SCCS

PhD Consortium (Autumn) 2024

Bringing academia and
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GeoEnergy Group

HERIOT WATT UNIVERSITY

Leveraging AI for Uncertainty Quantification in Subsurface CO2 Leakage Risk Assessment

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ECO-AI project: Enabling CO_2 Capture and Storage using AI

(Grant Ref: EP/Y006143/1)

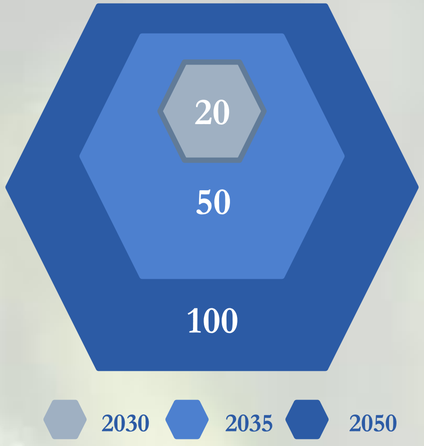
02/12/2024

Reliability in Subsurface CO2 Storage

Why does it matter ?

- Net-Zero goal by 2050: hundreds of Gt of CO_2 captured
- Extensive CCS deployment to meet the IPCC 1.5 °C target
- Storage capacity potential VS Leakage risk assessment

UK CCS goal (Mt/year)



Integrity & Relibability

- Geological Faults & Fracture damaged zones
- Mineral Reactivity & Geochemical concerns

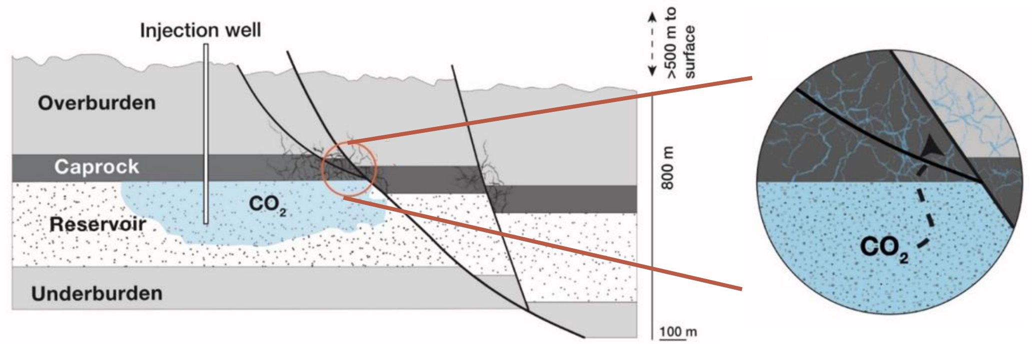
Lack of data

Multi-scale Uncertainties

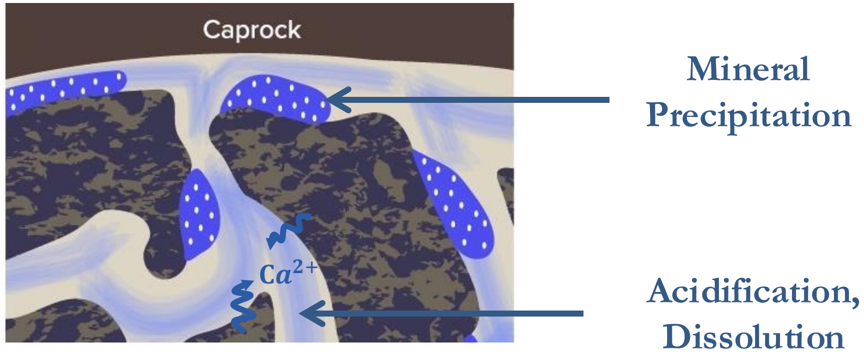
https://www.nstauthority.co.uk/the-move-to-net-zero/carbon-capture-and-storage/
https://www.nao.org.uk/wp-content/uploads/2024/07/carbon-capture-usage-and-storage-programme.pdf

Multi-scale Uncertainties in Leakage Risk

Reliability of subsurface CO2 storage models



Rizzo *et al.* (2024)



- Structural uncertainties
- Subseismic fractures & network distribution
- Hydraulic conductivities ? Empirical Laws

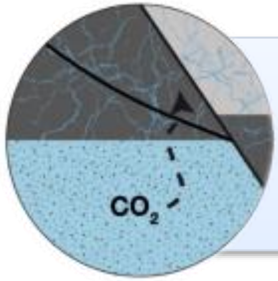
- Model Calibration:
  mineral reaction rates, kinetic factors
- Geological uncertainties:
  sub-resolved features, macro-properties ?

Data Uncertainty + Modeling Uncertainty

? Bridge the scales

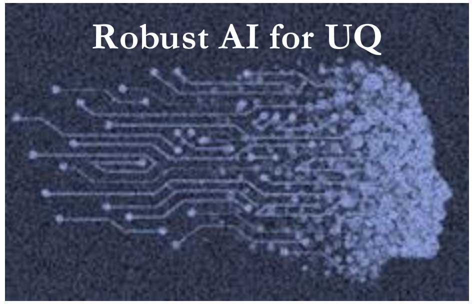
R. E. Rizzo, N. F. Inskip, H. Fazeli, P. Betlem, K. Bisdom, N. Kampman, et al. (2024), International Journal of Greenhouse Gas Control (https://doi.org/10.1016/j.ijggc.2024.104105)

AI-driven Uncertainty Quantification

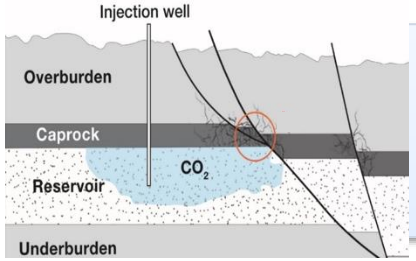


- Experimental Data
- Pore-scale Uncertainties
- Physical Models

1. Leverage local interactions

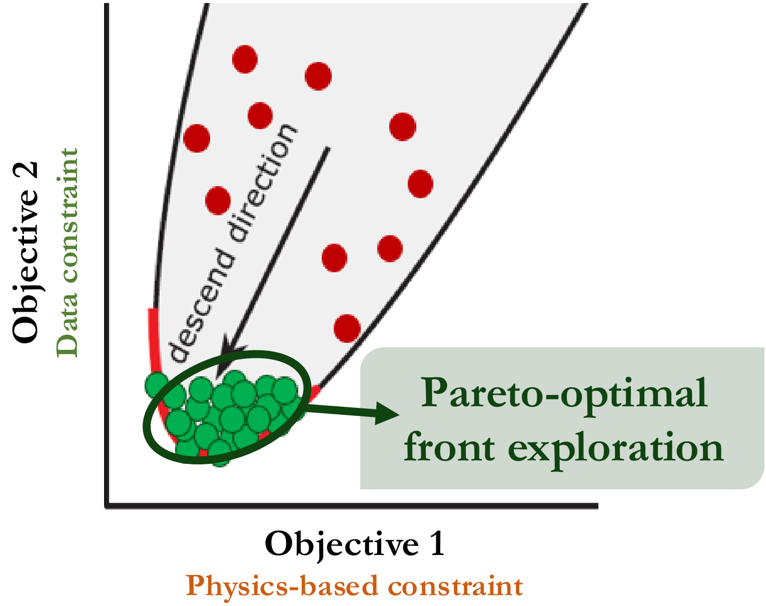


2. Bayesian Inference & Inverse Problems



- Upscaling & ML
- Macro-scale Uncertainties
- Model Calibration

3. Propagate the uncertainties

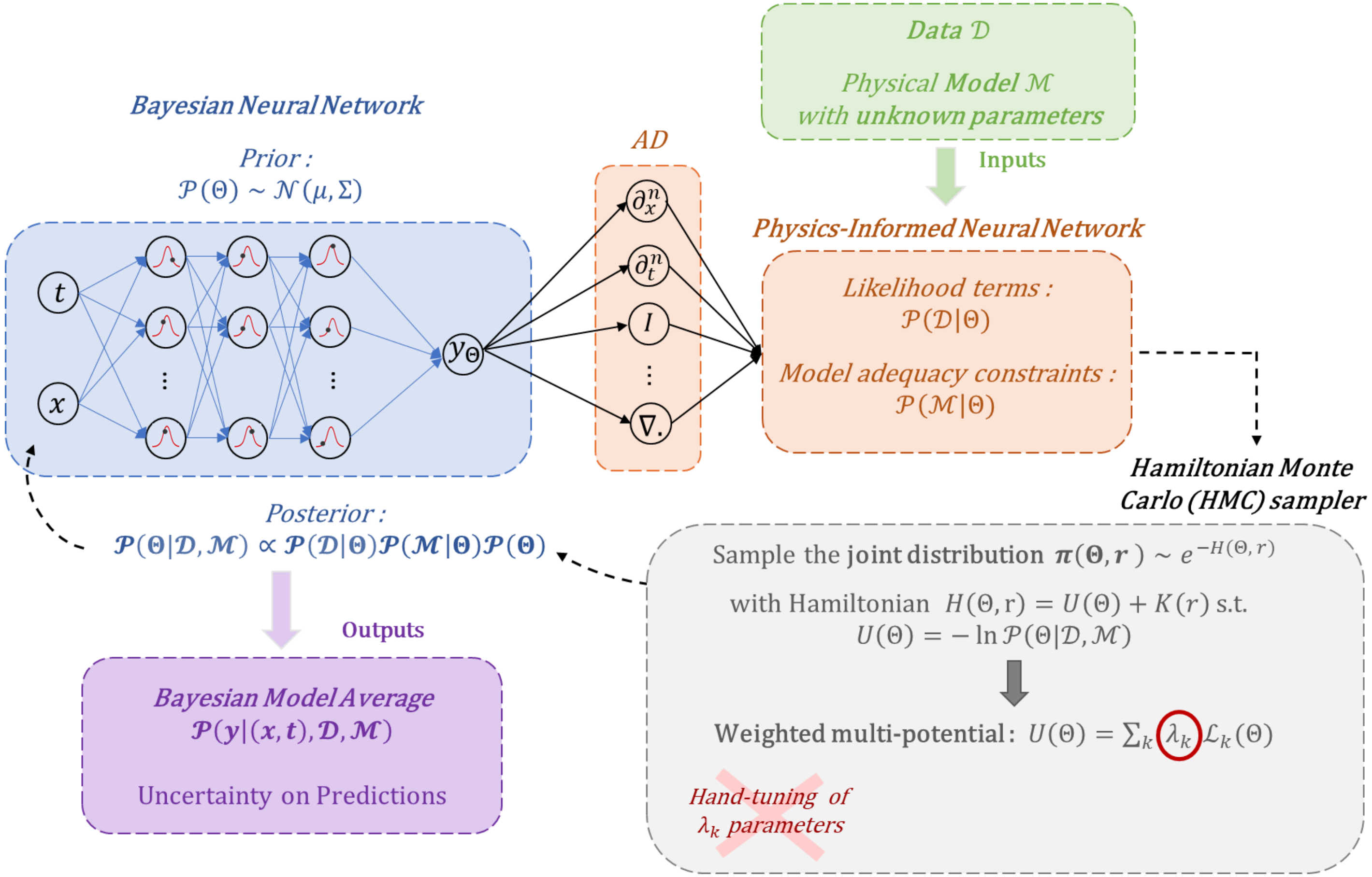


- Data & Modelling Uncertainties
- Data-driven & Physics-based
- Multi-scale & Multi-objective

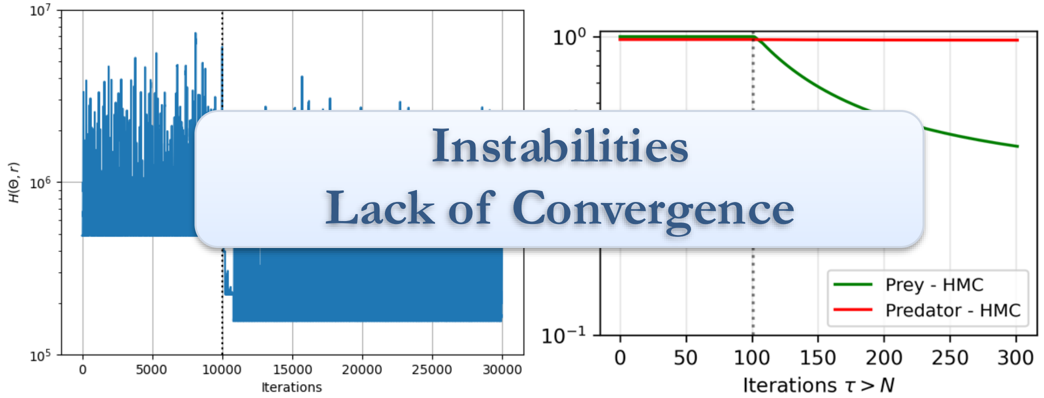
Balance the objectives

AI-driven Uncertainty Quantification

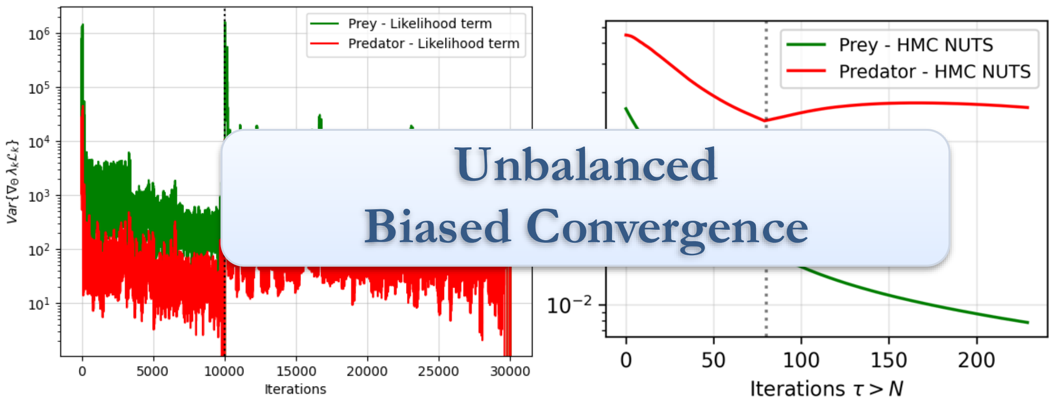
Robust Bayesian Physics-Informed Neural Networks



HMC with uniform λ_k



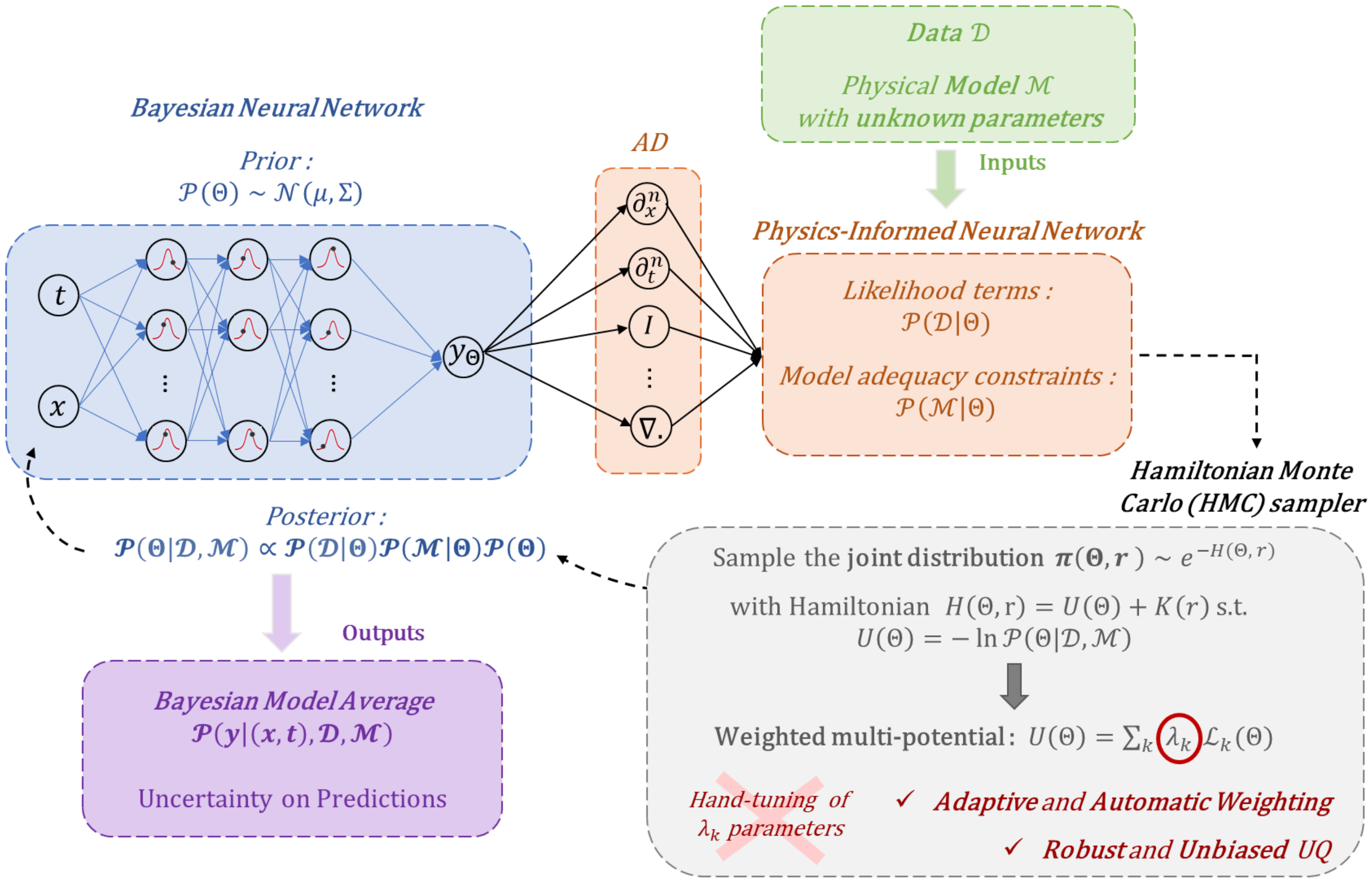
HMC NUTS with hand tuning



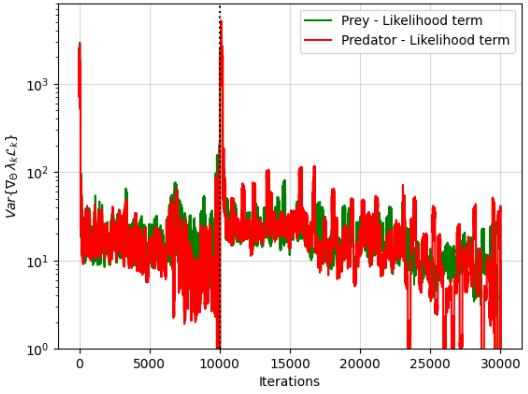
L. Yang, X. Meng, and G.E. Karniadakis (2021), Journal of Computational Physics (https://doi.org/10.1016/j.jcp.2020.109913)

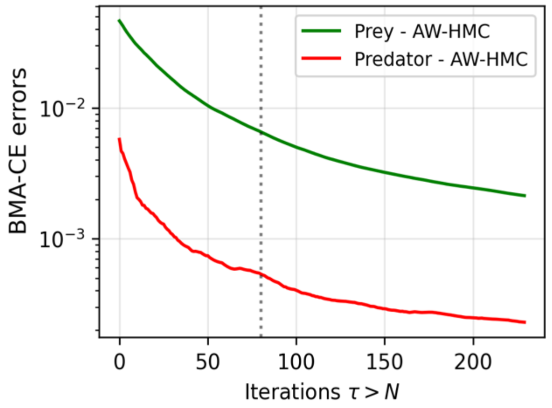
AI-driven Uncertainty Quantification

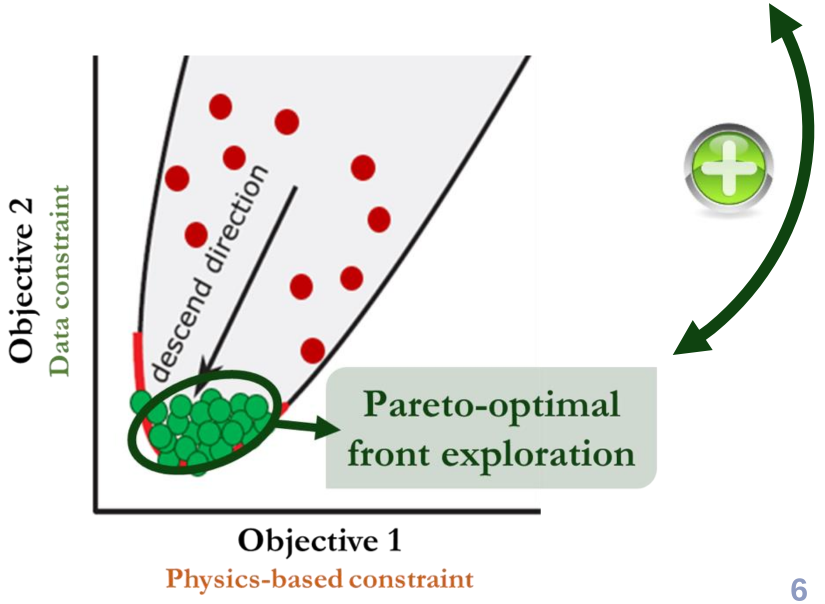
Robust Bayesian Physics-Informed Neural Networks



AW-HMC with $\lambda_k = \left(\frac{\min_i(Var\{\nabla_\Theta \mathcal{L}_i\})}{Var\{\nabla_\Theta \mathcal{L}_k\}}\right)^{1/2}$



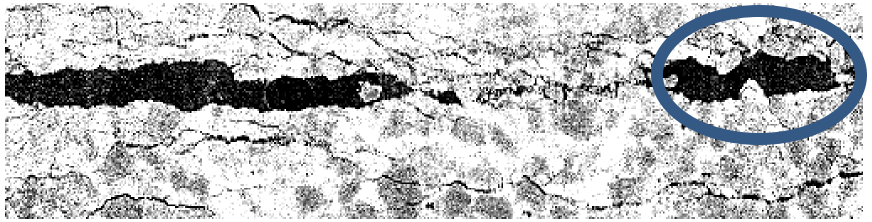


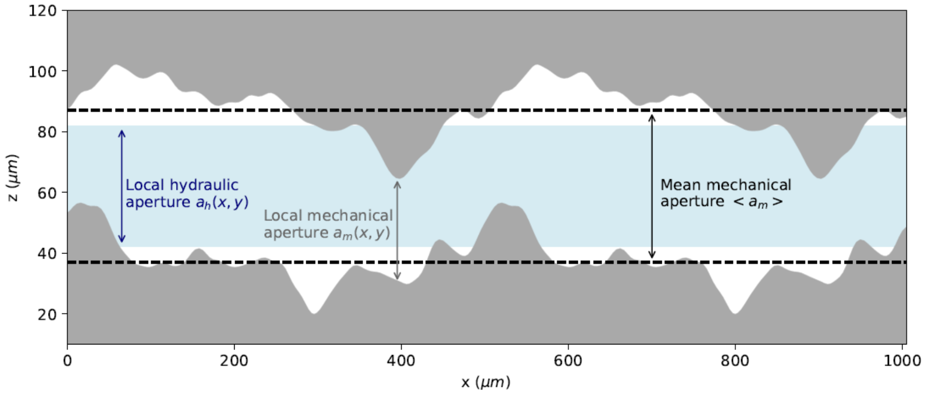


S. Perez, S. Maddu, I. F. Sbalzarini, P. Poncet (2023)
"Adaptive weighting of Bayesian physics informed neural networks for multitask and multiscale forward and inverse problems"
Journal of Computational Physics

Uncertainty on Fault-Related Leakage

Correct model misspecification on hydraulic conductivity





$$K_{CL} = \frac{< a_m >^2}{12}$$

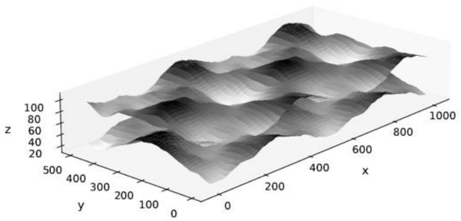
$$JRC \in [4.86, 10.31]$$

$$< a_m > \simeq 50\ \mu m$$

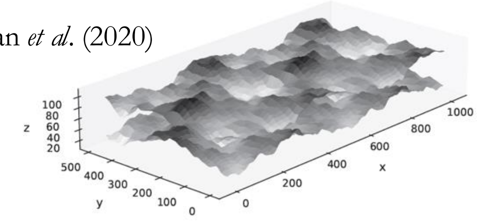
$$K_{CL} \simeq 208\ \mu m^2$$

$$K_D^{a_m} \simeq 201\ \mu m^2$$

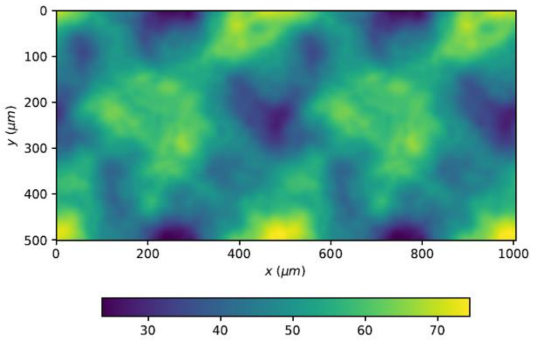
$$K_{CL}^{a_m}(x,y) = \frac{a_m(x,y)^2}{12} \xrightarrow{\text{2D Darcy flow-based upscaling}} K_D^{a_m}$$

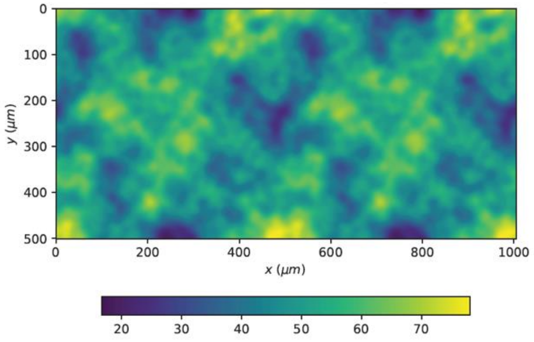


Guiltinan *et al.* (2020)



Mechanical aperture maps $a_m(x,y)$





$$K_{NS} = 195.98\ \mu m^2$$

$$K_{NS} = 174.31\ \mu m^2$$

No roughness effects & Overestimation of fracture conductivity

Cubic Law K_{CL} & Darcy Upscaling $K_D^{a_m}$ fail !

E. J. Guiltinan, J. E. Santos, M. B. Cardenas, D. N. Espinoza, Q. Kang (2020), Water Resources Research (https://www.digitalrocksportal.org/projects/314)

Uncertainty on Fault-Related Leakage

Correct model misspecification on hydraulic conductivity

Bayesian Inference Problem:

Infer latent hydraulic aperture field $a_h(x, y)$

such that $\boldsymbol{a_m(x,y) = a_h(x,y)} + \boxed{\xi_d}$ Data uncertainty

with $a_h(x, y) \leq a_m(x, y)$ and

$$\boldsymbol{K_{NS}} = \frac{\mathbf{1}}{|\boldsymbol{\Omega_f}^{\mathbf{2D}}|} \int_{\Omega_f^{2D}} \boldsymbol{K_{NN}^{a_h}(x,y)\, dx\, dy} + \boxed{\xi_m}$$

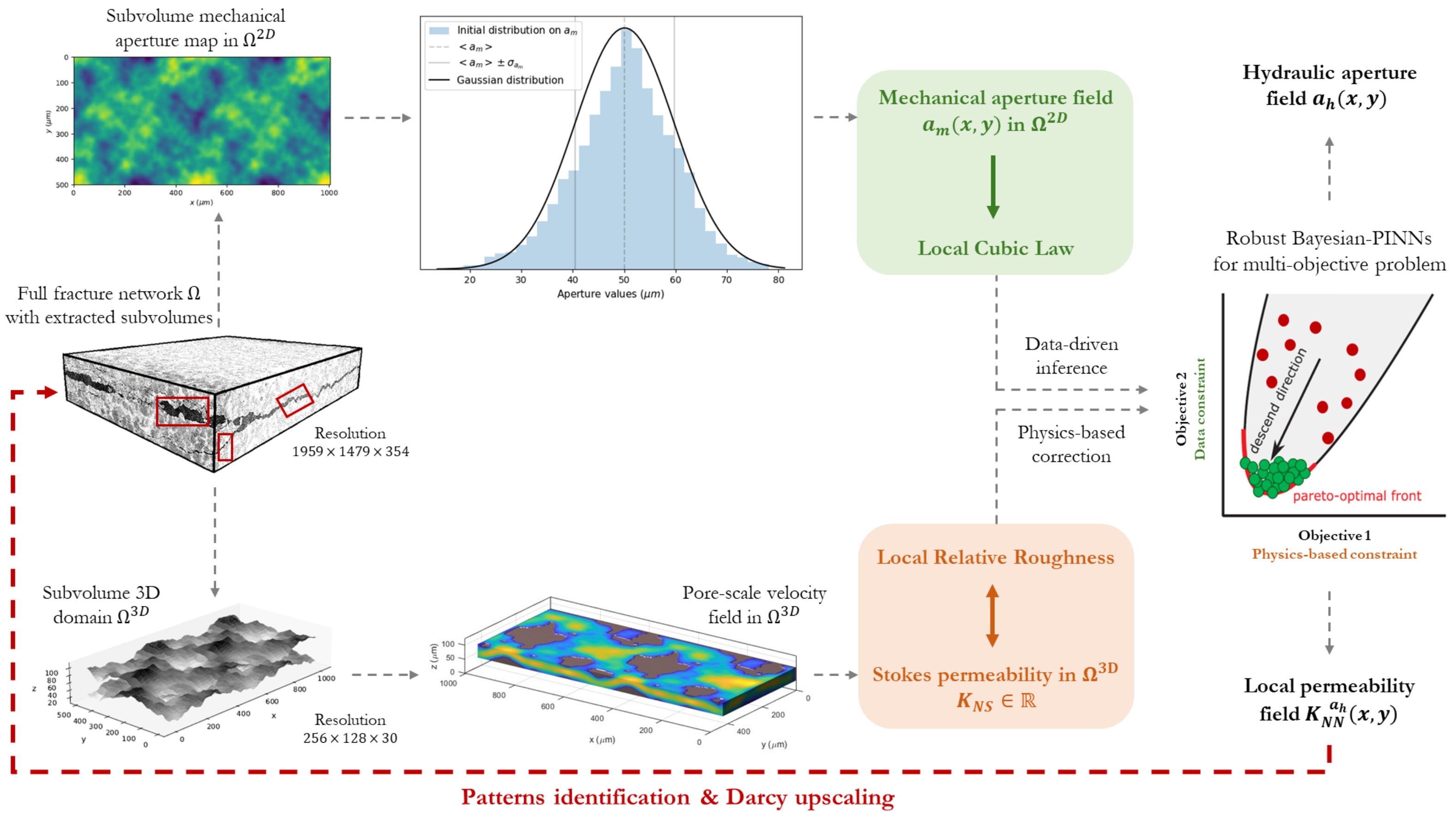
Model uncertainty

where $$K_{NN}^{a_h}(x, y) = \frac{a_h(x,y)^2}{12}\left(1 + \boldsymbol{\alpha}\, \frac{|\,a_h(x,y) - <a_m>|}{\sigma_{am}}\right)$$

Local Cubic Law

Local Relative roughness

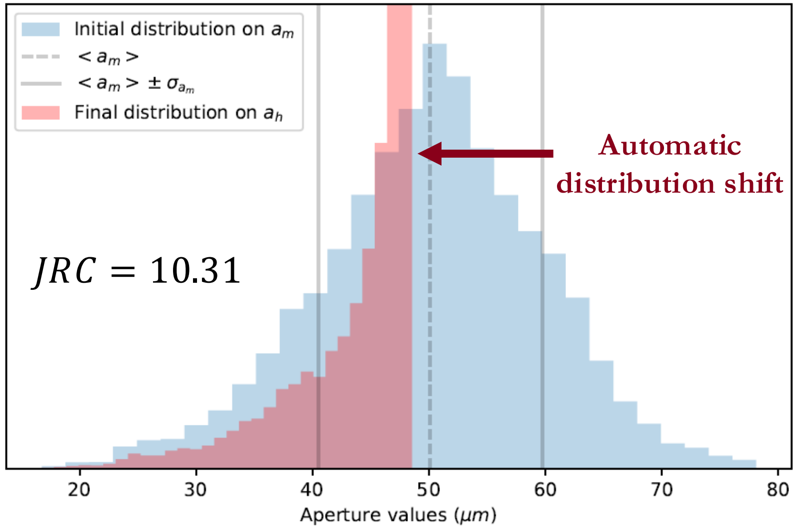
Workflow:



S. Perez, F. Doster, J. Maes, H. Menke, A. ElSheikh, A. Busch
Paper in Preparation

Uncertainty on Fault-Related Leakage

Correct model misspecification on hydraulic conductivity

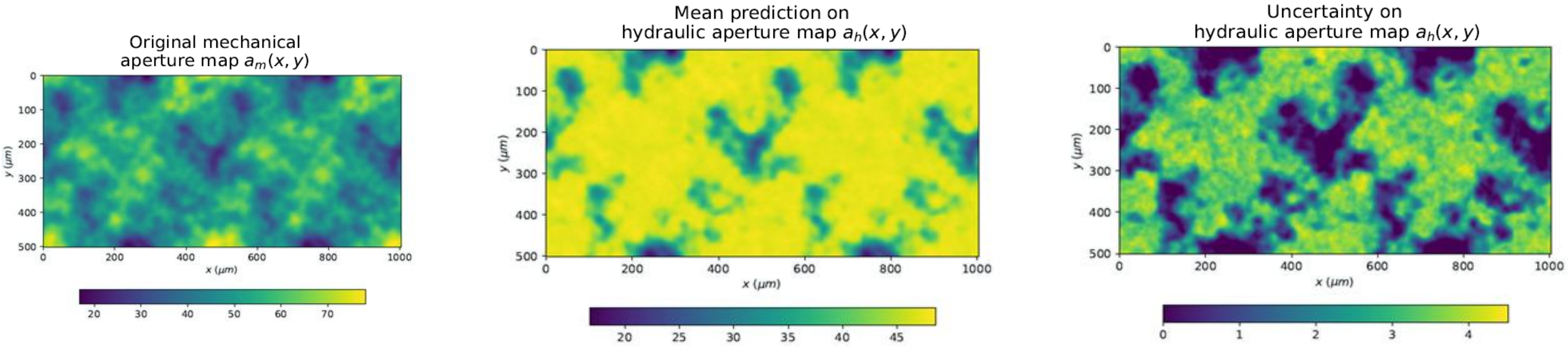


✓ **Adaptive correction given mechanical aperture maps**

Data-based, Geometric & Local

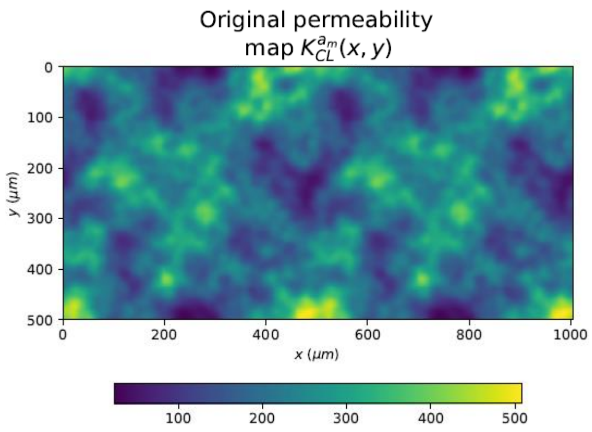
✓ **Uncertainties on hydraulic aperture $a_h(x, y)$**

Automatically account for roughness



Uncertainty on Fault-Related Leakage

Correct model misspecification on hydraulic conductivity

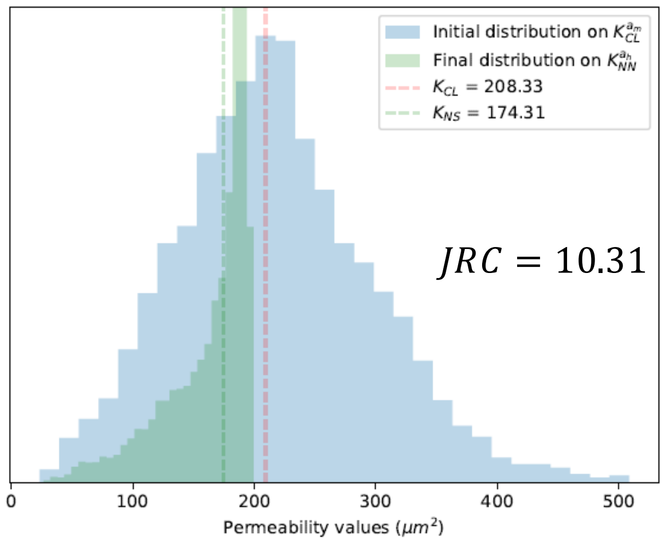


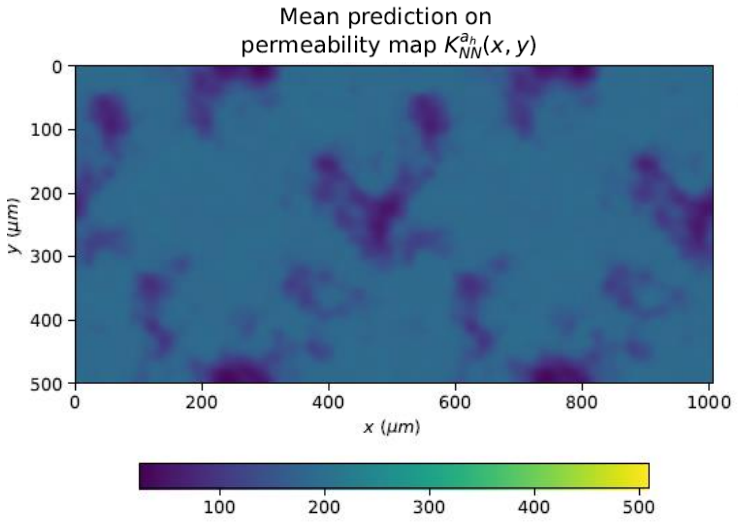
✓ **Uncertainties on fracture permeability**

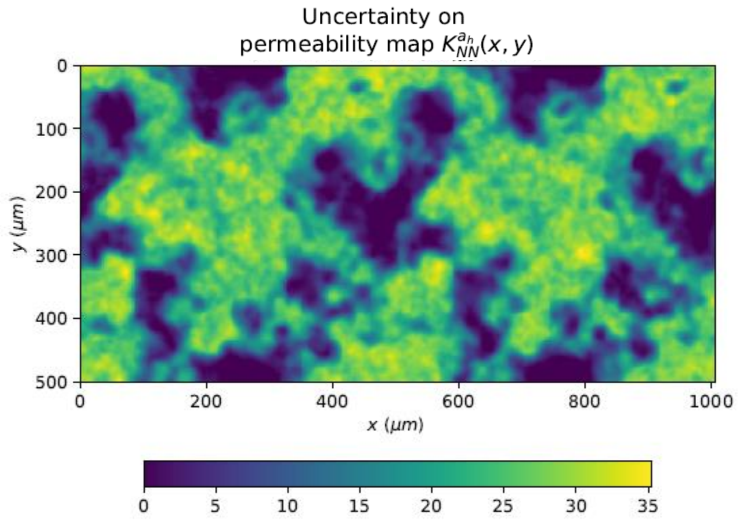
Automatically account for roughness

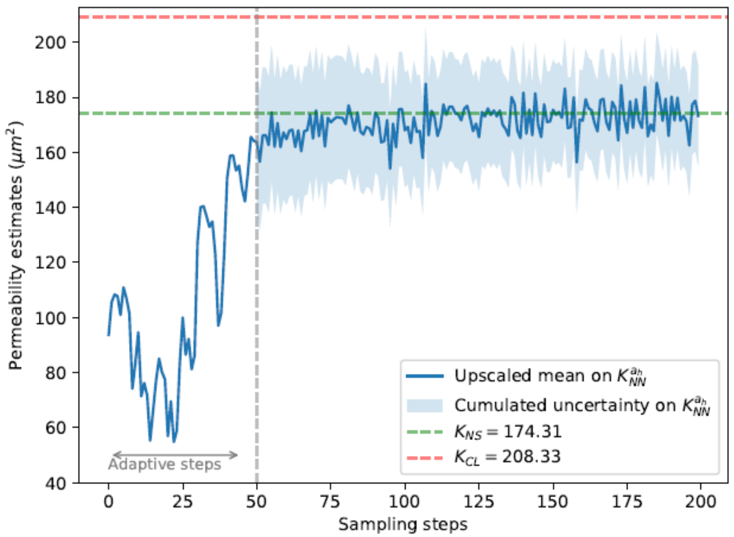
✓ **Infer local permeability field $K_{NN}^{a_h}(x, y)$**

Compatible with Stokes and Darcy upscaling









Uncertainty on Fault-Related Leakage

Roughness Effects and Uncertainties on Fracture Permeability

$< a_m >$ ↓ $a_m(x,y)$ ↓ $\cancel{K_{CL}^{a_m}(x,y)}$ ↓ Ω^{3D} ↓ $a_m(x,y)$ ↓

Increase Roughness

Roughness	Cubic Law	Darcy	(Navier) Stokes	Bayesian PINN	
JCR	K_{CL}	$K_D^{a_m}$	K_{NS}	Mean on $K_{NN}^{a_h}$	UQ on $K_{NN}^{a_h}$
/	μm^2	μm^2	μm^2	μm^2	μm^2
0		208.33	209.94	208.33	[208.3328; 208.3333]
4.86		201.98	195.98	189	[178; 199]
5.85	208.33	201.75	190.36	191	[184; 199]
7.52		201.61	184.92	187	[177; 196]
10.31		201.55	174.31	171	[153; 189]

$$\mathrm{K_{CL}} > \mathrm{K}_D^{a_m} > \mathrm{K}_{NS} \simeq \mathrm{K}_{NN}^{a_h} \simeq K_D^{a_h}$$

$K_D^{a_h}$ (mean + UQ)

$a_h(x,y)$ and $K_{NN}^{a_h}(x,y)$ (mean + UQ)

2D Darcy flow-based upscaling

S. Perez, F. Doster, J. Maes, H. Menke, A. ElSheikh, A. Busch
Paper in Preparation

Uncertainty on Mineral Reactivity

Reactive inverse problem at the pore-scale

$$CaCO_3\,(s) + H^+ \rightarrow Ca^{2+} + HCO_3^-$$

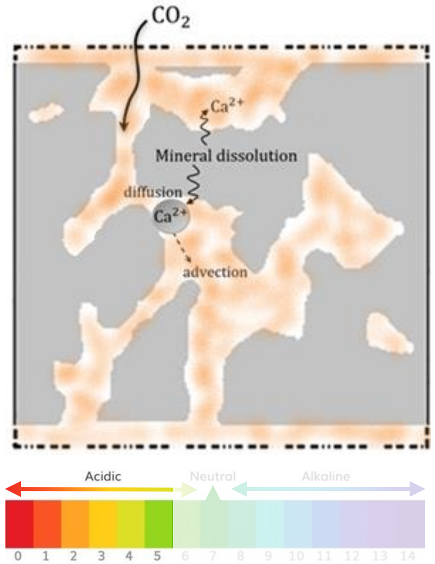
C_{H^+} : *Acid concentration*

$C_{CaCO_3(s)}$: *Calcite concentration*

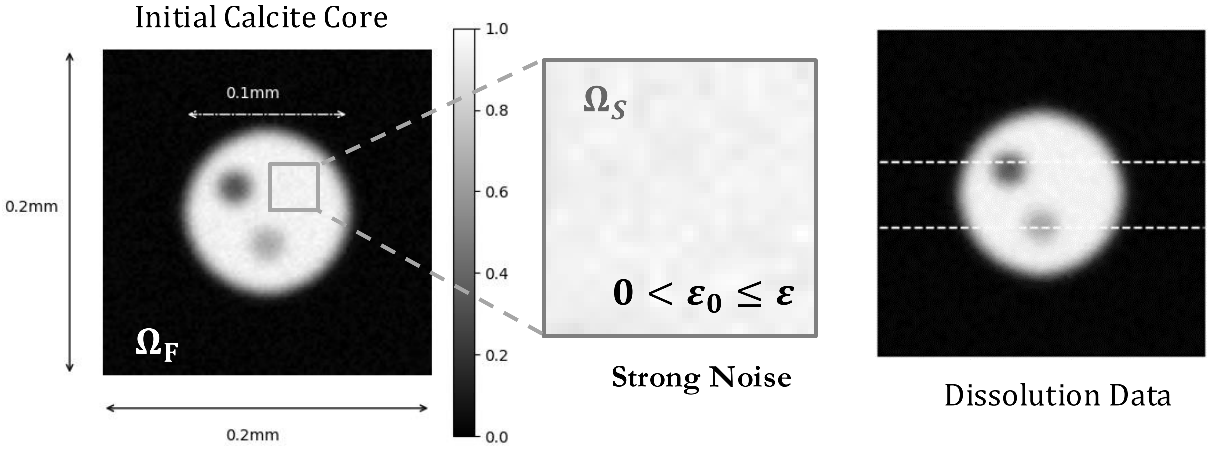
υ : *molar volume*

ε : *micro-porosity field*

$$C_{CaCO_3(s)} = (1-\varepsilon)/\upsilon$$



Dynamical data with uncertainties



Reactive model with **unknown parameters D_m^* & Da_{II}^***

$$\begin{cases} \dfrac{\partial C_{H^+}^*}{\partial t^*} - D_m^* \nabla \cdot \left(\varepsilon^{1+\eta} \nabla\left(\varepsilon^{-1} C_{H^+}^*\right)\right) + Da_{II}^* C_{H^+}^* \mathbb{1}_{\{(1-\varepsilon)>0\}} = 0 \\ \dfrac{1}{C_0 \upsilon} \dfrac{\partial \varepsilon}{\partial t^*} = Da_{II}^* C_{H^+}^* \mathbb{1}_{\{(1-\varepsilon)>0\}} \\ + \text{ initial and boundary conditions} \end{cases}$$

✓ **Morphological uncertainties on the data**

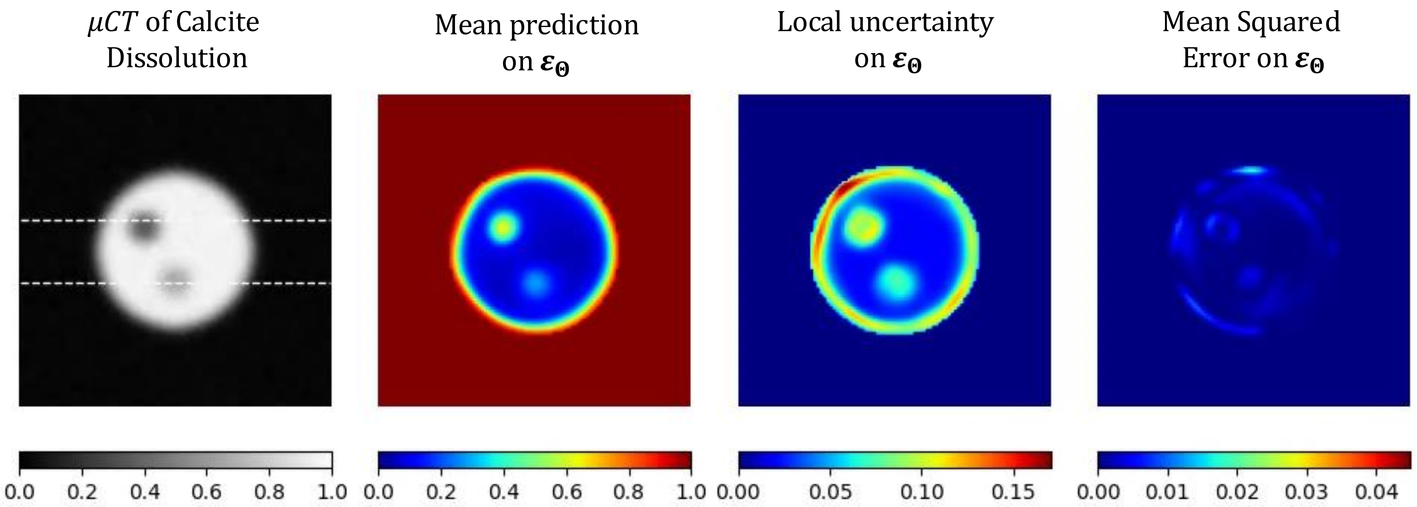
Learn from the dynamics ? UQ on initial state

✓ **Assimilation of reactive parameters**

PDE model, Noisy measurements

Uncertainty on Mineral Reactivity

Reactive inverse problem at the pore-scale

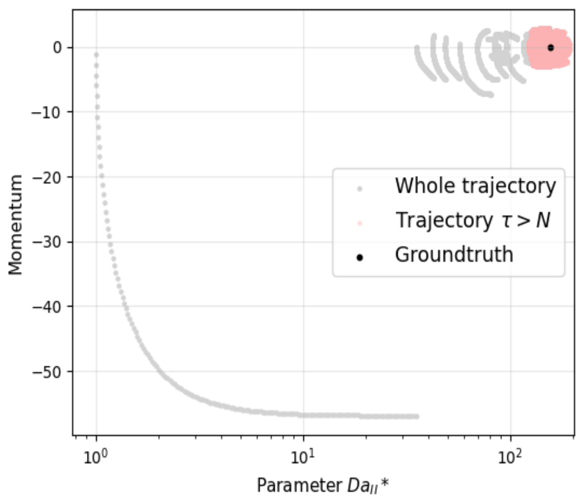


$$\begin{cases} \dfrac{\partial C^*_{H^+}}{\partial t^*} - \boldsymbol{D^*_m} \nabla \cdot \left(\varepsilon^{1+\eta} \nabla \left(\varepsilon^{-1} C^*_{H^+} \right) \right) + \boldsymbol{Da^*_{II}} C^*_{H^+} \mathbb{1}_{\{(1-\varepsilon)>0\}} = 0 \\ \dfrac{1}{C_0 \boldsymbol{v}} \dfrac{\partial \varepsilon}{\partial t^*} = \boldsymbol{Da^*_{II}} C^*_{H^+} \mathbb{1}_{\{(1-\varepsilon)>0\}} \\ + \text{ initial and boundary conditions} \end{cases}$$

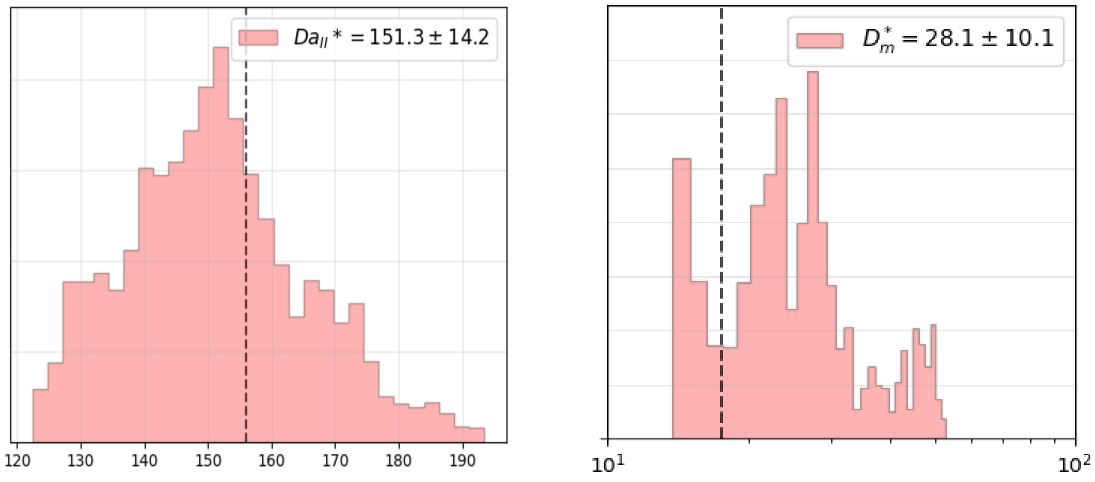
Sequential Reinforcement of PDE constraints

1) ε_Θ 2) ε_Θ , C_Θ and $\boldsymbol{Da^*_{II}}$ 3) ε_Θ , C_Θ , $\boldsymbol{Da^*_{II}}$ and $\boldsymbol{D^*_m}$

Phase Space Trajectory



Marginal Posterior Distributions



Posterior range of physical Damköhler

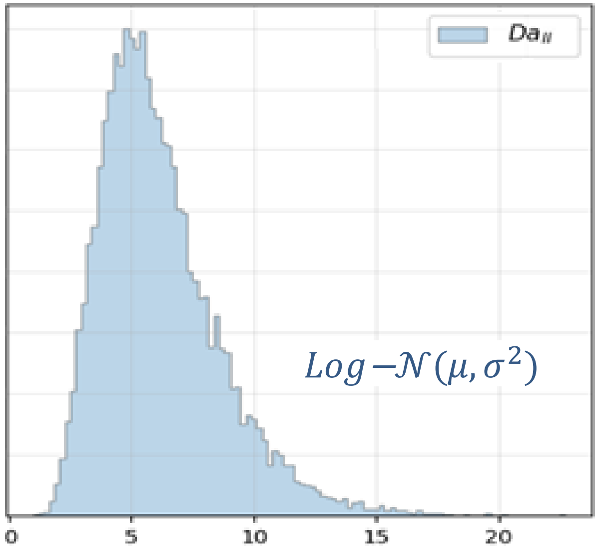
$$Da_{II} = \frac{Da^*_{II}}{D^*_m}$$

Uncertainty on Mineral Reactivity

✓ **Pore-scale calibration of mineral reaction rates**

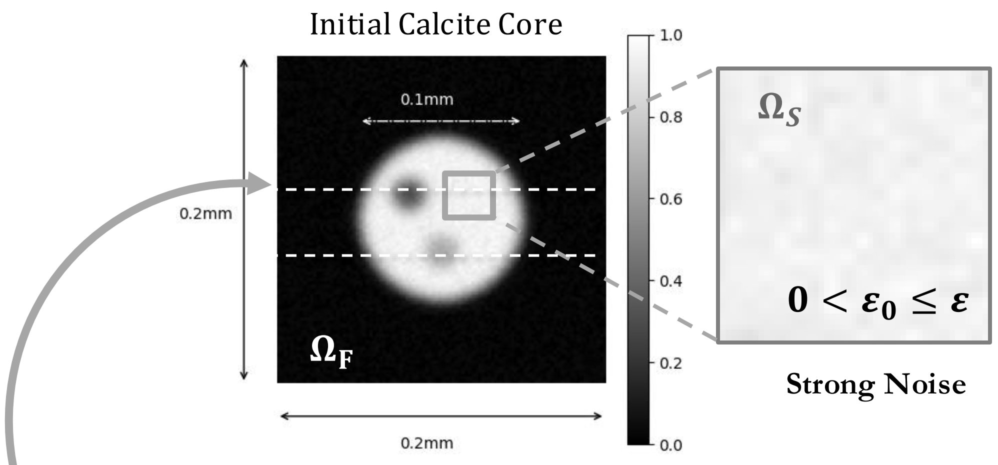
Regime identification & upscaling

$$Da_{II} = 6.14^{+8.72}_{-3.03} \quad (95\%\ \mathrm{CI})$$

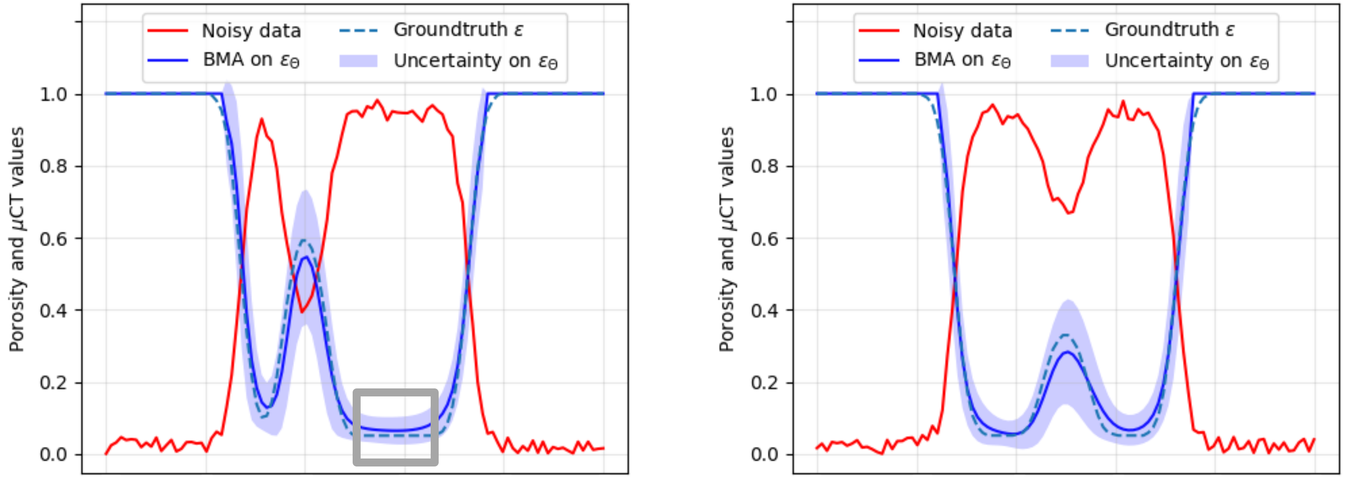


✓ **Quantify sub-resolved micro-porosity ε_0**

Upscale uncertainty ranges on ϕ



ε initial state $(t = 0)$ along the white dotted lines



$$3\% \leq \varepsilon_0 \leq 10\% \quad (95\%\ \mathrm{CI})$$

S. Perez, P. Poncet (2024)
"Auto-weighted Bayesian Physics-Informed Neural Networks and robust estimations for multitask inverse problems in pore-scale imaging of dissolution"
Computational Geosciences

SCAN ME

CONCLUSION

AI-driven uncertainty quantification for reliable leakage risk assessment

- Correct **model misspecification**
- **Model calibration** - Parameters ?
- **Data uncertainties**, noise & sparsity
- Learn from **models & experiments**
- **Multi-scale & Multi-objective** inference
- **Propagation of uncertainties**

Develop new methods

Mathematical understanding

Reliability, Robustness & Upscaling

Thank you !

Questions