

# PHYSICS-INFORMED ADAPTIVE TRAINING FOR 3D ACOUSTIC WAVE PROPAGATION

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## ABSTRACT

Physics-informed neural networks (PINNs) provide an implicit, meshless approach to solving high-dimensional partial differential equations while avoiding the curse of dimensionality. Despite recent progress, their application to three-dimensional wave propagation problems in time domain remains limited. In this study, a novel stable training scheme that combines adaptive sampling, absorbing boundary conditions, and neural tangent kernel (NTK) dynamical loss balancing is proposed. Exploiting strong space–time localization of wavefields allows accurate propagation modeling, while avoiding the exponential growth of the number of collocation points with the dimension that is inherent to classical numerical methods.

## 1 INTRODUCTION

Wave propagation in heterogeneous media is a central problem in seismology, radiophysics, optics, underwater acoustics, and exploration geophysics (Virieux & Operto, 2009). While classical numerical methods provide accurate solutions, their computational cost grows rapidly with the problem dimension and required resolution. This is especially true when simulating an acoustic wave in time over three-dimensional space. The use of neural networks to solve these equations is a promising way to overcome these challenges.

Physics-Informed Neural Networks (PINNs) (Raissi et al., 2019) offer a meshless, implicit representation of the solutions of partial differential equations (PDEs) as continuous functions of the spatial coordinates and the time, alleviating some aspects of the curse of dimensionality (Wu et al., 2023). This formulation has motivated increasing interest in applying PINNs to wave propagation problems in heterogeneous media, both in time- and frequency-domain formulations (Moseley et al., 2023; Sethi et al., 2023; Zhang et al., 2023; Song et al., 2021; Alkhalifah & Huang, 2024). Nevertheless, applications of PINNs to the simulation of wave phenomena in three-dimensional environments remains limited, mostly focusing on reconstruction (Lü & Duan, 2025) and on the frequency-domain approaches (Schoder, 2025), or relying on mesh-dependent techniques (Zou et al., 2025; Bizzi et al., 2025).

Despite some promising results, time-domain wave propagation still presents intrinsic challenges for PINNs. For instance, solutions of the wave equation are usually highly localized in space and time due to the concentration of their energy is near propagating wavefronts, that leads to severe gradient imbalance in residual-based training. Moreover, standard neural networks suffer from spectral bias and lack built-in causality (Wang et al., 2022; Xu et al., 2019; Wang et al., 2024; Yu et al., 2022). As a result, training may often converge to incorrect and physically meaningless solutions (Mishra & Shekar, 2025; Krishnapriyan et al., 2021).

Several architectural and training strategies have been proposed to mitigate these effects, including Fourier feature embeddings (Tancik et al., 2020), absorbing boundary conditions and hard enforcement of initial conditions (Ding et al., 2025), causal architectures (Zhao et al., 2024; Bizzi et al., 2025), and hybrid approaches with finite difference methods (Zou et al., 2025). Recent studies further show that adaptive sampling combined with the neural tangent kernel (NTK) establishes a

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stable training regime in two-dimensional problems by concentrating collocation points in dynamically important regions, such as wavefronts and media interfaces, where the reflected waves are generated (Marques et al., 2025). This framework mitigates gradient imbalance and spectral bias, leading to improved training stability and accuracy, particularly in two-dimensional environments.

In the case of non-stationary wave equation in three-dimensional spatial domain, adaptive sampling becomes even more critical as the complexity of the problem scales. We propose using an **adaptive sampling** strategy on the meshless PINN framework, whereby we can leverage the sparse structure of wavefields so that the training can focus mostly in a relatively small spacetime region of interest. The use of such strategies makes training substantially more stable, leading to higher accuracy of the resulting solutions.

## 2 PHYSICS-INFORMED NEURAL NETWORKS

Physics-Informed Neural Networks (PINNs) (Raissi et al., 2019) approximate the solution of partial differential equations (PDE) through a meshless, implicit neural representation over the domain. Instead of relying on structured meshes, the PINN framework allows a more flexible approach to choosing collocation points, including the use of adaptive sampling that focuses on dynamically important regions, such as wavefronts and media interfaces. This flexibility enables accurate resolution of critical solution features without uniformly increasing the sampling density.

In this study, we consider the application of PINNs to wave propagation modeling in the context of underwater acoustics (for the sake of concreteness). The propagation of acoustic waves in a three-dimensional heterogeneous medium is described, in the time domain, by the wave equation

$$\frac{\partial^2 p(\mathbf{x}, t)}{\partial t^2} - c^2(\mathbf{x})\Delta p(\mathbf{x}, t) = S(\mathbf{x}, t, \mathbf{x}_s), \quad (1)$$

where  $p(\mathbf{x}, t)$  is unknown acoustic pressure, while  $c(\mathbf{x})$  is known sound velocity distribution. We adopt a common setup in seismic simulations, where a point source located at  $\mathbf{x}_s$  is approximated by a separable space-time source term  $S$ , consisting of a Gaussian spatial kernel, and a source waveform  $s(t)$ , given by a Ricker wavelet. We assume that the system is initially at rest, i.e.  $p(\mathbf{x}, 0) = 0$  and  $\partial_t p(\mathbf{x}, 0) = 0$ , and that the propagation domain is infinite, therefore we employ high-order Higdon’s absorbing boundary conditions (BCs) (Higdon, 1986). A similar approach was taken in Marques et al. (2025) and Ding et al. (2025). For a more precise description, see Appendix A.

In this context, we represent the acoustic wavefield by a multilayer perceptron (MLP) enhanced by Fourier feature mapping (Tancik et al., 2020). More precisely, we adopt a hard-constrained formulation, following the architectures used by Ding et al. (2025) and Marques et al. (2025). The output of the neural network is here multiplied by a  $t^2$  factor, which enforces both a vanishing wavefield and a zero time derivative at  $t = 0$ . As a result, the initial conditions are satisfied exactly by construction. This contrasts with the widely used strategy in the PINN literature of enforcing initial conditions as soft constraints (Raissi et al., 2019; Hu et al., 2024), which may lead to unstable training dynamics due to unbalanced or competing gradients and does not guarantee a solution satisfying the initial conditions (Wang et al., 2021).

In the resulting framework, the governing physics is enforced through a weighted sum of residuals of the wave equation and absorbing boundary conditions (Higdon, 1986) evaluated at collocation points  $\mathbf{v}_i = (\mathbf{x}_i, t_i)$ ,

$$\mathcal{R}_{\text{PDE}}(\theta, \mathbf{v}_i) = \left( \frac{\partial^2}{\partial t^2} - c^2 \Delta \right) p(\mathbf{v}_i) - S(\mathbf{v}_i), \quad \mathcal{R}_{\text{ABC}}(\theta, \mathbf{v}_i) = \prod_{j=1}^N \left( \frac{\partial}{\partial t} + C_j \frac{\partial}{\partial \mathbf{n}} \right) p(\mathbf{v}_i), \quad (2)$$

where  $C_j = c(\mathbf{v}_i)$  for all  $j$ . The associated loss terms are defined as empirical mean-squared residuals over the collocation sets  $\mathcal{X}_{\text{PDE}}$  and  $\mathcal{X}_{\text{ABC}}$ , containing  $N_{\text{PDE}}$  and  $N_{\text{ABC}}$  points, respectively,

$$\mathcal{L}_{\text{PDE}}(\theta, \mathcal{X}_{\text{PDE}}) = \frac{1}{N_{\text{PDE}}} \sum_{\mathcal{X}_{\text{PDE}}} |\mathcal{R}_{\text{PDE}}(\theta, \mathbf{v}_i)|^2, \quad \mathcal{L}_{\text{ABC}}(\theta, \mathcal{X}_{\text{ABC}}) = \frac{1}{N_{\text{ABC}}} \sum_{\mathcal{X}_{\text{ABC}}} |\mathcal{R}_{\text{ABC}}(\theta, \mathbf{v}_i)|^2. \quad (3)$$

### 3 SAMPLING STRATEGIES AND BALANCING

The traditional uniform strategy used in PINNs samples collocation points using a regular grid, drawing from a uniform distribution or Latin hypercubes (Raissi et al., 2019; Ding et al., 2025). An interesting alternative is to use adaptive sampling, where the points distribution density is defined by the residual Wu et al. (2023); Daw et al. (2022); Bonfanti et al. (2025).

In particular, for three-dimensional wave problems the solution tends to be localized in space and time and to contain highly varying degrees of complexity throughout the domain. This suggests that sampling in a way that attributes equal importance to all regions of spacetime is inefficient at best, and unfeasible at worst. We adopt the adaptive sampling strategy of Marques et al. (2025), which we outline below.

After every 100 training steps, the wave equation residue is evaluated on a regular grid of collocation points. An adaptive distribution for each grid cube is constructed, where the probability of a cube is proportional to the residue at its center point. We then sample from a uniform distribution the box centered on this point. This approach leads to sampling primarily on regions where the PINN residue is high, thus locating complex parts of the solution, such as media interfaces or complex waveforms, that the PINN is currently in the process of learning, as shown in Figures 1b and 1d.

The adaptive distribution is used to sample a set  $\mathcal{X}_A$  of adaptive points. We also sample a set  $\mathcal{X}_U$  of uniform points, so as to keep the model from forgetting parts of the solution where the residue is currently low. The loss is then obtained as a combination of losses on these two sets:

$$\mathcal{L}_{PDE}(\theta) = \mathcal{L}_{PDE}(\theta, \mathcal{X}_U) + \beta \mathcal{L}_{PDE}(\theta, \mathcal{X}_A), \quad (4)$$

where  $\beta$  is a weight parameter. In order to keep adaptive points’ influence stable throughout training, we dynamically adjust the value of  $\beta$  using the Neural Tangent Kernel (Jacot et al., 2018).

The Neural Tangent Kernel of PINNs (Wang et al., 2022) describes the evolution of separate loss terms throughout training as coupled dynamical systems, which leads to an algorithm for adjusting the weights of different losses and ensuring that no single loss term dominates the training. This algorithm has been applied in many PINN problems to weigh different loss terms (Wu et al., 2024; Zhongkai et al., 2024), and is adapted by Marques et al. (2025) to the context of adaptive sampling.

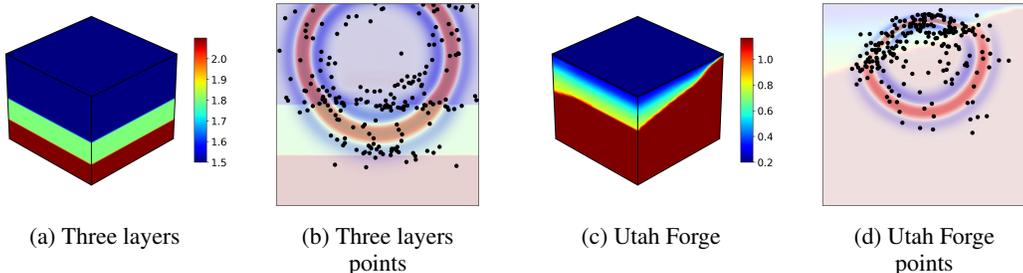


Figure 1: (a) and (c): Sound velocity  $c(\mathbf{x})$  distribution in the three-dimensional domains used in the experiments. (b) and (d): A vertical slice of the solution  $p(\mathbf{x}, t)$  at  $t = 0.35$  showing adaptive points after 10000 training steps. In both domains, the adaptively sampled points follow the wavefront and focus on the interfaces between media.

### 4 EXPERIMENTS AND RESULTS

As the objective of this paper is to extend the PINN techniques from Marques et al. (2025) to three-dimensional problems, we consider two propagation domains. **Three layers** environment consists of parallel horizontal layers with sharp interfaces, leading to transmitted and reflected waves that present a nontrivial benchmark for PINNs, even in two dimensions (Bizzi et al., 2025). **Utah Forge** case is a real-world seismic field described by Vasco & Chan (2022), leading to a solution with a more pronounced three-dimensional effects. In order to normalize the problem dimensions, we divide the original velocities and lengths in Utah Forge by a factor of 5. Due to the linearity of the

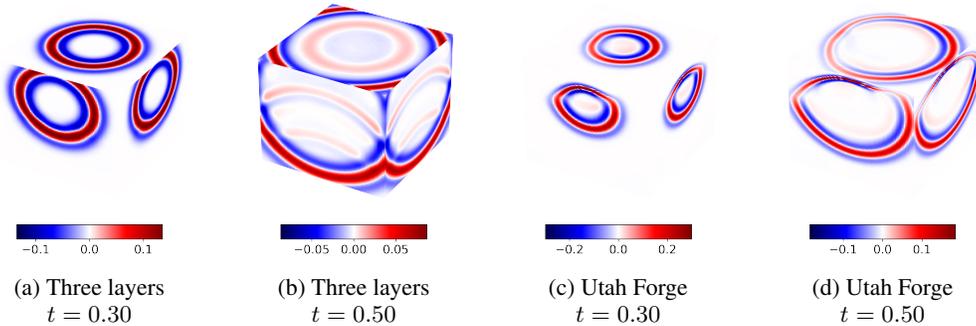


Figure 2: PINN solutions obtained for the Three-layered medium (a and b) and Utah Forge (c and d). Using adaptive sampling, NTK dynamic weights and the other techniques described, the PINN is able to accurately learn the correct form of the wave and its reflections.

wave equation, this scaling does not affect the true solution, but PINNs strongly benefit from this normalization (Xu et al., 2025). These domains are depicted in Figure 1 and in Appendix B.

Each domain has coordinates  $\mathbf{x} \in [0, 1]^3$  and  $t \in [0, 0.5]$ . For the forcing term, the Gaussian kernel has width  $\sigma = 0.025$  and is centered at  $\mathbf{x}_0 = (0, 0, 0.25)$ , and the Ricker wavelet  $s(t)$  has amplitude  $M_0 = 10^4$  and frequency  $f_0 = 10$ .

We use the same architecture as in Marques et al. (2025), with 180 random Fourier features and 5 hidden layers of each 150 neurons each. At each training step, we calculate the PDE residue on 20000 collocation points and the absorbing boundary conditions on 3000 points per boundary. In the case of adaptive sampling, the PDE points are split into 17500 uniform and 2500 adaptive points. The model is trained for 30000 steps, which is sufficient for the loss to become stable in every experiment.

Table 1: Relative  $L_1$  and  $L_2$  errors and training time (TT, in seconds) for wave propagation in both domains, with their average and standard deviation calculated over 5 different runs.

Sampler	Three layers			Utah Forge		
	L1RE ↓	L2RE ↓	TT	L1RE ↓	L2RE ↓	TT
Uniform	$1.165 \pm 0.515$	$1.024 \pm 0.376$	<b>2578 ± 62</b>	$0.959 \pm 0.165$	$0.849 \pm 0.187$	<b>2775 ± 5</b>
Adaptive	<b>0.067 ± 0.003</b>	<b>0.062 ± 0.002</b>	4358 ± 52	<b>0.048 ± 0.012</b>	<b>0.037 ± 0.005</b>	4622 ± 11

For each trained model, we evaluate the relative  $L_1$  and  $L_2$  errors against a reference solution as described in Appendix B, as in Zhongkai et al. (2024). The results, shown in Table 1 show that the adaptive training successfully converges to the correct wavefield, while the uniform strategy fails to converge even after 30000 steps. Despite the greater visual complexity of the Utah forge medium the three layer medium introduces higher frequencies when reflection occurs as it has a sharper discontinuity. This leads both methods to have more ease finding accurate representations of the solution for the Utah Forge dataset. We observed that adaptive training was able to track this physical phenomenon qualitatively as it is able to capture reflection at the media, as shown in Figure 2 above.

## 5 CONCLUSION

We introduced a stable Physics-Informed Neural Network framework for three-dimensional time-domain wave propagation in heterogeneous media. By combining adaptive collocation sampling, absorbing boundary conditions, and Neural Tangent Kernel (NTK)-guided dynamic loss balancing, the proposed approach addresses key challenges in training PINNs for wave equations, including gradient imbalance, spectral bias, and the lack of causality in standard neural architectures.

By exploiting the strong space-time localization of wavefields, the method focuses computational effort on dynamically relevant regions of the domain, enabling accurate wave propagation without the exponential growth in collocation points typical of mesh-based discretizations. These results suggest that implicit, meshless PINN formulations equipped with suitable stabilization and sampling strategies provide a promising foundation for extensions to more complex geometries, higher-frequency regimes, and data-informed wave modeling problems. As future work directions, we believe that applying adaptive sampling training strategies and weight balancing schemes for other complex partial differential equations and setups is merited.

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## A ACOUSTIC WAVE PROPAGATION IN A THREE-DIMENSIONAL MEDIUM

The propagation of acoustic waves in a three-dimensional heterogeneous medium is described, in the time domain, by the scalar wave equation. The acoustic pressure field  $p(\mathbf{x}, t)$  satisfies

$$\frac{\partial^2 p(\mathbf{x}, t)}{\partial t^2} - c^2(\mathbf{x})\Delta p(\mathbf{x}, t) = S(\mathbf{x}, t) := G(\mathbf{x}, \mathbf{x}_s) s(t), \quad (5)$$

where  $c(\mathbf{x})$  denotes the heterogeneous acoustic wave speed. A point source located at  $\mathbf{x}_s$  is approximated by a separable space-time source term, consisting of a Gaussian spatial kernel and a source time function,

$$G(\mathbf{x}, \mathbf{x}_s) = e^{-\frac{\|\mathbf{x}-\mathbf{x}_s\|^2}{2\alpha^2}} \quad \text{and} \quad s(t) = M_0 \left( 1 - 2\pi^2 f_0^2 \left( t - \frac{1}{f_0} \right)^2 \right) e^{-\pi^2 f_0^2 \left( t - \frac{1}{f_0} \right)^2}, \quad (6)$$

with  $t_0 = 1/f_0$ , where  $f_0$  denotes the dominant frequency and  $M_0$  the source amplitude.

We assume that the system is initially at rest, i.e.  $p(\mathbf{x}, 0) = 0$  and  $\partial_t p(\mathbf{x}, 0) = 0$ . Therefore, to simulate an infinite domain, we employ high-order Higdon’s absorbing BCs Higdon (1986), which can be written as

$$\prod_{j=1}^N \left( \frac{\partial}{\partial t} + C_j \frac{\partial}{\partial \mathbf{n}} \right) p = 0, \quad (7)$$

where  $N$  is the order of the condition, and  $\mathbf{n}$  is the outward-normal vector at the given point of the boundary.

## B EXPERIMENTAL SETUP

We consider propagating a wave using PINNs in the two media detailed in Figure 3.

The PINN solutions are evaluated by comparing them to a reference solution obtained by a pseudo-spectral method with discretization  $\Delta x = \Delta y = \Delta z = 10^{-2}$ , and an explicit fourth-order Runge-Kutta solver with  $\Delta t = 5 \times 10^{-4}$ .

Models are evaluated on the relative L1 and L2 errors as in Zhongkai et al. (2024), defined as:

$$L1RE = \frac{\sum_i |u_{pred}(t_i, \mathbf{x}_i) - u_{ref}(t_i, \mathbf{x}_i)|}{\sum_i |u_{ref}(t_i, \mathbf{x}_i)|}, \quad (8)$$

$$L2RE = \sqrt{\frac{\sum_i (u_{pred}(t_i, \mathbf{x}_i) - u_{ref}(t_i, \mathbf{x}_i))^2}{\sum_i u_{ref}(t_i, \mathbf{x}_i)^2}}. \quad (9)$$

where the summations are over a regular grid of 100 points in each space and time dimension.

All experiments were run on the same machine, having an i9-13900K CPU, an RTX 4090 GPU and 128GB RAM. In order to mitigate random effects, each experiment was repeated using 5 different random seeds.

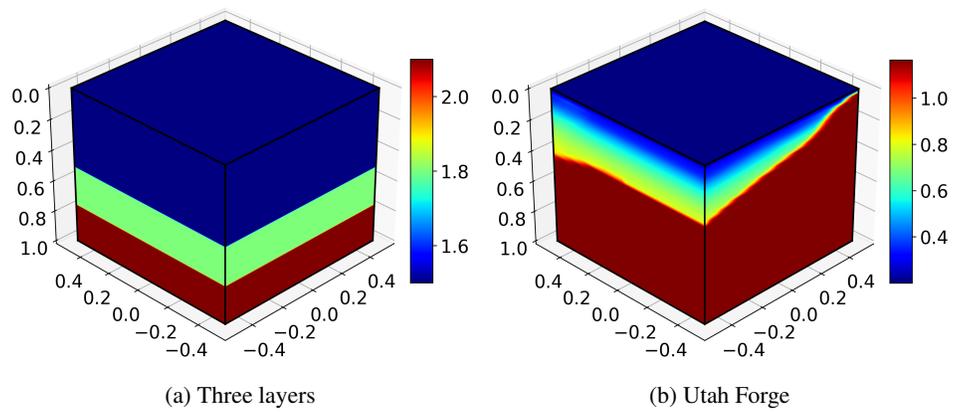


Figure 3: Wave propagation velocity in both domains considered in the experiments.