ONE Planet
Doctoral Training Partnership

Natural Environment Research Council

Project title: Modelling Atmospheric Chemicals for Climate Change Using Data-driven and Physics-informed Artificial Intelligence

Ref: OP2423

Keywords: Climate Change, AI, Data-driven, Atmopheric Chemistry

One Planet Research Theme: Climate & Climate Change ☒ | Earth System Processes ☒ |

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Key Research Gaps and Questions: 1. How to use data-driven and physics-informed machine learning to model atmospheric chemsitry (supported by the CASE partner NVIDIA's)? 2. How to optimize AI models to achive improved performances such as higher dimensionality, excellent stability and less reginal biases for long-term climate change prediction

Project Description: We can already see some of the effects of climate change. However, it is still uncertain what changes we might see in the future. To understand these, climate models are used to simulate potential futures. A lot of time, effort and money has been spent on the atmosphere/ocean components of these models. Less effort has been spent on the other components of the earth system which, while not directly contributing to the physical changes we experience, are fundamental in the feedbacks which determine the overall size of climate change. Why are these components missing? They are complex and including them in full earth system models (ESMs) is a hard problem. This is particularly the case for chemistry [1-6]. To comprehensively incorporate atmospheric chemistry into an ESM requires almost doubling the computational cost over an atmosphere/ocean model. For this reason, ESMs which simulate chemistry are often run at lower spatial resolution [7] degrading their representation of climate changes. This project aims to take a different approach to simulating atmospheric chemistry in ESMs.

This project aims to use cutting edge AI techniques to reduce the complexity of simulating atmospheric chemistry. It will use data driven and physics-informed machine learning techniques, based on super supercomputing resources supported by NVIDIA, to accurately simulate the global chemistry cycles and interactions. There are three broad objectives:[1] To tackle the limitations on dimensionality that restrict current methods to a subset of chemical species.[2]To improve the long-term stability of prediction of AI-based methods that is essential for climate-scale timescales.[3]To reduce regional bias in global chemistry models to improve the accuracy of the prediction.

To tackle the curse of dimensionality and address the full chemistry problem, we will explore novel DNN strategies shown in the current SOTA for large dimension, data-driven models such as transformer-based network schemes. Then, we will apply a hybrid approach that couples AI DNNs with physical knowledge of the system through such models as physics informed Neural Networks (PINN), Physics Constrained Networks, and variations such as Physics Informed Neural Operators. Regional bias is primarily a fidelity issue and simply increasing fidelity is not a practical solution. We will study possible approaches where DNN can aid with fidelity such as Generative Adversarial Networks and the very new GAN Operators.

The proposed CASE partner NVIDIA AI Technology Centre, NVIDIA will support the project by providing training and supercomputing resources for hundreds of TB data processing and training in AI.

References:[1]10.1175/AMSMONOGRAPHS-D-18-0018.15.[2] 10.5194/acp-5-2497-2005.[3] 10.5194/acp-23-1131-2023.[410.1038/s41561-020-0582-5.[5]10.1029/2021MS002926.[6]10.5194/acp-23-3471-2023 [7] 10.1029/2019MS001739

Prerequisites: Excellent programming skills using Python, MATLAB, or R. Knowledge of any of the following are desirable: Atmosphere chemistry: machine learning, earth system process.

Newcastle University

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