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PNNL-36697

Machine-learning based model reduction for partial differential equations

September 2024

Panos Stinis
Saad Qadeer

U.S. DEPARTMENT OF ENERGY

Prepared for the U.S. Department of Energy
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Abstract

We develop a novel synergistic approach between model reduction and machine learning. The specific goal of this project is to aid in the construction of reduced order models for basis functions that are custom-made to represent the solution of partial differential equations.

Partial differential equations (PDEs) are one of the main mathematical tools for describing physical phenomena. However, due to either efficiency or necessity, for many real-world problems, we are interested in constructing reduced order models (ROMs) which focus only on the explicit computation of subsets of the active spatio-temporal scales in the problem, while treating the interaction with the rest of the scales approximately. The task of accurate representation of such interactions (usually called memory terms) constitutes a vast area of research known as model reduction.

PI Stinis has significant expertise in the construction of ROMs for complex systems. In addition, in recent work with the project key participant Qadeer, they have utilized machine learning to acquire custom-made basis functions (CBFs) to expand the solutions of PDEs. In the proposed work, we will merge the two concepts by constructing ROMs for subsets of the CBFs needed to represent the solution of a PDE. Specifically, we will use the Mori-Zwanzig model reduction formalism to construct ROMs for subsets of CBFs for nonlinear PDEs of various complexity, as well as investigate the usage of CBFs in the spectral vanishing viscosity method for problems that can form shocks in finite time. The outcome of the research is aimed to be proof-of-concept about a novel synergistic approach between model reduction and machine learning, thus advancing the field of scientific machine learning. Such a capability will benefit the efficient modeling of physical systems appearing in various areas of interest to the DOE.

Summary

We can only report limited deliverables as Saad Qadeer, the project key participant, was absent from the US from March 2023 to August 2024 and, as a result, has only been able to make partial progress on this project.

The custom-made basis functions (CBFs) [1] obtained from training DeepONets on the viscous Burgers' equation were used in a spectral vanishing viscosity approach (SVV) to solve the inviscid Burgers' equation on a periodic domain. The initial conditions studied lead to the occurrence of shock waves and, in principle, require an infinite number of basis functions. The SVV formulation enables faithful representations of the solution while employing a finite basis by providing an energy ejection mechanism. In particular, this method requires damping to be introduced only on the high-frequency modes at a strength carefully tuned to yield the correct rate of energy decay.

In our work, we implemented this technique for CBFs acquired from multiple DeepONets, and with various choices for the viscosity magnitude and the frequency threshold. We found that the resulting computations are stable well beyond the time at which the shock forms, and for suitably chosen parameters, can correctly reproduce the rate of energy ejection.

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References

[1] Meuris, Brek, Saad Qadeer, and Panos Stinis. "Machine-learning custom-made basis functions for partial differential equations." arXiv preprint arXiv:2111.05307 (2021).

[2] Maday, Yvon, Sidi M. Ould Kaber, and Eitan Tadmor. "Legendre pseudospectral viscosity method for nonlinear conservation laws." SIAM Journal on Numerical Analysis 30, no. 2 (1993): 321-342.

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