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Machine learning based surrogates for particle-resolved direct numerical simulation

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In atmospheric physics, particle-resolved direct numerical simulation (PR-DNS) models constitute an important tool to study aerosol-cloud-turbulence interactions which are central to the prediction of weather and climate . They resolve the smallest turbulent eddies as well as track the development and motion of individual particles [1,2]. PR-DNS is expected to complement experimental and observational facilities to further our understanding of the cloud dynamics. With a sufficient computational speed and scale, it can also be part of the digital twin to the experimental facilities such as the cloud chambers [2,3]. The original version of PR-DNS does not scale well on multi-core CPUs, thereby limiting the scale it can simulate. There is therefore a great need to accelerate the PR-DNS solver with tools from traditional high performance computing (HPC) as well as replacing computationally expensive modules with machine learning models. In this study, we exploit the potential of Fourier Neural Operators (FNO) [4] learning to yield fast and accurate surrogate models for the velocity and vorticity fields. We have investigated two classes of FNO −2D FNO which has two spatial dimensions with a recurrent structure in time and 3D FNO with two spatial and one temporal dimensions. We discuss results from numerical experiments designed to assess the performance of these architectures as well as their suitability for capturing the behavior of relevant dynamical systems.

[1] Zheng Gao et al. Investigation of turbulent entrainment-mixing processes with a new particle-resolved direct numerical simulation model. J. Geophys. Res. Atmos. 123(4), 2018.
[2] Lulin Xue et al. Progress and challenges in modeling dynamics–microphysics interactions: From the Pi chamber to monsoon convection. Bull Am Meteorol Soc, 103(5), 2022.
[3] K. Chang et al. A laboratory facility to study gas–aerosol–cloud interactions in a turbulent environment: The ⊠ chamber. Bull Am Meteorol Soc, 97(12), 2016.
[4] Z. Li et al. Fourier neural operator for parametric partial differential equations, 2021. https://arxiv.org/abs/2010.08895

Significance

This presentation discusses the speedup gained by using a machine learning (ML) model as a surrogate for a traditional partial differential equation solver. The corresponding errors from two different ML architectures in the context of atmospheric physics, climate science, and turbulence will also be discussed.

References

https://arxiv.org/pdf/2312.12412.pdf
https://d197for5662m48.cloudfront.net/documents/publicationstatus/143045/preprint_pdf/6e1cbcdcef459f235515059f1011391b.pdf

Experiment context, if any

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