Surrogate Modeling for Methane Dispersion Simulations Using Fourier Neural Operator

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Abstract

Methane leak detection and remediation are critical for tackling climate change, where methane dispersion simulations play an important role in emission source attribution. As 3D modeling of methane dispersion is often costly and time-consuming, we train a deep-learning-based surrogate model using the Fourier Neural Operator to learn the PDE solver in our study. Our preliminary result shows that our surrogate modeling provides a fast, accurate and cost-effective solution to methane dispersion simulations, thus reducing the cycle time of methane leak detection.

1 Introduction

Methane (CH_4) is a potent greenhouse gas (GHG) and the second largest contributor to global warming (next to CO_2). CH_4 lasts in the atmosphere for nearly a decade, which is much less time than CO_2. However, it absorbs energy much more effectively than CO_2. Methane's severe impact on Earth's warming is reflected in its value of Global Warming Potential (GWP), an index for comparisons of the global warming impacts of different gases. Methane is estimated to have a GWP of 84–87 over 20 years [1]. This highlights the importance of methane remediation for tackling climate change.

The global oil and gas industry is one of the primary sources of methane emissions. From its operations, around 70% of today's methane emissions are technically possible to be avoided, according to the International Energy Agency (IEA)'s estimate [2]. This speaks of the strong motivation of leveraging methane detection technologies to mitigate emissions. Emerging methane-sensing technologies developed for this purpose include satellites, aerial surveys and IoT sensors, among others. For example, ground sensor grids can provide real-time/near real-time measurements of methane concentration over an area, in order to track emission sources and leak rates [3, 4]. This is an inverse problem whose corresponding forward process is methane dispersion modeling, that is, computing the downstream pollutant concentration given source leak locations and rates, together with meteorological variables.

The methane dispersion modeling or simulation belongs to the category of atmospheric dispersion modeling where a combination of advection (due to the wind) and diffusion (due to turbulent eddy motion) occurs in the air near surface. It is governed by the 3D advection-diffusion equation which is a 2^{nd} order Partial Differential Equation (PDE) [5]. The forward modeling of methane dispersion is the most computationally expensive component of a non-linear Bayesian regression approach for methane source attribution, where Markov Chain Monte Carlo (MCMC) simulations based on the 3D advection-diffusion PDE need to be performed numerous times (e.g., thousands) [4]. As the 3D dispersion modeling is costly and time-consuming, we will investigate a deep-learning-based proxy model to speed up the modeling by a few orders of magnitude. To be more specific, we will evaluate the Fourier Neural Operator (FNO) [6], a state-of-the-art approach for expediting our PDE-based modeling of methane dispersion.

2 Methodology

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2.1 Deep learning for PDEs

Recently we have seen the emergence of a new way of utilizing deep learning to provide faster AI surrogate models for physics-based numerical simulation or optimization problems. Those scientific simulations usually involve solving complex PDEs, where conventional numerical solvers typically require fine discretization (e.g., in space and time) to achieve accurate solutions. Therefore, conventional PDE solvers can often be computationally expensive and time-consuming, especially for a large-scale problem. To address the cost and speed challenge, innovative AI-based emulators are brought up to learn the solution operators of parametric PDEs. One category of approaches is to take advantage of the physics constraints defined in PDEs, such as Physics Informed Neural Network (PINN), where the underlying PDE formulation is coded in the loss function to train a deep learning model [7]. Another category is data-driven without using physics constraints. Among this category, a recent novel method named Fourier Neural Operator (FNO) shows great efficiency and state-of-the-art performance in directly approximating PDE operators [6]. The success of the FNO in learning highly non-linear and complex PDE operators relies on its spectral convolution in the Fourier domain, as spectral methods are widely used for deriving PDE solutions.

In this study, we will build a proxy FNO model for the methane dispersion PDE and validate its performance by comparing the FNO predictions to the traditional numerical solutions. We will experiment with some modifications of the FNO architecture and check their relative performance in future work. A high-speed and accurate AI-based simulator would dramatically expedite methane dispersion simulations, leading to a fast and cost-effective workflow of emission source attribution and sensor placement optimization.

Another contribution to emphasize in our study is that our methane dispersion modeling belongs to a more challenging class of PDEs whose solution operator appears more complex for an AI model to learn. In Li et al.'s FNO examples [6], the inputs to PDEs are static or not varying over time. However, we have time-variant input arguments to the methane dispersion PDE, such as the wind direction and speed. A rapid change in the wind condition can result in a dramatic change of methane concentration distribution in a non-smooth fashion and a short amount of time. Non-smooth temporal variations in inputs and outputs pose a big challenge for deriving a surrogate model.

2.2 Surrogate modeling using FNO

The governing PDE for the methane dispersion simulation is a 3D advection-diffusion equation [5]:

$$\frac{\partial C}{\partial t} + \nabla \cdot (C\vec{v}) = \nabla \cdot (D\nabla C) + S$$

Where $C(x,t)$ is the methane concentration field at location x and time t, a variable of interest to be solved. The term $\vec{v}(x,t)$ is the wind velocity field that methane is moving with. S describes methane leak sources and D is the diffusion coefficient matrix.

We use the above methane dispersion PDE, together with a conventional physics-based approach, to generate 1000 pairs of input and output data in our preliminary experiment. The inputs consist of the methane leak rate, wind direction, wind speed, atmospheric stability class, temperature, and pressure. The output data is the 3D methane concentration field as a function of time. Each simulation sample is performed in a time length of one day with one hour as a time-step. Therefore, our input and output data for surrogate modeling is 4D, in the form of (x, y, z, t) where nt = 24. The most impactful inputs are methane leak rate, wind direction and wind speed, and we consider only those three for our proof-of-concept surrogate modeling. Hence, we use a channel number of 3 to provide those 3 variables in our input data. Our output data has only one variable (methane concentration), so the channel number of output data is 1. All 1000 samples of the leak rate, wind direction and wind speed are randomly populated for training data generation. The wind direction and speed vary hour by hour, but the methane leak rate is kept constant within a day for now. In our preliminary surrogate model, we only consider one methane emission source, at the center of our 3D model with a fixed elevation.

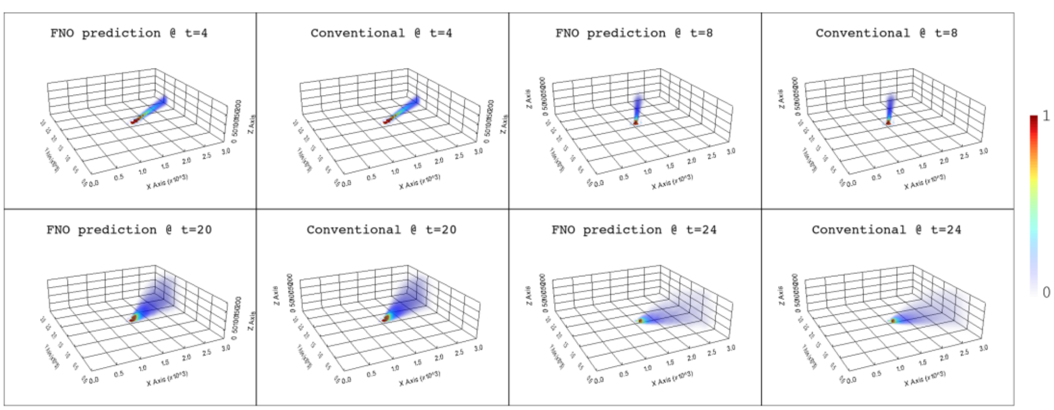
Once we obtain our training samples, we feed them to the FNO algorithm to train a surrogate model for our dispersion PDE operator. The original FNO architecture consists of 3 main components: (1) a time-domain encoder with Fully Connected (FC) layers to lift the channel dimension; (2) A series of repeatable Fourier layers combining Fourier-domain spectral convolution and time-domain 1x1 convolution; (3) a time-domain decoder with FC layers to project back to the target dimension. Our data size for 3D methane dispersion simulations over time is (nx, ny, nz, nt) = (57, 58, 40, 24), and 4D FFT and inverse FFT over those four dimensions are performed in the FNO. We also take advantage of distributed training using DeepSpeed [8] to expedite our training with 8 GPUs. Once a surrogate model is derived, we can predict the 3D methane concentration field at all 24 time-steps in a single pass of inference which takes less than a second.

2.3 Cloud HPC for training data generation

After our preliminary experiment, we would like to generate thousands more training data with the conventional physics-based solution to build a generalized and robust FNO surrogate model. This can be computationally intensive, and we rely on the cloud-native HPC technology for distributed 3D simulations. We use a combination of Dask and Kubernetes [9] for running methane dispersion modeling in a containerized fashion on cloud, which provides great features such as scalability, fault-tolerance, and auto-scaling. It can also take advantage of the spot virtual machines to significantly reduce the computational cost (up to 90%).

3 Preliminary results

We split our 1000 training samples into training (800 samples) and test (200 samples) datasets. We train a FNO proxy model with the 800 training samples using an Adam optimizer and a relative MSE loss function [6]. After a few hundred epochs, both training and testing losses are reduced to a few percent (relative to the ground truth). We run inference on test samples (unseen by training) and plot one sample result in the figure below. Displayed are 3D methane dispersion plumes from our FNO inference and the conventional physics-based solution at various time steps. Although the time-variant wind causes rapid changes in the plume orientation and shape, our FNO surrogate model is capable of learning the complex non-linear PDE operator very accurately, producing high-fidelity simulation results at all time steps in one pass of inference.



4 Conclusion

We have developed a preliminary surrogate model based on the FNO for methane dispersion modeling. The initial result shows that it emulates the highly non-linear PDE solver from the 3D advection-diffusion equation very well, producing accurate simulation results comparing to the conventional physics-based solution. Our FNO surrogate modeling is also capable of handling the time-variant inputs and temporally non-smooth outputs. The FNO model provides a fast and accurate alternative solution to methane dispersion simulations, thus reducing the cycle time for emission source attribution and quantification.

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