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Physics-Informed Neural Network Modeling of Heat Transfer and Phase Change in Permafrost for Sustainable Shallow Geothermal Energy Systems

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ABSTRACT

This study examines the potential of a Physics-Informed Neural Network (PINN) framework for simulating thermal processes in permafrost during shallow geothermal system operation, with particular emphasis on capturing soil freezing dynamics. The model incorporates nonlinear phase-change behavior, enabling the direct coupling of ice formation with heat and mass transport governed by temperature-dependent thermal and hydraulic conductivities. The governing energy conservation equation with phase-change terms is embedded within the PINN loss function to ensure physical consistency. The framework is validated against benchmark analytical and numerical solutions, showing excellent agreement. Results demonstrate that the PINN can accurately reproduce the transient evolution of temperature and unfrozen water content while providing a mesh-free alternative to conventional finite element methods. Overall, this work highlights the promise of PINNs for modeling complex thermal processes in frozen soils and establishes a foundation for efficient, reliable geothermal system design and safety assessment in permafrost environments.

1 INTRODUCTION

The growing demand for thermal energy storage (TES) as a sustainable heating and cooling solution has underscored the need for accurate modeling of thermal processes in frozen and partially frozen ground (Sojoudi et al., 2024). In cold regions, shallow geothermal systems interact directly with permafrost, where even slight thermal disturbances can lead to significant changes in ground behavior (Khaksar and Li, 2025). The ongoing warming climate accelerates a permafrost thaw, resulting in borehole instability and damage to local built environments (Norouzi et al., 2024). This is particularly concerning since permafrost plays a vital role in maintaining ground stability. Evidence of permafrost degradation, such as increased active layer thickness, reflects the growing influence of climatic forcing (Perreault et al., 2021). In permafrost-affected areas, the design and long-term performance of geothermal energy systems depend critically on the coupled dynamics of heat transfer and phase change within the soil (Vadiee et al., 2025).

In permafrost regions, the coexistence of ice and water phases, along with nonlinear latent heat effects, introduces additional complexity to the numerical modeling of geothermal heat exchangers and the surrounding ground thermal response (Khaksar and Li, 2026). These processes lead to moving phase boundaries and sharp thermal gradients that are difficult to resolve numerically. Conventional numerical methods such as finite difference, finite volume, and finite element methods have been widely used to simulate such problems. However, these approaches require spatial discretization, mesh refinement near phase fronts, and careful numerical stabilization to ensure convergence and accuracy.

Recent advances in machine learning have introduced new approaches for solving partial differential equations (PDEs) (Amini et al., 2022; Xing et al., 2025). Neural networks have been used as universal function approximators capable of representing complex physical fields. However, purely data-driven neural networks require large training datasets and often fail to enforce physical consistency. These datasets are often not available nor reliable due to the nature of the granular materials, like soils and rocks, which differs from location to location. As a result, purely data-driven neural networks may produce solutions that violate conservation laws or exhibit poor generalization outside the training dataset (Karniadakis et al., 2021; Wang et al., 2024).

Physics-Informed Neural Networks (PINNs), first introduced by (Raissi et al., 2019) address these limitations by embedding the governing physical equations directly into the training process. In PINNs, the residual of the governing PDE is incorporated into the loss function, allowing the neural network to learn solutions that satisfy

the underlying physical laws. Automatic differentiation enables the exact evaluation of spatial and temporal derivatives required for the PDE residual, eliminating the need for numerical discretization.

Despite their advantages, PINNs also present several challenges. Training can become difficult for stiff or highly nonlinear problems, and the accuracy of solutions may depend strongly on network architecture, sampling strategies, and loss balancing. Furthermore, steep gradients and moving interfaces, such as those encountered in phase-change problems, can introduce additional difficulties for neural network convergence.

In this study, a Physics-Informed Neural Network framework is developed to simulate heat transfer and phase change processes relevant to shallow geothermal systems operating in permafrost environments. The model incorporates an enthalpy-based formulation that accounts for latent heat effects and temperature-dependent phase saturation. The framework is validated using the classical one-dimensional Stefan problem, which provides an analytical benchmark for evaluating the accuracy of phase-change simulations.

2 METHODS

2.1 Governing Equations

The thermal behavior of frozen ground undergoing phase change is described by the transient energy balance equation in enthalpy form, which accounts for latent heat release during freezing and thawing processes (Norouzi et al., 2022):

$$\left(\rho C_p\right)_{\text{eff}} \frac{\partial T}{\partial t} - \nabla \cdot (\lambda_{\text{eff}} \nabla T) - L_f n \rho_i \frac{\partial S_i}{\partial t} = 0 \tag{1}$$

where $\left(\rho C_p\right)_{\text{eff}}$ is the equivalent volumetric heat capacity that integrates contributions from soil solids, liquid water, and ice phases:

$$\left(\rho C_p\right)_{\text{eff}} = (1-n)\rho_s C_p^s + n S_w \rho_w C_p^w + n S_i \rho_i C_p^i \tag{2}$$

Effective thermal conductivity λ_{eff} is expressed as a geometric mean of the thermal conductivities of each phase and their volumetric fractions:

$$\lambda_{\text{eff}} = {\lambda_s}^{1-n} {\lambda_w}^{nS_w} {\lambda_i}^{nS_i} \tag{3}$$

In this study, the phase change process is represented by defining the ice saturation as a function of temperature using a smooth transition that describes the gradual freezing and thawing:

$$S_i = \frac{1}{1+\exp[k(T-T_r)]} \tag{4}$$

Here, T_r is the reference freezing temperature and k controls the sharpness of the phase transition. The parameters n, ρ, and L_f denote porosity, density, and latent heat of fusion, respectively. This formulation captures both sensible and latent heat effects, allowing for accurate representation of freezing–thawing dynamics within geothermal heat exchange zones in permafrost soils.

2.2 Physics-Informed Neural Network (PINN) Formulation

To approximate the temperature field, a physics-informed neural network is employed. The network takes spatial and temporal coordinates as inputs and predicts the temperature field at those locations. The neural network architecture consists of multiple hidden layers with nonlinear activation functions. The network parameters are optimized to minimize a composite loss function that enforces both physical laws and boundary constraints.

The total loss function is defined as:

$$\mathcal{L} = \mathcal{L}_{\text{PDE}} + \mathcal{L}_{\text{BC}} + \mathcal{L}_{\text{IC}} \tag{5}$$

where:

- $\mathcal{L}_{\text{PDE}}$ enforces the energy balance equation at randomly sampled collocation points by penalizing the residual of the governing PDE,
- $\mathcal{L}_{\text{BC}}$ ensures compliance with prescribed thermal boundary conditions (e.g., geothermal heat flux or ground surface temperature),
- $\mathcal{L}_{\text{IC}}$ enforces the initial temperature distribution at $t = 0$.

The PDE loss is computed as

$$L_{PDE} = \frac{1}{N_c}\sum_{i=1}^{N_c}|R(x_i, t_i)|^2 \quad (6)$$

where $R(x,t)$represents the residual of the governing equation evaluated at collocation points.

The spatial and temporal derivatives required for evaluating the PDE residual are computed using automatic differentiation, ensuring exact gradients without numerical discretization.

2.3 Training Procedure

The PINN model was trained to approximate the temperature field $T(x,t)$over the spatial–temporal domain. The spatial domain was defined as $0 \le x \le 0.1$ m, and the simulation time extended to 72 hours. Dirichlet boundary conditions were imposed at both ends of the domain. A constant temperature was prescribed at the left boundary to represent the warm boundary condition, while the far-field temperature was defined using the analytical ice-side solution to ensure consistency with the Stefan problem formulation. The initial temperature field was obtained from the analytical solution evaluated at a small positive time to avoid incompatibilities at the initial phase boundary.

Training was performed using randomly sampled collocation points within the space–time domain. These collocation points were used to evaluate the residual of the governing energy equation. Additional sampling points were placed on the domain boundaries and at the initial time to enforce boundary and initial conditions.

The neural network consisted of multiple fully connected layers with nonlinear activation functions. Training was conducted in two stages. First, the Adam optimizer was used to perform stochastic gradient descent and capture the general structure of the solution. After the loss reached a plateau, the L-BFGS optimizer was applied to refine the solution and improve convergence accuracy.

The learning rate for the Adam optimizer was set to 5×10^{-5}, and the network was trained for 1000 epochs before switching to the L-BFGS optimizer. The total loss function included contributions from the PDE residual, boundary conditions, initial conditions, and additional snapshot supervision terms.

This two-stage optimization approach has been widely used in PINN implementations to improve training stability and convergence speed.

3 RESULTS

3.1 Benchmark Case: Stefan Problem for Ice Slab Melting

The proposed PINN framework was validated using the classical one-dimensional Stefan problem, which represents the melting of a semi-infinite ice slab. Initially, the slab is at a uniform subfreezing temperature $T_i < T_r$ and begins to melt when a constant boundary temperature is imposed at $x = 0$. The moving interface between ice and liquid water evolves according to the energy balance condition at the phase boundary, ensuring that the latent heat of fusion is properly captured. This benchmark problem provides a rigorous test for the PINN's ability to resolve phase-change fronts and nonlinear thermal gradients relevant to permafrost and shallow geothermal environments. The analytical solution can be found in (Hutter et al., 1990).

3.2 Material Properties

The thermophysical parameters adopted in the simulation are summarized in Table 1. These values correspond to a saturated porous medium composed of soil, water, and ice. The transition parameter $k = 2$ was selected to control the smoothness of the phase-change zone near the melting temperature in which the phase change between ice to liquid happens. This value for k ensures a gradual and physically consistent variation of ice saturation across the freezing front. The latent heat of fusion, $L_{\mathrm{f}} = 3.34 \times 10^5$(J/kg), represents typical values for water–ice systems encountered in permafrost soils.

Table 1. Material properties of the model

Properties	Value
Initial porosity	$n = 1$ (-)
Density of ice	$\rho_i = 910$ (kg/m3)
Density of water	$\rho_w = 1000$ (kg/m3)
Sharpness of the transition parameter	$k = 2$ (-)
Specific heat capacity of ice	$C_i = 2090$ (J/kg/K)
Specific heat capacity of water	$C_w = 4180$ (J/kg/K)
Latent heat of fusion	$L_f = 3.34 \times 10^5$(J/kg)
Reference temperature	$T_0 = 273.15$ (K)

3.3 Temperature Field and Interface Evolution

Figure 1 compares the temperature profiles predicted by the PINN with the analytical solution at various time steps ranging from 2 h to 72 h. The results show excellent agreement throughout the domain. The PINN successfully captures the nonlinear temperature evolution and accurately reproduces the motion of the melting front.

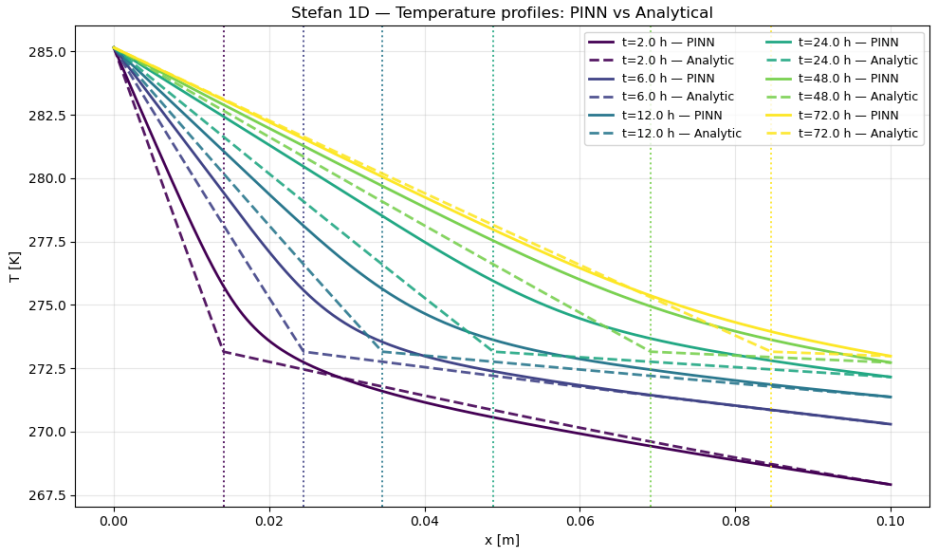


Figure 1. Comparison of temperature profiles predicted by the Physics-Informed Neural Network (PINN) and the analytical solution for the Stefan problem at different times.

Minor deviations occur near the early-time interface due to the steep temperature gradients, but these diminish as training progresses. The model demonstrates strong generalization across the spatial and temporal domain, effectively learning both solid and liquid regions through physics constraints without requiring labeled data. The results confirm that the PINN framework provides a mesh-free, data-efficient, and physically consistent approach for simulating heat transfer with phase change in frozen soils, an essential step toward geothermal system modeling in permafrost environments.

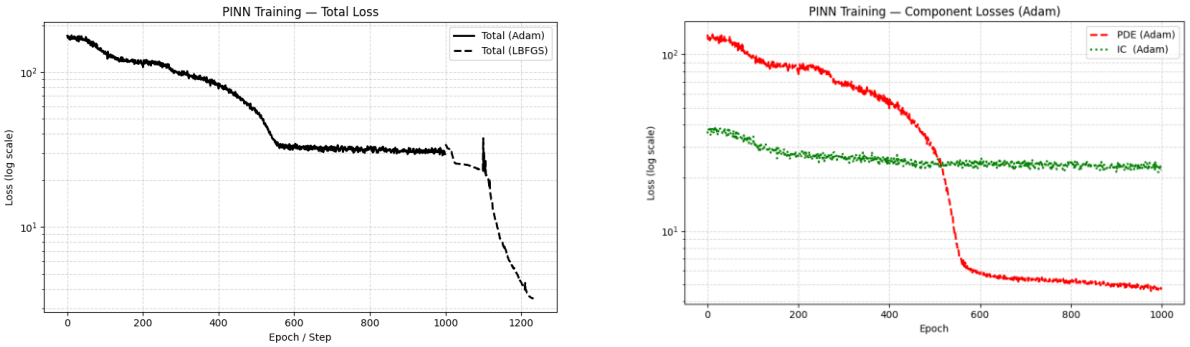
3.3.1 Loss function analysis

As mentioned earlier, the total loss of the system is a weighted combination of three individual components, which are the loss from PDE, from boundary condition, and from the initial condition. The PDE loss ensures that the learned solution satisfies the governing heat transfer equation, while the boundary and initial losses enforce the prescribed thermal conditions. This way of defining the total loss will ensures that the network learn physically consistent solution across the spatial-temporal domain.

Figure 2(a) shows the evolution of the total loss during training. A rapid decrease in the loss is observed during the early training phase using the Adam optimizer, indicating that the network quickly learned the overall structure of the temperature field. As training progressed, the rate of loss reduction became smaller, and the optimization entered a relatively flat region of the loss landscape. This plateau-like behavior is commonly observed in physics-informed neural networks when the solution approaches a physically consistent state.

To better understand the training process, the individual components of the loss function were also monitored. Figure 2(b) presents the evolution of the PDE, boundary condition, and initial condition. The PDE residual experienced the largest reduction during training, decreasing by more than one order of magnitude. This indicates that the network progressively improved its ability to satisfy the governing heat transfer equation.

The boundary condition loss remained consistently small throughout training due to the embedding of the Dirichlet boundary conditions within the network architecture. Similarly, the initial condition loss gradually decreased and stabilized at a low value, confirming that the predicted temperature field remained consistent with the prescribed initial state.



(a) (b)

Figure 2. (a) Total loss function, and (b) Decomposition of the loss function

To verify that the reduction in loss corresponds to meaningful physical learning, the trained PINN predictions were compared with the analytical solution of the classical Stefan problem. As shown in Figure 1, the temperature profiles predicted by the network closely match the analytical solution at all evaluated times. The agreement is observed across both the liquid and ice regions, and the predicted location of the phase-change front follows the analytical interface evolution closely.

The strong agreement between the PINN predictions and the analytical benchmark confirms that the decrease in the total and individual loss components corresponds to an accurate representation of the underlying physical processes rather than merely numerical minimization of the objective function.

3.4 Additional Sensitivity Analysis on Phase-Transition Sharpness

To further examine the robustness of the proposed PINN framework, additional simulations were conducted using larger values of the phase-transition sharpness parameter k, which controls the steepness of the ice-water saturation curve. While the baseline case employed moderate transition values ($k = 2$), supplementary tests explored sharper transitions up to $k = 4$. The results show that the network maintained excellent stability and accuracy even for these steep gradients, successfully resolving the abrupt changes in latent heat and temperature near the melting interface (Figure 3). This confirms the model's capacity to capture nonlinear freezing–thawing dynamics in highly sensitive thermal environments typical of natural permafrost layers.

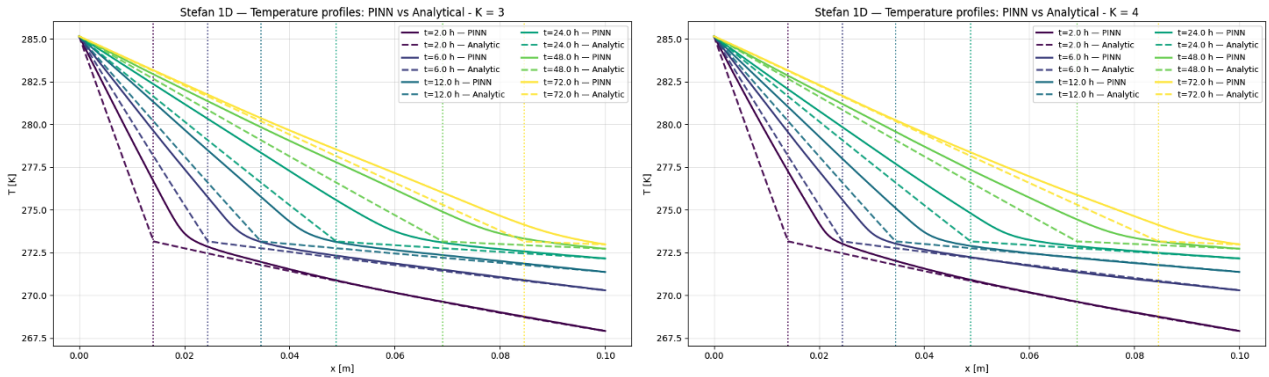


Figure 3. Temperature evolution predicted by the PINN for various sharpness parameters.

4 CONCLUSIONS

The results confirm that the Physics-Informed Neural Network (PINN) approach provides a powerful, mesh-free alternative for simulating heat transfer with phase change in frozen and partially frozen soils. By directly embedding the governing conservation laws and the nonlinear soil freezing characteristic curve (SFCC) into the learning process, the model achieves physically consistent solutions without relying on discretization schemes or numerical stabilization parameters.

The successful reproduction of the Stefan problem demonstrates that the proposed PINN can accurately capture both the temperature evolution and the movement of the melting/freezing front, matching analytical benchmarks with high precision. These findings highlight the ability of the PINN framework to resolve the strong nonlinearity associated with latent heat release, one of the key challenges in traditional finite element modeling of permafrost and geothermal systems.

From a geothermal perspective, the developed PINN methodology lays the foundation for modeling shallow geothermal energy systems in permafrost-affected regions, where ground temperature variations strongly influence the long-term performance of borehole heat exchangers and ground-source heat pumps. The mesh-free nature of PINNs enables efficient modeling of complex soil–structure interactions, heterogeneous ground conditions, and irregular geometries, while maintaining thermodynamic consistency.

Future work will extend the current one-dimensional formulation to coupled thermo-hydro-mechanical (THM) processes and three-dimensional geothermal field configurations. Integration with experimental and field datasets will further enhance predictive accuracy and allow for the development of data-driven digital twins of permafrost-geothermal systems. Overall, this study demonstrates that Physics-Informed Neural Networks offer a promising framework for sustainable geothermal energy design and climate-resilient infrastructure development in cold regions.

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