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Time Integration Schemes Based on Neural Networks for Solving Partial Differential Equations on Coarse Grids

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Abstract. In this work, we propose to learn time integration schemes based on neural networks which satisfy three distinct sets of mathematical constraints, i.e., unconstrained, semi-constrained with the root condition, and fully-constrained with both root and consistency conditions. We focus on the learning of 3-step linear multistep methods, which we subsequently applied to solve three model PDEs, i.e., the heat equation, the wave equation, and the Burgers' equation. The results show that the prediction error of the learned fully-constrained scheme is close to that of the Runge-Kutta method and Adams-Bashforth method. Compared to the traditional methods, the learned unconstrained and semi-constrained schemes significantly reduce the prediction error on coarse grids, with an overall better performance for the semi-constrained model. On a grid $4\times$ coarser than the reference, the mean square error (MSE) shows a reduction of up to two order of magnitude for some heat equation cases, and a substantial improvement in phase prediction for the wave equation. On a $32\times$ coarser grid, the MSE for the Burgers' equation can be reduced by up to 40% to 45%. Tests on the two-dimensional heat equation and wave equation show a good generalization capability for the constant optimized coefficients.

AMS subject classifications: 65L06, 65M08, 68T07

Key words: Time integration scheme, partial differential equation, numerical simulation on coarse grids, neural networks, mathematical constraints.

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1 Introduction

Many environmental and engineering problems, encompassing a broad spectrum of spatial and temporal scales, are described by partial differential equations (PDEs) of high dimension. Since resolving all the scales often demands exceedingly extensive computational resources, solving the high-dimensional PDEs poses a great challenge to the current computing systems. For example, direct numerical simulations of high-Reynolds number turbulent flows can be particularly challenging in this regard. Solving the PDEs on coarse grids, reducing the dimension of the problem, can substantially reduce the computational costs, while meanwhile introduces discretization errors. Discretization errors depend not only on the spatial discretization schemes but also on the time integration schemes. In this study, we propose to learn time integration schemes to reduce the error of solving PDEs on coarse grids.

The traditional approach to reduce the prediction error on coarse grid is to directly account for the effect of the physics of the unresolved scales. One way is to solve the spatially filtered PDEs instead of the original PDE. However, the filtering procedure on the nonlinear term often introduces a new unclosed term, i.e., the subgrid term. The subgrid term can be modelled explicitly by establishing its relation with the resolved scales. For instance, the eddy viscosity model for large-eddy simulation (LES) of turbulent flows governed by the Navier-Stokes (NS) equations [1, 2]. The subgrid term can also be modelled implicitly by changing the properties of the schemes for discretizing the spatial derivatives. One example is the Implicit Large-Eddy Simulation (ILES) method for solving turbulent flows [3]. The success of such approaches largely depends on our understanding of the physics of the unresolved scales. Moreover, the developed models are often valid for only a range of unresolved scales. When the dominant physics of the unresolved scales change from one to the other as the cut-off scale changes, a grey region appears where neither of the models in each regime works. For instance, the grey region in the microscale and mesoscale simulations of the atmospheric flow in the meteorology research [4, 5].

The machine learning methods are revolutionizing the numerical methods for solving PDEs [6–15]. Such approaches approximate the solution based on machine learning models [16, 17], e.g., neural networks [18], that a spatial discretization of the computational domain might not be needed. In the review paper by [19], three types of the methods based on neural networks were reviewed: 1) the physics-informed neural networks (PINN) [8, 20, 21], in which the PDEs with initial and boundary conditions are approximately enforced via loss functions; 2) the methods based on the Feynman–Kac formula [22], which approximate the solution of a PDE as the expectation of a stochastic process; and 3) the methods based on the solution of backward stochastic differential equations [23,24], in which deep neural networks (DNN) are employed for computing the gradient of solutions. As noted in the review [19], the last two methods showed promising results for high-dimensional linear and semilinear systems. The methods based on PINN are capable of handling complex nonlinear PDEs and inverse problems with in-