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Solving Diffusion Problems by a Random Feature Method

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Abstract. Solving diffusion problems requires numerical methods able to capture the heterogeneity over complex geometries and are robust in terms of positivity preserving, nonlinearity, and radiation diffusion. Current deep learning methods, although mesh-free, encounter difficulties in achieving convergence and exhibit low accuracy when confronted with these specific issues. In this paper, we develop a novel method to overcome these issues based on the recently proposed random feature method (RFM). Our contributions include: (1) for anisotropic and discontinuous coefficient problems, we rewrite a diffusion problem into a first-order system and construct the corresponding loss function and approximation spaces; (2) to avoid negative solutions, we employ the square function as the activation function to enforce the positivity and the trust-region least-square solver to solve the corresponding optimization problem; (3) for the radiation diffusion problem, we enrich the approximation space of random feature functions with the heat kernel. Various numerical experiments show that the current method outperforms the standard RFM as well as deep learning methods in terms of accuracy, efficiency, and positivity preserving.

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1. Introduction

Diffusion problems manifest across diverse scientific and industrial realms, encompassing applications such as inertial confinement fusion (ICF) [13, 15], reservoir engineering [24], and astrophysical systems [18]. Within the domain of diffusion problems, significant challenges arise, particularly given the complexities inherent in practical computational domains. Furthermore, the intricacies are compounded by the presence of diverse materials and localized physical variables — e.g. magnetic fields, leading to the emergence of anisotropic diffusion coefficients or discontinuous coefficients. For radiation diffusion problems, finding non-negative solutions leads to an additional layer of complexity. Simultaneously, optimization algorithm challenges arise due to the mismatch between the initial value condition and the boundary value condition, coupled with strong nonlinearity, thereby posing hurdles for convergence.

To address these challenges, various traditional numerical methods have been proposed over the past few decades. Notably, finite volume schemes based on multi-point stencils have been developed. The Kershaw scheme, introduced in [11] for smooth meshes, represents one such example. Subsequently, other methods, including the mimetic finite difference method [19], the nine-point scheme [3, 25], and the multi-point flux approximation (MPFA) [1], have been introduced to accommodate general distorted meshes. Additionally, several variants [7, 8] have been proposed to handle anisotropic diffusion tensors, incorporating improved heat flux approximations. More recently, to ensure numerical positivity, certain nonlinear finite volume schemes were presented in [14, 16, 27, 29]. These schemes require the application of Picard or Newton iteration methods to obtain their numerical solutions. For radiation diffusion problems, numerous studies have also presented a range of numerical algorithms, with the majority employing the finite volume method. Knoll *et al*. [10, 12, 20, 21] extensively investigated this problem. Sheng *et al*. [26] developed a monotone finite volume scheme designed for distorted meshes, specifically addressing multimaterial non-equilibrium radiation diffusion equations. In their approach, the Picard iteration was applied to solve the resulting nonlinear algebraic systems. Yuan *et al*. [31] provided a comprehensive review of recent advancements in numerical methods for the radiation diffusion equation. Their research primarily emphasizes the construction of nonlinear solvers tailored for large nonlinear algebraic systems. More recently, Yue *et al*. [33] introduced the Picard-Newton iterative method as a strategy to enhance efficiency and overcome the limitations of the Picard iteration.

However, mesh generation is still a huge problem for traditional methods. Therefore, deep learning methods with adaptability to high-dimensional problems and mesh-free characteristics have achieved rapid development. One of the noteworthy methods is the Physics-Informed Neural Network (PINN) approach [23]. To address the diffusion problems mentioned earlier, numerous variations of the PINN method have been proposed. Xie *et al*. [28] introduced a weighted function to handle potential discontinuities in the diffusion coefficient across material interfaces. In a related study, He *et al*. [9] underscored the inefficiency of relying on a single neural network structure to represent the interface. They proposed a piecewise neural network structure and an adaptive resampling strategy to effectively