Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2020-0164

Vol. **28**, No. 5, pp. 2002-2041
November 2020

Extended Physics-Informed Neural Networks (XPINNs): A Generalized Space-Time Domain Decomposition Based Deep Learning Framework for Nonlinear Partial Differential Equations

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Received 26 August 2020; Accepted (in revised version) 3 October 2020

Abstract. We propose a generalized space-time domain decomposition approach for the physics-informed neural networks (PINNs) to solve nonlinear partial differential equations (PDEs) on arbitrary complex-geometry domains. The proposed framework, named eXtended PINNs (*XPINNs*), further pushes the boundaries of both PINNs as well as conservative PINNs (cPINNs), which is a recently proposed domain decomposition approach in the PINN framework tailored to conservation laws. Compared to PINN, the XPINN method has large representation and parallelization capacity due to the inherent property of deployment of multiple neural networks in the smaller subdomains. Unlike cPINN, XPINN can be extended to any type of PDEs. Moreover, the domain can be decomposed in any arbitrary way (in space and time), which is not possible in cPINN. Thus, XPINN offers both space and time parallelization, thereby reducing the training cost more effectively. In each subdomain, a separate neural network is employed with optimally selected hyperparameters, e.g., depth/width of the network, number and location of residual points, activation function, optimization method, etc. A deep network can be employed in a subdomain with complex solution, whereas a shallow neural network can be used in a subdomain with relatively simple and smooth solutions. We demonstrate the versatility of XPINN by solving both forward and inverse PDE problems, ranging from one-dimensional to three-dimensional problems, from time-dependent to time-independent problems, and from continuous to discontinuous problems, which clearly shows that the XPINN method is promising in many practical problems. The proposed XPINN method is the generalization of PINN and cPINN methods, both in terms of applicability as well as domain decomposition approach, which efficiently lends itself to parallelized computation. The XPINN code is available on *https://github.com/AmeyaJagtap/XPINNs*.

AMS subject classifications: 35E05, 35E15, 68T99, 76J20, 74B05

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Key words: PINN, XPINN, domain decomposition, irregular domains, machine learning, physics-informed learning.

1 Introduction

Recently deep neural networks (DNNs) have gained a lot of attention in the field of scientific machine learning (SciML). Thanks to their universal approximation properties, they can be exploited to construct alternative approaches for solving PDEs. In particular, they offer nonlinear approximation through the composition of hidden layers, which does not limit the approximation to the linear spaces. The training of a DNN based model (black-box surrogate model) usually requires a large amount of labeled data, which are often unavailable in many scientific applications. However, when the governing PDEs are known, their solutions can be learned in a physics-informed fashion with relatively small amounts of data. The physics-informed loss functions are constructed based on PDE residuals and the DNN is trained by minimizing this loss function, which, in turn, satisfies the governing physical laws. The notion of a neural network to solve PDEs was proposed in 90's, see [1–4], and more recently in [5–7], which had rapid success due to remarkable advances in the GPU hardware but also the stochastic gradient descent algorithms such as Adam [20]. More broadly, Owhadi [33] constructed physics-informed learning machines that made use of systematically structured prior information about the solution. Brunton, et al. [34] proposed the SINDy framework for dictionary learning of dynamical systems. Ling et al. [39] uses DNN to model the Reynolds stresses in a Reynolds-averaged Navier-Stokes model. Wang et al. [29] proposed the physics-informed machine learning approach for turbulence modeling. Tompson et al. [40] used a convolutional neural network to solve a large sparse linear system for Navier-Stokes equations. In [38], the authors proposed a deep Galerkin method, which is a deep learning algorithm for solving PDEs. Recently, Raissi et al. [37] used automatic differentiation and proposed physics-informed neural networks (PINNs), where the PDE residual is incorporated into the loss function of fully-connected neural networks as a regularizer, thereby constraining the space of admissible solutions. In this setting, the problem of inferring solutions of PDEs is transformed into an optimization problem of the loss function. The major advantage of PINNs is providing a mesh-free algorithm as the differential operators in the governing PDEs are approximated by *automatic differentiation* [8]. PINNs require a modest amount of data, which can be properly enforced in the loss function. PINNs can solve forward problems, where the solution of governing physical laws is inferred, as well as inverse problems, where unknown coefficients or even differential operators in the governing equations are identified. The PINNs has been applied extensively to solve various PDEs such as fractional PDEs [13, 14], stochastic PDEs [11, 12], with limited training data. Moreover, it has been successfully employed to solve many problems in computational and engineering science like, geostatistical modeling [36], cardiovascular systems [42–44], vortex-induced vibrations [45], high Mach number compressible