NESTED FOURIER NEURAL OPERATOR FOR BASIN-SCALE 4D CO_2 STORAGE MODELING

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ABSTRACT

Carbon capture and storage (CCS) plays an essential role in global decarbonization. Scaling up CCS requires accurate and high-resolution modeling of the storage reservoir pressure buildup and the gaseous plume migration. However, such modeling is very challenging at scale due to the high computational costs of existing numerical methods. This challenge leads to significant uncertainty in evaluating storage opportunities which can delay the pace of global CCS deployments. We introduce a machine-learning approach for dynamic basin-scale modeling that speeds up flow prediction nearly 700,000 times compared to existing methods. Our framework, Nested Fourier Neural Operator (FNO), provides a general-purpose simulator alternative under diverse reservoir conditions, geological heterogeneity, and injection schemes. It enables unprecedented real-time high-fidelity modeling to support decision-making in basin-scale CCS projects.

1 INTRODUCTION

Carbon capture and storage (CCS) is an important climate change mitigation technology that captures carbon dioxide (CO_2) and permanently stores it in subsurface geological formations. It provides a tangible solution for decarbonizing hard-to-mitigate sectors and can generate negative emissions when combined with direct air capture or bioenergy technologies (Pathways, 2019; Luderer et al., 2018; Fankhauser et al., 2022). However, the current pace of CCS deployment scale-up has failed to meet expectations (Reiner, 2016). One of the critical challenges contributing to the delay is the uncertainties in storage prospects and injection capacities (Lane et al., 2021). The geological storage of CO_2 leads to pressure buildup and gaseous plume migration in the storage formation (NAS, 2018). Forecasts of these dynamic responses are used to determine CO_2 storage capacities and guide important engineering decisions. The modeling of these processes requires multi-phase (Pruess et al., 1999; Blunt, 2017), multi-physics (Pruess & Garcia, 2002), and multi-scale simulations, which are very expensive with current numerical approaches. As a result, they are inadequate to provide rigorous computation supports that are needed for accelerating CCS project deployments around the world (Lane et al., 2021).

An especially challenging characteristic of CO_2 storage modeling is that it demands both high-resolutions and extremely large spatial-temporal domains. The CO_2 plume and near-well pressure buildup require highly resolved grids (Pruess & Müller, 2009; André et al., 2014; Doughty, 2010; Wen & Benson, 2019). Meanwhile, pressure buildup can travel hundreds of kilometers beyond the

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CO_2 plume and interfere with other injection operations (Chadwick et al., 2004). Due to these multi-scale responses, many CCS-related analyses are forced to use inaccurate simulations with coarsened grid resolution (Kou et al., 2022) and/or simplified physics (Cavanagh & Ringrose, 2011).

One approach for reducing the computational costs of numerical simulations is to use non-uniform grids to capture different responses with different resolutions. A popular method, known as local grid refinement (Bramble et al., 1988) (LGR), has enabled simulations of real-world three-dimensional (3D) CO_2 storage projects, where the fine-grid responses capture the plume migration while the coarser grid responses capture the far-field pressure buildup (Eigestad et al., 2009; Faigle et al., 2014; Kamashev & Amanbek, 2021). However, even with non-uniform grid approaches, these numerical models are still too expensive to be used for important CCS tasks that require probabilistic/repetitive forward stimulation such as site selection (Callas et al., 2022), optimization (Nghiem et al., 2010; Zhang & Agarwal, 2012), and inversion (Strandli et al., 2014).

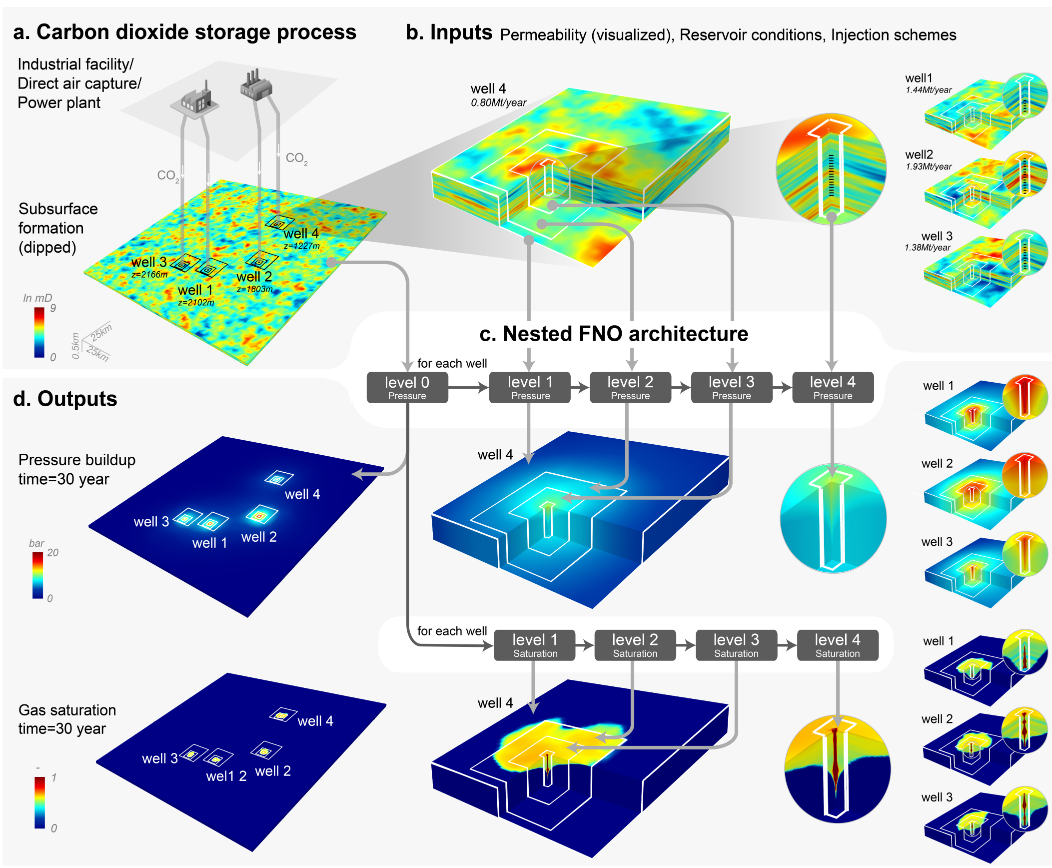

Figure 1: **a-b.** Permeability for a dipped 3D reservoir with four injection wells; white and black lines indicate level 0 to 4's boundary; the black dotted lines in the zoomed-in circles show the locations of injection perforation intervals. **c.** Each grey block represents an FNO model; light grey arrows point to the input and output's level; dark grey arrows show when one model's output is used as another model's input. **d.** Pressure buildup and gas saturation at 30 years.

In recent years, machine learning approaches are emerging as a promising alternative to numerical simulation for subsurface flow problems (Tang et al., 2020; Wen et al., 2021b;a). Machine learning models, trained with numerical simulation data, are usually much faster than numerical simulators because inferences are very cheap. However, for CO_2 storage problems, the challenge of the multi-scale response has limited developments of machine learning models. Previous studies either focus on 2D problems with a single injection well (Wen et al., 2021a; 2022), or 3D problems with very coarse resolutions that fail to capture essential physics (Tang et al., 2022; Yan et al., 2022).

In addition, standard machine learning methods suffer from the lack of generalization (Kovachki et al., 2021). This limits the usage of machine learning in CO_2 storage modeling as it requires generalization under diverse input conditions. Fourier neural operator (FNO) is a type of neural operators (Li et al., 2020b;c) that overcome these generalization challenges by directly learning the solution operator for the governing equation family. As a result, it provides great potential towards the development of a realistic general-purpose simulator alternative for CO_2 storage problems (Wen et al., 2022; Witte et al., 2022).

Here we present a machine learning framework with an unprecedented capability of high-resolution, full-physics, dynamic 3D CO_2 storage modeling. We integrate the FNO machine learning architecture with the LGR modeling approach and introduce the Nested Fourier Neural Operator (Nested FNO) architecture. As shown in Figure 1, five levels of FNOs are used to predict flow responses in five different resolutions. This approach vastly reduces the computational cost needed during data collection as well as overcomes the memory constraints in model training. Using this approach, our prediction resolution exceeds many benchmark CO_2 storage simulations run with existing numerical models. Meanwhile, Nested FNO only needs less than 2,500 training data at the coarsest resolution and about 6,000 samples for the finer resolutions. Despite the small training size, it generalizes well to the large problem dimension with millions of cells and a diverse collection of practical input variables, making it a general-purpose simulator alternative for basin-scale CO_2 storage projects.

2 Data Overview

We consider CO_2 injection into basin-scale 3D saline reservoirs (Page et al., 2020) through multiple wells over 30 years, as shown in Figure 1 **a**. Our data set includes a comprehensive collection of variables for practical CO_2 storage projects, covering most realistic storage scenarios of potential CCS sites. Input parameters comprise reservoir conditions (depth, temperature, dip angle), injection schemes (number of injection wells, rates, perforation intervals), and permeability heterogeneity (mean, standard deviation, correlation lengths). The numerical simulation data is generated using a semi-adaptive LGR approach to ensure high fidelity and computational tractability. We use global (level 0) resolution grids in the large spatial domain to mimic typical saline storage formations with infinite boundary conditions. Next, we apply four levels of local refinements (levels 1 to 4) around each well to gradually increase the grid resolutions. Going from levels 0 to 4, we reduce the cell size by 80x on the x, y dimensions and 10x on the z dimension to resolve near-well responses.

3 Nested FNO Architecture

As shown in Figure 1, we use a sequence of FNO models to predict the 3D reservoir domain consisting of subdomains at levels 0 to 4. At each refinement level, we extend the original FNO (Li et al., 2020a) architecture into 4D to produce outputs for pressure buildup and gas saturation in the 3D space-time domain. The input for each model includes the permeability field, initial hydro-static pressure, reservoir temperature, injection scheme, as well as spatial and temporal encoding. Besides the global level model, each model in Nested FNO takes the input on its own domain together with the coarser-level prediction to predict the finer-level output.

4 Results & Pathway to Climate Impact

As shown in Figure 2 **a**, Nested FNO successfully captures the CO_2 plume migration in this nested locally refined grid. The shapes and saturation distribution of each plume are accurately predicted for each well. Such accuracy is well sufficient for most practical applications, such as forecasting plume footprints for land acquisition or monitoring program design. Similarly, as shown in Figure 3, Nested FNO precisely captures the local pressure buildup responses around each well, as well as the global interaction among them. The high-resolution refinements provide accurate estimates of the maximum pressure buildup, which is an essential indicator of reservoir integrity. These predictions are sufficient to guide important engineering decisions, such as choosing injection rates.

Nested FNO offers these dynamic 3D simulations in *real time* because the prediction speed is 700,000 times faster compared to the state-of-the-art numerical solver. This prediction speed enables many critical CCS tasks that were prohibitively expensive. For example, we present a rigorous

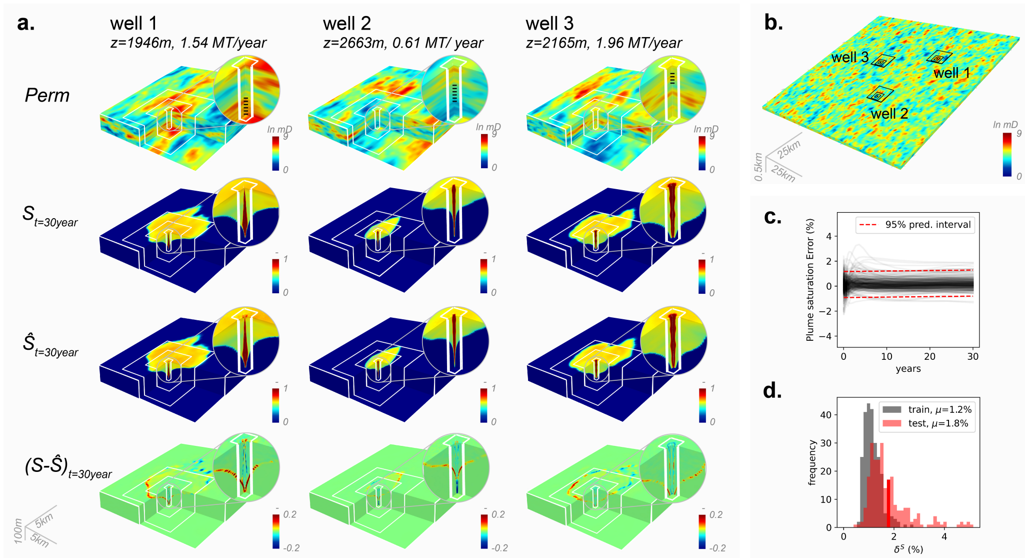

Figure 2: **Gas saturation prediction. a.** Visualizations of gas saturation predictions at 30 years for a 3-well case. Each row shows permeability, gas saturation ground truth, prediction, and error. The white lines indicate the boundary between each level. **b.** Reservoir permeability and the location of each well. **c.** Testing set plume saturation error versus time for 250 random cases. The red dotted line shows the 95% prediction bands of the error. **d.** Error histograms for 250 cases in the training and test set. The solid red column indicates the error for the example shown in a.

probabilistic assessment for maximum pressure buildup and CO_2 plume footprint (Appendix A). Such assessment can reduce uncertainties in capacity estimation and injection designs (NAS, 2018); however, it would have taken nearly two years with numerical simulators. Using Nested FNO, this assessment took only 2.8 seconds. The high-quality real-time predictions of Nested FNO can greatly enhance our ability to develop safe and effective CCS projects.

Notably, by releasing the trained Nested FNO to the public, our approach promotes equity in CCS project development and accelerates knowledge adoption for CO_2 storage. This especially benefits small- to mid-sized developers, as well as communities desiring independent evaluation of projects being proposed. Such high-quality forecasts and probabilistic assessments of reservoir dynamics were previously unattainable to these important players.

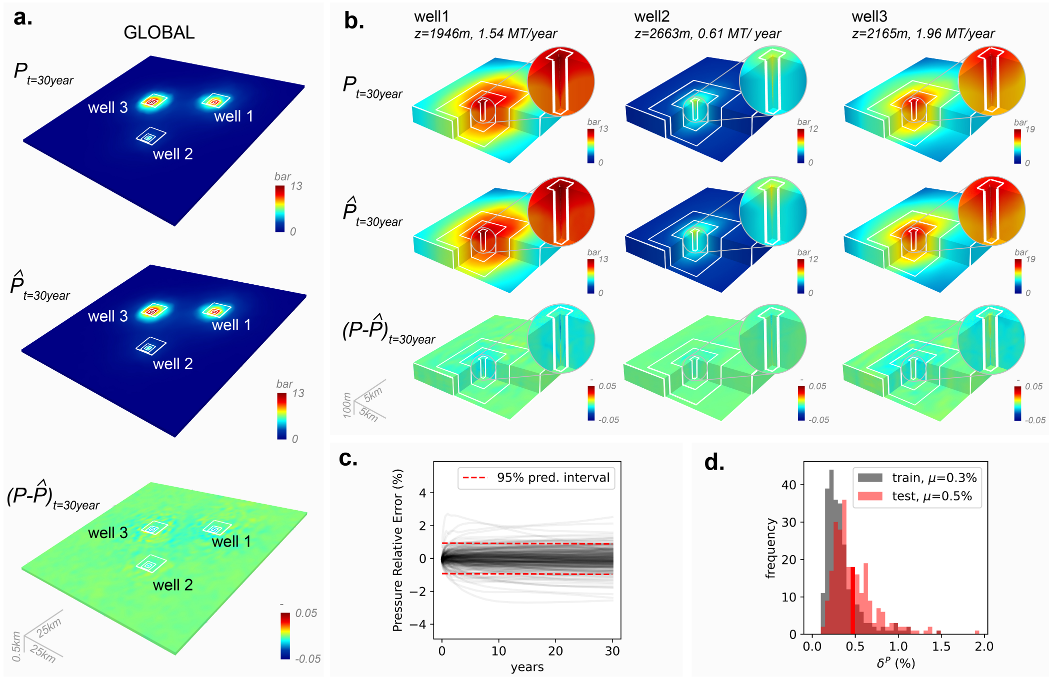

Figure 3: **Pressure buildup prediction. a.** Global and **b.** well pressure buildup predictions at 30 years. Each row shows pressure buildup ground truth, prediction, and relative error. The white lines indicate the boundary between each level. **c.** Testing set pressure relative error versus time for 250 random cases. The red dotted line shows the 95% prediction bands of the error. **d.** Error histograms for 250 cases in the training and test set. The solid red column indicates the error for the visualized example.

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A Probabilistic Assessment

Nested FNO's fast prediction speed enables rigorous ensemble modeling and probabilistic assessments that were previously unattainable. As an example, we conducted a probabilistic assessment for the maximum pressure buildup and CO_2 plume footprint for a four-well CCS project where each well injects at a 1MT/year rate. To investigate the influence of permeability heterogeneity, we generate 1,000 realizations using a fixed set of distribution and spatial correlations, then use Nested FNO to predict gas saturation plumes and pressure buildup for each realization. As shown in Figure 4, we obtained probabilistic estimates of the CO_2 plume footprint and maximum pressure buildup, which can help project developers and regulators manage uncertainties (Pawar et al., 2016). For example, the plume footprint helps determine the area of the land lease acquisition required (NETL, 2017); the maximum reservoir pressure buildup helps evaluating the safety of a certain injection scheme and ensures reservoir integrity. Running this assessment takes only 2.8 seconds with Nested FNO but requires nearly two years with traditional numerical simulators.

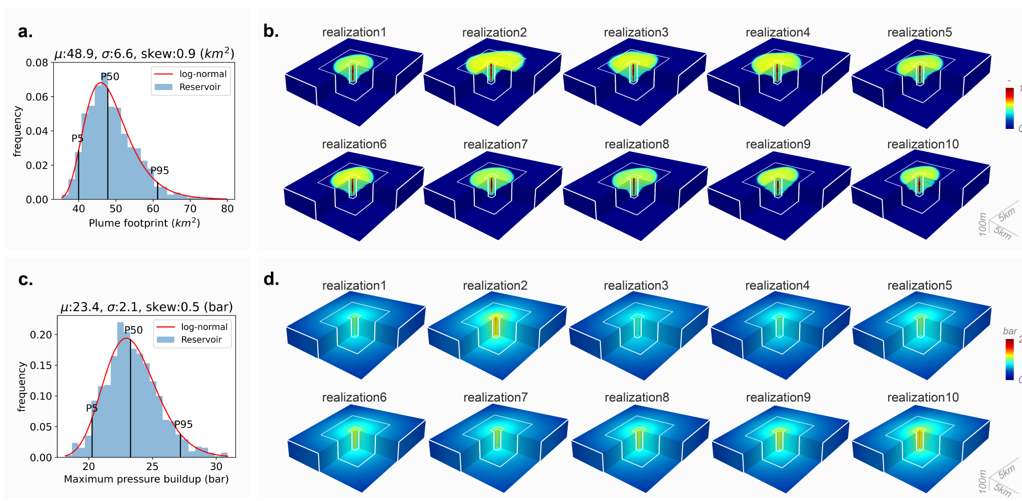

Figure 4: **Probabilistic assessment. a.** Histogram of CO_2 plume footprint predictions given 1,000 permeability realizations from the same geological parameters. The result satisfies a log-normal distribution; P5, P50, and P95 are marked on the distribution. **b.** Ten realizations of CO_2 plume at 30 years. **c.** Histogram of CO_2 pressure buildup predictions given the same 1,000 permeability realizations. The result satisfies a log-normal distribution; P5, P50, and P95 are marked on the distribution. **d.** Ten realizations of pressure buildup at 30 years.