Proceedings of the 1st international Symposium on AI and Fluid Mechanics
Paper No S11 P5

MBPINN: Mesh-based Physics-Informed Neural Networks for Global and Local Hyperbolic Conservation

Lin Lu [1 3], Yiye Zou [1 3], Jingyu Wang[2 3] *, Xiaogang Deng [3];

[1] School of Computer Science, Sichuan University, Chengdu, 610065, China
[2] College of Aerospace Science and Engineering, Sichuan University, Chengdu, 610200, China
[3] National key laboratory of Fundamental Algorithms and Models for Engineering Simulation, Sichuan University, Chengdu, 610207, China

Abstract. In recent years, Physics-Informed Neural Networks (PINNs) have emerged as a prominent framework for solving partial differential equations (PDEs) using neural networks. However, conventional PINNs often fail to rigorously satisfy both global and local conservation, which are critical for many PDE problems. This study introduces a novel PINN approach that embeds conservation laws into the loss function, ensuring local and global conservation constraints. A key limitation of conventional PINNs lies in their mesh-free nature, which relies on sum-based global optimization and lacks the mechanisms necessary to preserve global conservation. To address this issue, our method discretizes the global conservation law numerically and incorporates it into the loss function. Additionally, while automatic differentiation implicitly encodes partial derivatives at each point using the network parameters over the entire domain, this implicit treatment fails to ensure strict local conservation. In contrast, our approach explicitly establishes the connections between each point and its neighbors, thereby ensuring local conservation when approximating differential operators. Our method transitions from a mesh-free framework to a mesh-based one by enforcing both global and local conservation laws through numerical discretization within the loss function. This paper presents an approach for solving conservation laws by combining PINN (Physics-Informed Neural Networks) with traditional grid-based numerical methods. To demonstrate the limitations and solution accuracy of this approach, we selected three equations and compared the prediction errors and conservation errors for PINN, global conservation-based PINN, MBPINN-G, and local conservation-based PINN, MBPINN-L. Our results show that after adding the conservation constraints, the conservation of the PINN method is significantly submitted, which leads to an improvement in the solution accuracy as well. However, we find that in the intermittent problem, due to the inherent limitation of automatic differentiation, the addition of the conservation constraints does not significantly improve the solution accuracy.

Keywords: Mesh-based; Numerical method; Conservation laws; Physics-informed neural network;

1. Introduction

In physics, most phenomena are described by partial differential equations (PDEs) [5]. Physics-Informed Neural Networks (PINNs) [1] constitute a framework that leverages neural networks to efficiently learn and solve these governing laws—that is, the PDEs. Essentially, PINNs embed the known PDE into the loss function at interior points, while at the boundaries a limited set of real boundary data constrains the boundary loss [2]. Together, these terms form the overall objective function for the neural network, which is then optimized using various optimizers. The advent of PINNs has revolutionized traditional numerical methods for solving PDEs [10], achieving impressive accuracy across diverse fields. This success is attributed to a novel approach: imposing soft constraints at the boundaries and enforcing the governing equations at interior points to balance the respective strengths of data and physics. Such a strategy offers several conveniences [4], including greater flexibility regarding the geometry of the computational domain and simpler code implementation compared to conventional solvers, thereby garnering significant attention from researchers.

In addition to investigating the mathematical forms of the governing equations, the study of conservation laws is another critical approach for addressing real-world physical problems. Most physical phenomena adhere to conservation laws [8]; for instance, in problems involving shock waves [3], the original governing equations are often insufficient for accurately capturing the dynamics of high-speed shocks. However, standard PINNs and their variants tend to struggle with conservation law equations. This shortcoming arises from the discretization strategy and the global optimization [9] over interior points inherent in PINNs. In contrast, traditional numerical methods often modify both the equation formulations and discretization schemes to enhance the conservation properties of the overall numerical framework. Given that the PINN approach is somewhat analogous to mesh-free methods in traditional numerical analysis, we draw inspiration from these methods to demonstrate that incorporating a grid-discretization concept—augmented by conservation-law loss functions—can improve the conservation properties of the original PINN framework and, consequently, enhance solution accuracy.

In this work, we propose a grid-discretization-based PINN that integrates hard constraints for conservation laws into the loss function, drawing on the ideas of both global and local conservation from numerical methods. This enhancement addresses the shortcomings of the standard PINN with respect to conservation, and we refer to the proposed method as MBPINN. The MBPINN method is further divided into two variants: the global conservation-based MBPINN-G and the local conservation-based MBPINN-L. The MBPINN-G variant enforces global conservation across the entire domain, which is particularly effective for problems involving discontinuities, while the MBPINN-L variant applies local conservation principles, which is better suited for smooth, non-discontinuous problems. The core idea is to combine the conservation principles of traditional numerical methods with the gradient-based optimization framework of PINNs guided by the PDE loss. First, we modify the discretization strategy. Conventional PINNs typically employ randomly scattered collocation points over the computational domain—a strategy akin to a mesh-free approach. In mesh-free numerical methods, conservation can be guaranteed provided that the discretized coefficient matrix satisfies certain conditions. We then incorporate a global conservation law into the discretized domain to ensure global conservation. More importantly, these mesh-free methods usually explicitly express the relationship between a discretization point and its neighboring points, thereby approximating finite-difference terms. In contrast, the conventional PINN framework does not inherently incorporate such a strategy. To overcome this, we introduce a local conservation loss function that explicitly represents the relationships between points and their neighbors, thereby facilitating more effective information exchange between points and achieving local conservation.

To validate the effectiveness of our method in enforcing conservation laws, we compare the performance of the original PINN and the Mb-PINN in solving the one-dimensional convection equation with sine initial conditions, the convection equation with discontinuous initial conditions, and the viscous Burgers' equation. We define both global and local conservation loss functions, along with corresponding evaluation metrics. Our results demonstrate that the MBPINN exhibits superior conservation properties compared to the traditional PINN across various experiments.

2. Related work

In traditional numerical methods [5], mesh-free approaches can still maintain both global and local conservation [7]. The computational domain Ω is discretized using a cloud of NNN points, covering the boundary $\partial\Omega$ as well. Each point is assigned vector coordinates x_i, $i = 1,2, \dots, N$. The outward-facing vector normal n_i on the boundary is defined as positive, and each point is associated with a set of neighboring points S_i that does not include the point itself. The discrete first-order derivative is defined as follows:

$$m_i \partial^k \phi_i \approx m_i \delta^k \phi_i = a_{ii}^k \phi_i + \sum_{j \in s_i} a_{ij}^k \phi_j \tag{1}$$

Here, k denotes a spatial direction, and ∂^k and δ^k represent the analytical and discrete first-order derivative operators along that direction, respectively. The matrix m_i can denote the area associated with each point, while a_{ij}^k represents the coefficients corresponding to each point and its neighbors. Kwan-yu et al.[6] demonstrates that if the matrices m and a satisfy the following two definitions, then this derivative operator satisfies the conservation law.

The first definition concerns the reciprocccity of the coefficients—in simple terms, it states that:

$$\begin{aligned} a_{ij}^k &= -a_{ji}^k, i \neq j (j \in s_i \Leftrightarrow i \in s_j) \\ a_{ii}^k &= 0, i \notin s_B \\ a_{ii}^k &= \frac{1}{2} n_i^k, i \in s_B \end{aligned} \tag{2}$$

For non-boundary points, the diagonal entries are zero, and at the discrete level, the entire matrix exhibits an antisymmetric structure.
The second definition is the consistency of a given order L, which requires that the operator exactly reproduces the analytical derivative for all multivariate polynomials p of degree no greater than L.

$$a_{ii}^{k} p(x_i) + \sum_{j \in s_i} a_{ij}^{k} p(x_j) = m_i \partial^k p(x_i) \tag{3}$$

3. Method

This section is divided into three parts. First, we introduce the mathematical definition of global conservation; next, we explain why the PINN method fails to enforce global conservation; finally, we propose an improved approach. Initially, we consider the case where the equation has no source term and is subject to Dirichlet boundary conditions. In this scenario, global conservation can be defined as:

$$\frac{d}{dt}\int_{\Omega} u(x,t)dV = -\int_{\partial\Omega} f(g(x,t)) \cdot \vec{n}dS \tag{4}$$

Its physical significance can be described as the connection between interior and boundary points across the entire computational domain—that is, the change in the interior field quantity is equal to the change in flux at the boundary. From the definition of global conservation, it is evident that the PINN loss function primarily consists of the PDE loss at interior points and the discrepancy with the boundary conditions at the boundary. However, the relationship between the boundary and interior points is not explicitly defined within the PINN loss function, which makes it difficult for PINN to achieve global conservation when solving partial differential equations. Our proposed improvement is to incorporate the aforementioned global conservation as a hard constraint to guide the descent gradient of the entire neural network. Clearly, due to the random point scattering discretization in PINN, it is challenging to directly introduce such a loss function. Therefore, inspired by traditional numerical methods such as the finite difference method, we first discretize the computational domain into uniformly distributed points, convert the global conservation law into its discrete form through numerical methods, and finally integrate it as a hard constraint into the original loss function.

3.2.

Similar to the previous subsection, this part first defines the local conservation law under the same conditions:

$$\frac{d}{dt}\int_{V} u(x,t)dV + \int_{\partial V} f(u(x,t)) \cdot \vec{n}dS = 0 \tag{5}$$

Unlike global conservation, local conservation focuses on the conservation relationship between interior points and their neighboring nodes. Here, V denotes the volume of each control cell, which implies that within each control cell the change in the physical quantity equals the difference between the physical flux entering and exiting the cell. Compared to the PINN method, this relationship explicitly captures the conservation among interior points. However, in PINN, the summation over interior points is optimized to reduce the loss function; this approach does reflect the relationships between points—primarily by connecting each point's information through the neural network's parameters—but it has several limitations. First, such connections are implicitly represented through the neural network parameters and are not explicitly manifested in the loss function. Moreover, the summation performed is not a true summation based on conservation laws but merely a sum of the equation errors. Lastly, in terms of global conservation, the key interactions occur only among neighboring nodes; points that are far apart contribute little to conservation. Yet, PINN calculates relationships involving all points and then optimizes the sum over the entire domain. Similarly, inspired by traditional numerical methods, we incorporate the relationship between each point and its neighboring nodes as a hard constraint into the original PINN loss function, thereby ensuring that the model satisfies local conservation.

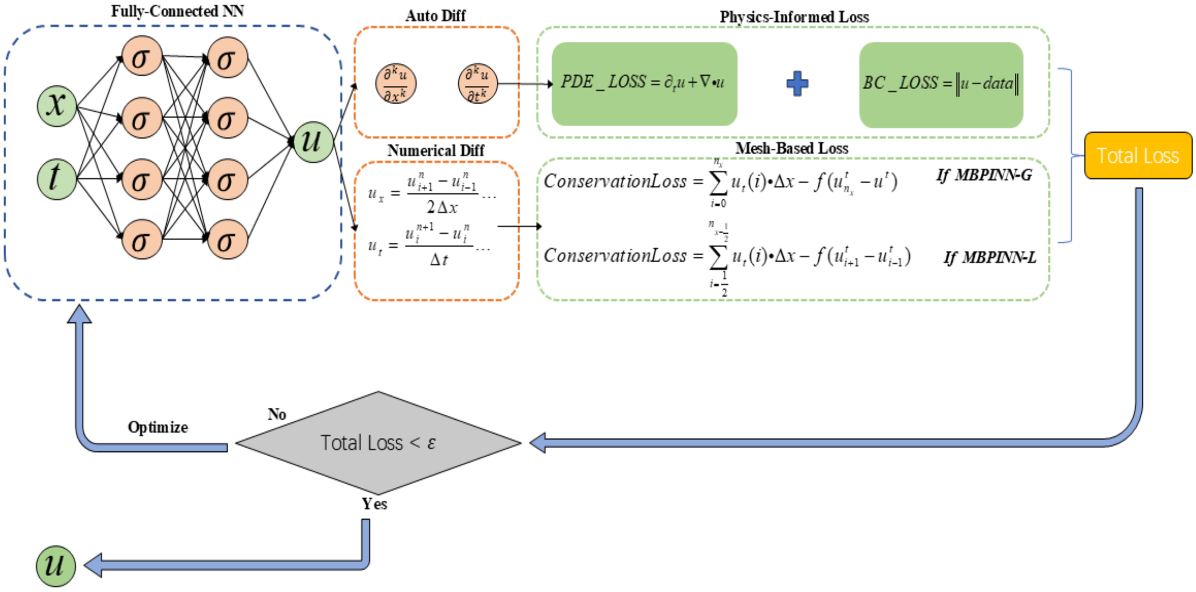

Figure 1. Schematic of MBPINN-G and MBPINN-L.

3.3. Experimental Setup

We study the conservation problem using three model equations: the one-dimensional convection equation with continuous initial conditions, the one-dimensional convection equation with discontinuous initial conditions, and the Burgers equation. For these three equations, we train PINN, MBPINN-G, and MBPINN-L. The training processes of MBPINN-L and MBPINN-G are similar to PINN, where we add global and local conservation as hard constraints to the original loss function. It is important to emphasize that the main difference between our models and PINN is not just the addition of new loss functions, but rather the change in the discretization approach, from a mesh-free method to a traditional numerical discretization method, allowing conservation laws to be incorporated into the loss function. The model takes spatiotemporal coordinates x and t as input and outputs u. For all the problems, we set 200 spatial points and 100 time points, making a total of 20,000 points in the solution domain. The optimizer used is the Adam optimizer. It should be noted that our sampling points are evenly distributed within the solution domain, so all the data comes from our own dataset.

3.4. Evaluation

First, the benchmark for all our results is the exact solution of the equation. When selecting equations, we choose those that have exact solutions to facilitate the comparison of experimental results. We primarily compare the error in the prediction solution $Error\ u$, the global conservation error $Error\ c-g$, and the local conservation error $Error\ c-l$ for each model on different equations. Our main goal is to explore which conservation scheme provides more accurate solutions for different equations.

4. Results

Table 1. L2 error for prediction (Error u), global conservation (Error c-g), and local conservation

		Advection Eq with sin	Advection Eq with discontinuities	Burgers'Eq
PINN	Error u	2.36E-04	1.37E-03	9.11E-04
	Error c-g	6.08E-05	3.36E-01	7.31E-04
	Error c-l	9.234E-08	1.8E-03	8.01E-03
MBPINN-G	Error u	1.48E-06	**1.27E-03**	**3.77E-06**
	Error c-g	**6.46E-07**	**6.25E-10**	**1.44E-07**
	Error c-l	1.65E-02	1.83E-01	8.03E-04
MBPINN-L	Error u	**1.39E-06**	1.33E-03	1.34E-03
	Error c-g	2.59E-06	6.01E-04	2.1E-04
	Error c-l	**1.94E-09**	**6.26E-06**	**4.12E-04**

Table 1 presents our experimental results. The first column shows the results for the experiment with continuous initial conditions, the second column presents the results for the convection equation with discontinuous initial conditions, and the third column shows the results for the burgers equation. From the results, it is evident that MBPINN-G achieves the best error in global conservation across all three equations, while PINN performs the worst. On average, MBPINN-G improves global conservation by nearly 6 orders of magnitude compared to PINN, and by 4 orders of magnitude compared to MBPINN-L. On the other hand, MBPINN-L excels in local conservation error across all three equations. This highlights that adding a conservation loss function significantly enhances the precision and consistency of PINN, proving the effectiveness of our method.
Moreover, we find that adding the conservation constraints works better on the convective and burgers equations with sinusoidal initial conditions, both solved with two orders of magnitude accuracy, but not so well on the convective equations with intermittent initial conditions. We believe that this is due to the limitations of automatic differentiation in dealing with interrupted problems. Automatic differentiation forces a gradient to be computed at the point of interruption, however, there is no gradient at this location itself, thus causing some error, so it can be seen that none of the three methods improved their accuracy significantly in the second experiment.

5. Conclusion

In this paper, we present a method for solving conservation laws by combining PINN (Physically Informed Neural Networks) with traditional grid-based numerical methods. In order to demonstrate the limitations and the solution accuracy of this method, we select three equations and compare the prediction error, the global conservation error, and the local conservation error for PINN, MBPINN-G, and MBPINN-L. Our results show that the addition of further conservation constraints improves the conservation of PINN and improves the solution accuracy of the model. Some of these numerical methods are inherently conservative compared to traditional methods such as finite volume methods and finite differences, e.g., finite volume methods. The finite difference methods, on the other hand, can be constructed in a format that maintains the conservation. But PINN can only achieve the same effect by adding additional constraints, such a problem is that the optimizer is difficult to converge during multi-objective optimization, which is also a limitation of this method. In addition, the inherent problems of automatic differentiation on intermittent problems also constrain the method in this paper, and these will be the direction we will address in the future.

6. References

[1]. Raissi M, Perdikaris P, Karniadakis G E. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations[J]. Journal of Computational physics, 2019, 378: 686-707.
[2]. Lu L, Pestourie R, Yao W, et al. Physics-informed neural networks with hard constraints for inverse design[J]. SIAM Journal on Scientific Computing, 2021, 43(6): B1105-B1132.
[3]. Stevens B, Colonius T. Enhancement of shock-capturing methods via machine learning[J]. Theoretical and Computational Fluid Dynamics, 2020, 34(4): 483-496.
[4]. Baez A, Zhang W, Ma Z, et al. Guaranteeing Conservation Laws with Projection in Physics-Informed Neural Networks[J]. arXiv preprint arXiv:2410.17445, 2024.
[5]. Farlow S J. An introduction to differential equations and their applications[M]. Courier Corporation, 2006.
[6]. Kwan-yu Chiu E, Wang Q, Hu R, et al. A conservative mesh-free scheme and generalized framework for conservation laws[J]. SIAM Journal on Scientific Computing, 2012, 34(6): A2896-A2916.
[7]. Chiu E K, Wang Q, Jameson A. A conservative meshless scheme: general order formulation and application to Euler equations[C]//49th AIAA Aerospace Sciences Meeting including the New Horizons Forum and Aerospace Exposition. 2011: 651.
[8]. Dafermos C M, Dafermos C M. Hyperbolic conservation laws in continuum physics[M]. Berlin: Springer, 2005.
[9]. Baydin A G, Pearlmutter B A, Radul A A, et al. Automatic differentiation in machine learning: a survey[J]. Journal of machine learning research, 2018, 18(153): 1-43.
[10]. Huang S, Feng W, Tang C, et al. Partial differential equations meet deep neural networks: A survey[J]. arXiv preprint arXiv:2211.05567, 2022.