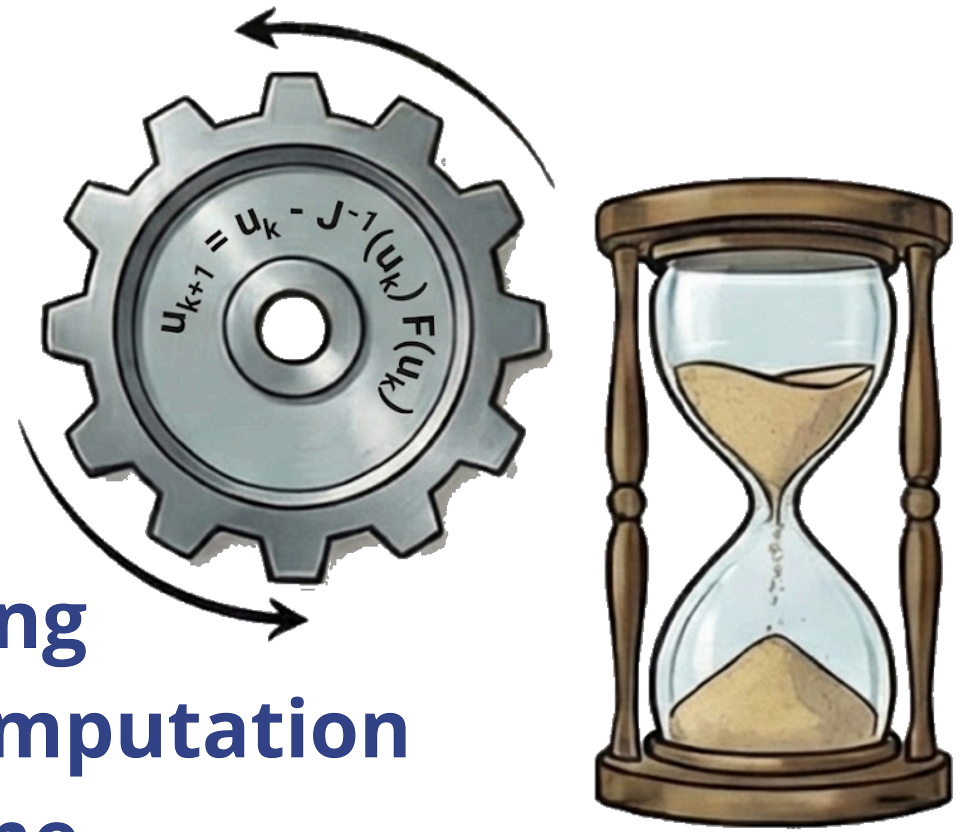
How to accelerate the convergence of nonlinear solvers?

Rémy Vallot - Lightning talk

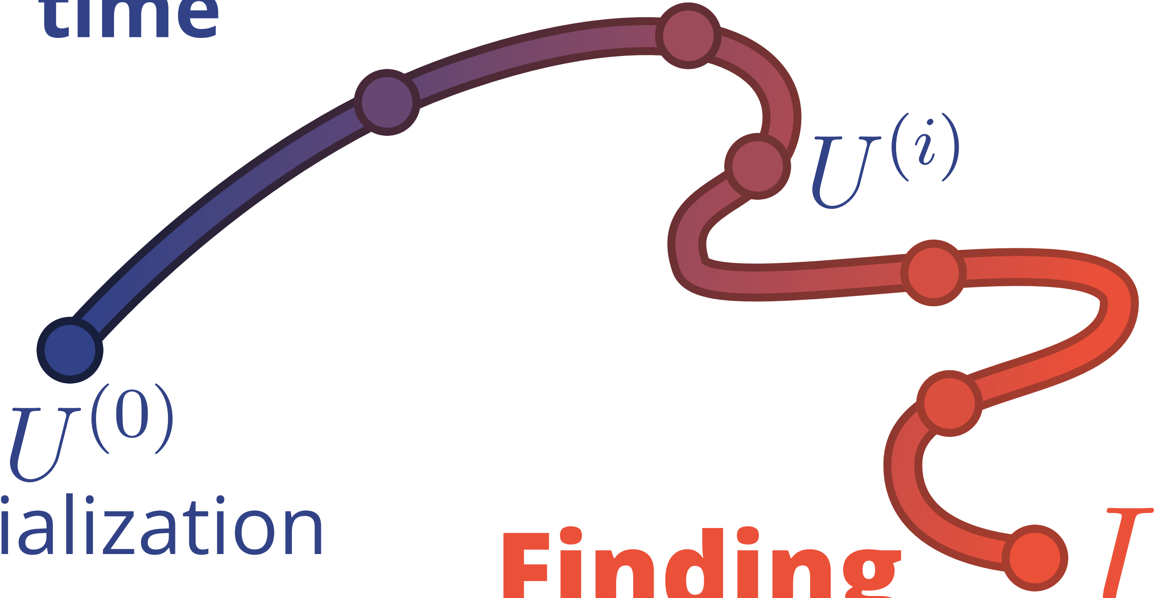
Application of Digital Twins to Large-Scale Complex Systems,
IMSI, Chicago, December 1 — 5, 2025

How to accelerate the convergence of nonlinear solvers?

Traditional solvers



Long computation time



$U^{(i)}$

$U^{(0)}$
initialization

Finding $U^\star$ **such that** $F(U^\star, \lambda) = 0$

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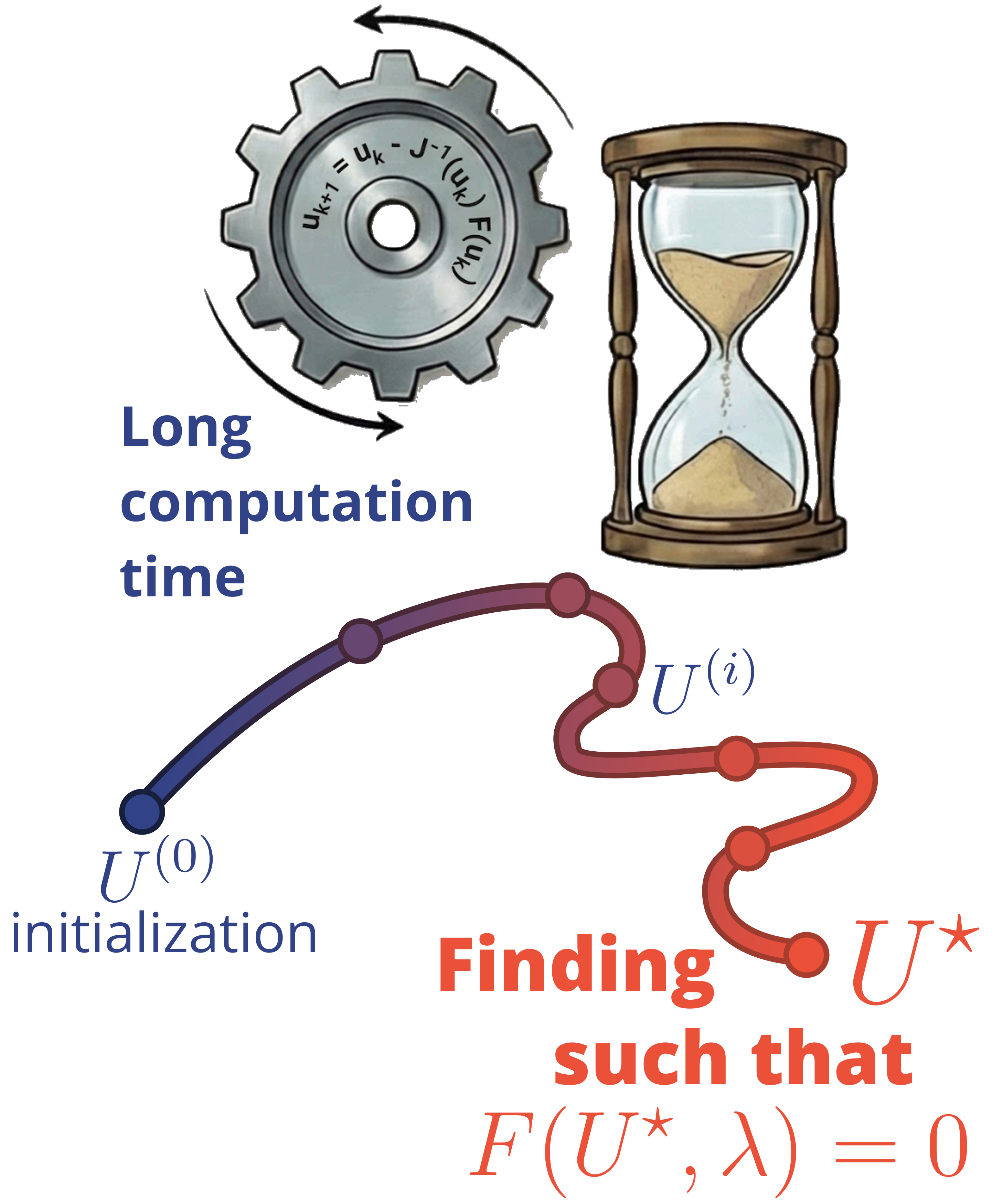
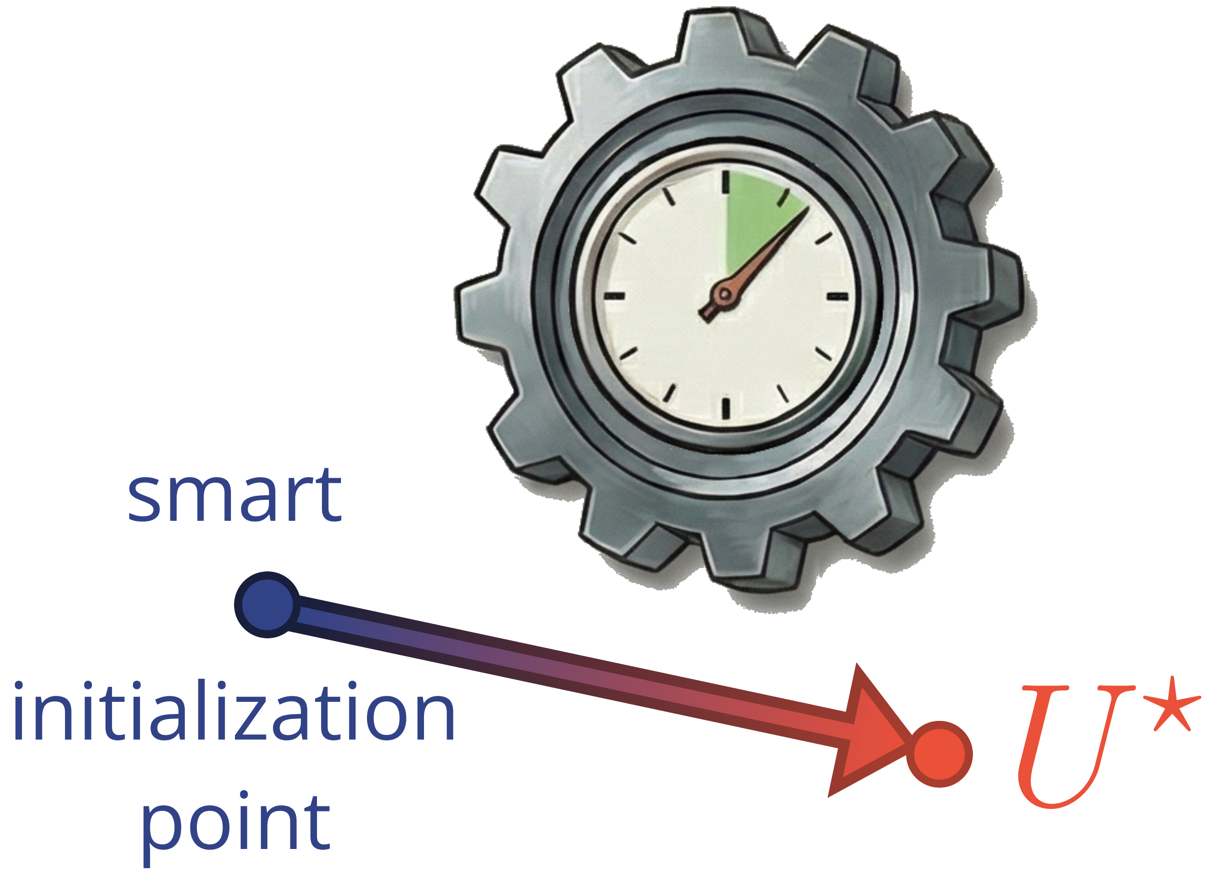
Traditional solvers



Initialization strategy



Applied methods

- Nearest solution in train set
- Proper Orthogonal Decomposition
- Neural Network
- DeepONet

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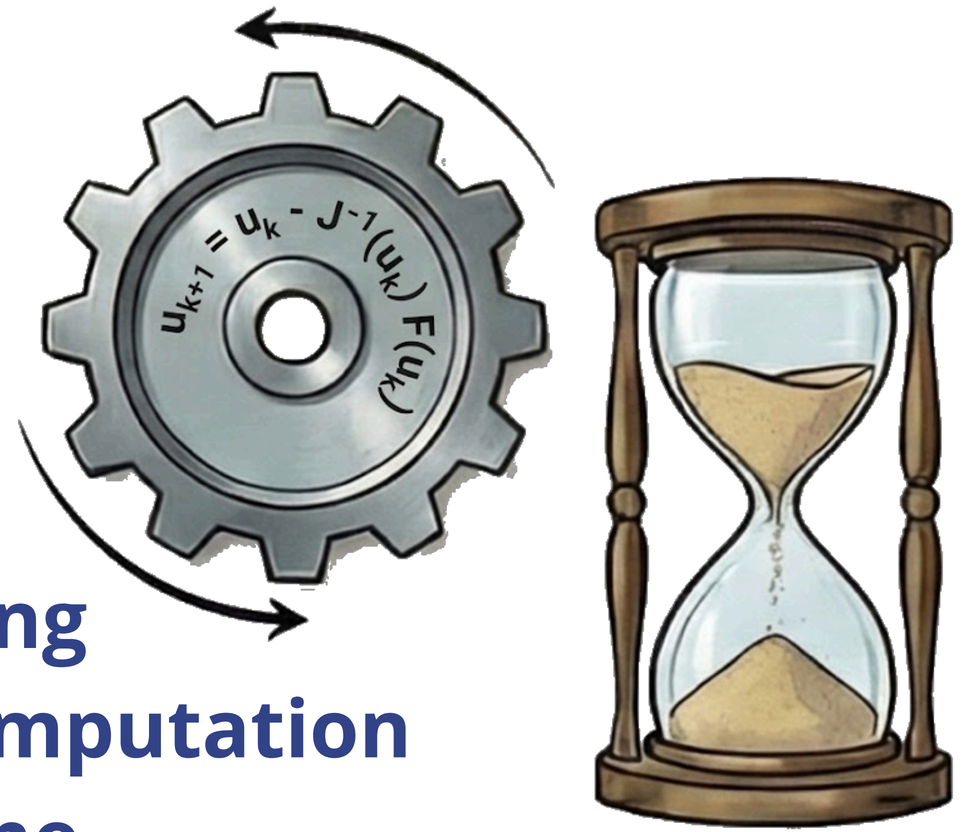
Traditional solvers



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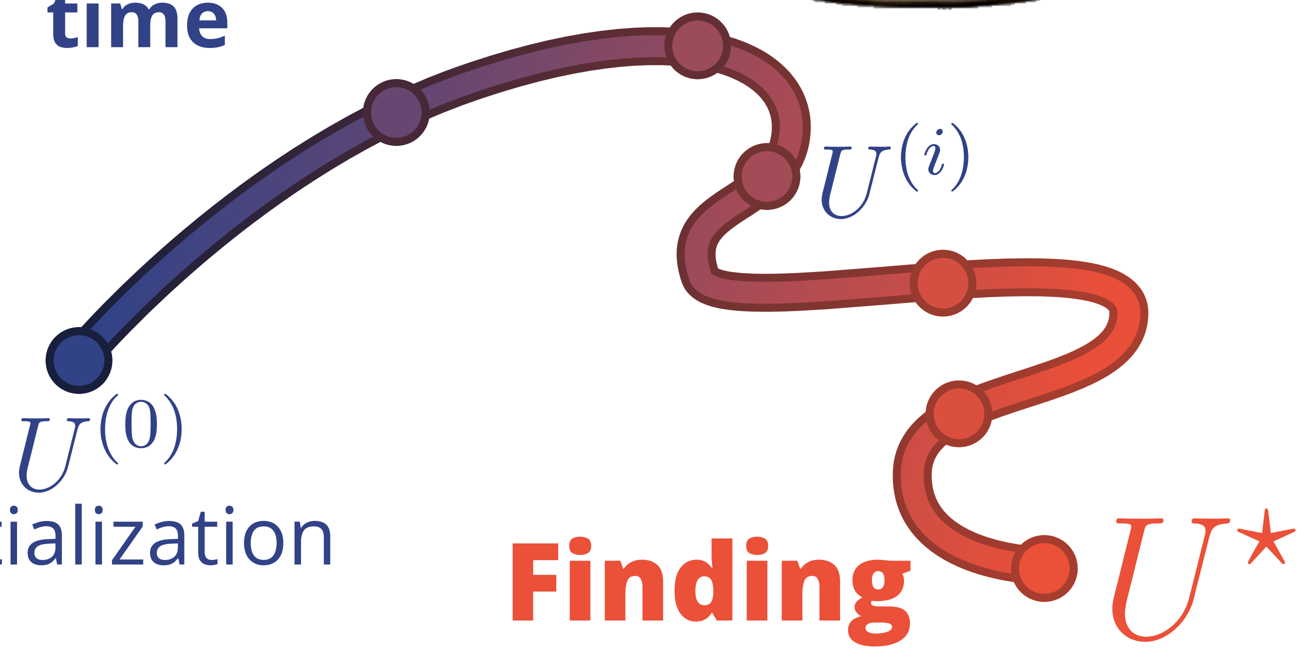
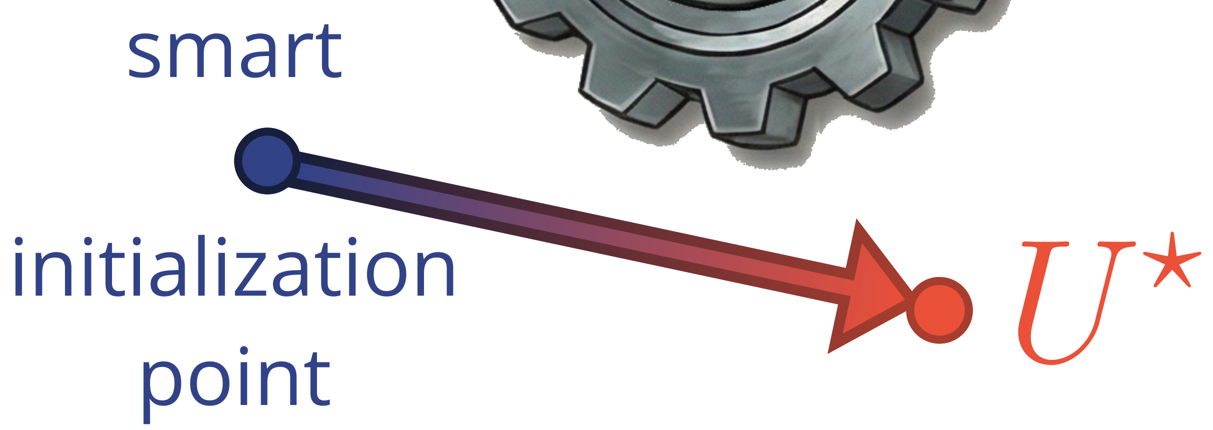


Finding $U^{\star}$ such that

$$F(U^{\star}, \lambda) = 0$$

Initialization strategy



Applied methods

- **Nearest solution in train set**
- **Proper Orthogonal Decomposition**
- **Neural Network**
- **DeepONet**

Use cases:

1D Nonlinear Poisson equation

$$\begin{cases} -\frac{\partial}{\partial x}\left[q(u)\frac{\partial}{\partial x}u\right] = g(x,\lambda) & \text{in } \Omega \\ u = u_D & \text{on } \partial\Omega \end{cases}.$$

Calendering process

Rubber process manufacturing : compress material between two counter-rotating rolls.

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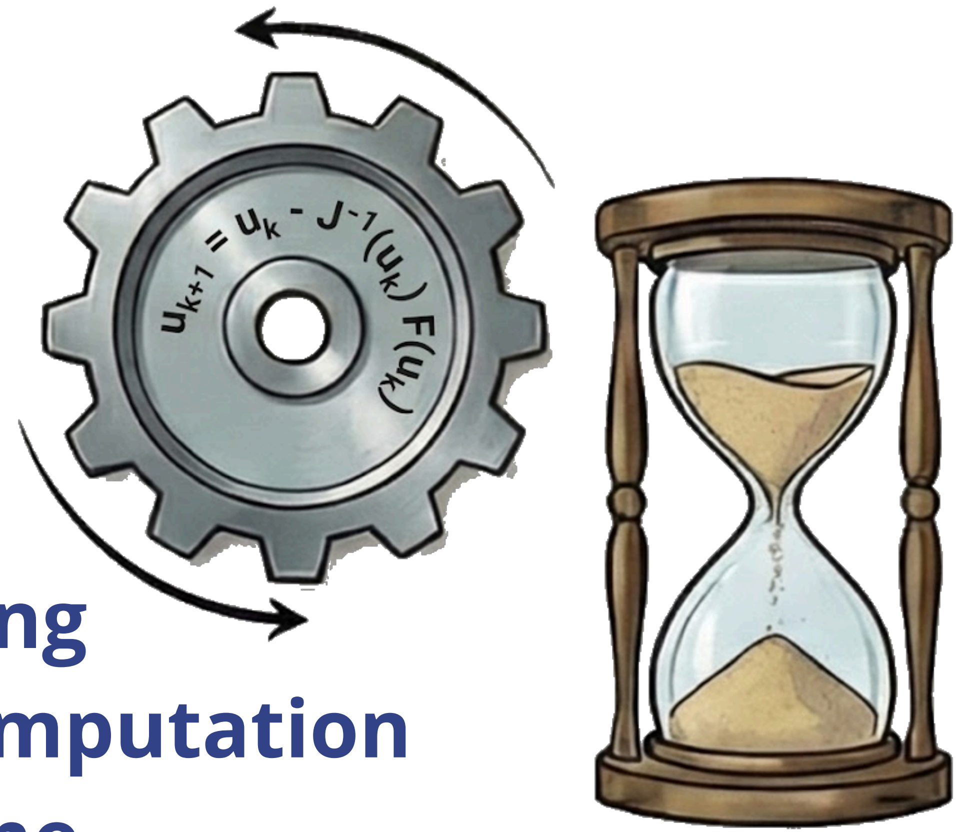
Traditional solvers



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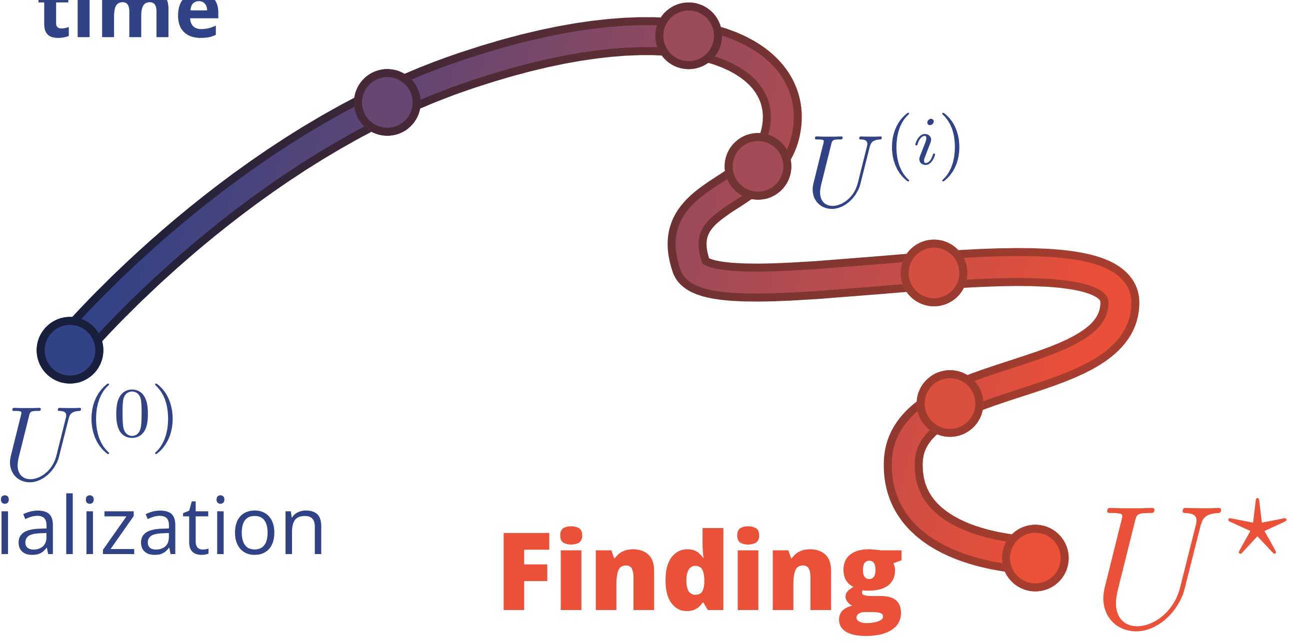
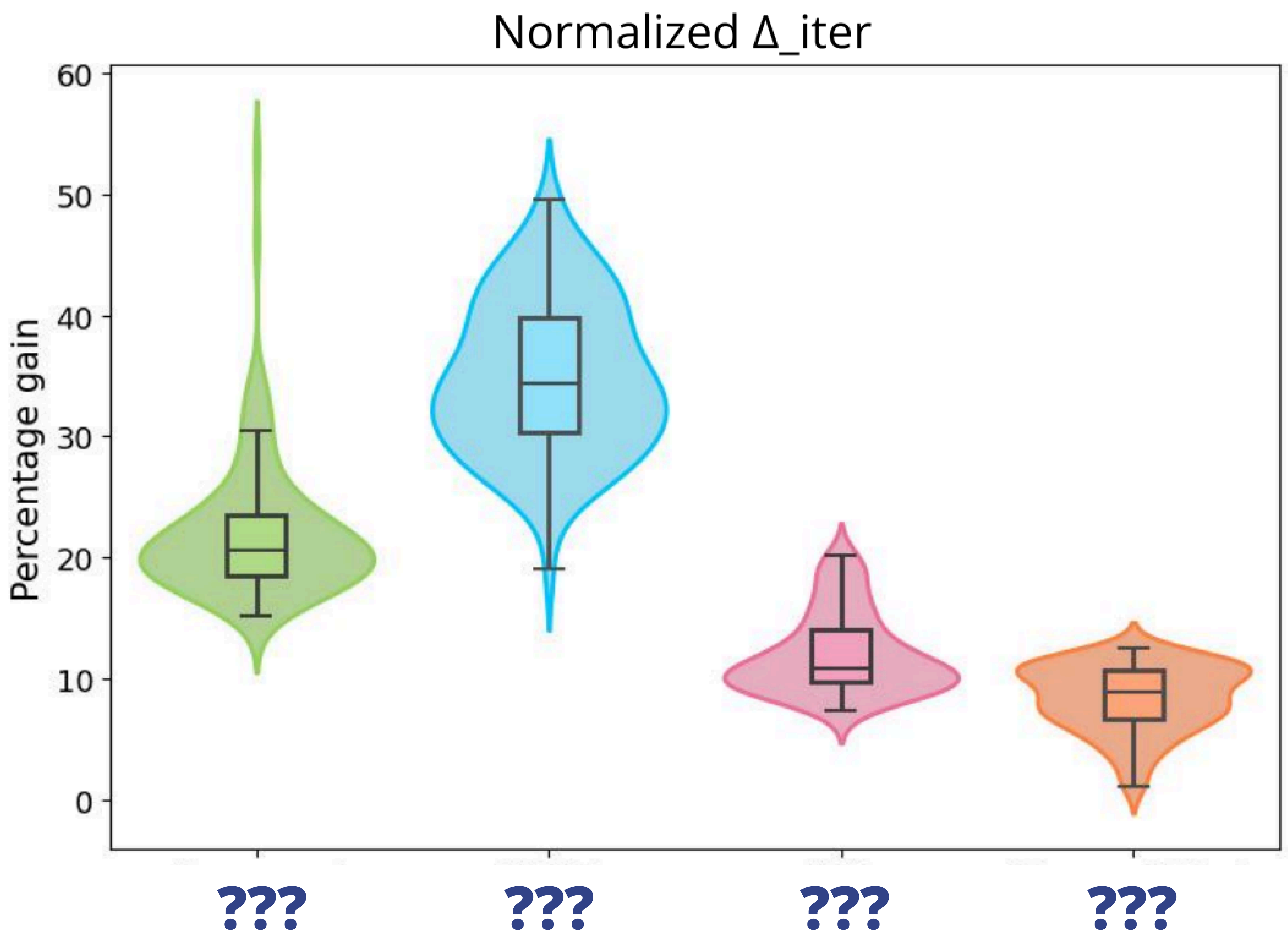


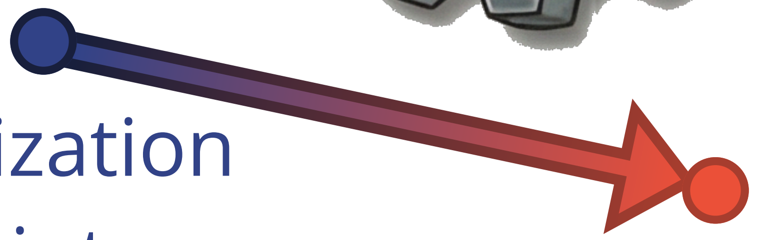
$U^{(0)}$ initialization

Finding $U^{\star}$ such that

$$F(U^{\star}, \lambda) = 0$$



Initialization strategy



smart initialization point $U^{\star}$

Applied methods

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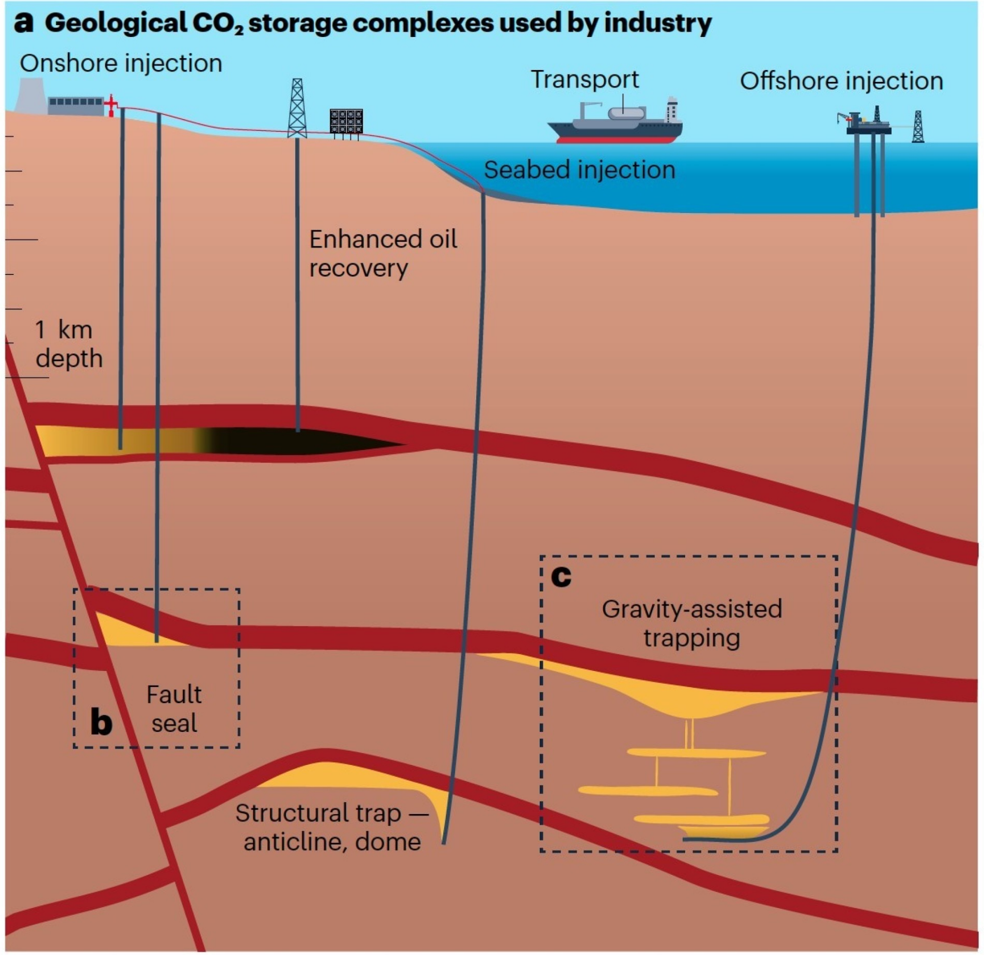
Calendering process

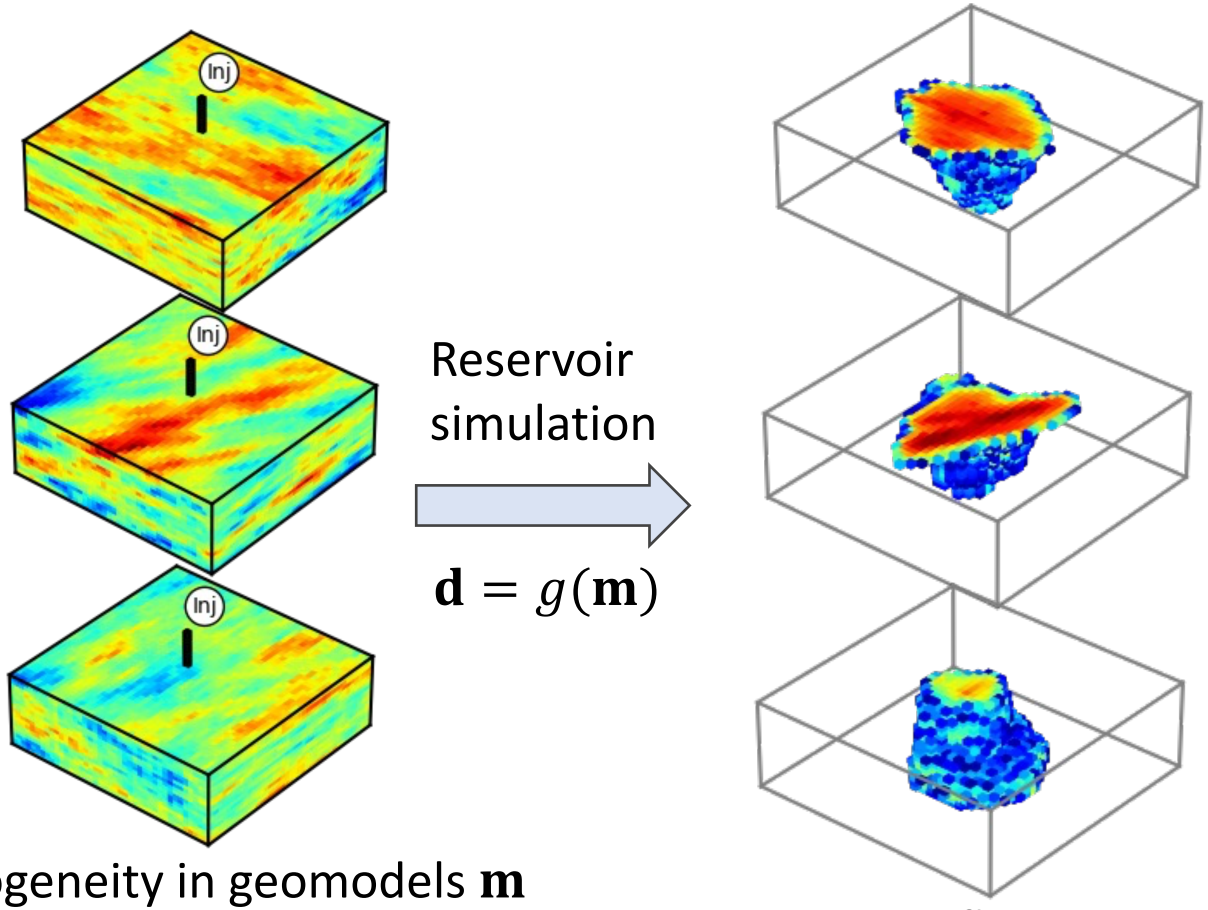
Rubber process manufacturing : compress material between two counter-rotating rolls.

Latent Score-based Diffusion Model for Data Assimilation in Geological Carbon Storage

Su Jiang (sujiang@andrew.cmu.edu), Carnegie Mellon University



(Krevor et al., 2023)

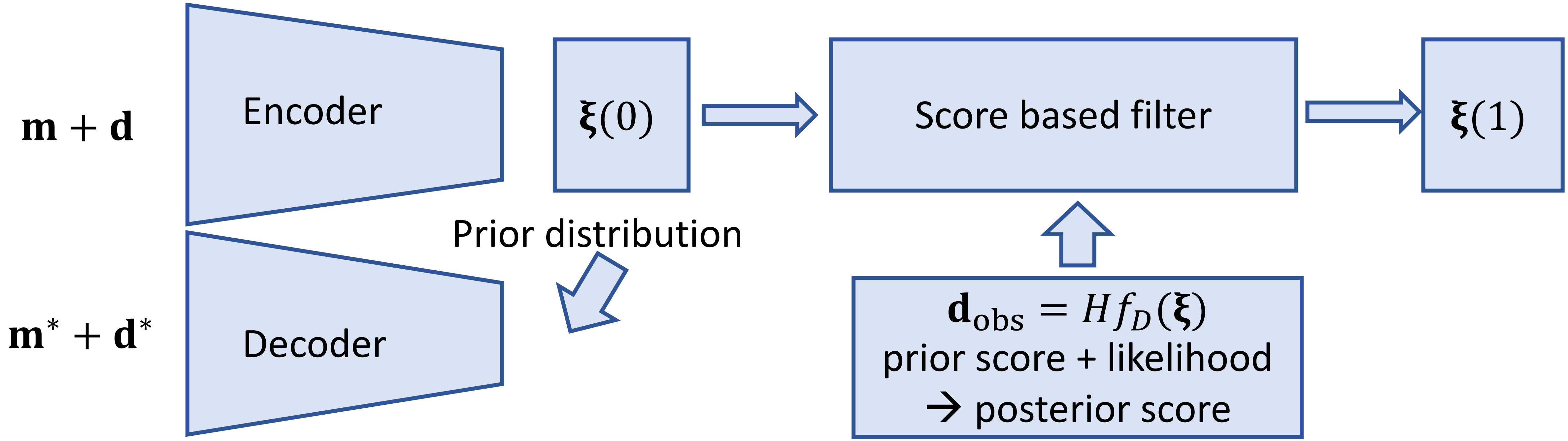


Heterogeneity in geomodels $\mathbf{m}$ (e.g., permeability)

Uncertainty in flow responses $\mathbf{d}$ (e.g., CO_2 plumes)

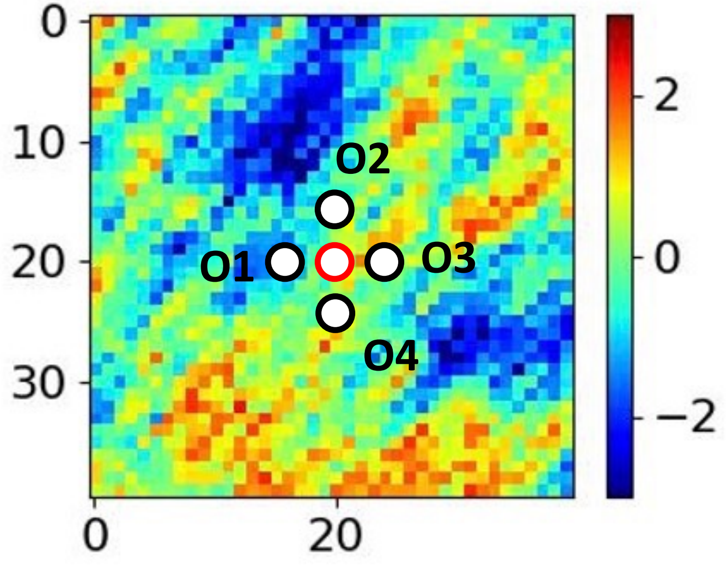
Latent Ensemble Scored-based Filter for Joint Inversion

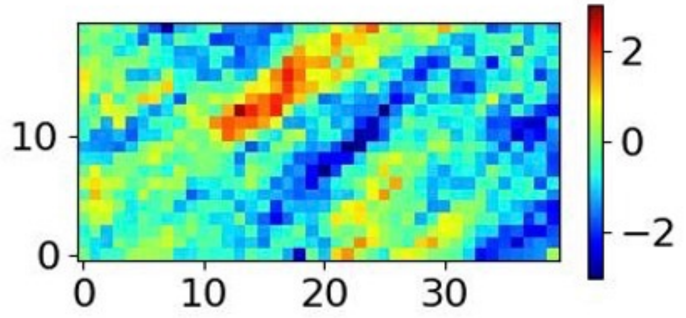
Goal: Develop latent score-based diffusion model for joint inference of model parameters and dynamic state variables



- Forward SDE: $d\boldsymbol{\xi}(t) = b(t)\boldsymbol{\xi}(t)dt + \sigma(t)d\mathbf{W}(t)$
- Reverse SDE: $d\boldsymbol{\xi}(t) = \left[b(t)\boldsymbol{\xi}(t) - \sigma^2(t)\nabla_\xi \log p\big(\boldsymbol{\xi}(t)\big)\right]dt + \sigma(t)d\mathbf{W}(t)$
- Posterior score function: $S(\boldsymbol{\xi}(t), t|\mathbf{d}_{\text{obs}}) = S(\boldsymbol{\xi}(t), t) + \nabla_\xi \log p(\mathbf{d}_{\text{obs}}|\boldsymbol{\xi}(t))$

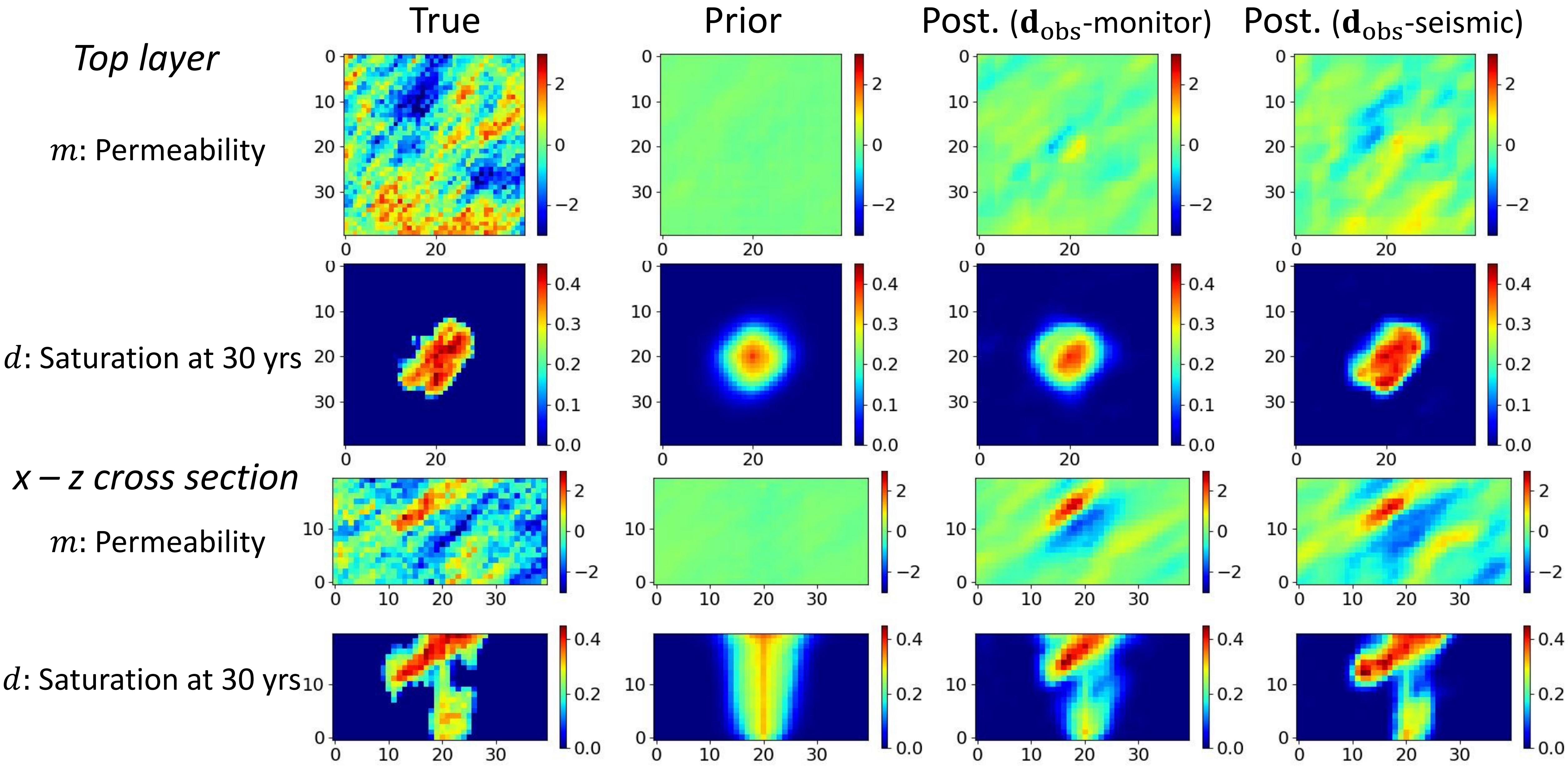
Test Case Setup: 3D Gaussian Geomodel



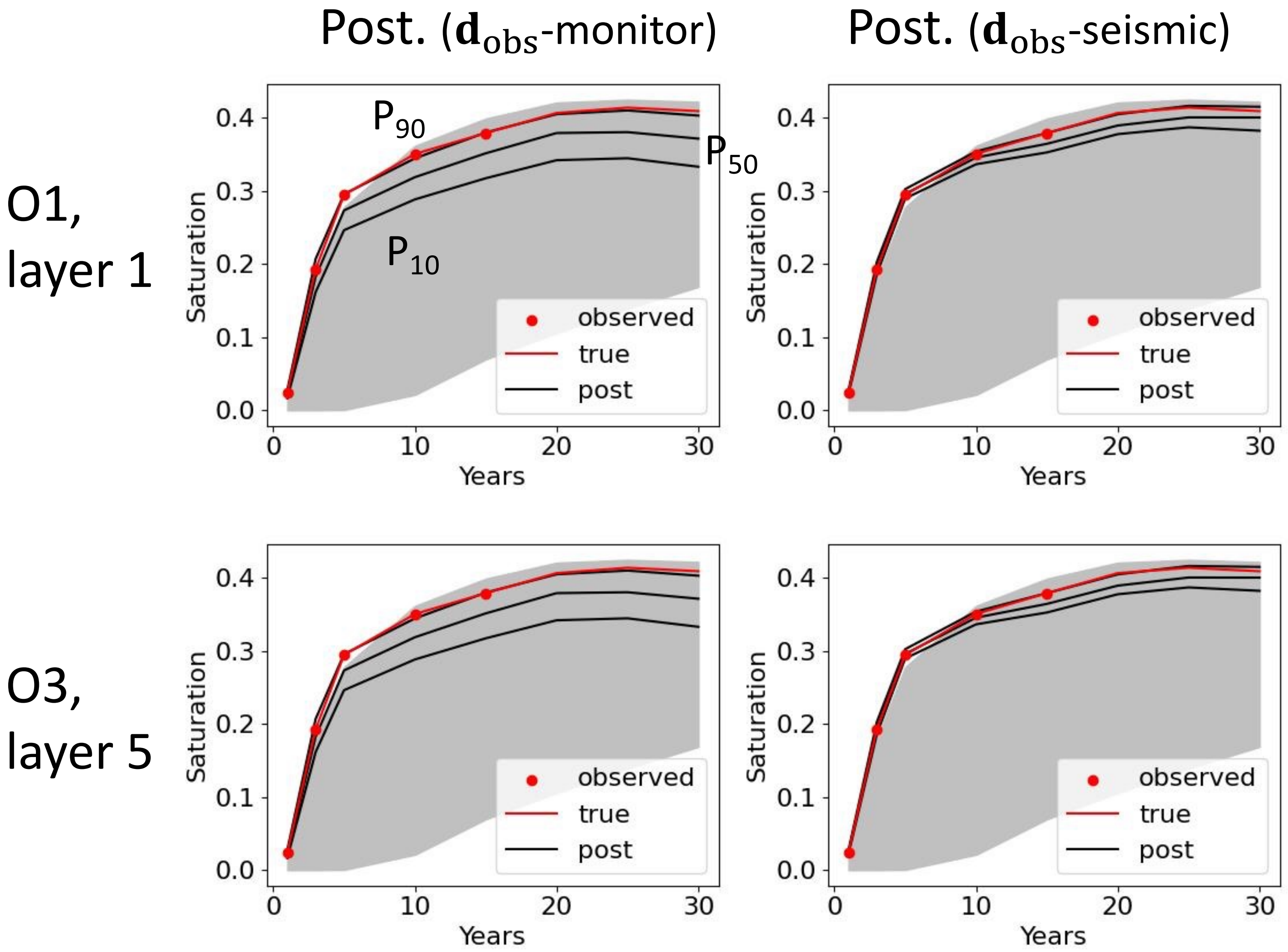


- Storage aquifer: 12 km x 12 km x 100 m, 40 x 40 x 20
- 1 vertical well, 2 Mt CO_2/year total for 30 years
- 2000 realizations to train
- Observations
  - 4 monitors from years 1, 3, 5, 10, 15
  - Saturation map (ideally 4D seismic) from years 1, 3, 5, 10, 15

Posterior Results (m and d, Mean Value)



Posterior Results and Summary



- Developed latent ensemble score-based filter to jointly update geological models and predict the flow dynamics
- Applied the data assimilation method to a 3D heterogenous case and achieved significant uncertainty reduction
- Extend this method to more realistic cases, coupled systems

Tire grip potential estimation under limited excitation conditions.

iMSi Workshop *Application of Digital Twins to Large-Scale Complex Systems* - Chicago

December 3, 2025

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Digital twin of a tire

Figure: Digital twin of a tire throughout its vehicle lifecycle

A tire is a complex physical system ...

multi-physics **(material, mechanical, thermal);**
diversity **of (size, rubber, usage...);**
operating conditions **(load, pressure, temperature, road conditions...);**
limited number of sensors **(or none) on the tire itself.**

... with multiple time scales to consider during its lifecycle ...

short-term **(road conditions, temperature, pressure, load...);**
long-term **(wear, aging...).**

... and making informed decisions can optimize its performances.

predictive maintenance **(pressure, wear, damage);**
optimize vehicle performance **(fuel consumption, ADAS...);**
inform the driver.

Context and motivations - Tire-road friciton

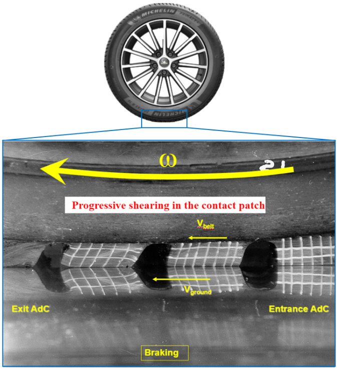

Figure: Tire longitudinal slip: Slippage & Shear phases during braking

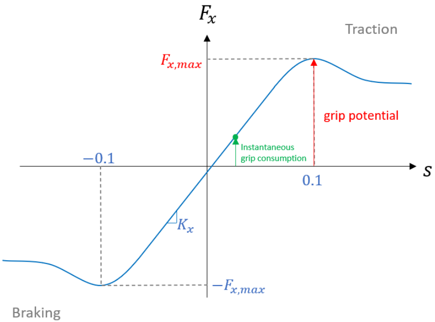

Figure: Tire longitudinal characteristic

$$s_x = \frac{R_e\omega - v_x}{v_x} \quad (1)$$

$$\mu = \frac{F_x}{F_z}. \quad (2)$$

The force generated depends on the tire slip $\rightarrow F_x = f(s_x, \cdots)$.

Context and motivations - Available grip potential

...road surface, water, ice, tire wear, tire pressure, tire temperature...

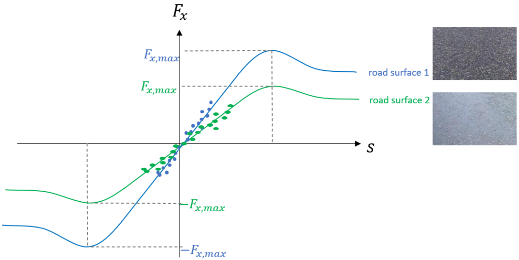

Figure: Grip potential changes detection with a slip-slope approach (Gustafsson 1997; Mussot 2022)

Problem formulation

Problem formulation

$\underbrace{\textbf{Estimate tire grip potential online,}}_{\text{only signals from the vehicle's CAN bus}}$ $\underbrace{\textbf{under standard driving conditions}}_{\text{straight line trajectory } + \mu(t) = F_x/F_z \leq 0.5}$ **and for** $\underbrace{\textbf{any vehicle}}_{\text{no prior knwoledge on the tire}}$**, in order to** $\underbrace{\textbf{improve the vehicle dynamics control}}_{\text{to be defined a bit later}}$**.**

Possible applications:

- Inform the driver in real-time about the road and/or tire conditions.
- Improve the vehicle chassis control with tire grip potential informed control strategies (such as shortening braking distance).

Efficient Adaptation of GNNs to Simulate Deformable Materials Across Parametric Families of Constitutive Models

Hassan Iqbal

Joint work with Naveen Manoharan and Krishna Kumar
The University of Texas at Austin

Manoharan, Naveen Raj, Hassan Iqbal, and Krishna Kumar. "Parameter-Efficient Conditioning for Material Generalization in Graph-Based Simulators." *arXiv preprint arXiv:2511.05456* (2025).

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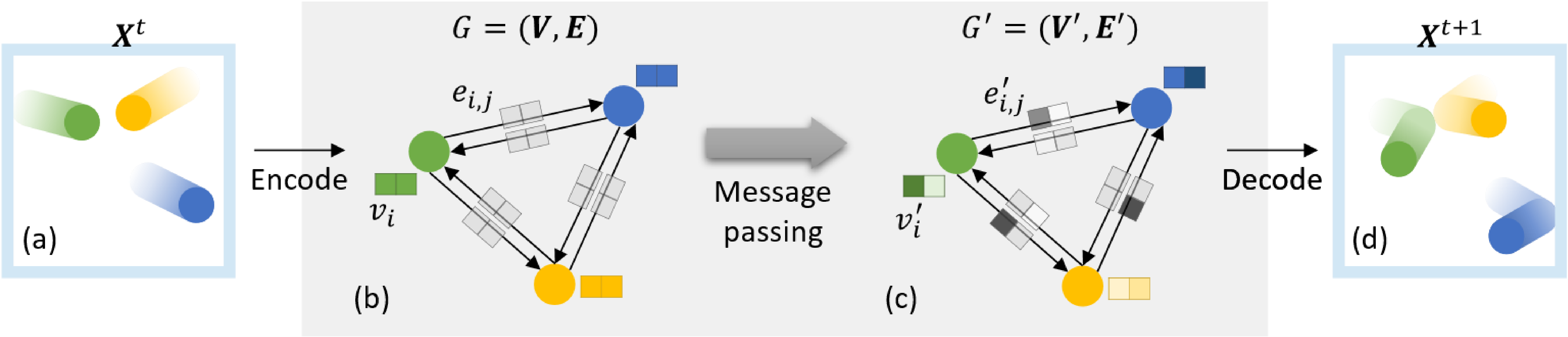
Graph neural network-based simulator (GNS)



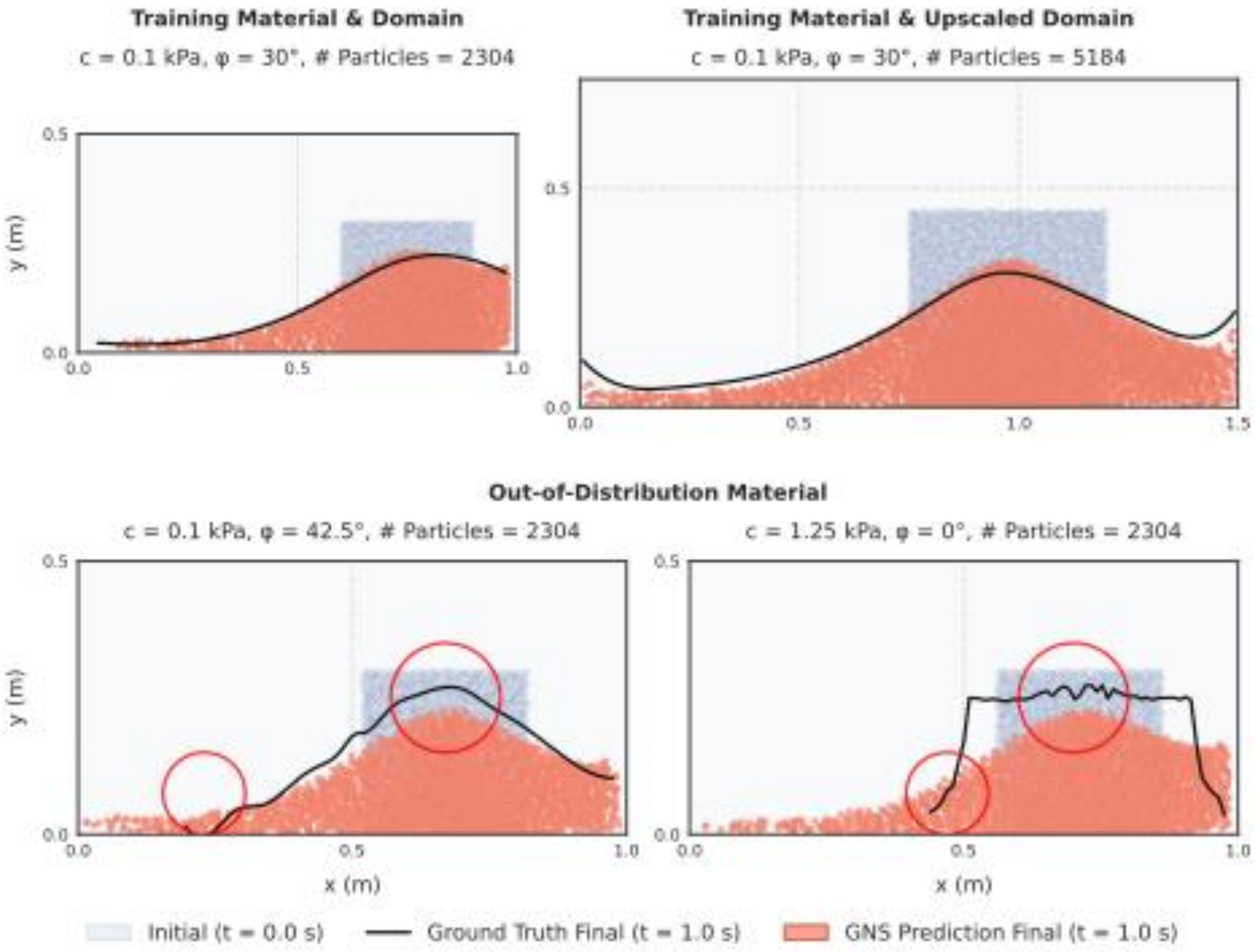
$$v_i^{(l)} = f_\theta^{(l)}\left(v_i^{(l-1)}, \bigoplus_{j \in N(i)} g_\theta^{(l)}\left(v_j^{(l-1)}, v_i^{(l-1)}, e_{i,j}^{(l-1)}\right)\right)$$

$$e_{i,j}^{(l)}(w, v) = g_\theta^{(l)}\left(v_j^{(l-1)}, v_i^{(l-1)}, e_{i,j}^{(l-1)}\right)$$

Limitations of GNS

“Most GNN applications in this domain often exclude material properties from their input tensors and have minimal material variations in their training dataset,” Zhao, Yingxue, et al. (2025).

Objective
Using granular flows as a running example, formulate a parameter-efficient conditioning mechanism that adapts GNS model to varying material parameters like internal friction and cohesion.



Manoharan, Naveen Raj, Hassan Iqbal, and Krishna Kumar. "Parameter-Efficient Conditioning for Material Generalization in Graph-Based Simulators." *arXiv preprint arXiv:2511.05456* (2025).

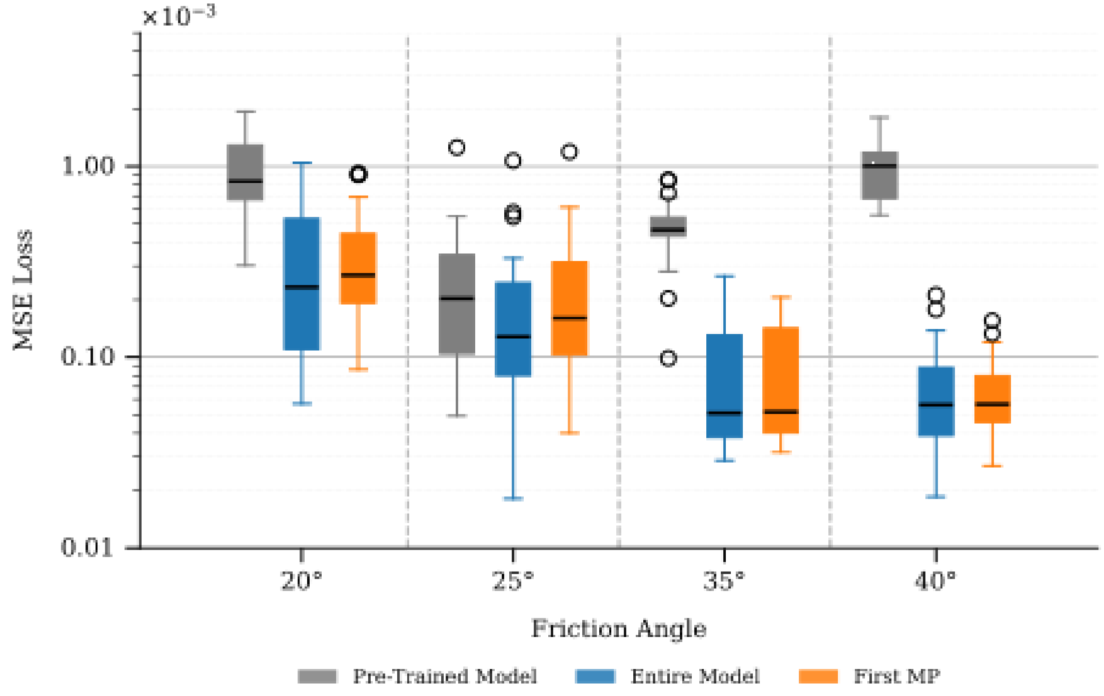
Identifying material-specific message-passing blocks

Mohr-Coulomb is the most commonly used constitutive model for soil. It acts locally, but global failures emerge from collective particle behavior.

$$F = R_{mc} q + p' \tan \phi - c$$

$$R_{mc}(\theta, \phi) = \frac{1}{\sqrt{3} \cos \phi} \sin\left(\theta + \frac{\pi}{3}\right) + \frac{1}{3} \cos\left(\theta + \frac{\pi}{3}\right) \tan \phi$$

where p' is the effective mean pressure, q is the magnitude of deviatoric stress, θ is the Lode's angle, ϕ is the effective friction angle, c is the effective cohesion.

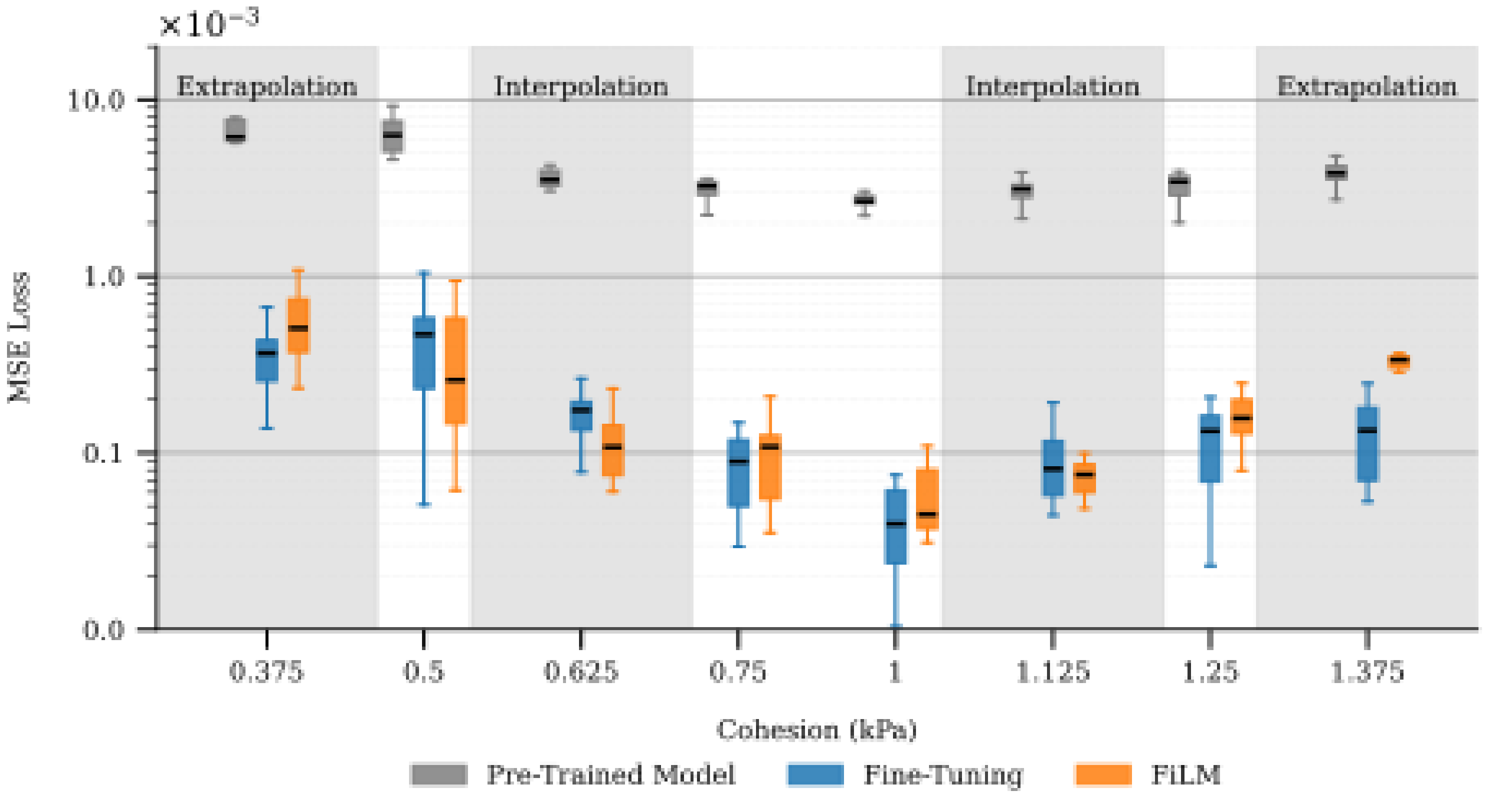


Feature-wise Linear Modulation (FiLM):

FiLM modifies the conditioned network using learned scale and shift parameters

$$\mathrm{FiLM}(\mathrm{h}\,|\gamma, \beta) = \gamma \odot h + \beta$$

where $\gamma, \beta \in R^d$ are computed from a small conditioning MLP.



Bayesian optimization of the cohesion parameter *c*