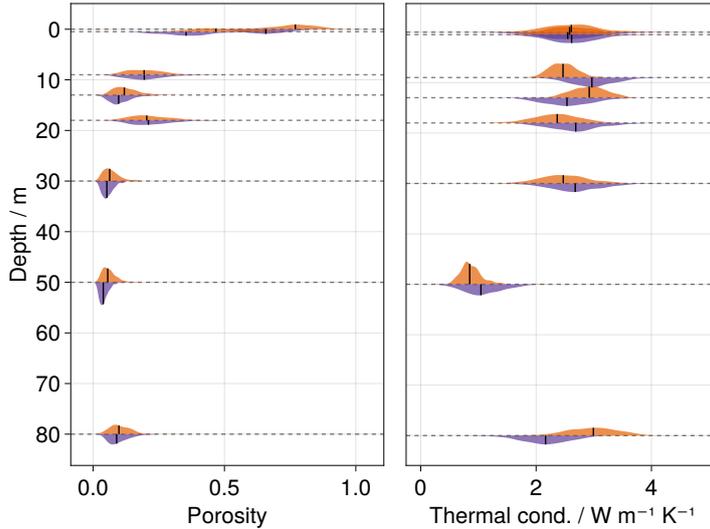


Figure B1. Posterior densities for the porosity and thermal conductivity parameters in each stratigraphy layer. The top (orange) density in each layer corresponds to the model without seasonal thaw, while the bottom (purple) density corresponds to the model with seasonal thaw included.

709 between the two model variants, e.g. in the thermal conductivities of layers 3-5. The pos-
 710 terior densities for the variant with seasonal thaw appear to have shifted (increasing in
 711 layer 3 and decreasing in layer 4) which is likely to compensate for the impacts of freez-
 712 ing and thawing on the thermal properties of the upper layers. In the bottom-most layer,
 713 the posterior density for the first model variant (excluding seasonal thaw) indicates a
 714 higher thermal conductivity which would result in a smaller geothermal gradient. This
 715 is consistent with the smaller bias in the predicted temperature profiles shown in Fig-
 716 ure 4b. The reason for the decrease in the posterior estimate of this conductivity for the
 717 model variant with seasonal thaw is, however, less clear. It could be that this is a com-
 718 pensating effect for the model having a slight cold bias at the 80 m sensor, or it may sim-
 719 ply be an artifact of the sampling method failing to adequately adjust these parameters.
 720 The inclusion of the annual signal increases the difficulty of the optimization problem
 721 since it adds an additional parameter (i.e. the seasonal amplitude) and makes the re-
 722 sponse of the near-surface ground temperatures to the GST signal more nonlinear.

723 Appendix C Open Research

724 The data and code repository used to generate the results in this work is available
 725 on Zenodo (Groenke, Langer, et al., 2024). The code for the forward model, CryoGrid.jl,
 726 is available as open source software on both GitHub and Zenodo (Groenke, Nitzbon, &
 727 Langer, 2024). The historical air temperature forcing data used in the synthetic exper-
 728 iments can be downloaded from Zenodo (Langer et al., 2022a). The model outputs from
 729 Nitzbon et al. (2023) and Langer et al. (2024) used in Figure 1 are also available on Zen-
 730 odo (Langer et al., 2022b). Air temperature data from Tiksi can be obtained directly
 731 from the NOAA Climate Data Center (NOAA National Centers of Environmental In-
 732 formation, 1999).

733 **Acknowledgments**

734 Brian Groenke acknowledges the funding and support of the Helmholtz Einstein Inter-
 735 national Berlin Research School in Data Science (HEIBRiDS) as well as the German Aca-
 736 demic Exchange Service (DAAD).

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