

TensorDiffEq: Scalable Multi-GPU Forward and Inverse Solvers for Physics Informed Neural Networks

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domain-specific knowledge
customized architecture optimization
transfer learning

Abstract

Physics-Informed Neural Networks promise to revolutionize science and engineering practice, by introducing domain-aware deep machine learning models into scientific computation. Several software suites have emerged to make the implementation and usage of these architectures available to the research and industry communities. Here we introduce

★ TensorDiffEq, built on Tensorflow 2.x, which presents an intuitive Keras-like interface for problem domain definition, model definition, and solution of forward and inverse problems using physics-aware deep learning methods. TensorDiffEq takes full advantage of Tensorflow 2.x infrastructure for deployment on multiple GPUs, allowing the implementation of large high-dimensional and complex models. Simultaneously, TensorDiffEq supports the Keras API for custom neural network architecture definitions. In the case of smaller or simpler models, the package allows for rapid deployment on smaller-scale CPU platforms with negligible changes to the implementation scripts. We demonstrate the basic usage and capabilities of TensorDiffEq in solving forward, inverse, and data assimilation problems of varying sizes and levels of complexity. The source code is available at <https://github.com/tensordiffeq>.¹

Keywords: Scientific Machine Learning, PINNs, Neural PDEs, Scientific Computation, Numerical Methods, Neural Networks, Physics-Informed Deep Learning

1. Introduction

As part of the burgeoning field of scientific machine learning (Baker et al., 2019), physics-informed neural networks (PINNs) have emerged recently as an alternative to traditional partial differential equation (PDE) solvers (Raissi et al., 2019; Raissi, 2018; Wight and Zhao, 2020; Wang et al., 2020b), and have given rise to the larger field of study in neural network approximation of PDE systems, generally referred to as Neural PDEs. Typical black-box

1. Package documentation is available at <https://docs.tensordiffeq.io>

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framework
deep NN

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deep learning methodologies do not take into account the underlying physics of the problem domain. The Neural PDE approach is based on constraining the output of a deep neural network to satisfy a physical model specified by a PDE. PINNs typically perform this task via PDE-constrained regularization of a residual function defined by the approximation of the solution network u and forward-pass calculations through the physics of the PDE model, with the applicable derivatives of u calculated via reverse-mode automatic differentiation in a modern deep learning framework such as Tensorflow (Abadi et al., 2016).

The potential of using neural networks as universal function approximators to solve PDEs had been recognized since the 1990's (Dissanayake and Phan-Thien, 1994; Lagaris et al., 1998). However, Physics-Informed Neural Networks promise to take this approach to a different level through deep neural networks, the exploration of which is now possible due to the vast advances in computational capabilities and training algorithms since that time (Abadi et al., 2016; Revels et al., 2016) and modern congenial automatic differentiation software (Baydin et al., 2017; Paszke et al., 2017).

A great advantage of the PINN architecture over traditional time-stepping PDE solvers is that the entire spatial-temporal domain can be solved at once using collocation points distributed quasi-randomly (rather than on a grid) across the spatial-temporal domain, in a process that can be massively parallelized via GPU. As we have continued to see GPU capabilities increase in recent years, a method that relies on parallelism in training iterations could begin to emerge as the predominant approach in scientific computing. To this end, while other software suites exist to define and solve PINNs (Rackauckas and Nie, 2017; Lu et al., 2021; Hennigh et al., 2020; Haghighat and Juanes, 2021), many of those platforms are either restricted to single-GPU implementation or are not fully open-source. Additionally, with full support and customization capabilities of the Keras neural network ecosystem built in to the package, researchers and practitioners can define and train their own custom neural network architectures to approximate the solution of their problem domains. *TensorDiffEq* provides these scalable, modular, and customizable multi-GPU architectures and solvers in a fully open-source platform, tapping into the collective intelligence of the field to improve the implementation of the software and provide input on the direction, structure, and feature coverage of the framework.

2. Mathematical Underpinnings of PINNs

Consider a general nonlinear PDE of the form:

$$\begin{cases} \mathcal{N}_{x,t}[u(x,t)] = 0, & \text{spatial temporal} \\ u(x,t) = g(x,t), & x \in \partial\Omega, t \in [0,T], \text{boundary condition} \\ u(x,0) = h(x), & x \in \Omega, \text{initial condition} \end{cases} \quad (1)$$

where $\mathbf{x} \in \Omega$ is a spatial vector variable in a domain $\Omega \subset \mathbb{R}^d$, t is time, and $\mathcal{N}_{x,t}$ is a spatial-temporal differential operator. Following Raissi et al. (2019), let $u(\mathbf{x}, t)$ be approximated by the output $u(\mathbf{x}, t; \mathbf{w})$ of a deep neural network with inputs \mathbf{x} and t . Define the residual network $r(\mathbf{x}, t; \mathbf{w})$, which share the same network weights \mathbf{w} as the approximation network $u(\mathbf{x}, t; \mathbf{w})$, and satisfies:

$$\{ r(\mathbf{x}, t; \mathbf{w}) := \mathcal{N}_{x,t}[u(\mathbf{x}, t; \mathbf{w})], \text{residual} \} \quad (4)$$

weight²

physic
constraint

where all partial derivatives can be computed by automatic differentiation methods (Baydin et al., 2017; Paszke et al., 2017). The shared network weights \mathbf{w} are trained by minimizing a loss function that penalizes the output for not satisfying (1)-(3):

$$\mathcal{L}(\mathbf{w}) = \mathcal{L}_s(\mathbf{w}) + \mathcal{L}_r(\mathbf{w}) + \mathcal{L}_b(\mathbf{w}) + \mathcal{L}_0(\mathbf{w}), \quad (5)$$

where \mathcal{L}_s is the loss corresponding to sample data (if any), \mathcal{L}_r is the loss corresponding to the residual (4), \mathcal{L}_b is the loss due to the boundary conditions (2), and \mathcal{L}_0 is the loss due to the initial conditions (3):

$$\mathcal{L}_s(\mathbf{w}) = \frac{1}{N_s} \sum_{i=1}^{N_s} |u(\mathbf{x}_s^i, t_s^i; \mathbf{w}) - y_s^i|^2, \text{ sample data} \quad (6)$$

$$\mathcal{L}_r(\mathbf{w}) = \frac{1}{N_r} \sum_{i=1}^{N_r} r(\mathbf{x}_r^i, t_r^i; \mathbf{w})^2, \quad (7)$$

$$\mathcal{L}_b(\mathbf{w}) = \frac{1}{N_b} \sum_{i=1}^{N_b} |u(\mathbf{x}_b^i, t_b^i; \mathbf{w}) - g_b^i|^2, \text{ boundary condition} \quad (8)$$

$$\mathcal{L}_0(\mathbf{w}) = \frac{1}{N_0} \sum_{i=1}^{N_0} |u(\mathbf{x}_0^i, 0; \mathbf{w}) - h_0^i|^2, \text{ initial condition} \quad (9)$$

where $\{\mathbf{x}_s^i, t_s^i, y_s^i\}_{i=1}^{N_s}$ are sample data (if any), $\{\mathbf{x}_0^i, h_0^i = h(\mathbf{x}_0^i)\}_{i=1}^{N_0}$ are initial condition point, $\{\mathbf{x}_b^i, t_b^i, g_b^i = g(\mathbf{x}_b^i, t_b^i)\}_{i=1}^{N_b}$ are boundary condition points, $\{\mathbf{x}_r^i, t_r^i\}_{i=1}^{N_r}$ are collocation points randomly distributed in the domain Ω , and N_s, N_0, N_b and N_r denote the total number of sample data, initial points, boundary points, and collocation points, respectively. The network weights \mathbf{w} can be tuned by minimizing the total training loss $\mathcal{L}(\mathbf{w})$ via standard gradient descent procedures used in deep learning.

tune \mathbf{w}

3. Using *TensorDiffEq* for Forward Problems

TensorDiffEq has a boilerplate model that can loosely be followed in most instances of usage of the package. In forward problems, this process is generally described in the following order:

1. Define the problem domain
2. Describe the physics of the model
3. Define the Initial Conditions and Boundary Conditions (IC/BCs)
4. Define the neural network architecture
5. Select and define the solver
6. Solve the PDE using the fit method

Each of these steps has multiple options and definitions in the *TensorDiffEq* solution suite. The following sections will provide a brief overview of some of the built-in functionality of the package.

①

3.1 Define the Problem Domain

A **Domain** object is the first essential component of defining a problem in *TensorDiffEq*. The domain object contains **primitives** for defining the problem scope used later in your definitions of boundary conditions, initial conditions, and eventually to sample collocation points that are fed into the PINN solver.

The Domain object is defined iteratively. As many dimensions as are required can simply be added to the domain using the **add method**. This means *TensorDiffEq* can be used to solve spatial (steady-state) or spatiotemporal 2D, 3D, or ND problems.

②

3.2 Describe the Physics of the Model

Since *TensorDiffEq* is built on top of Tensorflow (Abadi et al., 2015) physics of the model can be defined via a **strong-form PDE**, with **gradients** defined using the built-in `tf.gradients` function. This allows for a definition similar to that seen in Raissi et al. (2019). An example of defining the PDE for a viscous Burger's system is shown below:

```
1 def f_model(u_model, x, t):
2     u = u_model(tf.concat([x, t], 1))
3     u_x = tf.gradients(u, x)
4     u_xx = tf.gradients(u_x, x)
5     u_t = tf.gradients(u, t)
6     f_u = u_t + u * u_x (0.01 / tf.constant(math.pi)) * u_xx
7     return f_u
```

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}$$

u: fluid velocity
v: kinematic viscosity

Due to the nature of how the PDE system is defined in *TensorDiffEq*, one could define a separate system of **u** and allow for a coupled PDE definition using a similar style as the one shown above.

③

3.3 Define the ICs/BCs

TensorDiffEq supports various types of ICs and BCs and the list will continue to grow. The ICs and BCs that require functions allow for intuitive definitions of those functions of system variables as a Python function, which allows for nonlinear and non-continuous function definitions of state variables. One could define piece-wise functions, Boolean functions, etc using this verbiage and it would be valid input to *TensorDiffEq*'s solvers. At the time of this writing, *TensorDiffEq* supports **constant Dirichlet**, **Function Dirichlet**, and **periodic BCs**, as well as function-based ICs. *TensorDiffEq* takes the ICs and BCs as a list, therefore one can add as many as necessary to define the system. If a BC is not defined on a particular boundary or it is overlooked in the problem definition then the solver will attempt to approximate that boundary using PDE-constrained regularization of the inner points on or around that boundary.

solution fixed at boundary fixed
1D domain [a, b] x=a u(a)=c

BC

not fixed point, function at boundary

④

3.4 Define the Neural Network Architecture

The default architecture of the neural network is a **fully connected MLP** defined in the Keras API (Chollet et al., 2015). To take advantage of the built-in MLP, a list of **hidden layer** sizes is passed into the solver. However, this baseline architecture can be overwritten by any Keras neural network. Currently, the solver requires the number of inputs of the neural network to be the same as the number of dimensions of the system, and the output is the

no. input = no. dim

multilayer perceptron

output = $u(\mathbf{X})$

scalar value of the approximation of $u(\mathbf{X})$ at that combination of input points. However, this “single-network” output architecture is actively being expanded at the time of this writing.

In the event one desires to add batch norm residual blocks, etc, then the Keras API could be used to define the model and the internal parameters of *TensorDiffEq*'s solvers could be modified to use that network as the solution network for $u(\mathbf{X})$. In this way, so long as the input to the neural network has the correct dimensionality for the system (i.e. 3 nodes for a problem with \mathbf{x} , \mathbf{y} , \mathbf{t} dimensions) and the output node is the correct number of dimensions then one could build any architecture the Keras API allows and pass it into the solver. This features also allows for custom neural network layer support using the Keras lambda layer ecosystem, allowing for complete autonomy in the definition of the neural network model internals and training via built-in Keras optimizers.

⑤

3.5 Select and Define The Solver

Stochastic Gradient
Descent

TensorDiffEq is a suite designed to provide forward and inverse PINN solvers. As such, there are various solvers to perform these tasks. At the time of this writing, there are Collocation Method solvers for forward modeling and the Discovery Model for inverse modeling.

set before
learning

Hyperparameter selection can be modified by the user by overwriting the default Adam optimizer (Kingma and Ba, 2014) with any of the other available optimizers in Keras, to include AdaDelta (Zeiler, 2012), Root-Mean-Square Propagation, SGD, and others. Some of these different optimization techniques prove more stable in training than others, and there exist various methods of modifying the loss function of the collocation solver to improve convergence (Wang et al., 2020b,a). To this end, *TensorDiffEq* supports self-adaptive training methods, which have proven to be effective in helping semi-linear PDE systems, such as Allen-Cahn (Allen and Cahn, 1972), converge where the baseline collocation method fails (McClenny and Braga-Neto, 2020). Other methods of improving convergence in Neural PDE and PINN training are continuously being considered.

learning
rate &
hyperparameter

⑥

3.6 Solve the PDE

Each solver has a compile and fit method, to give the package a feel similar to modern popular machine learning or deep learning frameworks such as Keras (Chollet et al., 2015) or scikit-learn (Pedregosa et al., 2011). In most instances, the compile function places parameters such as the domain size and shape, neural network sizes, BCs/ICs, etc. into the solver and the fit function takes only the number of iterations of Keras optimizer runs or newton solver runs.

A feature unique to *TensorDiffEq* is that the Keras neural network model can be exported and saved for later use. This could allow for training on a data center platform, but inference on a local machine. Additionally, being able to export the Keras neural network model opens the door to transfer learning possibilities previously difficult with the versions of Neural PDE solvers currently in circulation. In the case of *TensorDiffEq*, this is a natural result of leaning on the Tensorflow/Keras APIs.

4. Solving Inverse Problems

TensorDiffEq comes with a **base class solver** for inverse problems. Inverse problems can imply parameter estimation or even estimate the interactions between nonlinear operators (Lu et al., 2019) from data. *TensorDiffEq* contains solvers that perform parameter estimation in a PDE system. These parameters can be mobility parameters, diffusivity parameters, etc, where there is some level of a priori physical knowledge about the system in question, but a specific parameter may be unknown. *TensorDiffEq* contains built-in support for solving of such systems that can be solved in ND cases. Parameters are defined as variables that are learned over the course of the training, therefore a natural output is a trained $u(\mathbf{X}, t)$ solution as well as the estimate of the parameters in question.

n-dim

5. Conclusion

In this article, the authors introduce *TensorDiffEq*, a **scalable multi-GPU solver** for PINNs/NeuralPDEs. Some of the main highlights of the software are covered, and more features are currently underway. *TensorDiffEq* contains support for various types of initial conditions, boundary conditions, and allows the user to custom-define their PDE system for their specific problem. In the event that inverse modeling is required, *TensorDiffEq* contains solvers that will accommodate parameter estimation of a PDE system. Currently, *TensorDiffEq* is the only software suite to support self-adaptive solving, demonstrated to improve training convergence and accuracy of the final solution. *TensorDiffEq* takes a step forward in modern implementations of PINN solvers, and fills a unique niche of being a fully open-source multi-GPU PINN solver in the current ecosystem of Scientific Machine Learning software offerings.

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PINN: NN = solution to PDE & w/ physics constraints
 Loss func: $\left\{ \begin{array}{l} \text{data-fitting:} \\ \text{NN prediction} - \text{observed data} \\ \text{physics-constraint:} \\ \text{deviation from PDE} \end{array} \right.$

Neural PDES: $NN \rightarrow \text{approx. solution to PDE}$
 $\star \text{ Input } (x, t) \xleftrightarrow{\text{map}} \text{solns.}$

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