





# **ML Based Newton preconditioner**

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## Numerical simulation of Carbon storage

Advantages	Drawbacks
Safety	Model uncertainties
Parametric studies	Parameters uncertainties
Cost and time efficiency	Computational resources

CO<sub>2</sub> storage requires important amount of simulations

 $\rightarrow$  Modify parameters to test scenarios

Explore recent breakthroughs in Artificial Intelligence to accelerate numerical simulation



2) Bicherg Yan et al.

## Outline

- Mathematical model and numerical resolution
- Global Hybrid Newton
- Results
- Conclusion



## Mathematical model and Numerical resolution



## Mathematical model

• Incompressible two-phase flow in porous medium

$$\begin{split} \phi \frac{\partial}{\partial t} (1 - S) + div(\mathbf{v}_{w}) &= 0, \quad \phi \frac{\partial}{\partial t} (S) + div(\mathbf{v}_{g}) = q_{g}, \quad \text{Mass conservation} \\ \mathbf{v}_{w} &= -\frac{Kkr_{w}(1 - S)}{\mu_{w}} \nabla P, \quad \mathbf{v}_{g} = -\frac{Kkr_{g}(S)}{\mu_{g}} \nabla P, \quad \text{Darcy's law} \\ S &= S_{g} = 1 - S_{w}, \end{split}$$



## Numerical Resolution



#### P, S as main unknowns

 $S_w = 1 - S$  auxiliary unknown



#### Discretization

- Finite volume in space
- Implicit Euler in time



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- P, S as main unknowns
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#### Discretization

- Finite volume in space
- Implicit Euler in time

#### • Fully Implicit scheme

$$egin{aligned} & R_g(S^{n+1},P^{n+1}) &= 0, \ & R_w(1-S^{n+1},P^{n+1}) &= 0. \end{aligned}$$

- → Non-linear system of equations solved using Newton's method
- Unconditionnaly stable but large time steps can prevent Newton's method from converging



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#### Discretization

- Finite volume in space
- Implicit Euler in time

Python library: Yads: Yet Another Darcy Solver



- ➔ Non-linear system of equations solved using Newton's method
- Unconditionnaly stable but large time steps can prevent Newton's method from converging



## Reservoir geometries

200 cells

**1D** 

Variable parameters :

- Well injection flow rate: **q**<sub>g</sub>
- Time-step: dt





## Reservoir geometries

#### 200 cells

**1D** 

**2D** 

Variable parameters :

- Well injection flow rate: **q**<sub>g</sub>
- Time-step: dt

SHPCO2 benchmark<sup>1</sup>

95 X 60 cells Variable parameters :

- Initial saturation: S<sub>0</sub>
- Well injection flow rate: **q**<sub>g</sub>
- Time-step: dt



1) Florian Haeberlein 2011 Time Space Domain Decomposition Methods for Reactive Transport — Application to CO2 Geological Storage.



#### • Scenario :









#### **Computational cost?**

- 0.8

-0.6

-0.4

-0.2





## Hybrid initialization: 1D example





## Hybrid initialization: 1D example

200





**Implicit Pressure Solver**  $\rightarrow$  Solve linear system

$$div(v_w(P^{n+1},1-S^n))=0, \ \ div(v_g(P^{n+1},S^n))=q_g,$$



### Hybrid initialization: 1D example



Implicit Pressure Solver
→ Solve linear system

$$div(v_w(P^{n+1}, 1-S^n)) = 0, \quad div(v_g(P^{n+1}, S^n)) = q_g.$$

Well events are similar in space and time

#### $\rightarrow$ Machine Learning model



# Workflow



→ Cover large range of well events

- $\rightarrow$  Fourier Neural operator
  - $S_{guess} = f_{\theta}(P_{imp}, S, q_g, dt)$

→ Compare Hybrid with Standard Newton's method



# Data Generation

- Variable parameters
  - Well injection flow rate:  $q_g \in [10^{-5}, 10^{-3}] \text{ m}^2/\text{s}$
  - Well opening time:  $dt \in [1, 10]$  years
  - Reservoir gas saturation:  $S \in [0, 0.6]$
- Generate realistic saturations S
  - Consecutive well opening and closing
  - 3 600 parameters combination
  - 18 000 samples
- Computational cost
  - Run in parallel using MPI
  - 360 CPUs
  - ≈36 hours



# Fourier Neural Operator<sup>1</sup>





1) Zongyi Li, et al 2020. Fourier neural operator for parametric partial differential equations.

## Saturation model - Architecture



# Saturation model - Training

- Dataset
  - 80% train / 20% test
- Computational cost
  - 132 hours on NVIDIA V100 GPU
- Hyperparameters
  - Loss:  $\frac{1}{N} \sum_{i=1}^{N} \frac{\|s_i \hat{s}_i\|_2}{\|s_i\|_2}$
  - Batch size: 128
  - Adam optimizer
  - Starting learning rate: 10<sup>-4</sup>
  - Momentum: 0.9
  - Weight decay: 10<sup>-4</sup>



CSSR



**Saturation initializations :** 



Standard



Hybrid



Saturation initializations :

Hybrid





Solution



#### Saturation initializations :



Hybrid



# Summary of Global Hybrid Newton

Advantages	Drawbacks
Acceleration of numerical simulation for a large range of well events Online phase affordable	Offline phase expensive : <ul> <li>Data generation</li> <li>Model training</li> </ul> Constant well location



# Conclusion and perspectives

- Integration of Hybrid Newton preconditioning in OPM
- Challenges:
  - More complex physical model
  - Training data generation cost
  - Multi-well handling
  - Heterogeneities
  - Discretization
- Current developments:
  - Local Hybrid Newton  $\rightarrow$  Reduce training cost / Multi-well handling
  - Generalized well model  $\rightarrow$  Reduce Dataset generation cost



# References

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  - https://github.com/PINN-Well-opening-and-closing-events/Yads.git







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CSSR is a Petrocentre financed by NFR (nr: 331841) NORCE lead, UiB partner, 170 MNOK budget, start-up 2022. Supported by major operators and technology providers





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