U-FNO - an enhanced Fourier neural operator based-deep learning model for multiphase flow

Gege Wen¹, Zongyi Li², Kamyar Azizzadenesheli³, Anima Anandkumar², Sally M. Benson¹

¹Stanford University, ²California Institute of Technology, ³Purdue University
Numerical simulation of the **multiphase flow processes** are used throughout project planning, monitoring, optimization...

### Challenges

- Highly nonlinear governing PDEs
- Multi-physics in the problems
- Multiscale heterogeneity
- Need for high grid resolution
- Inherent uncertainty in geology
## Summary to ML approaches available for CO$_2$-water multiphase flow problem

| Approach    | Example                        | Method                                           | Advantage            | Problem                  |
|-------------|--------------------------------|--------------------------------------------------|----------------------|--------------------------|
| Neural-FEM  | Physics-informed neural networks (Raissi et al, 2019; Fuks et al, 2020) | Formulate PDE/initial cond. in loss function     | PDE-based            | Expensive, convergence   |
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| Neural-FEM       | Physics-informed neural networks             | Formulate PDE/initial cond. in loss function | PDE-based             | Expensive, convergence    |
|                  | (Raissi et al, 2019; Fuks et al, 2020)       |                                      |                       |                           |
| Data-driven CNN  | CCSNet                                       | Learn empirical input-output mapping | Very fast prediction  | Lots of data              |
|                  | (Wen et al, 2021)                           |                                      |                       |                           |
### Neural-FEM
- **Example:** Physics-informed neural networks (Raissi et al, 2019; Fuks et al, 2020)
- **Method:** Formulate PDE/initial cond. in loss function
- **Advantage:** PDE-based
- **Problem:** Expensive, convergence

### Data-driven CNN
- **Example:** CCSNet (Wen et al, 2021)
- **Method:** Learn empirical input-output mapping
- **Advantage:** Very fast prediction
- **Problem:** Lots of data

### Neural operator
- **Example:** FNO (Li et al, 2021)
- **Method:** Learn infinite-dimensional integral operator with NN
- **Advantage:** Very fast prediction, data efficient
- **Problem:** To be investigated

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Summarizing ML approaches available for CO$_2$-water multiphase flow problem:

| Approach            | Example                                | Method                                           | Advantage                      | Problem                          |
|---------------------|----------------------------------------|--------------------------------------------------|--------------------------------|----------------------------------|
| Neural-FEM          | Physics-informed neural networks        | Formulate PDE/initial cond. in loss function     | PDE-based                      | Expensive, convergence           |
|                     | (Raissi et al, 2019; Fuks et al, 2020) |                                                   |                                |                                  |
| Data-driven CNN     | CCSNet                                 | Learn empirical input-output mapping             |                                |                                  |
|                     | (Wen et al, 2021)                      |                                                   |                                |                                  |
| Neural operator     | FNO                                    | Learn infinite-dimensional integral operator with NN | Very fast, data efficient      | To be investigated               |
|                     | (Li et al, 2021)                       |                                                   |                                |                                  |

**U-FNO:**

an enhanced FNO
Let's take a closer look at the model architecture of original Fourier Neural Operator (Li et al, 2021)
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The transform is conducted utilizing Fast Fourier Transform (FFT).

After the transform, the discrete pixel data becomes **continuous function**.
Closer look at the model architecture of Fourier Neural Operator (Li et al, 2021)

\[(\mathcal{K}(\phi)v_t)(x) = \mathcal{F}^{-1} \left( R_{\phi} \cdot (\mathcal{F}v_t) \right)(x) \]

\[(\mathcal{F}f)_j(k) = \int_D f_j(x) e^{-2i\pi \langle x, k \rangle} dx \]
Closer look at the model architecture of Fourier Neural Operator (Li et al, 2021)

\[(\mathcal{F}f)_j(k) = \int_D f_j(x)e^{-2i\pi\langle x,k \rangle}dx\]

\[(\mathcal{F}^{-1}f)_j(x) = \int_D f_j(k)e^{2i\pi\langle x,k \rangle}dk\]
U-FNO instead of FNO to enhance the predictability of higher frequencies information
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Note 1: CNN U-Net to enhance higher frequencies information
U-FNO instead of FNO to enhance the predictability of higher frequencies information

Note 2:
Fourier and U-Fourier layer split is a hyper-parameter that can be tuned for specific problem

Note 1:
CNN U-Net to enhance higher frequencies information
Training general-purposed numerical simulator alternative with data set contains 4,500 input/output mappings

Input: parameters covering nearly all realistic scenarios for CO₂ storage in saline aquifers

- Pressure: 100-300 bar
- Temperature: 35-170 °C
- Formation thickness: 15-200m
- Rel perm (S_wi): 0.1-0.3
- Capillary pressure (λ): 0.3-0.7
- Injection rate: 0.2-2 Mt/yr
- Perforation interval: 10-200m
- Permeability map
- Anisotropy map
- Porosity map

![Diagram of CO₂ storage in saline aquifers]
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Output: gas saturation and pressure buildup in temporal-3d volumes
Result: CO$_2$ gas saturation plume prediction greatly improved with U-FNO comparing to CNN
Result: Pressure buildup prediction greatly improved with U-FNO comparing to CNN
**Result:** U-FNO is 46% more accurate in gas saturation, and 24% more accurate in pressure buildup.

A. Gas saturation

B. Pressure buildup
Remark: U-FNO is as much as 3.4 times more data efficient than CNN

Lower the test error we want to achieve, more CPU hours we can save.
**Computational efficiency**: prediction speed up is 60000x vs. numerical simulation; even faster than CNN

|        | # Parameter (-) | Training (s/epoch) | Testing |             | Speed-up vs. numerical simulation (times) |
|--------|-----------------|--------------------|---------|-------------|------------------------------------------|
| CNN    | 33,316,481      | 562                | 0.050   | 0.050       | $1 \times 10^4$                          |
| FNO    | 31,117,541      | 711                | 0.005   | 0.005       | $1 \times 10^5$                          |
| Conv-FNO | 31,222,625    | 1,135              | 0.006   | 0.006       | $1 \times 10^5$                          |
| U-FNO  | 33,097,829      | 1,872              | 0.010   | 0.010       | $6 \times 10^4$                          |
Thank you for listening!