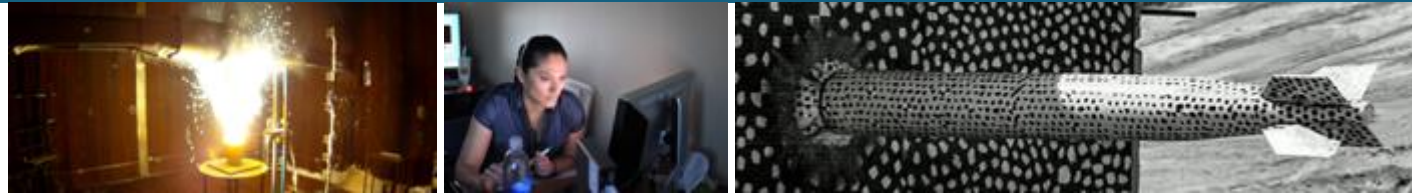




Continuous conditional generative adversarial networks for data-driven solutions of poroelasticity with heterogeneous material properties



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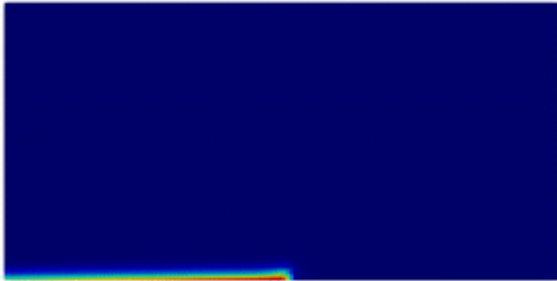


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Why reduced order model?



Full order model (FOM) is computationally demanding



This would take 1-2 hours^{1,2}

Imagine if you do 100,000 times of this

FOM is computationally very expensive for large-scale uncertainty quantification, optimization, or inverse modeling

¹Kadeethum T, Ballarin F, Choi Y, O'Malley D, Yoon H, Bouklas N. Non-intrusive reduced order modeling of natural convection in porous media using convolutional autoencoders: comparison with linear subspace techniques. arXiv preprint arXiv:2107.11460. 2021 Jul 23. [Avd. Water Res. In review after moderate revision]

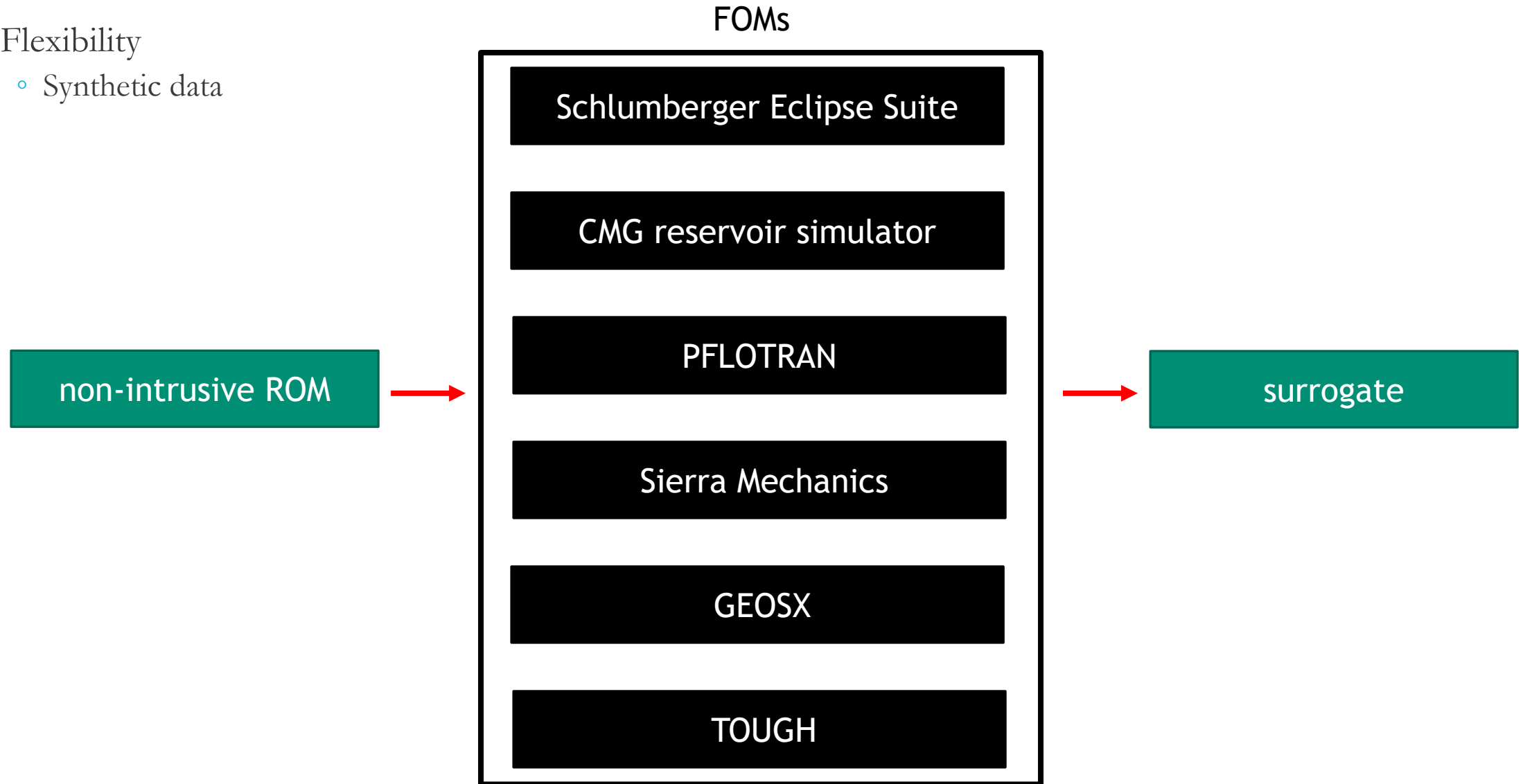
²Kadeethum T, Lee S, Ballarin F, Choo J, Nick HM. A locally conservative mixed finite element framework for coupled hydro-mechanical-chemical processes in heterogeneous porous media. Computers & Geosciences. 2021 Jul 1;152:104774.

Why non-intrusive approach?



Flexibility

- Synthetic data

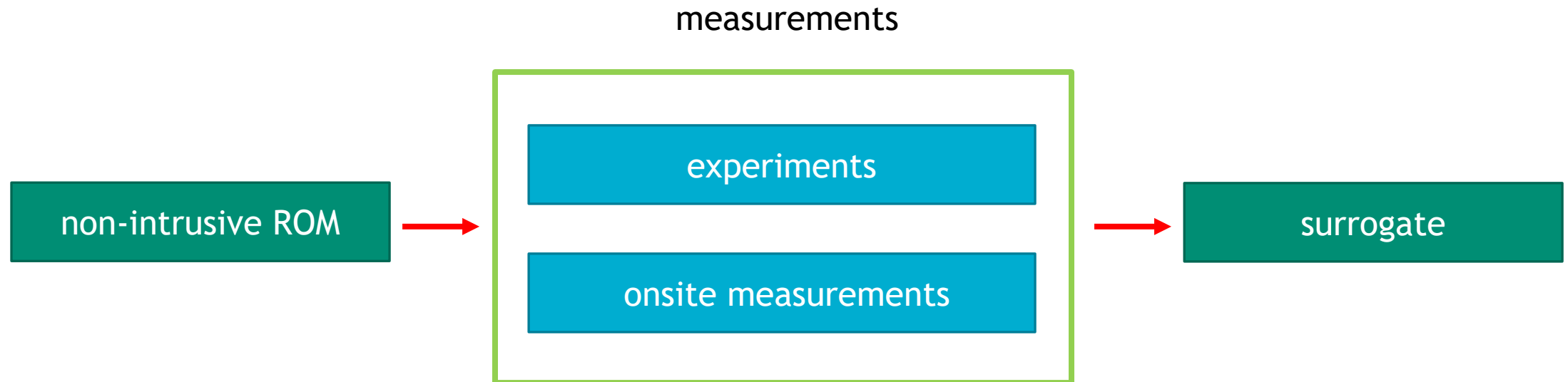


Why non-intrusive approach? - continued



Flexibility

- measurement

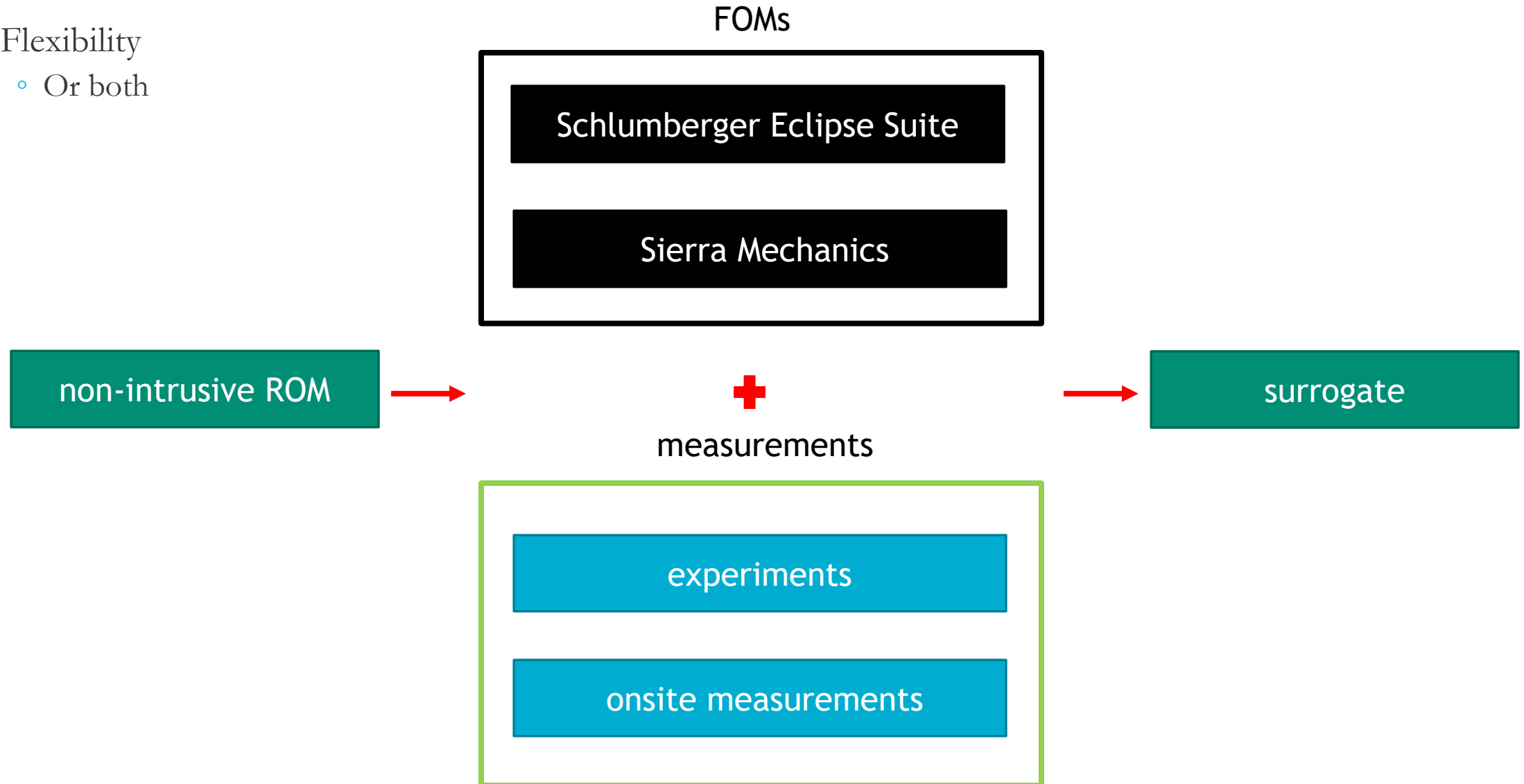


Why non-intrusive approach? - continued

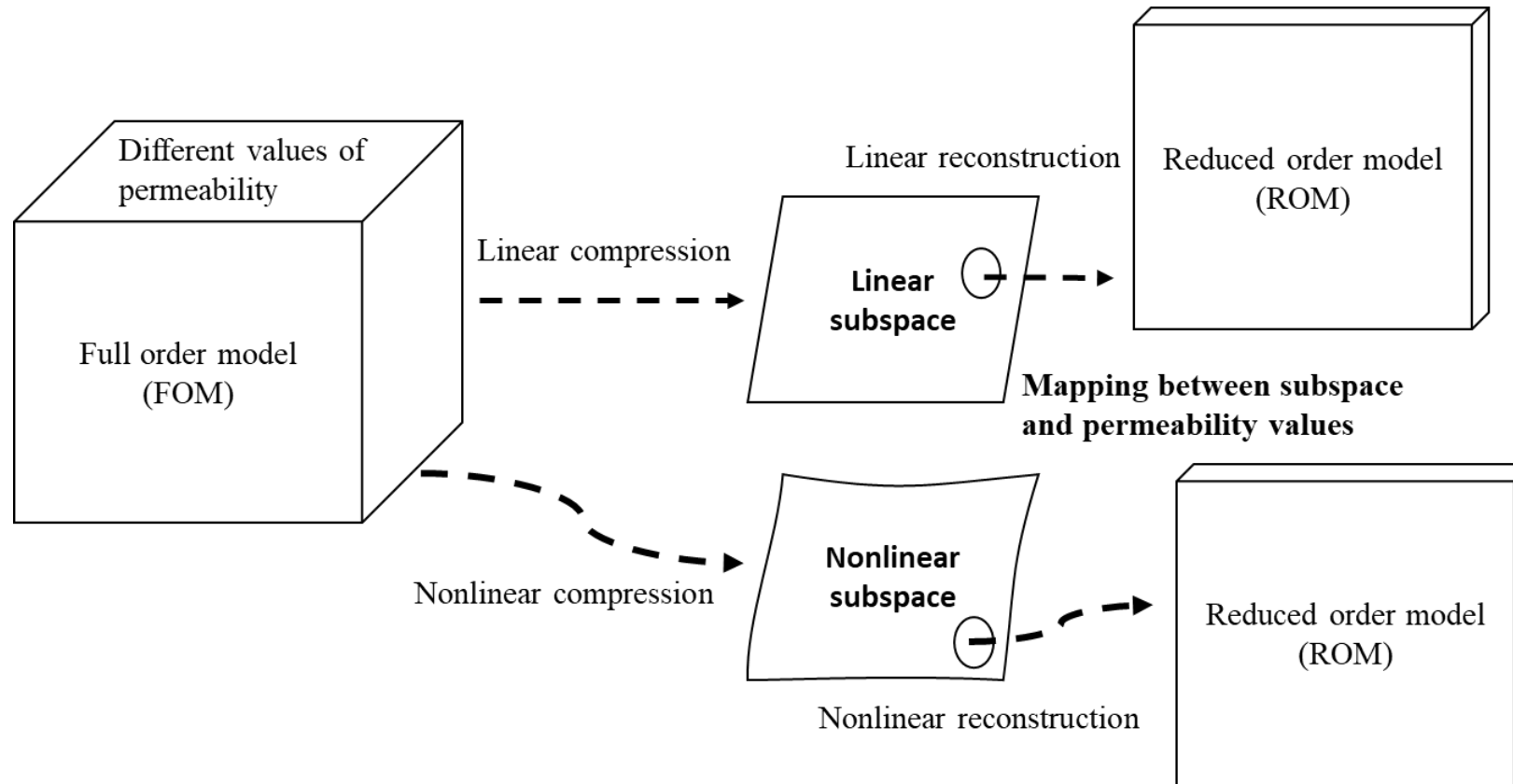


Flexibility

- Or both



ROM typically works on ‘parameterized PDEs’ and ‘reduced subspace’

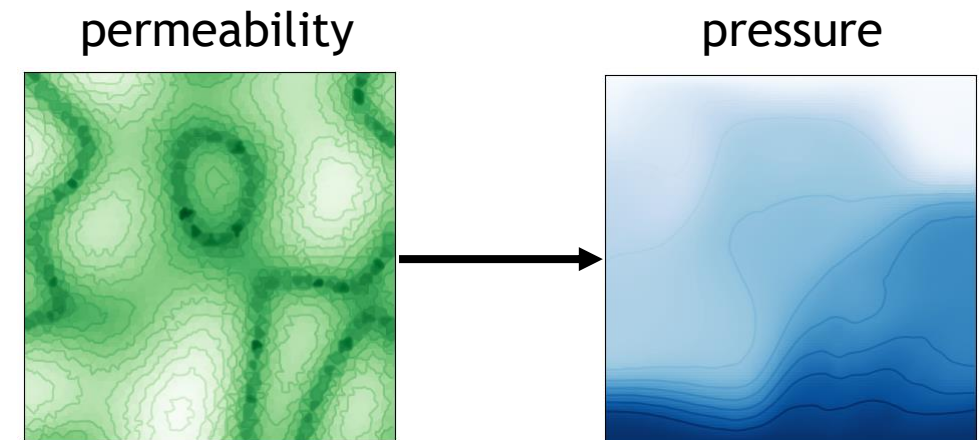
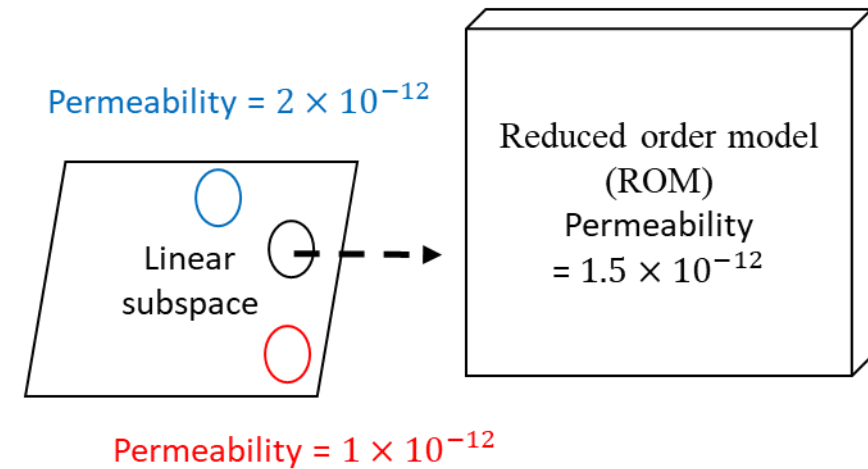


Motivation - continued

Parameterization for a single value (low dimension) is straightforward

However, how could we parameterize the whole heterogeneous field?

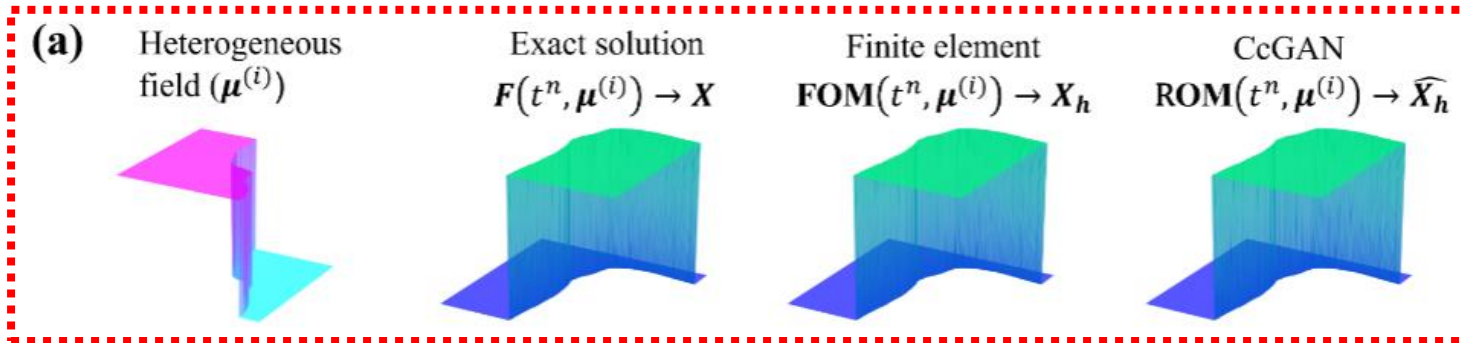
Mapping between subspace and permeability values



Methodology



We want to create a **surrogate model** that can provide a good accuracy comparable to that of **finite element model** with a much cheaper computational cost



(b) 1. Initialization

Training set: $\mu = [\mu^{(1)}, \mu^{(2)}, \dots, \mu^{(M-1)}, \mu^{(M)}]$



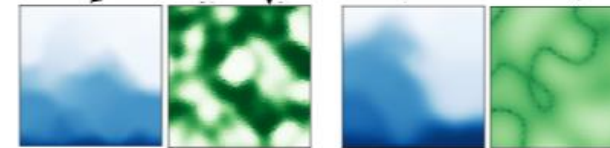
The same goes for validation and test sets.

3. Training CcGAN (ROM)



2. Full order model (FOM)

$FOM = X_h^{(1)}(t^n, \mu^{(1)}) \dots X_h^{(M)}(t^n, \mu^{(M)})$



For each $t^n \in [0 =: t^0 < t^1 < \dots < t^N := \tau]$

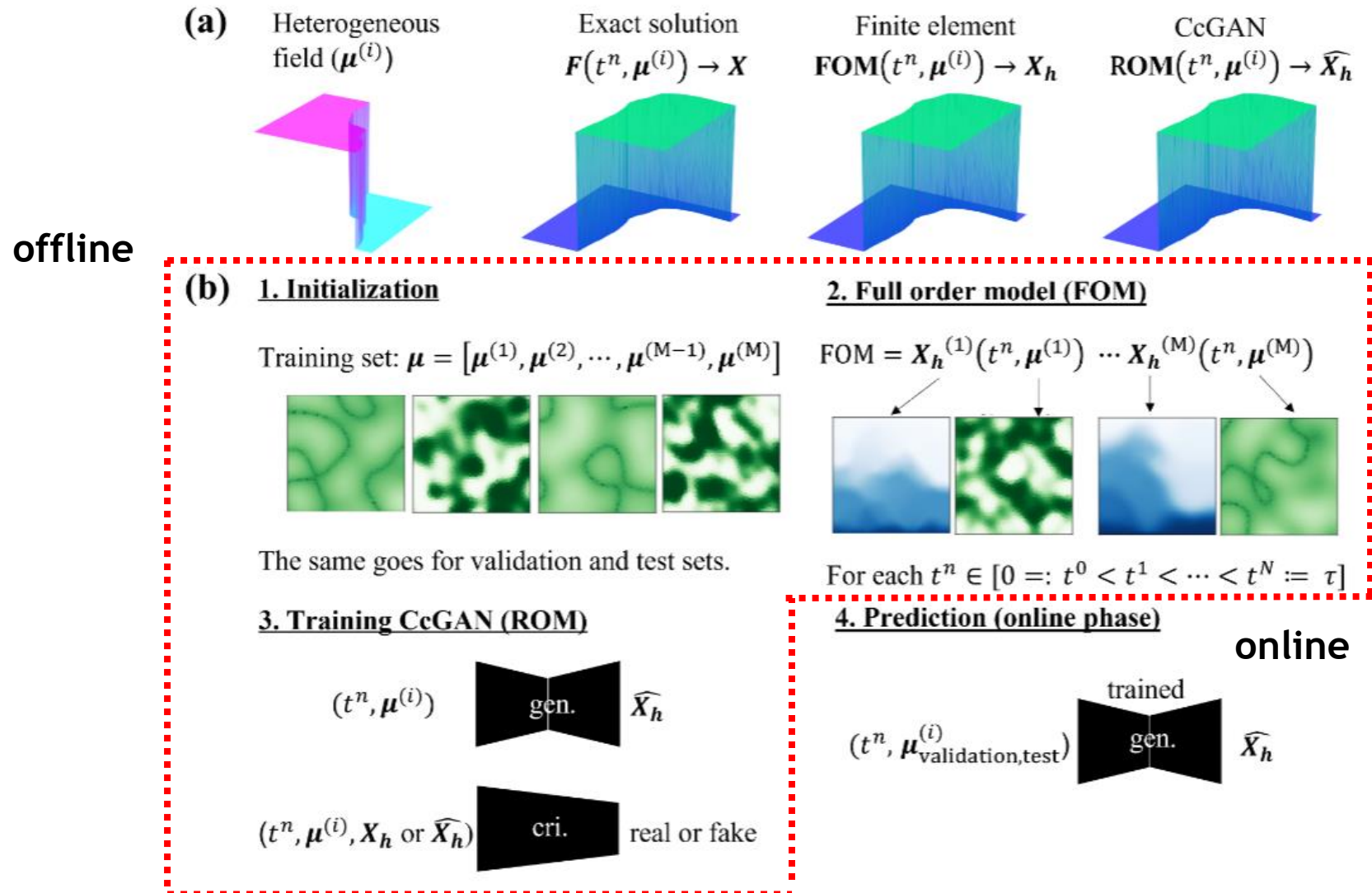
4. Prediction (online phase)



Methodology - continued



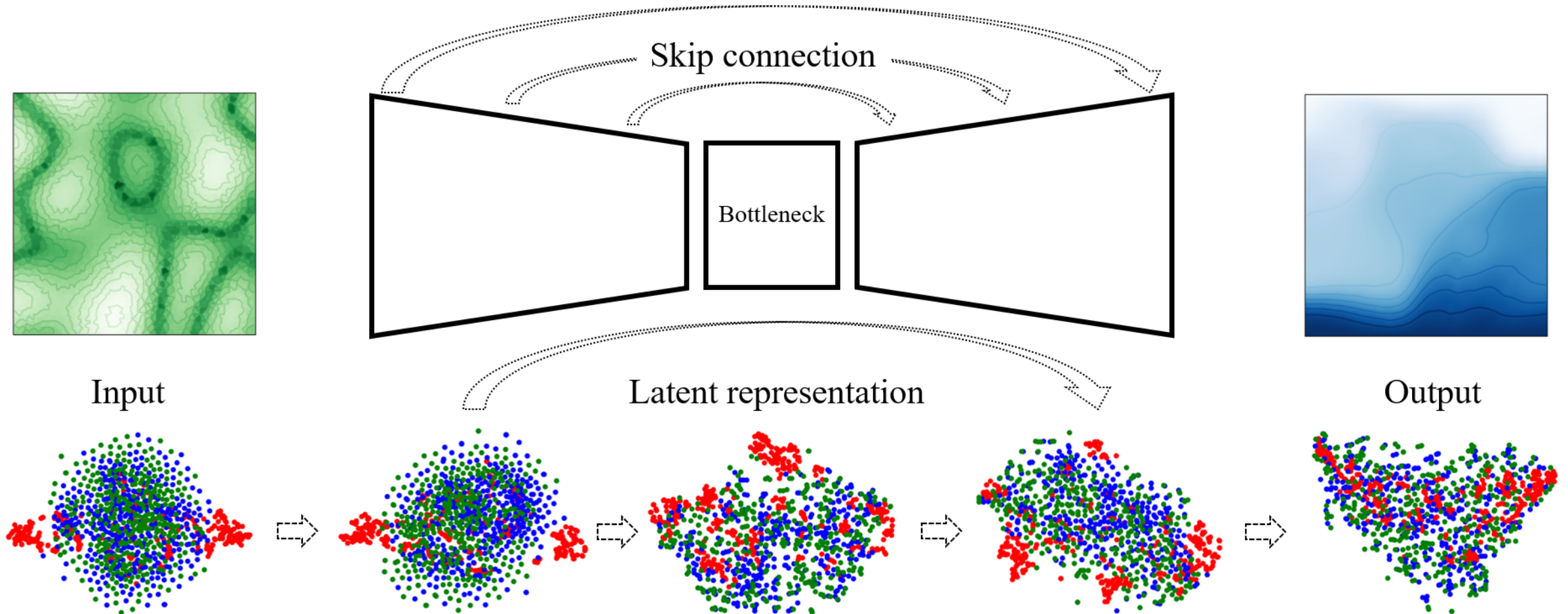
Our framework is developed for **parameterized** coupled **multiphysics** processes based on **offline** and **online** phases



Methodology - continued



In short, we extend the work done by Kadeethum et al. (2021) to time-dependent problems.



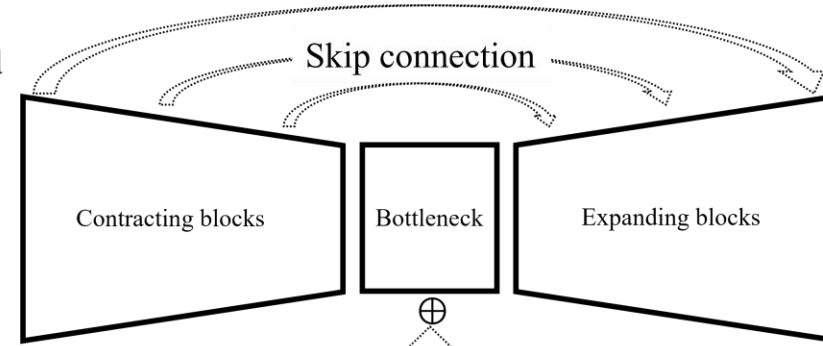
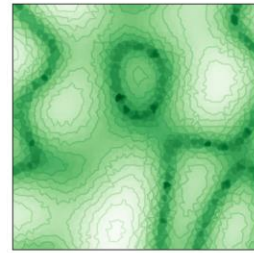
Methodology - continued

We have two models:

1. naive label input (NLI)
2. Improved label input (ILI)

Both models use the same critic.

Generator: with NLI Input: heterogeneous field

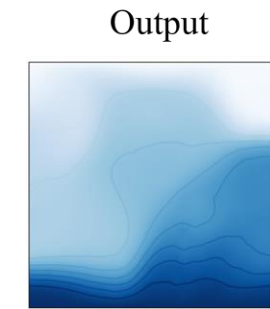
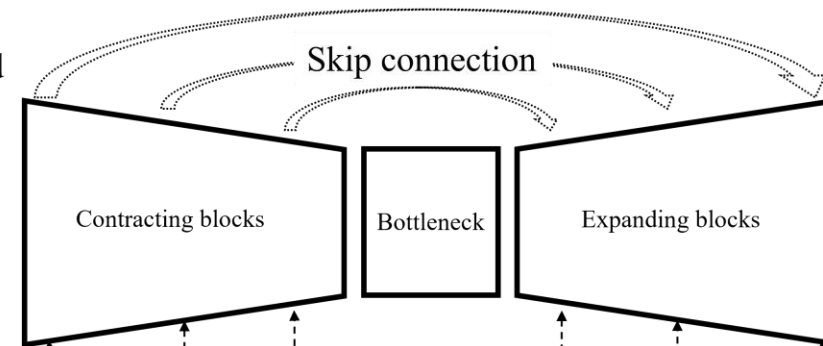
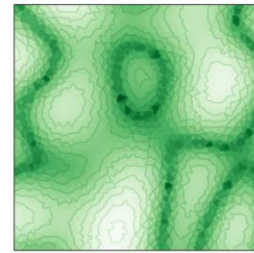


Input: time (t^n)

$$0 =: t^0 < t^1 < \dots < t^N := \tau$$

Element-wise addition

Generator: with ILI Input: heterogeneous field

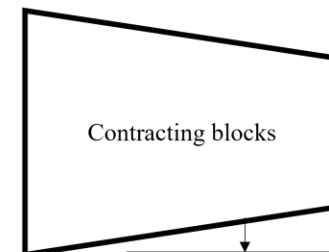
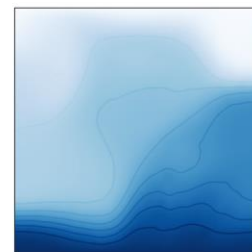
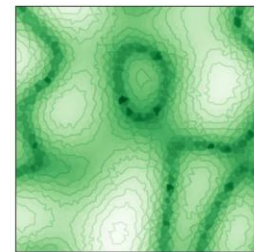


Input: time (t^n)

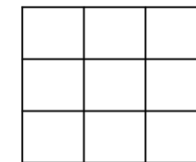
$$0 =: t^0 < t^1 < \dots < t^N := \tau$$

Conditional batch normalization

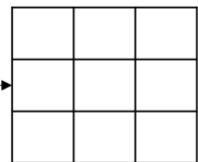
Critic Heterogeneous field + Output (fake) or real



Patch score



Final score



Inner product

Element-wise addition

Input: time (t^n)

$$0 =: t^0 < t^1 < \dots < t^N := \tau$$

1st linear layer

2nd linear layer

Element-wise addition

Methodology - continued



Generator architecture - Batch normalization is used by NLI, and it is replaced by ‘conditional batch normalization’ for ILI model

Table S1. Generator: NLI’s detail used in this study (input and output sizes are represented by $[B, C, \tilde{N}_h^p, \tilde{N}_h^p]$. We use hidden layers $H = 32$). BN refers to batch normalization.

Block	Input size	Output size	BN	Dropout
1 st convolutional layer	$[B, C, 128, 128]$	$[B, 32, 128, 128]$		
1 st contracting block	$[B, 32, 128, 128]$	$[B, 64, 64, 64]$	✓	✓
2 nd contracting block	$[B, 64, 64, 64]$	$[B, 128, 32, 32]$	✓	✓
3 rd contracting block	$[B, 128, 32, 32]$	$[B, 256, 16, 16]$	✓	✓
4 th contracting block	$[B, 256, 16, 16]$	$[B, 512, 8, 8]$	✓	
5 th contracting block	$[B, 512, 8, 8]$	$[B, 1024, 4, 4]$	✓	
6 th contracting block	$[B, 1024, 4, 4]$	$[B, 2048, 2, 2]$	✓	
1 st expanding block	$[B, 2048, 2, 2]$	$[B, 1024, 4, 4]$	✓	
2 nd expanding block	$[B, 1024, 4, 4]$	$[B, 512, 8, 8]$	✓	
3 rd expanding block	$[B, 512, 8, 8]$	$[B, 256, 16, 16]$	✓	
4 th expanding block	$[B, 256, 16, 16]$	$[B, 128, 32, 32]$	✓	
5 th expanding block	$[B, 128, 32, 32]$	$[B, 64, 64, 64]$	✓	
6 th expanding block	$[B, 64, 64, 64]$	$[B, 32, 128, 128]$	✓	
2 nd convolutional layer	$[B, 32, 128, 128]$	$[B, C, 128, 128]$		

Critic architecture

Table S3. Critic: NLI and ILI's detail used in this study (input size is represented by $[B, C, \tilde{N}_h^p, \tilde{N}_h^p]$, and output size is represented by $[B, C, \text{PATCH}_X, \text{PATCH}_Y]$. We use hidden layers $H = 8$).

Block	Input size	Output size	BN
1 st convolutional layer	$[B, C+1, 128, 128]$	$[B, 8, 128, 128]$	
1 st contracting block	$[B, 8, 128, 128]$	$[B, 16, 64, 64]$	
2 nd contracting block	$[B, 16, 64, 64]$	$[B, 32, 32, 32]$	✓
3 rd contracting block	$[B, 32, 32, 32]$	$[B, 64, 16, 16]$	✓
4 th contracting block	$[B, 64, 16, 16]$	$[B, 128, 8, 8]$	✓
2 nd convolutional layer	$[B, 128, 8, 8]$	$[B, C, 8, 8]$	

Governing equations



Momentum balance equation

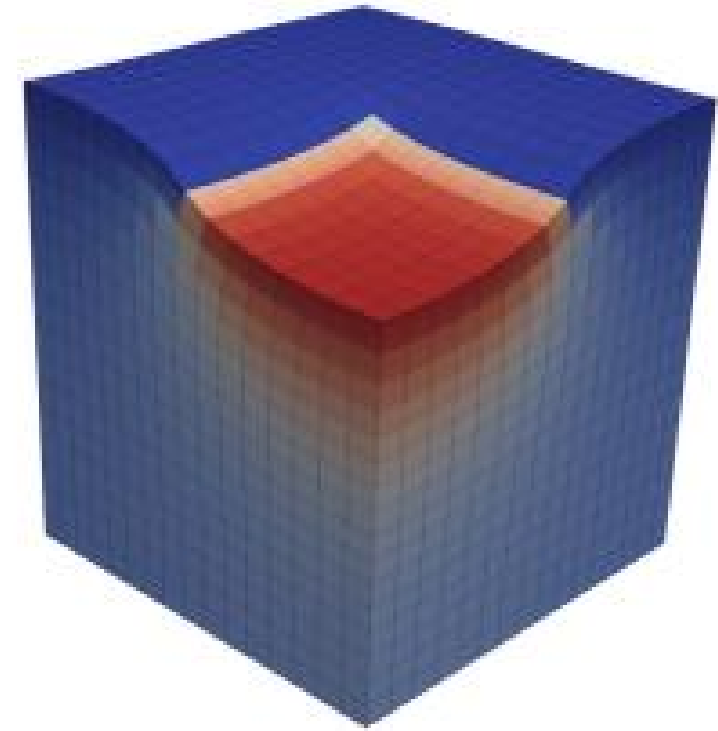
$$\begin{aligned}\nabla \cdot \boldsymbol{\sigma}'(\mathbf{u}) - \alpha \nabla \cdot (p\mathbf{I}) + \mathbf{f} &= \mathbf{0} \quad \text{in } \Omega \times \mathbb{T}, \\ \mathbf{u} &= \mathbf{u}_D \quad \text{on } \partial\Omega_u \times \mathbb{T}, \\ \boldsymbol{\sigma}(\mathbf{u}) \cdot \mathbf{n} &= \mathbf{t}_D \quad \text{on } \partial\Omega_t \times \mathbb{T}, \\ \mathbf{u} &= \mathbf{u}_0 \quad \text{in } \Omega \text{ at } t = 0,\end{aligned}$$

where $\boldsymbol{\sigma}'$ is the effective stress, p is the pore pressure, \mathbf{u} is bulk displacement, α is the Biot coefficient, \mathbf{f} is the body force.

Mass balance equation

$$\begin{aligned}\left(\frac{1}{M} + \frac{\alpha^2}{K}\right) \frac{\partial p}{\partial t} + \frac{\alpha}{K} \frac{\partial \boldsymbol{\sigma}_v}{\partial t} - \nabla \cdot (\boldsymbol{\kappa} \nabla p) &= g \quad \text{in } \Omega \times \mathbb{T}, \\ p &= p_D \quad \text{on } \partial\Omega_p \times \mathbb{T}, \\ -\boldsymbol{\kappa} \nabla p \cdot \mathbf{n} &= q_D \quad \text{on } \partial\Omega_q \times \mathbb{T}, \\ p &= p_0 \quad \text{in } \Omega \text{ at } t = 0,\end{aligned}$$

where M is the Biot modulus, $\boldsymbol{\sigma}_v$ is the volumetric stress, K is bulk modulus, $\boldsymbol{\kappa}$ is the porous media conductivity



Pic from: J.Choo. Stabilized mixed continuous/enriched Galerkin formulations for locally mass conservative poromechanics. CMAME. 2019.

Results

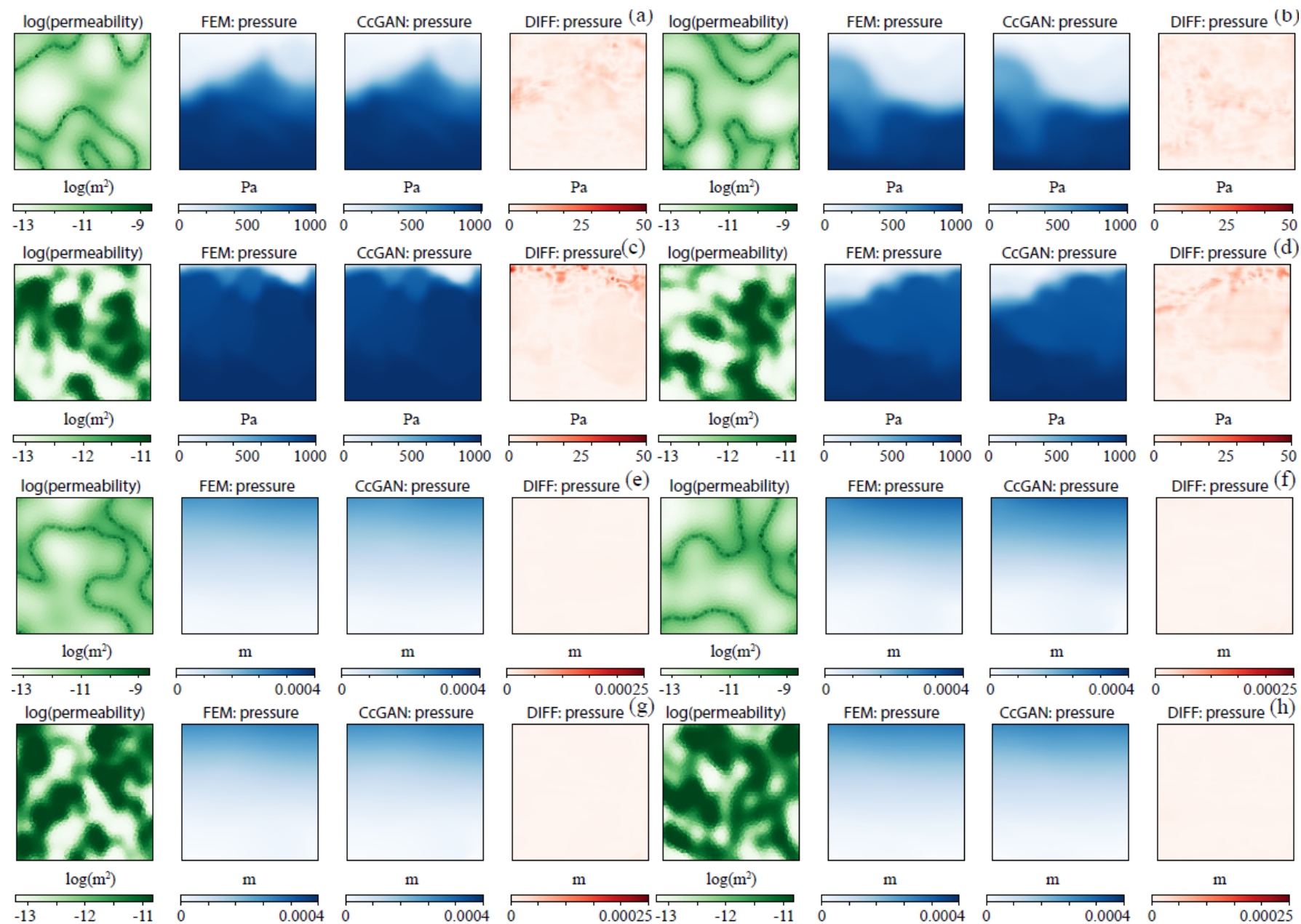


Table 1. The relative RMSE (Eq. (9)) results for testing data of three example cases as a function of the number of training data (M) for pressure and magnitude of displacement. Each example is evaluated with both NLI and ILI models.

Pressure	Example 1	M = 1250	M = 2500	M = 5000	M = 10000
	NLI (%)	4.63	3.24	2.34	1.74
	ILI (%)	4.55	3.15	2.30	1.67
	Example 2	M = 1250	M = 2500	M = 5000	M = 10000
	NLI (%)	3.60	2.61	1.83	1.24
	ILI (%)	3.73	2.55	1.67	1.22
	Example 3	M = 2500	M = 5000	M = 10000	M = 20000
	NLI (%)	3.36	2.31	1.65	1.32
	ILI (%)	3.07	2.24	1.63	1.29
Displacement	Example 1	M = 1250	M = 2500	M = 5000	M = 10000
	NLI (%)	4.32	2.98	2.14	1.57
	ILI (%)	4.13	2.78	2.03	1.33
	Example 2	M = 1250	M = 2500	M = 5000	M = 10000
	NLI (%)	3.60	2.51	1.47	1.10
	ILI (%)	3.37	2.07	1.26	0.83
	Example 3	M = 2500	M = 5000	M = 10000	M = 20000
	NLI (%)	3.28	2.28	1.27	1.27
	ILI (%)	2.74	2.15	1.18	1.05

Example 3: a total number of M is the sum of training data from both Examples 1 and 2.

x_i and \hat{x}_i are the ground truth (FOM result) and approximated values (ROM result)

$$\text{relative RMSE} = \frac{\sqrt{\frac{\sum_{t=1}^M (x_t - \hat{x}_t)^2}{M}}}{\sqrt{\frac{\sum_{t=1}^M x_t^2}{M}}}$$

Table S4. Comparison of the wall time (seconds) used for each operation presented in Figure 1 (main text). μ is a set of parameterize spatial fields, and $\mu_i \in \mu$.

	NLI	ILI	remark
Build FOM snapshots	40	40	per μ_i for $N^t = 10$
Train ROM with $M = 1250$	12600	12600	approximately 3.75 hours
Train ROM with $M = 2500$	25200	25200	approximately 7.5 hours
Train ROM with $M = 5000$	50400	50400	approximately 15 hours
Train ROM with $M = 10000$	108000	108000	approximately 30 hours
Train ROM with $M = 20000$	216000	216000	approximately 60 hours
Prediction	0.001	0.001	per testing (l^n, μ_i)

FOM: 36 cores AMD Ryzen Threadripper 3970X
 ROM: a single Quadro RTX 6000,

Conclusions



1. High dimensional parameterization – the whole heterogeneous field.
2. Reduced order model that could provide much faster calculation and maintain reasonable accuracy.
3. ILI provides a better accuracy than NLI without additional computational cost.
4. Including physics-information (PDEs) is in progress.