Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2023-0180

Vol. **35**, No. 2, pp. 467-497
February 2024

A Conservative and Positivity-Preserving Method for Solving Anisotropic Diffusion Equations with Deep Learning

Hui Xie[1], Li Liu[1], Chuanlei Zhai[1], Xuejun Xu[2,3] and Heng Yong[1,*]

[1] *Institute of Applied Physics and Computational Mathematics, Beijing, 100094, China.*

[2] *LSEC, Institute of Computational Mathematics, Academy of Mathematics and System Sciences, Chinese Academy of Sciences, P.O. Box 2719, Beijing, 100190, China.*

[3] *School of Mathematical Sciences, Tongji University, Shanghai, China.*

Received 4 July 2023; Accepted (in revised version) 15 November 2023

Abstract. In this paper, we propose a conservative and positivity-preserving method to solve the anisotropic diffusion equations with the physics-informed neural network (PINN). Due to the possible complicated discontinuity of diffusion coefficients, without employing multiple neural networks, we approximate the solution and its gradients by one single neural network with a novel first-order loss formulation. It is proven that the learned solution with this loss formulation only has the $\mathcal{O}(\epsilon)$ flux conservation error theoretically, where the parameter ϵ is small and user-defined, while the loss formulation with the original PDE with/without flux conservation constraints may have $\mathcal{O}(1)$ flux conservation error. To keep positivity with the neural network approximation, some positive functions are applied to the primal neural network solution. This loss formulation with some observation data can also be employed to identify the unknown discontinuous coefficients. Compared with the usual PINN even with the direct flux conservation constraints, it is shown that our method can significantly improve the solution accuracy due to the better flux conservation property, and indeed preserve the positivity strictly for the forward problems. It can predict the discontinuous diffusion coefficients accurately in the inverse problems setting.

AMS subject classifications: 65M08, 35R05, 76S05

Key words: Anisotropic diffusion, physics-informed neural network, first-order loss, flux conservation, positivity.

---

*Corresponding author. *Email addresses:* `xiehui@lsec.cc.ac.cn` (H. Xie), `liu_li@iapcm.ac.cn` (L. Liu), `zhai_chuanlei@iapcm.ac.cn` (C. Zhai), `xxj@lsec.cc.ac.cn` (X. Xu), `yong_heng@iapcm.ac.cn` (H. Yong)

1 Introduction

Anisotropic diffusion equations exist in the mathematic modeling of many practical applications such as inertial confinement fusion (ICF) [19, 23], reservoir engineering [33], astrophysical systems [28]. Generally, the computational domain is quite complicated for these practical applications. The traditional mesh-based method will be time-consuming even just for the mesh generation. In addition, the different materials and localized physical variable (e.g., magnetic field) may result in the multiscale diffusion transport coefficients, thus introducing an anisotropic diffusion equation defined on the complex computational domain.

For solving this multiscale diffusion problem on the general computational meshes, many traditional mesh-based numerical methods have been investigated in the last decades. As we know, some finite volume scheme based on the multi-point stencil are developed. The Kershaw scheme was proposed in [16] for the smooth meshes. After that, the mimetic finite difference method [29], nine-point scheme [4, 34] and multi-point flux approximation (MPFA) [1] were introduced on general distorted meshes. Also some variants [9, 11] were proposed for anisotropic diffusion tensors with improved heat flux approximation. Recently, for keeping positivity numerically, some nonlinear finite volume schemes were proposed in [24, 30, 38, 41], where Picard or Newton iteration must be employed to find their numerical solutions. To make ease of simulation on the complex domain, the PINN methodology [32] is a promising alternative method, but the physics embedded in the standard PINN may be insufficient for these multiscale problems.

In the context of scientific computing, the idea of PINN for solving PDEs can be tracked to some pioneer papers [18, 20] in the 1990s. It is free of mesh generation and less sensitive to the dimensionality of the problems. As the vast advance of computing power and machine learning platform (e.g. TensorFlow), recently, Raissi et al. [32] proposed PINN for the solution and parameters discovery of PDE. The main idea behind the PINN is that the governing equation is used in the loss function to constraint the neural network approaching the strong solution of PDEs. PINNs have been successfully used in solving a large number of nonlinear PDEs, including Burgers, Schröinger, Navier-Stokes, Allen-Cahn, Euler equations, etc [6, 13, 21, 25, 27, 37, 39, 40, 43, 44].

As for the second-order elliptic problems, the convergence analysis was developed for the linear elliptic and parabolic equation in [36] and [14]. Solving a class of second-order boundary-value problems on the complex geometries was studied in [2] and [35], where the boundary condition is trained with a separate neural network in the latter paper. A comprehensive review of different boundary condition enforcement manners was given by [5]. In [12], solving advection-diffusion equations were addressed for high Péclet number. An extreme machine learning method [7] with only one hidden layer was proposed for 1D diffusion problems. To alleviate the high-order derivatives of neural network approximation, the variational PINN was introduced in [17]. Similarly, the deep mixed residual method [26] and deep least-squares methods [3] have been introduced. The asymptotic-preserving first-order deep neural network for one special anisotropic