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Plasma-Simulation Physics Informed Neural Networks (PS-PINNs) for Global Discharge Models

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Abstract. We consider the global discharge model in plasma simulations using physics-informed neural networks (PINNs). Our method, named Plasma-Simulation PINNs (PS-PINNs), effectively addresses the inherent stiffness and multiphysics aspects of the global model. Logarithmically equidistant points are employed to capture the steep behaviour in state variables during early stages. This distribution, while typical for handling stiffness in standard numerical methods, can hinder neural network (NN) training. To overcome this, we introduce a pre-processing layer featuring logarithmic transformation and standardization, significantly improving neural network training efficiency. In addition, our model addresses the complex interactions between multiple species common in the plasma problem, resulting in numerous physics loss terms. It is important to balance among various loss terms during training. To this end, we employ a self-adaptive loss balanced method to adaptively choose the weights, enhancing training robustness and effectiveness. The effectiveness of the proposed framework is demonstrated through several examples, including the forward and inverse problems in the chlorine global discharge model, and parameter dependency analysis.

AMS subject classifications: 65M10, 78A48

Key words: Plasma simulation, global discharge model, physics-informed neural networks, multi-task optimization.

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1. Introduction

Plasma, often referred the fourth state of matter, consists of free charged particles such as ions and electrons and is characterized by its quasi-neutrality, where positive and negative charges are generally balanced. Plasma discharge, which involves processes such as ionization and attachment, plays a significant role in semiconductor manufacturing, particularly in film etching and decomposition [6, 16]. Particle-level studies, focusing on individual collisions, face impractical computational demands. Consequently, researchers have developed simpler models, from kinetic [14] and fluid models [4] to the most simplified global models [15]. Global models omit spatial aspects and concentrate on time-dependent changes, which is valuable for examining species density changes, especially in steady-state reactions. Despite their simplicity, these models provide crucial insight into the overall plasma behavior. Our study focuses on the Cl_2 global discharge model, widely used in the etching of materials such as polysilicon, silicon oxide, and aluminum [15].

In plasma simulation, global models are typically represented as systems of ordinary differential equations (ODEs) that capture species interactions and fundamental physics principles such as mass and energy conservation. Characterized by nonlinear terms and multiple species, these ODEs often result in stiff dynamical behavior. Traditional numerical methods, such as the Euler method, have been widely used [2, 23]. Recent advances in machine learning have led to its application in plasma simulations, with studies such as [9, 22] utilizing autoencoders (AEs) for dimensionality reduction in reaction equations and neural ODEs. Deep operator networks (DeepONets) have also been used to create surrogate models for ODE systems [8], although these often require ground truth data, which can be inaccessible or expensive. Our method builds upon physics-informed neural networks (PINNs) [12, 19], leveraging the underlying physical laws and existing data to address a broad spectrum of scientific and engineering problems [10, 11, 17, 21]. Since then, many PINN variants has been developed to overcome the limitations of the original PINN framework [7, 8, 24, 25].

We apply PINNs to the global discharge model of chlorine gas (Cl_2) and demonstrate its potential to address various related tasks. To this end, we introduce an enhanced method, termed plasma-simulation PINNs (PS-PINNs). This method addresses two limitations of the naive PINN approaches. The first challenge is the stiffness of the solution functions near the initial time ($t = 0$). Species densities and electron temperature exhibit rapid changes in the initial phase, which is effectively captured by the dense distribution of points near $t = 0$. This necessitates the selection of collocation points that are logarithmically equidistant. However, their skewed distribution poses challenges for neural network (NN) training [1, 3]. To overcome this, PS-PINNs employ a pre-processing layer with logarithmic transformation and standardization, effectively normalizing these distributions for improved training convergence. Another challenge arises from managing a large number of species and their associated loss terms in the PINN framework. PS-PINNs incorporate self-adaptive loss-balanced PINNs (lbPINNs) [25], which automatically adjust the weights for each loss term to maximize the likelihood function, establishing a balance with regu-