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Physics informed neural networks based on sequential training for CO₂ utilization and storage in subsurface reservoir

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Summary

The energy transition is unavoidable because energy production accounts for roughly two-thirds of current global emissions. To achieve this goal, active carbon emission reduction is required. Carbon dioxide capture, utilization, and storage (CCUS) is a promising technology to mitigate global warming. In order to operate CCUS intelligently, there must be a robust simulation technology that captures physics and the expected scenario. Machine learning (ML) techniques have recently been applied to a wide range of nonlinear computational problems. Recently, Physics informed neural network (PINN) has been proposed for solving partial differential equations. Unlike typical ML algorithms that require a large dataset for training, PINN can train the network with unlabelled data. The applicability of this method has been explored for flow and transport of multiphase in porous media. However, for strongly nonlinear hyperbolic transport equation, the solution degrades significantly. In this work, we propose a sequential training PINN to simulate two-phase transport in porous media. The main concept is to retrain neural network to solve the PDE over successive time segments rather than train for the entire time domain at once. We observe that, sequential training can capture the solution more accurately with respect to standard training method.

Introduction

It is inevitable to overlook the role of carbon emission reduction while the world attempts to mitigate global warming. One of the key technologies for reducing the amount of greenhouse gases in the atmosphere is carbon dioxide capture, utilization, and storage (CCUS). Carbon dioxide and its associated compounds are captured from producing sources, compressed, transported, and used for operations such as permanent storage in deep underground geological formations and increased hydrocarbon recovery in existing oil fields. To reduce the risk of the operation, a model that can captures multiphase transport in subsurface reservoir is required.

Machine learning (ML) techniques, particularly deep learning (LeCun et al, 2015), are gaining popularity in the computational science and engineering communities. Especially, physics-informed neural networks (PINNs) have been used to target problems where engineering conservation equations and constitutive closure relationships are known without having a labelled data (Raissi et al, 2019). To approximate complex nonlinear solutions, neural networks are constructed with several hidden layers accompanied by nonlinear activation functions.

Standard PINN has been used to model two-phase immiscible flow in porous media. They demonstrated that for PINN cannot find the solution in case of the steep saturation front with the nonconvex flux function. Only when an artificial diffusion term was added to the original conservation equation, could the neural networks solution approximate the true solution (Fraces et al., 2020; Tchelepi and Fuks, 2020).

In this work, we propose the novel sequential training approach in which unlike training for the entire spatio-temporal domain, we discretise the time domain and march in time to reach to the end time. The approach is motivated by classic techniques used in such as finite volume methods (FVMs) in solving partial-differential equations. We observe that sequential training can predict the solution more accurately comparing to standard training approach.

Method and/or Theory

We consider the general form of conservation of two-phase immiscible fluid flow (water – CO_2) in one-dimension space as:

$$\frac{\partial S_\alpha}{\partial t} + u_t \frac{\partial (f_\alpha(s))}{\partial x} = 0, t \in (0, T], x \in \Omega, \alpha \in \{water, CO_2\} \quad (1)$$

$$f_\alpha = \frac{\lambda_w}{\lambda_w + \lambda_{CO_2}} \quad (2)$$

Where u_t is a total velocity and where $\lambda_\alpha = \frac{(k k_{r\alpha})}{\mu_\alpha}$ stands for phase mobility, μ_α is the viscosity of the phase, $k_{r\alpha}(S_\alpha)$ is the relative phase permeability, and q_w is the source and sink terms.

Std-PINN Solution

(Raissi et al, 2019) proposed that the solution of the PDE could be approximated by a deep neural network through the loss function of the neural network. In standard PINN solution, a Neural network is trained for the entire spatial-temporal domain. The equation 1 in residual form is written as:

$$r(t, x) = (S_\alpha)_t + (f_\alpha)_x = 0, \quad (3)$$

The initial and boundary conditions are

$$S(x, t) = 0, \forall x \text{ \& } t = 0 \quad (4)$$

$$S(x, t) = 1, \quad x = 0 \text{ \& } t > 0$$

The loss function of the PINN is made of three error conditions:

$$L_{tot} = L_i + L_{ii} + L_{iii} \tag{5}$$

$$\begin{cases} L_i = \frac{\sum_{k=1}^{N_i} (S(x_k^i, 0) - S_k^i)}{N} \\ L_{ii} = \frac{\sum_{k=1}^{N_b} (S(x_k^b, t_k) - S(x_k^b, t_k))}{N} \\ L_{iii} = \frac{\sum_{k=1}^{N_b} (R(x_k^r, t_k))}{N} \end{cases} \tag{6}$$

Seq-PINN Solution

Unlike standard PINN training, we train for the entire domain at once, we discretise the time domain into several segments. We use a marching-time scheme to predict next timestep.

$$[T_0 = 0, T_1], [T_1, T_2], \dots, [T_{n-1}, T_n], \dots, [T_{n_{max-1}} - T_{n_{max}}] \tag{7}$$

Figure 1 illustrates schematically the sequential training strategy versus standard training scheme.

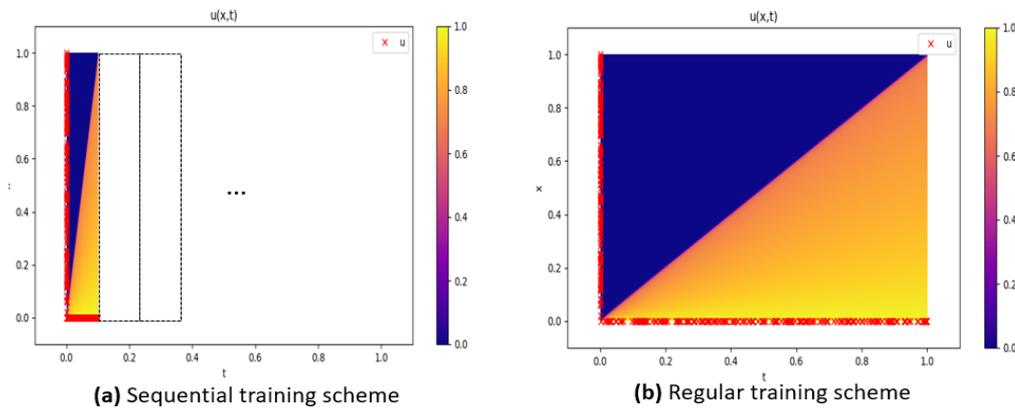


Figure 1 Regular training scheme Versus Sequential training

Note that this behaviour also has analogues with numerical methods used in scientific computing, where space time problems are typically harder to solve, as compared to time marching methods. To motivate our sequential approach, we consider the discretised single cell implicit transport equation as:

$$R = S^{n+1} + \frac{\Delta t}{\Delta x} (f_R(S^{n+1}) - f_L(S_L)), \tag{8}$$

We analyse the nonlinearity of the residual for 4 different progressive time steps. Figure 4 shows that the larger the timestep the higher the nonlinearity of the residual. The nonlinearity of the residual is dictated by the nonlinearity of the flux function for the larger timesteps.

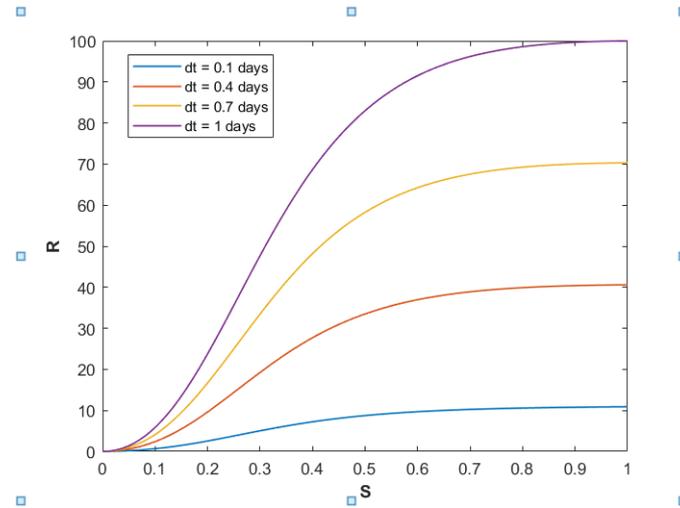


Figure 2 residual function for single cell, fix boundary conditions for different timesteps

Examples (Optional)

Here we compare the solution of Seq-PINN and Std-PINN for two phase immiscible test case. Initially, the 1D domain is fully saturated by non-wetting phase and we inject a wetting phase at the left boundary. Figure 3, we compared the solution of PINN for two different timesteps and compare the solution of the PINN train sequentially and standard approach. We observe that the Seq-PINN can approximate the solution more accurately. Table 1 summarized the loss function value after training. We observe that optimizer reduce the loss function by almost 2 orders of magnitudes in the case of sequential training for the smaller timestep and one order of magnitude for the bigger timestep with respect to standard approach. Another observation is that the bigger the time step interval for training the larger the loss function and the bigger the error.

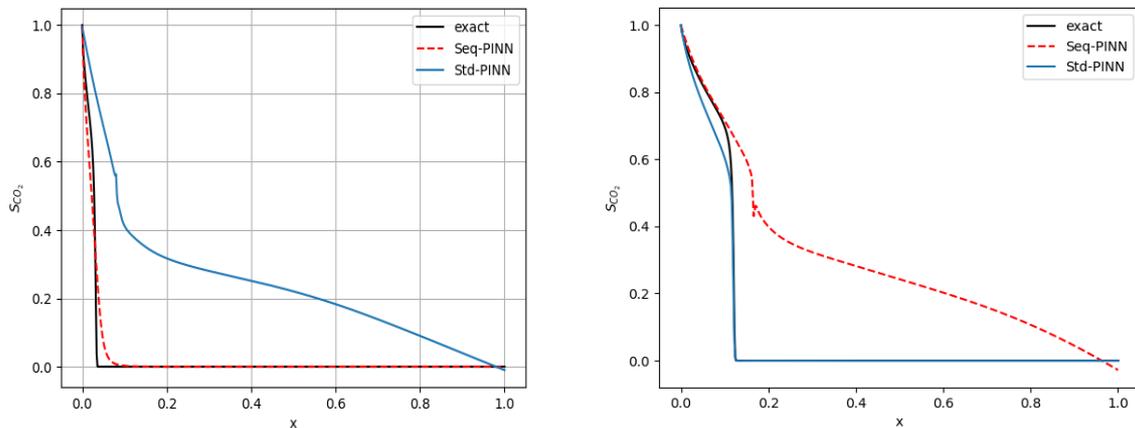


Figure 3 Solution comparison between std-PINN, Seq-PINN, and analytical solution left for for two different timesteps dt = 0.01 (left) dt= 0.1 (right)

Table 1 Final loss function value after training for sequential and standard methods (make it 3)

| Training method | Final loss function value |
|------------------------|---------------------------|
| Sequential (dt = 0.01) | 7.4e-4 |
| Sequential (dt = 0.1) | 1.2e-3 |
| Standard | 2.2e-2 |

Conclusions

carbon dioxide capture, utilization, and storage (CCUS) are required in addition to innovative low-carbon energy solutions to mitigate global warming. For simulation of CO₂ use and storage (CCUS) in subsurface reservoirs with complicated heterogeneous structures, a model that includes multiphase compositional flow and transport is needed. We investigated the application of a Physics informed neural network (PINN) for two phase fluid in porous media. We proposed the sequential training scheme as an alternative to standard training scheme. We observe that Seq-PINN can capture the solution more accurately compared to the standard approach. In the future work, we will focus on adding more complex physics by including miscibility and compositional transport.

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