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Asymptotic-Preserving Neural Networks for Multiscale Kinetic Equations

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Abstract. In this paper, we present two novel Asymptotic-Preserving Neural Networks (APNNs) for tackling multiscale time-dependent kinetic problems, encompassing the linear transport equation and Bhatnagar-Gross-Krook (BGK) equation in all ranges of Knudsen number. Our primary objective is to devise accurate APNN approaches for resolving multiscale kinetic equations, which is also efficient in the small Knudsen number regime. The first APNN for linear transport equation is based on even-odd decomposition, which relaxes the stringent conservation prerequisites while concurrently introducing an auxiliary deep neural network. We conclude that enforcing the initial condition for the linear transport equation with inflow boundary conditions is crucial for this network. For the Boltzmann-BGK equation, the APNN incorporates the conservation of mass, momentum, and total energy into the APNN framework as well as exact boundary conditions. A notable finding of this study is that approximating the zeroth, first, and second moments—which govern the conservation of density, momentum, and energy for the Boltzmann-BGK equation, is simpler than the distribution itself. Another interesting phenomenon observed in the training process is that the convergence of density is swifter than that of momentum and energy. Finally, we investigate several benchmark problems to demonstrate the efficacy of our proposed APNN methods.

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Key words: Asymptotic-Preserving Neural Networks, even-odd decomposition, conservation laws, multiscale.

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1 Introduction

In scientific modeling, kinetic equations describe the dynamics of density distribution of particles that collide between themselves, or interacting with a medium or external fields. These equations are defined in the phase space, thus suffer from curse-of-dimensionality. In addition, they typically involve multiple spatial and/or temporal scales, characterized by the Knudsen number, as well as high dimensional nonlocal operators, hence present significant computational challenges in numerical simulations. For a comprehensive overview, please refer to the literature sources [1–4] for a review.

Deep learning methods and deep neural networks (DNNs) have garnered immense attention within the scientific community, including the possibility of resolving partial differential equations (PDEs) [5–12]. To explore alternative machine learning approaches for solving partial differential equations, we refer to the exemplary review article [5]. The key motivation behind such methods is to parameterize the solutions or gradients of PDE problems using deep neural networks. These methods ultimately culminate in a minimization problem that is typically high-dimensional and nonconvex. Unlike classical numerical methods, deep learning methods are mesh-free and can solve PDEs in high dimension, complex domains and geometries. It is also advantageous to possess flexibility and ease of execution. Nonetheless, deep learning methods have several potential drawbacks, including lengthy training times, a lack of convergence, and reduced accuracy. The idea of operator learning, on the other hand, offers a method to resolve a class of PDEs by training the neural network just *once* [13–18]. It is important to note, however, that a number of issues regarding the convergence theory remain unclear.

In recent years, there has been extensive research conducted on multiscale kinetic equations and hyperbolic systems by employing deep neural networks. This research includes, but is not limited to the works cited in references [19–21, 23–27]. In the design of DNNS, the definition of loss functions is crucial. There are numerous choices available to build the loss when given a PDE. For instance, the variational formulation (DRM), the least-squares formulation (PINN, DGM), the weak formulation (WAN), etc. Due to the presence of small scales, the vanilla Physics-Informed Neural Networks (PINNs) can perform poorly for resolving multiscale kinetic equations where small scales present [21,23]. A natural question is what kind of loss is "good". One important feature is to preserve important physical properties, such as conservation, symmetry, parity, entropy conditions, and asymptotic limits, etc. In our previous work [21], we developed a DNN for multiscale kinetic transport equations (with possible uncertainties) by creating a loss that can capture the limiting macroscopic behavior, as the Knudsen number approaches zero, satisfying a property known as Asymptotic-Preserving (AP), an asymptotic property known to be important in designing efficient numerical methods for multiscale kinetic equations [3, 22], hence justifies the need to use Asymptotic-Preserving Neural Networks (APNNs). This APNN method is based on the micro-macro decomposition, and we demonstrated that the loss is AP with respect to the Knudsen number when it tends