# A STABLE AND SCALABLE METHOD FOR SOLVING INITIAL VALUE PDEs WITH NEURAL NETWORKS

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## ABSTRACT

Unlike conventional grid and mesh based methods for solving PDEs, neural networks have the potential to break the curse of dimensionality, providing approximate solutions to high-dimensional PDEs. While global minimization of the PDE residual over the network parameters works well for boundary value problems, catastrophic forgetting limits its applicability to initial value problems. In an alternative local in time approach, the optimization problem can be converted into an ODE on the network parameters and the solution propagated forward in time; however, we demonstrate that current methods utilizing this idea suffer from two key issues. First, following the ODE produces an uncontrolled growth in the conditioning of the problem, ultimately leading to unacceptably large numerical errors. Second, as the ODE methods scale cubically with the number of model parameters, they are restricted to small neural networks, significantly limiting their ability to represent intricate PDE initial conditions and solutions. Building on these insights we develop Neural-IVP, an ODE based IVP solver which prevents the network from getting ill-conditioned and runs in time linear in the number of parameters, enabling us to evolve the dynamics of challenging high-dimensional PDEs with neural networks.

## 1 INTRODUCTION

Partial differential equations (PDEs) are needed to describe many phenomena in the natural sciences. PDEs that model complex phenomena cannot be solved analytically and many numerical techniques need to be emploted to computer their solutions. Classical techniques such as finite differences rely on grids and provide efficient solutions when the dimensionality is low ($d = 1, 2$). Yet, the computational and memory costs of using grids or meshes scales exponentially with the dimension, making it extremely challenging to solve PDEs accurately in more that 3 dimensions. Even sophisticated techniques such as fast multipole or adaptive-mesh refinement methods fail when the dimension is high enough.

Neural networks have shown considerable success in modeling and reconstructing functions on high-dimensional structured data such as images or text, but also for unstructured tabular data and spatial functions. Neural networks sidestep the "curse of dimensionality" by learning representations of the data that enables them to perform efficiently. In many ways, neural networks have the benefits and drawbacks of being Monte Carlo methods. Rather than compute costs which scale exponentially in the dimension, they instead typically have error $\epsilon \propto 1/\sqrt{N}$, or equivalently: $N \propto e^{2 \log 1/\epsilon}$, a compute which grows exponentially in the number of significant digits. For many problems this tradeoff is favorable, an approximate solution is much better than no solution.

Thus, it is natural to consider neural networks for solving high-dimensional PDEs. While first investigated in Dissanayake & Phan-Thien (1994) and Lagaris et al. (1998), recent developments by (Yu et al., 2018) and Sirignano & Spiliopoulos (2018) have shown that neural networks can successfully approximate the solution by forcing them to satisfy the dynamics of the PDE on collocation points in the spatio-temporal domain. In particular, the previous paradigm has proven useful for solving boundary value problems where the neural network can successfully approximate the solution by treating time as another spatial dimension. However, for initial value problems (IVPs) time should not be treated symmetrically to the spatial dimension and doing so results in training complications for the neural network such as catastrophic forgetting. Some heuristics have been develop to ame-

liorate this latter problem, such as increasing the collocation points as time progresses, but then the computational cost of training the neural network becomes impractical.

Recently, Du & Zaki (2021) and Bruna et al. (2022) have provided two methods that follow a novel *local in time* paradigm for training neural networks to solve IVPs by updating the parameters sequentially through time rather than by having some fixed set of parameters to model the whole spatio-temporal domain. These methods has proven successful for a variety of high-dimensional PDEs but they currently suffer from two shortcomings. First, the conditioning of the linear systems required to follow the ODE on the network parameters degrades over time, leading to longer solving times and ultimately to a complete breakdown of the solution. Second, the current methodologies lack the capacity to represent difficult initial conditions and solutions as their runtime scales cubically in the number of parameters limiting their ability to use large neural networks. In this work we provide a *local in time* IVP solver (*Neural-IVP*) that circumvents the shortcomings of Du & Zaki (2021) and Bruna et al. (2022) and thus enable us to solve challenging higher dimensional PDEs. In particular we make the following contributions:

- We show how our method can be implemented with fast matrix vector multiplies, scaling only linearly in the number of parameters, allowing us to use much larger neural networks
- We further improve the representational power and quality of initial condition fits through the use of last layer linear solves and sinusoidal embeddings
- We show how following the parameter ODE leads the network parameters to an increasingly poorly conditioned part of the parameter space, and how this relates to exact and approximate parameter symmetries in the network
- Using regularization, restarts, and last layer finetuning, we are able to prevent this phenomenon from happening thereby stabilizing the method

## 2 BACKGROUND

Given a spatial domain $\mathcal{X} \subseteq \mathbb{R}^D$, we will consider the evolution of a time-dependent function $u : \mathcal{X} \times [0, T] \to \mathbb{R}^k$ which at all times belongs to some function space $\mathcal{U}$ and whose dynamics are governed by

$$\begin{aligned} \partial_t u(x,t) &= \mathcal{L}[u](x,t) && \text{for } (x,t) \in \mathcal{X} \times [0,T] \\ u(x,0) &= u_0(x) && \text{for } x \in \mathcal{X} \\ u(x,t) &= h(x,t) && \text{for } x \in \partial\mathcal{X} \times [0,T] \end{aligned}$$

where $u_0 \in \mathcal{U}$ is the initial condition, $h$ is spatial boundary condition, and $\mathcal{L}$ is the (possibly non-linear) operator containing spatial derivatives. We can represent PDEs with higher order derivatives in time such as the wave equation $\partial_t^2 \phi = \Delta\phi$ by reducing them to a system of first order in time equations $u := [\phi, \partial_t \phi]$ where in this example $\mathcal{L}[u_0, u_1] = [u_1, \Delta u_0]$.

**Global Collocation Methods** The first approaches for solving PDEs via neural networks are based on the idea of sampling uniformly from the whole spatio-temporal domain and ensuring that the neural network obeys the PDE by minimizing the PDE residual (or a proxy for it). This approach has roots going back to Dissanayake & Phan-Thien (1994); Lagaris et al. (1998) exploring some initial solutions using neural networks. However, recent advances in automatic differentiation, compute, and neural network architecture have enabled successful applications such as the Deep Galerkin Method (Sirignano & Spiliopoulos, 2018), Deep Ritz Method (Yu et al., 2018), and PINN (Raissi et al., 2019) which have revitalized interest in using neural networks to solve PDEs.

**Learning From Simulations** Not all approaches use neural networks as a basis function to represent the PDE solution. Some approaches focus on directly learning the PDE operator as in Lu et al. (2019) or Kovachki et al. (2021), which can be learned from simulation. However as these methods typically use grids, the purpose is more focused on speeding up existing solvers rather tackling problems that existing solvers cannot tackle. Other approaches that do not rely on collocation points exploit specific information of elliptic and semi-linear parabolic PDEs such as (E. et al., 2017) and (Han et al., 2018).

### 2.1 GLOBAL PDE RESIDUAL MINIMIZATION

The most straightforward method for producing a neural network solution to initial values PDEs is similar to the approach used for boundary value problems of treating the temporal dimensions as if they were spatial dimensions and parametrizing the solution simultaneously for all times $u(x,t) = \mathrm{NN}_\theta(x,t)$. The initial and boundary conditions can be enforced through appropriate parametrization of the network architecture (Berg & Nyström, 2018), whereas the PDE is enforced through minimization of the training objective:

$$S(\theta) = \int_{\mathcal{X}\times[0,T]} r_\theta(x,t)^2 d\mu(x)dt = \int_{\mathcal{X}\times[0,T]} [(\partial_t u_\theta(x,t) - \mathcal{L}\left[u_\theta\right](x,t))^2] d\mu(x)dt$$

where the expectation is estimated via Monte Carlo samples over a chosen distribution of $\mu$ and times $t$.

Initial value PDEs have a local temporal structure where only values on the previous spatial slice are necessary to compute the next; however, the global minimization approaches do not share this property. The weights of the neural network must be used to represent the solution simultaneously at all times, and care must be taken that the PDE solution at earlier times is not catastrophically forgotten as later time values are determined. While Sirignano & Spiliopoulos (2018) and Sitzmann et al. (2020) take this approach, the downsides of avoiding forgetting requiring increasing computation spent on remembering old points are significant.

### 2.2 LOCAL IN TIME METHODS

To circumvent the inherent inefficiency of the global methods, (Du & Zaki, 2021) and (Bruna et al., 2022) propose a local in time method whereby the minimization problem gets converted into an ODE that the parameters satisfy at each time point. In this approach, the PDE solution is given by $u(x,t) = \mathrm{N}(x,\theta(t))$ for the neural network $N$, where the time dependence comes from the parameter vector $\theta(t)$ rather than as an input to the network. Thus, the network only represents the solution at a single time, rather than simultaneously at all times, and subsequently $\theta(t)$ can be recorded and no representational power or computational cost is incurred preserving previous solutions. Assuming the PDE is one-dimensional, the PDE residual at a single time can be written as,

$$L(\dot{\theta},t) = \int_{\mathcal{X}} r(x,t)^2 d\mu(x) = \int_{\mathcal{X}} (\dot{\theta}^\top \nabla_\theta \mathrm{N}(x,\theta(t)) - \mathcal{L}[\mathrm{N}](x,\theta(t)))^2 d\mu(x), \tag{1}$$

since the time derivative is $\partial_t u(x,t) = \dot{\theta}^\top \nabla_\theta \mathrm{N}(x,\theta)$.

Choosing the dynamics $\dot{\theta}$ of the parameters to minimize the instantaneous PDE residual error $L(\dot{\theta},t)$ yields the (implicitly defined) differential equation

$$M(\theta)\dot{\theta} = F(\theta) \quad \text{and} \quad \theta_0 = \arg\min_\theta \int_{\mathcal{X}} (\mathrm{N}(x,\theta) - u(x,0))^2 d\mu(x), \tag{2}$$

where $M(\theta) = \int_{\mathcal{X}} \nabla_\theta \mathrm{N}(x,\theta) \nabla_\theta \mathrm{N}(x,\theta)^\top d\mu(x)$ and $F(\theta) = \int_{\mathcal{X}} \nabla_\theta \mathrm{N}(x,\theta)^\top \mathcal{L}[\mathrm{N}](x,\theta) d\mu(x)$. Once we find $\theta_0$ to fit the initial conditions, we have a fully specified system of differential equations, where we can advance the parameters (and therefore the solution $u(x,\theta(t))$) forward in time.

Since both $M(\theta)$ and $F(\theta)$ involve integrals over space, one can estimate them with $n$ Monte Carlo samples, yielding $\hat{M}(\theta)$ and $\hat{F}(\theta)$, and then solve the linear system $\hat{M}(\theta)\dot{\theta} = \hat{F}(\theta)$ at each timestep for the dynamics $\dot{\theta}$ and use that for an ODE integrator such as RK45. For systems of PDEs such as the Navier Stokes equations, the method can be extended in a straightforward manner by replacing the outer product of gradients with the Jacobians of the multi-output network $N$: $M(\theta) = \int_{\mathcal{X}} D_\theta \mathrm{N}(x,\theta)^\top D_\theta \mathrm{N}(x,\theta) d\mu(x)$ and likewise for $F$, which results from minimizing the norm of the PDE residual $\int_{\mathcal{X}} \|r(x,t)\|^2 d\mu(x)$.

Introducing some additional notation, we can write the Monte-Carlo estimates $\hat{M}$ and $\hat{F}$ in a more illuminating way. Defining the Jacobian matrix of the network for different input points $J_{ik} = \frac{\partial}{\partial \theta_k} \mathrm{N}(x_i,\theta)$, and defining $f$ as $f_i = \mathcal{L}[\mathrm{N}](x_i,\theta))$, the PDE residual loss estimated via the $n$-sample Monte-Carlo estimator is just the least squares objective $\hat{L}(\dot{\theta},t) = \frac{1}{n}\|J\dot{\theta} - f\|^2$. The matrices

$\hat{M}(\theta) = \frac{1}{n}J^\top J$ and $\hat{F}(\theta) = \frac{1}{n}J^\top f$, revealing that the ODE dynamics is just the familiar least squares solution $\dot{\theta} = J^\dagger f = (J^\top J)^{-1}J^\top f$.

## 3 Diagnosing Local in Time Neural PDE solvers

The success of local in time method hinges on the PDE residual error $L(\dot{\theta}, t)$ being close to 0 as we follow the dynamics of $\dot{\theta} = \hat{M}(\theta)^{-1}\hat{F}(\theta)$. The lower the local error, the lower the global PDE residual $S(\theta) = \int L(\dot{\theta}, t)dt$ and the more faithfully the PDE is satisfied.

Even though $\dot{\theta}$ minimizes $L(\dot{\theta}, t)$ this does not mean that the PDE residual error takes a small value, and instead the value of $r(x, t)$ depends nontrivially on the network architecture and the values of the parameters themselves. While the local in time methods have been applied successfully in several cases, there are harder problems where they fail unexpectedly. For example, they fail with unacceptable large errors in second-order PDEs or problems with complex initial conditions. In the following section, we identify the reasons why this is the case.

### 3.1 Representational Power

The simplest reason why local in time methods can fail is because the networks do not have enough representational power. Having enough degrees of freedom and inductive biases in the network matters for being able to find a $\dot{\theta}$ in the span of $J$ which can match the spatial derivatives. The spatial derivatives $\mathcal{L}[N](x, \theta)$ of the PDE must be able to be expressed (or nearly expressed) as a linear combination of the derivative with respect to each parameter: $\frac{\partial}{\partial \theta_k}N(x, \theta)$, which is a different task than a neural network is typically designed for. The easiest intervention on this front is to make the problem easier is to increase the number of parameters $p$, yielding additional degrees of freedom.

Increasing the number of parameters also improves the ability of the network to reconstruct the initial conditions, which can have knock-on effects with the evolution later in time. However, increasing the number of parameters and evolving through time with Du & Zaki (2021); Bruna et al. (2022) immediately runs into a problem. The linear solves used to define the ODE dynamics run in time $O(p^3 + p^2 n)$ and use $O(p^2 + pn)$ memory, which means that networks with more than around $p = 5,000$ parameters cannot be used, and these are extremely small networks compared to modern deep learning standards. In contrast, in subsection 4.1 we show how our Neural-IVP method resolves this limitation, allowing us to use large neural networks with many parameters.

### 3.2 Stability and Conditioning

However, in additional to lacking sufficient representational power, there are more subtle reasons why the local in time methods can fail.

**Even when the solution is exactly representable, a continuous path $\theta^*(t)$ between them may not exist.** Even if a network is able to faithfully express the solution at a given time $u(x, t) = N(x, \theta^*)$ for some value of $\theta^*$ in the parameter space, that does not mean that there exists a continuous path between these $\theta^*$ for different times. This fact is related to the implicit function theorem. With the multi-output function $H_i(t, \theta) = N(x_i, \theta) - u(x_i, t)$, even if we wish to satisfy $H_i = 0$ only at a finite collection of points $x_i$, the existence of a continuous path $\theta^*(t) = g(t)$ in general requires that the Jacobian matrix $D_\theta H = J$ is invertible. Unfortunately this is not the case, there exist singular directions and nearly singular directions in the parameter space as we will now argue.

**There exist singular directions of $J$ and $M$ as a result of symmetries in the network.** Each continuous symmetry of the network will produce a right singular vector of $J$, regardless of how many points $n$ are used in the Monte Carlo estimate. Here we define a continuous symmetry as a parametrized transformation of the parameters $T_\alpha : \mathbb{R}^p \to \mathbb{R}^p$ defined for $\alpha \in (-\epsilon, \epsilon)$, in a neighborhood of the identity $T_0 = \mathrm{Id}$ and $T_\alpha$ has a nonzero derivative with respect to $\alpha$ at the identity. For convenience, consider reparametrizing $\alpha$ to be 'unit speed' so that $\|\partial_\alpha T_\alpha(\theta)\| = 1$.

**Theorem 1.** *Suppose the network $N(x, \theta)$ has a continuous parameter symmetry $T_\alpha$ which preserves the outputs of the function: $\forall \theta, x : N(x, T_\alpha(\theta)) = N(x, \theta)$, then*

$$v(\theta) = \partial_\alpha T_\alpha(\theta)\big|_{\alpha=0} \tag{3}$$

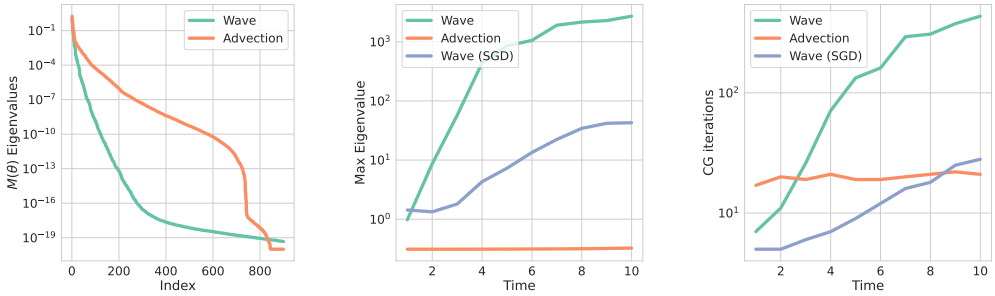


Figure 1: The conditioning of the linear systems needed to solve the ODE on the network parameters increases for challenging PDEs like the wave equation but not for others like the advection equation. (Left): Eigenvalue spectrum of $M(\theta)$ matrix at initialization. (Middle): Growth of largest eigenvalue of $M(\theta)$ over time. (Right): Number of preconditioned CG iterations required to solve the linear system to a specified tolerance of $\epsilon = 10^{-7}$.

*is a singular vector of both $J$ and $M$.*

***Proof:*** *Taking the derivative with respect to $\alpha$ at 0, from the chain rule we have: $0 = \partial_\alpha\big|_0 N(x, T_\alpha(\theta)) = \nabla_\theta N(x,\theta)^\top \partial_\alpha T_\alpha(\theta)\big|_{\alpha=0}$. As this expression holds for all $x$, $J(\theta)v(\theta) = 0$ and $M(\theta)v(\theta) = 0$.*

As Dinh et al. (2017) demonstrated, multilayer perceptrons using ReLU nonlinearities have a high dimensional group of exact parameter symmetries corresponding to a rescaling of weights in alternate layers. Furthermore even replacing ReLUs with alternate activation functions such as Swish (Ramachandran et al., 2017) does not solve the problem, as these will have approximate symmetries which will produce highly ill-conditioned $M$ and $J$ matrices.

**Theorem 2.** *An approximate symmetry $\forall x : \|N(x, T_\alpha(\theta)) - N(x,\theta)\|^2 \leq \epsilon\alpha^2$ will produce nearly singular vectors $v(\theta) = \partial_\alpha T_\alpha(\theta)\big|_{\alpha=0}$ for which*

$$v^\top M v < \epsilon, \tag{4}$$

*and therefore the smallest eigenvalue of $M$ is less than $\epsilon$.*

***Proof:*** *See Appendix A*

Additionally, the rank of the Monte Carlo estimate $\hat{M} = \frac{1}{n} J^\top J$ using $n$ samples is at most $n$, and there is a $p - n$ dimensional manifold of parameters which match the function values at the sample points $\forall i = 1, ..., n : N(x_i, \theta) = N_i$ rather than over the whole domain. In Figure 1 (left), we show empirically that the eigenspectrum of $\hat{M}$ is indeed deficient and highly ill-conditioned, with a long tail of small eigenvalues. Hence some form of regularization such as $[M(\theta) + \mu I]\,\dot{\theta}$ is necessary to have a bounded condition number, $\kappa\left(M(\theta) + \mu I\right) = (\lambda_1 + \mu) / (0 + \mu)$.

Furthermore, as seen in Figure 1 (middle) the conditioning of the linear system (equation 2) deteriorates over time. This deterioration tends to be more of a problem on more challenging PDEs like second-order wave equation in contrast to the easier advection equation. Even when using a dense solver, the quality of the solves will degrade over time, leading to increased error in the solution. When using an iterative method like CG shown in Figure 1 (right), the runtime of the method will increase during the evolution and eventually not be able to meet the desired error tolerance. In contrast, if we instead take snapshots of the solution at different times and fit it directly with SGD, we find that the conditioning is much better as shown by the green curve in Figure 1.

Making sense of this observation, we can learn from the ways that neural networks are typically used: in conjunction with stochastic gradient descent. In general when training neural networks with SGD, the initialization must be chosen carefully to make the problem well-conditioned (Mishkin & Matas, 2015). Many initializations, such as setting the scale of the parameters with drastically different values between layers, will lead either to diverging solutions or no progress on the objective. With the right initialization and a good choice of hyperparameters, the optimization trajectory will stay in a well-conditioned region of the parameter space. However, many bad regions of the

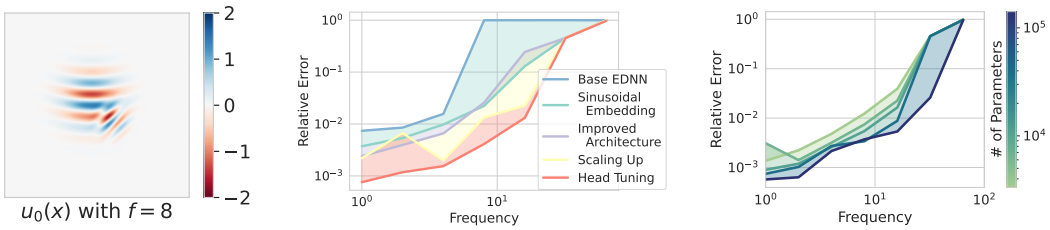


Figure 2: (Left): Example wave packet initial condition with varying levels of fine details parametrized by the frequency $f$. (Middle): Impact of Neural-IVP improvements in the model on the initial condition fit relative error across different levels of difficulty of the solution as parametrized by the frequency $f$, yielding an improvement of $1-2$ orders of magnitude. (Right): Initial condition fit with all Neural-IVP interventions but with varying number of parameters in the model. Note the the value of $5000$ parameters representing the largest matrices that can be used with the dense method.

parameter space exist, and a number of architectural improvements in deep learning such as batch normalization (Ioffe & Szegedy, 2015) and skip connections (He et al., 2016) were designed with the express purpose of improving the conditioning of optimization while leaving the expressive power unchanged. Unfortunately, while SGD optimizers stay in a well-conditioned region of the parameter space, Equation 2 does not.

To see this, consider a singular vector $v$ of $J$ which has a very small singular value $\sigma_v$ (due to an approximate symmetry or otherwise). Analyzing the solution, we see that the projection of the parameters along the singular vector evolves like: $v^\top \dot{\theta} = v^\top J^\dagger f = \sigma_v^{-1} u_v^\top f$, where $Jv = \sigma_v u_v$. A small singular value leads to a large change in that subspace according to the evolution of the ODE. Considering the approximate rescaling symmetry for swish networks, this points the dynamics directly into amplifying the difference between size of weights in neighboring layers and worsening the conditioning, precisely what was identified as *sharp minima* from Dinh et al. (2017). We describe how this problem can be circumvented by our method as described in subsection 4.2.

# 4 Neural IVP

Drawing on these observations, we introduce Neural IVP, a method for solving initial value PDEs that resolves the scalability and numerical stability issues limiting current local in time methods. Additionally, we present several aspects that increase the effectiveness of Neural IVP such as projections to different regions of the parameter space, fine-tuning procedures and inductive biases that increase the representation power of the neural networks.

## 4.1 Improving Representational Power and Scalability

To evaluate the representational power of the network, we examine fitting a complex initial condition typically present in the later evolution of an entangled system, and which will contain components at many different frequencies. We fit a sum of two Gaussians of different sizes modulated by frequencies pointing in different directions in 3-dimensions within the cube $[-1,1]^3$, with the slice through $z=0$ shown in Figure 2 (left). The function is defined as the sum of two Gaussian like wave packets, modulated by spatial frequencies pointing in different directions: $u_0(x) = 30\left(2\pi s_1^2\right)^{-1} e^{-||v||_2^2/(2s_1^2)} \cos\left(2\pi f x^\top \hat{n}\right) + 24\left(2\pi s_2^2\right)^{-1} e^{-||w||_2^2/(2s_2^2)} \cos\left(2\pi f x^\top \hat{m}\right)$ where $v = x - 0.5(\hat{x}_2 + \hat{x}_3)$, $w = x + (\hat{x}_1 + \hat{x}_2 + \hat{x}_3)/6$ also $\hat{n} = (\hat{x}_1 + \hat{x}_2)/\sqrt{2}$ and $\hat{m} = 2^{-1}(\hat{x}_2 + x_1\hat{x}_1/3)$

By changing the frequency parameter $f$, we can investigate how well the network is able to fit fine scale details. We introduce three substantial improvements to the models over those used in Evolutional Deep Neural Networks of Du & Zaki (2021) in order to improve their representational power, and we evaluate the impact of these changes in Figure 2 (middle), starting with the exact 4-layer 30 hidden unit tanh nonlinearity MLP architecture used in EDNN.

**Increasing Number of Parameters and Scalability** As shown in Figure 2 (right), the number of parameters of the network has a large impact on its representational power, not just for solving the initial conditions but also for finding a $\dot{\theta}$ that achieves low PDE residual error. Increasing the number of parameters substantially reduces the approximation error, and especially at high frequencies which are challenging for the model. While dense solves prohibit scaling past 5000 parameters, we show that the solves can be performed much faster making use of the structure of $\hat{M}$. Matrix vector multiplies with the matrix $\hat{M}(\theta) = \frac{1}{n}J^\top J$ can be implemented much more efficiently than using the dense matrix. Making use of Jacobian-vector-products implemented using automatic differentiation (such as in `JAX` (Bradbury et al., 2018)), we can implement a matrix vector multiply using 2 Jacobian-vector-products:

$$\hat{M}\left(\theta\right) v = \tfrac{1}{2n}\nabla_v \|Jv\|^2, \tag{5}$$

which takes $O(n+p)$ time and memory for a single matrix vector product, sidestepping memory bottlenecks that are usually the limiting factor. Then, with these efficient matrix vector products, we can use a scalable Krylov subspace routine of conjugate gradients (CG). To further accelerate the method, we construct a Nystrom preconditioner (Frangella et al., 2021), drasticaly reducing the number of CG iterations. Using this approach, each solve takes time $O((n+p)\sqrt{\kappa})$ where $\kappa(P^{-1}\hat{M})$ is the condition number of the preconditioned matrix $\hat{M}$, rather than $O(p^3 + p^2 n)$ time of dense solves. These improvements to the runtime using the structure of $\hat{M}$ mirror the sparse and Kronecker structures that are made use of by finite difference methods.

**Sinusoidal Embedding** We make several architectural enhancements to the networks used in Du & Zaki (2021); Bruna et al. (2022) which improve the quality of the initial condition fit and the error when evolving forward in time. Notably, we find that using the sinusoidal embedding (Mildenhall et al., 2021) substantially improves the ability of the network to represent higher frequency details in the solution. In contrast to the original form, we use the featurization

$$\gamma(p) = [\sin(2^k p \tfrac{\pi}{2})2^{-\alpha k}]_{k=0}^{L} + [\cos(2^k p \tfrac{\pi}{2})2^{-\alpha k}]_{k=0}^{L}, \tag{6}$$

which scales the magnitude of the high frequency (large $\omega$) components down by $1/\omega^\alpha$. While $\alpha = 0$ (the original sinusoidal embedding) works the best for fitting an initial signal (the only requirement needed for NEural Radiance Fields (Mildenhall et al., 2021)), if we do so then the derivatives will not be well behaved as the magnitude of the largest components of $\gamma'(p)$ will scale like $2^L$ and $\gamma''(p)$ will scale like $2^{2L}$. We find setting $\alpha = 1$ to be the most effective for both first order and 2nd order PDEs. As shown in Figure 2 (middle), the sinusoidal embedding provides a large improvement in the models ability to represent complex functions.

**Last Layer Linear Solves** To further improve the quality of the initial condition fit, after training the network on the initial condition, we recast the fitting of the last layer of the network as solving a linear least squares problem which we can solve using conjugate gradients. The network up until the last layer can be considered as features $N(x) = w^\top \phi_\theta(x) + b$, and over a fixed set of collocation points $X$, we can solve the minimization problem with respect to the final layer weights $w, b$ using linear methods

$$\min_{w,b} \|w^\top \phi_\theta(X) + b - u_0(X)\|^2, \tag{7}$$

which can be solved to a higher level of precision than possible with the full nonlinear and stochastic problem. Doing so enables further reductions to the fit error even if they are below the noisy ball threshold of stochastic optimizers like SGD.

Combining these three improvements of scalability, sinusoidal embeddings, and last layer linear solves (head tuning) we are able to reduce the representation error of the networks by 1-2 orders of magnitude across different difficulties of this challenging 3d problem.

### 4.2 Stability and Conditioning

**Preconditioning** In section 3.2 we discussed how even for easier PDEs, the symmetries in the neural networks generate badly conditioned linear systems for the ODE on the parameters. To counteract this negative effect on our CG solver, we use the highly effective and scalable randomized Nyström preconditioner Frangella et al. (2021). As discussed in Frangella et al. (2021), this preconditioner is close to the optimal truncated SVD preconditioner and it is empirically performant. To employ this preconditioner we first construct a Nyström approximation of $M(\theta)$:

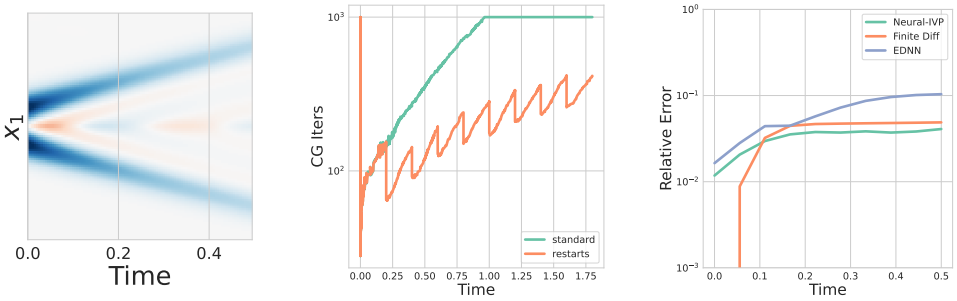


Figure 3: (Left): Neural-IVP fit of the wave equation through time. (Middle): Restarts improve the condition of the linear systems. Here we cap the number of CG iterations at 1000, but without restarts the number required to reach a desired error tolerance will only continue to increase. (Right): Neural-IVP performs slightly better than a finite difference method on the 3D wave equation.

$M_{\text{nys}}(\theta) = (M(\theta)\Omega)\left(\Omega^\top M(\theta)\Omega\right)^{-1}(M(\theta)\Omega)^\top$ using a Gaussian random subspace projection $\Omega \in \mathbb{R}^{p\times\ell}$, where $\ell$ denotes the subspace rank. Then, using the SVD of the approximation $M_{\text{nys}}(\theta) = U\hat{\Lambda}U^\top$ we can construct a preconditioner (where $\nu$ is a small regularization) as follows:

$$P = \frac{1}{\hat{\lambda}_\ell + \nu} U\left(\hat{\Lambda} + \nu I\right)U^\top + \left(I - UU^\top\right).$$

that will mimic the optimal truncated SVD preconditioner when the eigenspectrum $\hat{\Lambda}$ resembles that of the original problem. The cost of using this preconditoner are $\ell$ matrix-vector-multiplies (MVMs) and a Cholesky decomposition of $O\left(\ell^3\right)$, where in our problems $\ell \in \{100, 200, 300\}$.

**Projection to SGD-like regions** Following the ODE on the parameters leads to linear systems whose condition worsens over time as we saw on the middle panel of Figure 1. In that plot it is also visible how the conditioning of the systems is much lower and does not increase as rapidly when the neural network is trained to fit the PDE solution using SGD. In principle we would opt for the SGD behavior but we do not have access to fitting the ground truth PDE solution directly. Instead, when the condition number grows too large, we can refit against our neural predictions using SGD and thus start from another location in the parameter space. That is, every so often, we solve $\theta^{\text{SGD}}(t) = \arg\min_\theta \int_{\mathcal{X}} \left(N(\theta, x) - N(\theta(t), x)\right)^2 d\mu(x)$ where $\theta(t)$ is our current parameters at time $t$. Performing restarts in this way considerably improves the conditioning. As seen in Figure 3 (middle) the number of CG iterations increases substantially slower when using the SGD restarts.

### 4.3 Validating our Method

In order to validate our method, we employ it on the 3 dimensional wave equation $\partial_t^2 u = \Delta u$, which has a few well known analytic solutions, despite being computationally taxing for finite difference and finite element methods. We use the radially symmetric outgoing wave solution $u(x,t) = f(t - \|x\|)/\|x\|$ with $f(s) = 2s^2 e^{-200s^2}$ and integrate the initial condition forward in time by $T = .5$ seconds. In Figure 3 we compare to the analytic solution each of the solutions produced by[1] Neural-IVP, EDNN (Du & Zaki, 2021), and finite differences evaluated on a $100\times100\times100$ grid with RK45 set to a $10^{-4}$ tolerance. Despite the fact that this initial condition does not contain fine scale detail that Neural-IVP excels at, Neural-IVP performs the best among the three solvers, and faithfully reproduces the solution as shown in Figure 3 (left).

## 5 Solving High Dimensional Hyperbolic PDEs

Having validated the Neural-IVP solver on a PDE with analytic solution, we turn to a challenging hyperbolic PDE which does not have known analytic solutions: the wave maps equation. The wave

[1]While we would like to benefit from the improved sampling distribution proposed by (Bruna et al., 2022), unfortunately since the solution is not a probability distribution there is no clear measure to sample from, and we instead sample uniformly from the volume.

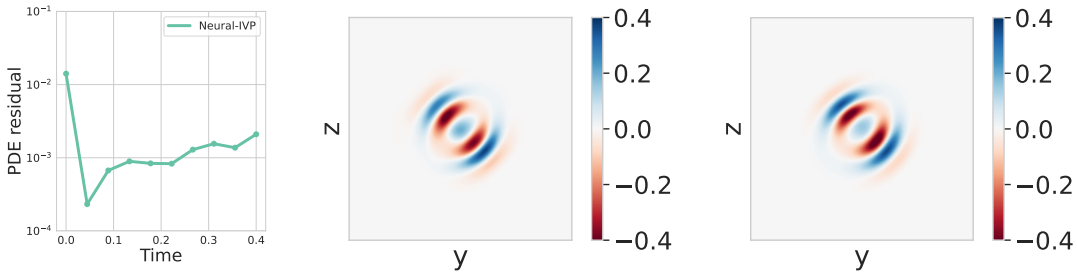


Figure 4: (Left): Neural-IVP's PDE residual over time for wave maps. (Middle): Neural-IVP solution for the wave maps at $t = 0.36$ at a $x = 0$ slice. (Right): Finite difference solution for the wave maps at the same slice.

maps equation is a second-order hyperbolic PDE that often arises in general relativity and that describes the evolution of a scalar field in a curved (3+1) dimensional spacetime. Following Einstein's tensor notation from differential geometry, the wave maps equation can be expressed as

$$g^{\mu\nu}\nabla_\mu\nabla_\nu\phi = g^{\mu\nu}\partial_\mu\partial_\nu\phi - g^{\mu\nu}\Gamma^\sigma_{\mu\nu}\partial_\sigma\phi = 0, \tag{8}$$

where $g$ is the metric tensor expressing the curvature of the space; $\Gamma^\sigma_{\mu\nu}$ are the Christoffel symbols, combinations of the derivatives of the metric, and $\partial_\mu$ are derivatives with respect to components of both space and time.

For the metric, we choose the metric from a Schwarzschild black hole located at coordinate value $c = -2\hat{x}$ in a Cartesian-like coordinate system:

$$g_{\mu\nu}dx^\mu dx^\nu = -(1 - r_s/r_c)dt^2 + [\delta_{ij} + \tfrac{1}{r_c^2(r_c/r_s - 1)}(x_i - c_i)(x_j - c_j)]dx^i dx^j,$$

where $r_c = \|x - c\| = \sqrt{\sum_i (x_i - c_i)^2}$ and $r_s = 2M$ is the radius of the event horizon of the black hole, and we choose the mass $M = 1/2$ so that $r_s = 1$. We choose a wave packet initial condition and evolve the solution for time $T = .5 = 1M$ inside the box $[-1, 1]^3$, with the artificial Dirichlet boundary conditions on the boundary $\partial[-1, 1]^3$. Here the event horizon of the black hole lies just outside the computational domain and boundary conditions meaning that we need worry about complications on and inside the horizon, and instead the scalar field only feels the effect of the gravity and is integrated for a time short enough that it is not yet pulled inside.

While we do not have an analytic solution to compare to, we plot the relative error of the PDE residual averaged over the spatial domain in Figure 4 which is consistently small. We also compare the solution at the time $T = 0.4$ of our solver solution against the finite difference solution run at a spatial grid size of $150 \times 150 \times 150$ which is the largest we were able to run with our optimized sparse finite difference solver before running out of memory. Despite the challenging nature of the problem, Neural-IVP is able to produce a consistent solution for this task.

## 6 Discussion

There are many interesting high-dimensional PDEs that are massively complex to simulate using classical methods due the challenges with scaling up grid and mesh based methods. At the same time, neural networks have shown promise for solving boundary value problems but the current methods for solving initial value problems can be unstable, deficient in scale and in representation power. To ameliorate these deficiencies, we presented Neural-IVP, a local in time method for solving high dimensional initial value PDEs. Neural-IVP can be competitively employed for problems that are computationally challenging to simulate for classical methods like the (3+1) dimensional wave maps equation in section 5. Continuous effort on this front will empower researchers and engineers to simulate high dimensional physical PDEs which lie at the boundary of what is possible with classical methods, allowing prototyping and experimentation without the massive complexity of modern large scale mesh and grid based solvers involving mesh generation, mesh refinement, boundaries, excision, parallelization, and communication.

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## A Approximate Symmetries Yield Small Eigenvalues

Suppose that the network $N$ has an approximate symmetry in the parameters, meaning that there exists a value $\epsilon$ for which

$$\forall x, \theta : \|N(x, T_\alpha(\theta)) - N(x, \theta)\|^2 \leq \epsilon\alpha^2. \tag{9}$$

holds for $\alpha$ in a neighborhood of $0$. If this is the case, we can rearrange the inequality and take the limit as $\alpha \to 0$:

$$\lim_{\alpha \to 0} \|N(x, T_\alpha(\theta)) - N(x, \theta)\|^2/\alpha^2 \leq \epsilon. \tag{10}$$

As the limit $\lim_{\alpha\to 0} \frac{N(x,T_\alpha(\theta))-N(x,\theta)}{\alpha} = \frac{\partial}{\partial\alpha} N(x, T_\alpha(\theta))$ exists, we can interchange the limit and norm to get

$$.\|\nabla_\theta N^\top v\|^2 = v\nabla_\theta N \nabla_\theta N^\top v \leq \epsilon, \tag{11}$$

since $\frac{\partial}{\partial\alpha} N(x, T_\alpha(\theta)) = \nabla_\theta N^\top v$ for $v(\theta) = \partial_\alpha T_\alpha(\theta)\big|_{\alpha=0}$. Recalling that $M(\theta) = \int \nabla_\theta N \nabla_\theta N^\top d\mu(x)$, we can take the expectation of both sides of the inequality with respect to $\mu$, producing

$$v^\top M v < \epsilon. \tag{12}$$