

PFNN-2: A Domain Decomposed Penalty-Free Neural Network Method for Solving Partial Differential Equations

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Abstract. A new penalty-free neural network method, PFNN-2, is presented for solving partial differential equations, which is a subsequent improvement of our previously proposed PFNN method [1]. PFNN-2 inherits all advantages of PFNN in handling the smoothness constraints and essential boundary conditions of self-adjoint problems with complex geometries, and extends the application to a broader range of non-self-adjoint time-dependent differential equations. In addition, PFNN-2 introduces an overlapping domain decomposition strategy to substantially improve the training efficiency without sacrificing accuracy. Experiments results on a series of partial differential equations are reported, which demonstrate that PFNN-2 can outperform state-of-the-art neural network methods in various aspects such as numerical accuracy, convergence speed, and parallel scalability.

AMS subject classifications: 65M55, 68T99, 76R99

Key words: Neural network, penalty-free method, domain decomposition, initial-boundary value problem, partial differential equation.

1 Introduction

In recent years, neural network methods are becoming an attractive alternative for solving partial differential equations (PDEs) arising from applications such as fluid dynamics [2–4], quantum mechanics [5–7], molecular dynamics [8], material sciences [9] and geophysics [10, 11]. In contrast to most traditional numerical approaches, methods based

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on neural networks are naturally meshfree and intrinsically nonlinear therefore can be applied without going through the cumbersome step of mesh generation and could be more potentially applicable to complicated nonlinear problems. These advantages have enabled neural network methods to draw increasingly more attention with both early studies using shallow neural networks [12–18] and recent works with the advent of deep learning technology [5, 19–25].

Despite of the tremendous efforts to improve the performance of neural network methods for solving PDEs, there are still issues that require further study. The first issue is related to the accuracy of neural network methods. It is still not fully understood how well a neural network can approximate the solution of a PDE in either theory or practice. Recent investigations were carried out to reveal some preliminary approximation properties of neural networks for simplified problems [26–29], or to improve the accuracy of neural network methods from various aspects such as by introducing weak form loss functions to relax the smoothness constraints [21, 30–34], by modifying the solution structure to automatically satisfy the initial-boundary conditions [15, 17, 18, 35, 36], by revising the network structure to enhance its representative capability [37–40], and by introducing advanced sampling strategies to reduce the statistical error [41, 42]. These improvements so far are usually effective in respective situations, but are not general enough to adapt with different types of PDEs defined on complex geometries.

Another difficulty for solving PDEs with neural network methods is related to the efficiency. It is widely known that training a neural network is usually much more costly than solving a linear system resulted from a traditional discretization of the PDE [43–45]. To improve the efficiency, it is natural and has been extensively considered [4, 46] to utilize distributed training techniques [47, 48] based on data or model parallelism, by which the training task is split into a number of small sub-tasks according to the partitioned datasets or model parameters so that multiple processors can be exploited. Although this distributed training is general and successful in handling many machine learning tasks [49–52], it is not the most effective choice for solving PDEs because no specific knowledge of the original problem is adopted throughout the training process.

Inspired by the idea of classical domain decomposition methods [53], it was proposed to introduce domain decomposition strategies into neural network based PDE solvers [54–62] by dividing the learning task into training a series of sub-networks related to solutions on sub-domains. This tends to be more natural than the plain distributed training approaches because by introducing domain decomposition the training of each sub-network only requires a small part of dataset related to the corresponding sub-domain, therefore can significantly decrease the computational cost. However, these methods may still suffer from issues related to low convergence speed and poor parallel scalability due in large part to the straightforward treatment of artificial sub-domain boundaries.

In this paper, we present PFNN-2, a new penalty-free neural network method that is a subsequent improvement of our previously proposed PFNN method [1]. Inheriting all advantages of PFNN in handling the smoothness constraints and essential bound-