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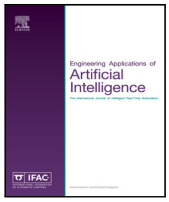

Research paper

Hierarchical deep learning-based adaptive time stepping scheme for multiscale simulations

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ABSTRACT

Multiscale is a hallmark feature of complex systems, presenting challenges for traditional numerical methods due to their reliance on local *Taylor* series constraints. Further, multiscale techniques often face limitations in identifying appropriate heuristic closures used to handle unresolved scales or processes within the system being modeled. In this study, we develop an efficient time-stepping strategy for multiscale problems. The proposed method's novelty lies in synergizing the hierarchical deep learning formalism with an adaptive step-size estimation process to approximate dynamical system flow maps across timescales efficiently. The model is purely data-driven and provides improved forecasting accuracy compared to fixed-step neural network time steppers. To demonstrate the effectiveness of the proposed scheme, we provide numerical simulations for several canonical nonlinear systems and source codes for their implementation. We believe the method has the potential to benefit multiscale analysis of complex systems and encourage further investigation in this area.

1. Introduction

Multiscale systems are ubiquitous in science and engineering. Modeling and controlling such systems is essential due to their prevalence in natural and engineered systems, and understanding their behavior requires a multidisciplinary approach that integrates models and experimental techniques at multiple scales (Weinan, 2011). These complex systems generally have dynamics operating at different spatiotemporal scales, such as a *fine* or microscale, and a *coarse* or macroscale. Microscale modeling usually involves analyzing the system behavior at fine resolutions, thus entailing a substantial computational cost while capturing the system's long-term behavior. On the other hand, the macroscopic models are efficient, but their accuracy hinges on the ability to capture the system dynamics effectively. Another challenge in studying multiscale systems is that the governing equations may be explicitly known at the microscopic/individual level. However, the closures required to translate them to high-level macroscopic descriptions remain elusive. For instance, at the microscale, the governing equations that describe the behavior of fluid particles can be modeled using molecular dynamics simulations, which consider the interactions between individual particles. However, at the macroscale, the behavior of fluid flows is mainly influenced by interactions between particles at larger length scales, such as turbulent eddies, which are challenging to model accurately due to their complex nature. Thus, multiscale analysis involves deriving representative models at different scales and coupling them to achieve the accuracy of the microscopic models, as well as the efficiency of the macroscopic models (Weinan, 2011).

Many of these multiscale systems may also exhibit chaotic behavior, implying that any initial inaccuracies in determining the system's state can lead to errors that increase exponentially over time. Furthermore, due to the limitations of finite precision, this exponential increase of errors can significantly reduce the accuracy of long-term predictions (Wang et al., 2019). Conventional forecasting methods for chaotic systems generally estimate the initial state and discover a reliable model that accurately represents the physical laws. If either component is inaccurate, the resulting forecast becomes unreliable due to the chaotic nature of the underlying system. Over recent years, there has been a transition towards data-driven modeling, facilitated by improvements in sensor technology and data measurement tools due to advancements in machine learning algorithms (Brunton et al., 2017; Fan et al., 2020; Weng et al., 2022; Brunton et al., 2016). Some of these methods are discussed as follows.

1.1. Related works

Various multiscale modeling techniques have been developed that combine different approaches to analyze and study the behavior of such systems. Some of these classical methods include the equation-free

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