Quantifying Uncertainties in Fracture Conductivity for CO_2 Storage: The Impact of Model Misspecifications

Sarah Perez, Florian Doster, Julien Maes, Hannah Menke, Ahmed ElSheikh & Andreas Busch

ECO-AI project – WP3 *(Grant Ref: EP/Y006143/1)*

Heriot-Watt University

"All models are wrong, but some are useful"

George E. P. Box (1979)

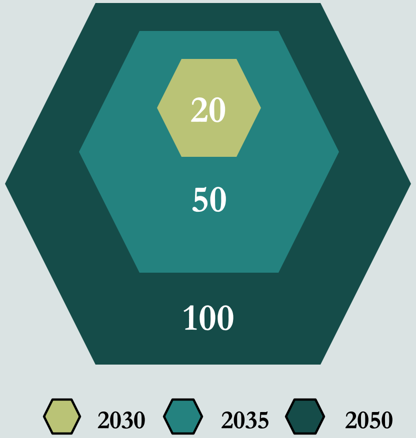
G.E.P. Box (1979) Robustness in Statistics

CO_2 storage as part of the Net Zero transition

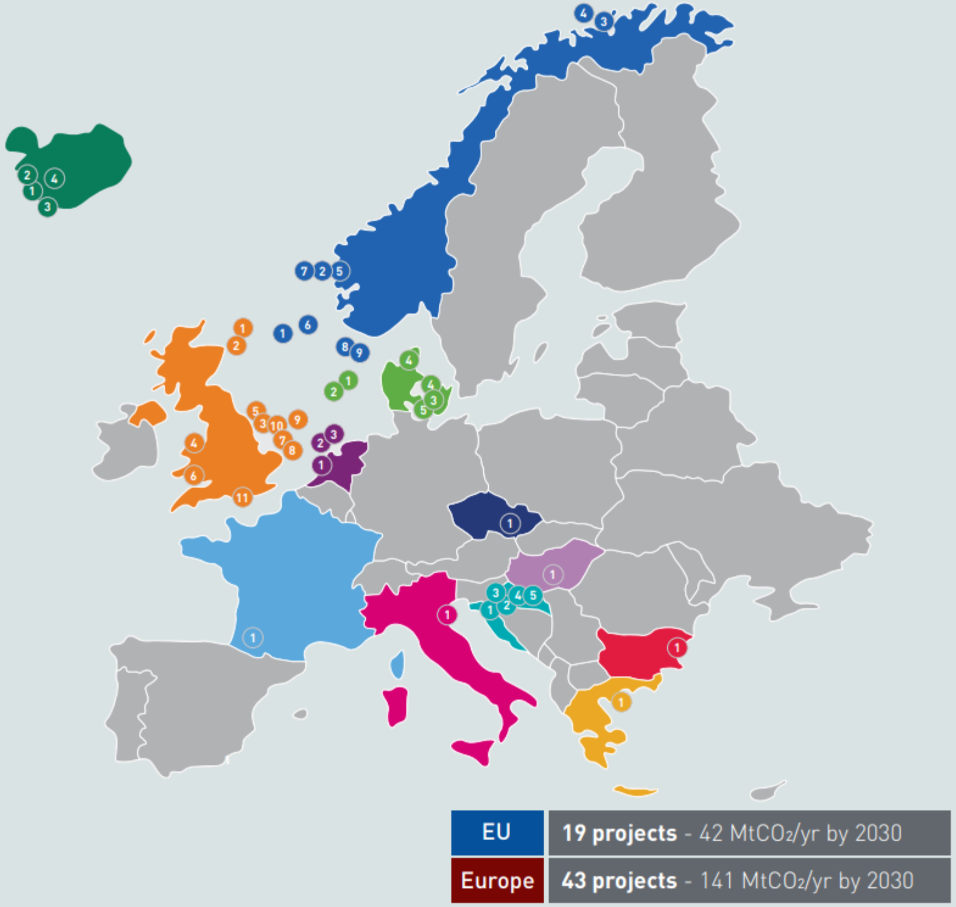
- **Net-Zero goal by 2050:**

hundreds of Gt of CO_2 captured worldwide

- Extensive CCS deployment to meet the **IPCC 1.5 °C target**



UK CCS targets (Mt/yr)

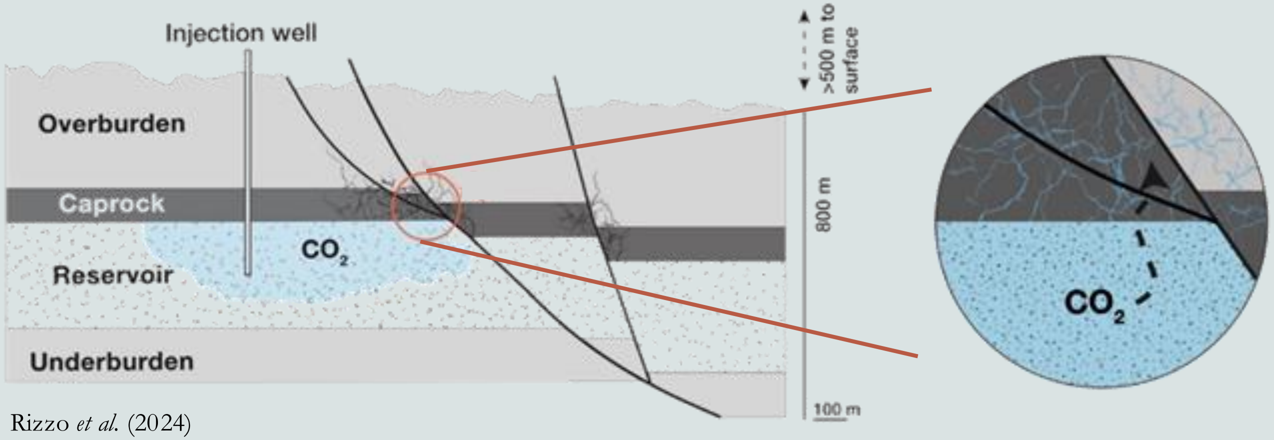


IOGP map of existing and planned CO_2 storage projects in Europe

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

De-risking of subsurface CO_2 storage

UNCERTAINTIES ON FAULT-RELATED LEAKAGE

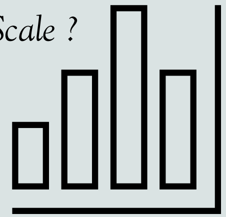


Rizzo *et al.* (2024)

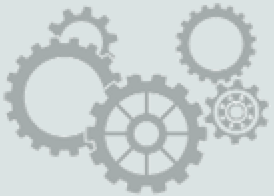
- **Geological Uncertainties**
- Deterministic VS Sensitivity Analyses
- **Trust the model ? Empirical Laws ?**
- Calibrating hydraulic conductivities

Data Uncertainties

Heterogeneities ?
Noise ?
Scale ?



Modelling Uncertainties

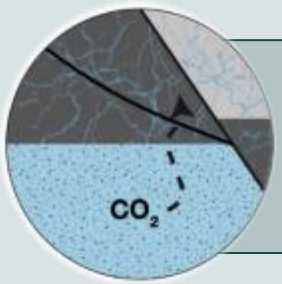


Fault Properties ?
Prior distributions ?

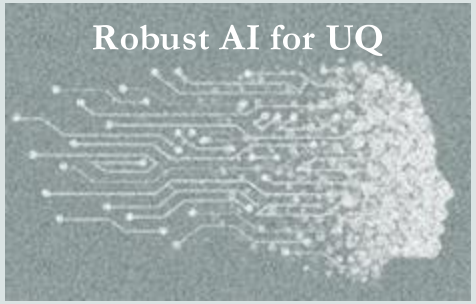
R. E. Rizzo, N. F. Inskip, H. Fazeli, P. Betlem, K. Bisdom, N. Kampman, et al. (2024), International Journal of Greenhouse Gas Control (https://doi.org/10.1016/j.ijggc.2024.104105)

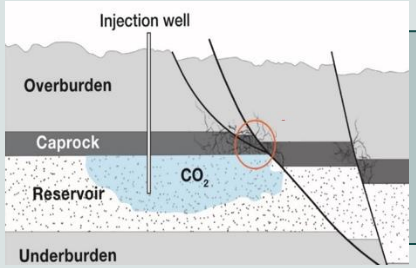
AI driven Uncertainty Quantification

BRIDGE THE SCALES – BALANCE THE OBJECTIVES



- Experimental Data
- Pore-scale Uncertainties
- Physical Models



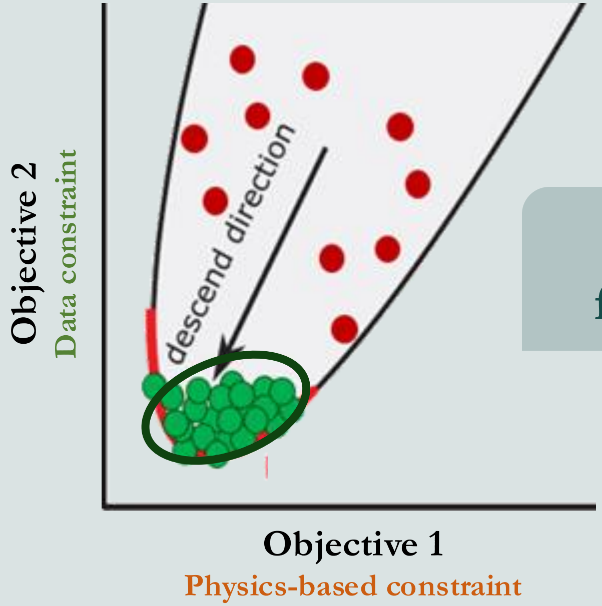


- Upscaling & ML
- Macro-scale Uncertainties
- Model Calibration

1. Leverage local interactions

2. Bayesian Inference & Inverse Problems

3. Propagate the uncertainties

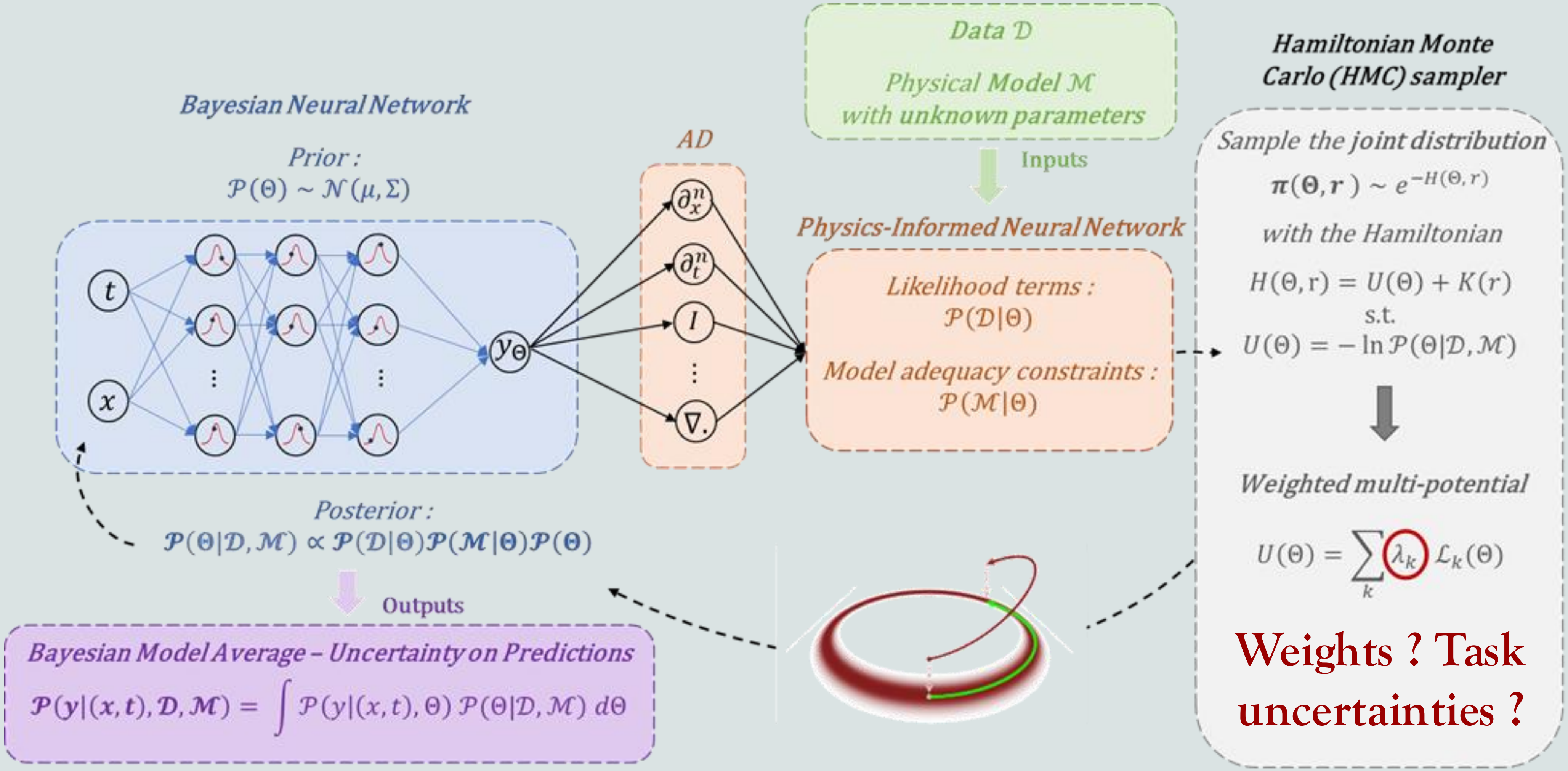


Pareto-optimal front exploration

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

AI driven Uncertainty Quantification

BAYESIAN PHYSICS-INFORMED NEURAL NETWORKS

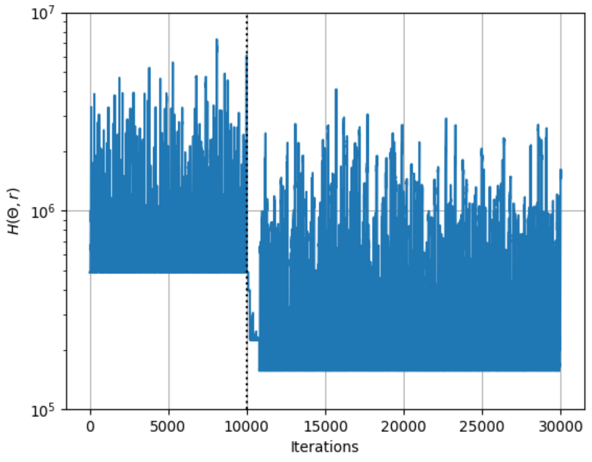


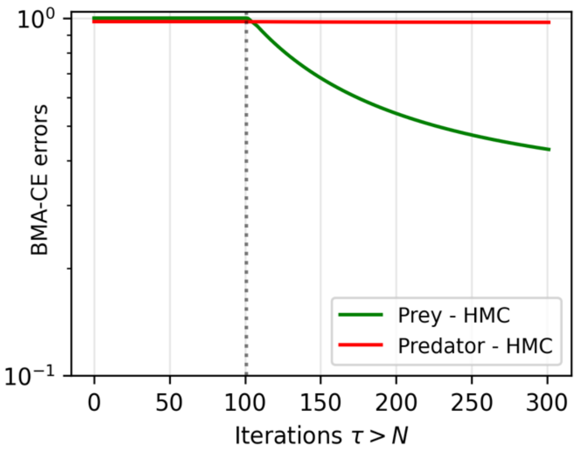
Weights ? Task uncertainties ?

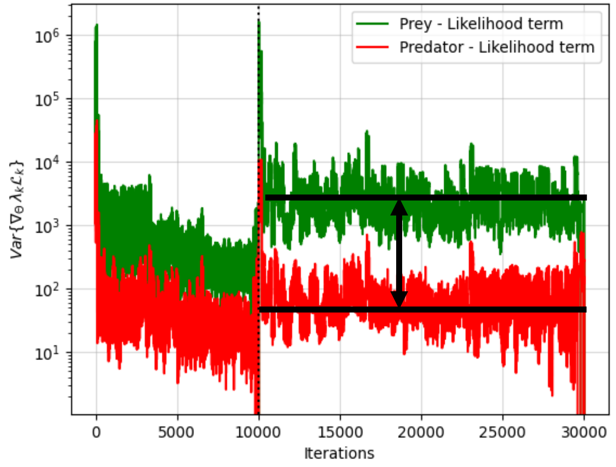
L. Yang, X. Meng, and G.E. Karniadakis (2021),
Journal of Computational Physics (https://doi.org/10.1016/j.jcp.2020.109913)

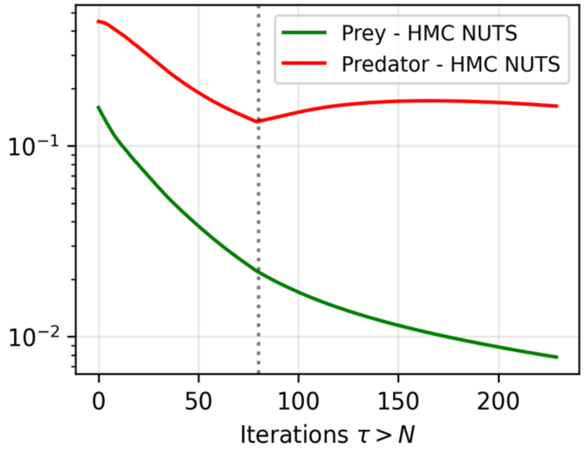
AI driven Uncertainty Quantification

CHALLENGES OF BAYESIAN PINNS – UNBIASED UQ ?









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HMC with uniform λ_k

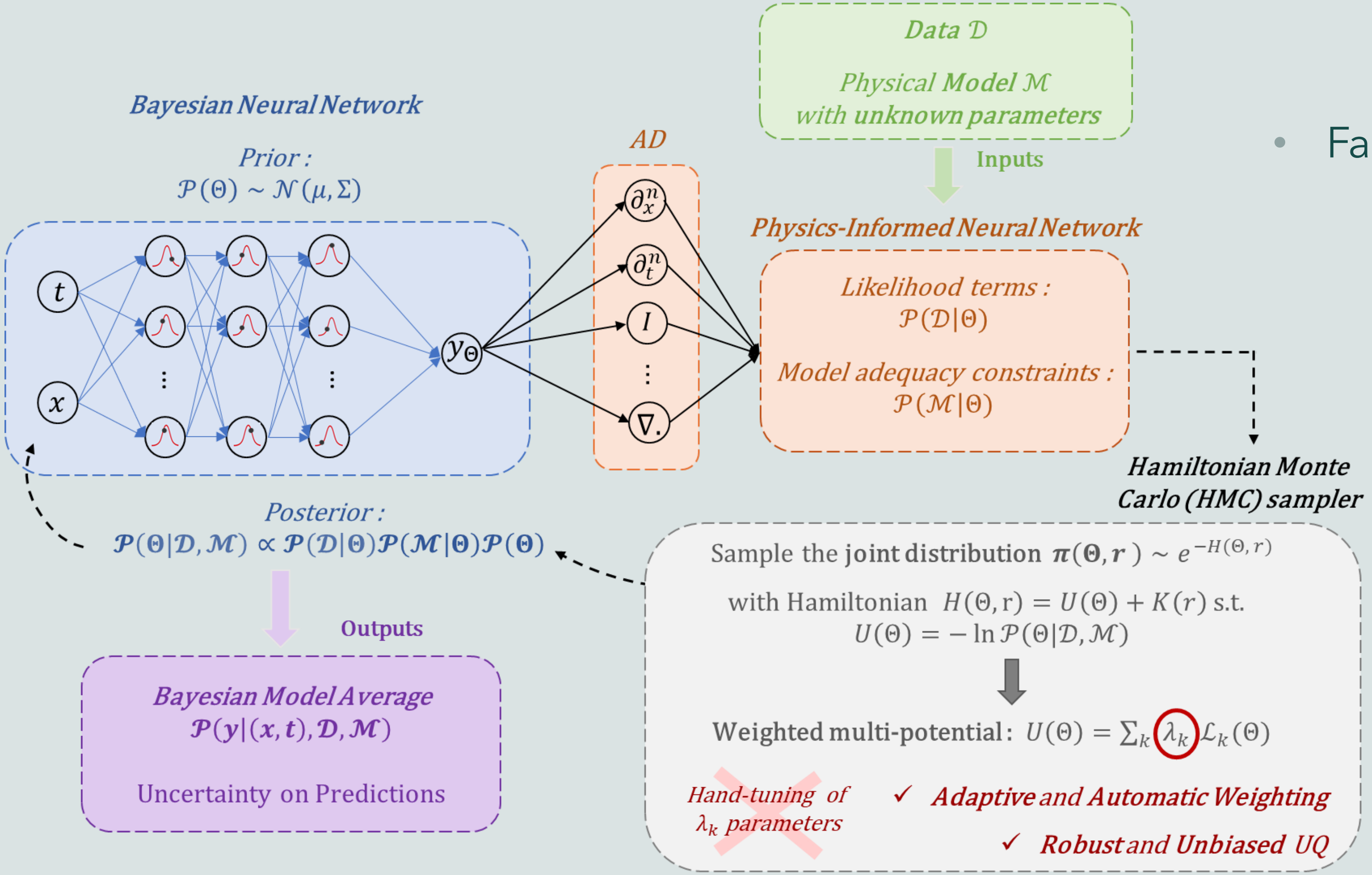
- Instabilities
- Poor exploration of the MCMC chain
- Lack of Convergence

HMC NUTS with hand-tuning

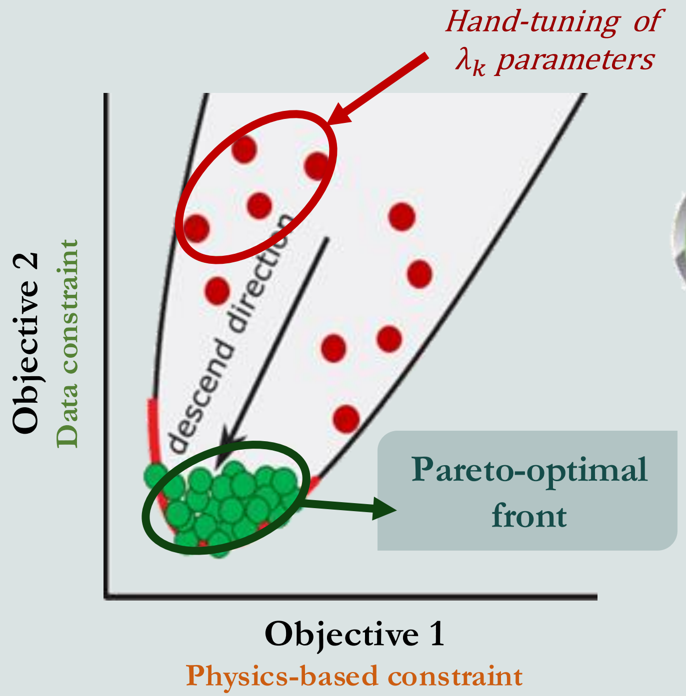
- Unbalanced conditions
- Biased Convergence
- Poor exploration of the Pareto front

AI driven Uncertainty Quantification

ROBUST UQ FOR THE BAYESIAN PINNS



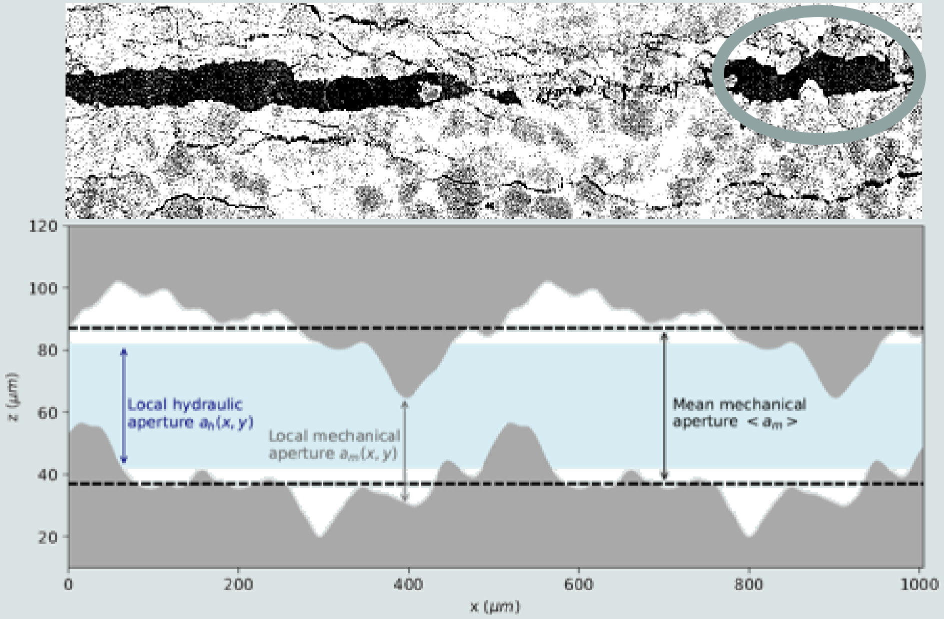
- Enhanced stability & accuracy
- Faster convergence & Pareto front exploration



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

MODEL MISSPECIFICATION ON HYDRAULIC CONDUCTIVITY



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

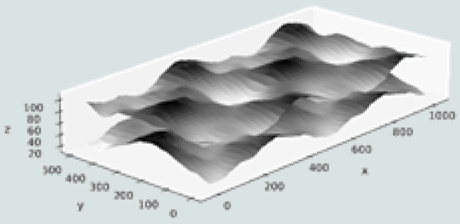
$$JRC \in [4.86, 10.31]$$

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

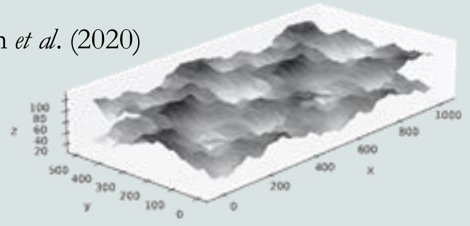
$$K_{CL} \simeq 208\ \mu m^2$$

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

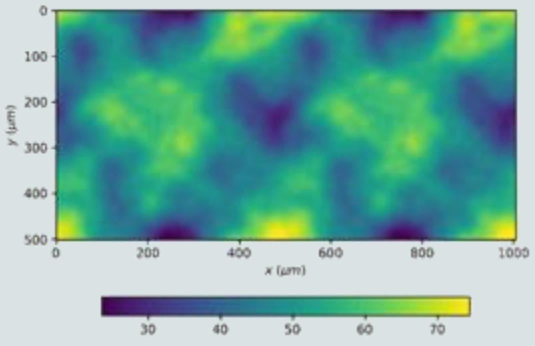
$$K_{CL}^{a_m}(x,y) = \frac{a_m(x,y)^2}{12} \xrightarrow{\text{2D Darcy flow-based upscaling}} \boldsymbol{K_D^{a_m}}$$

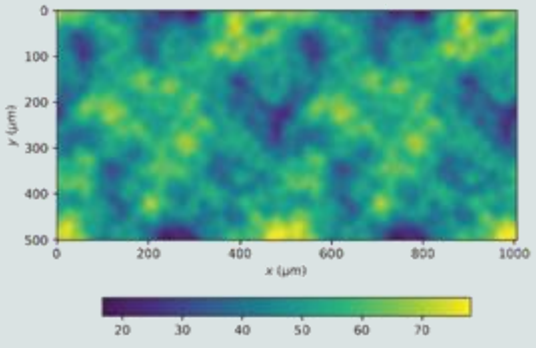


Guiltinan *et al.* (2020)



Mechanical aperture maps $a_m(x,y)$





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

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

No roughness effects & Overestimation of fracture conductivity

Cubic Law $\boldsymbol{K_{CL}}$ & Darcy $\boldsymbol{K_D^{a_m}}$ 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 $\boldsymbol{a_m(x,y)} = \boldsymbol{a_h(x,y)} + \boxed{\xi_d}$ Data uncertainty

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

Model uncertainty

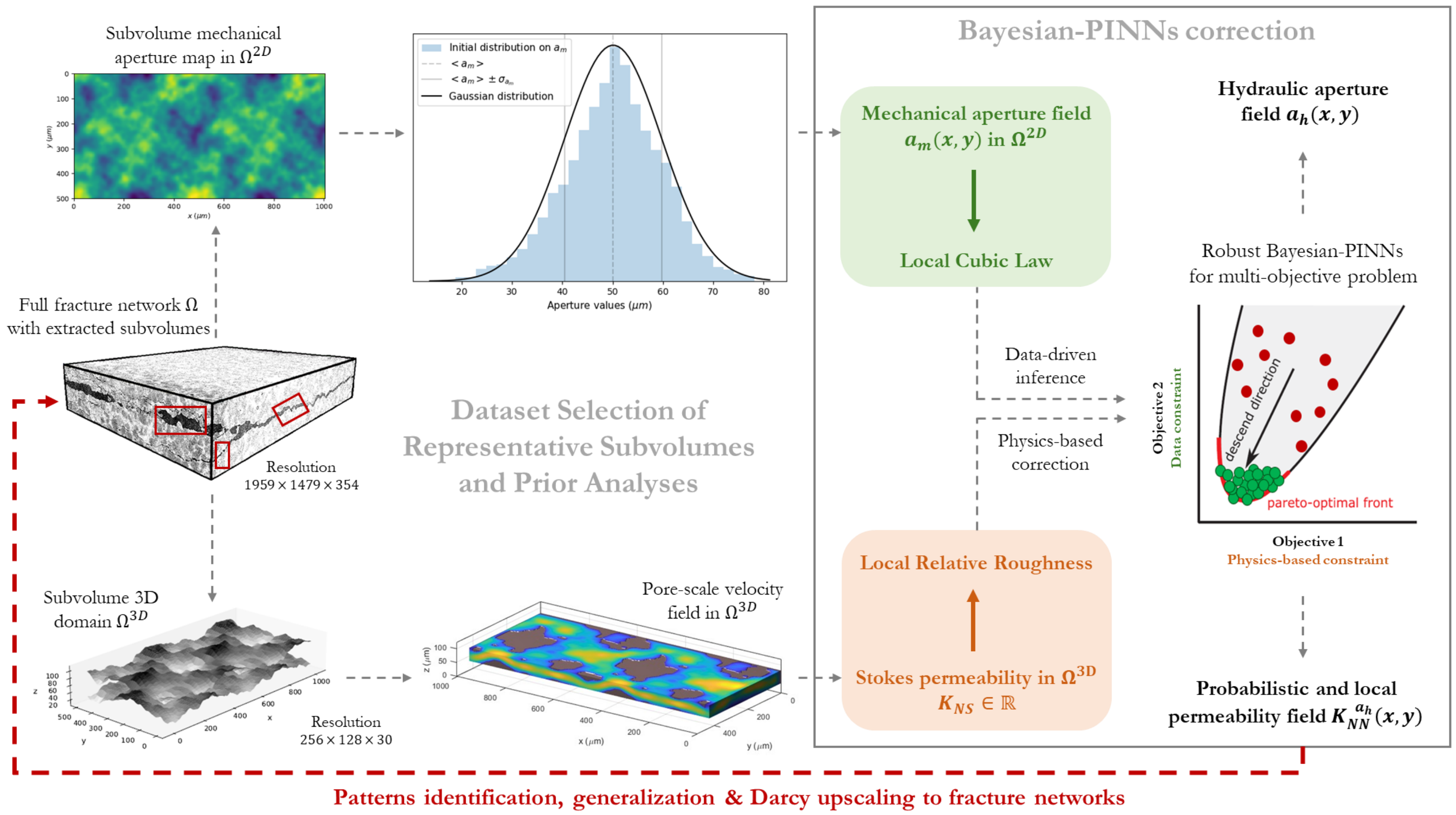
$$K_{NS} = \frac{1}{|\Omega_f^{2D}|}\int_{\Omega_f^{2D}} K_{NN}^{a_h}(x,y)\,dx\,dy + \boxed{\xi_m}$$

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

Local Cubic Law

Local Relative roughness

Workflow:



Uncertainty on Fault-Related Leakage

CORRECT MODEL MISSPECIFICATION ON HYDRAULIC CONDUCTIVITY

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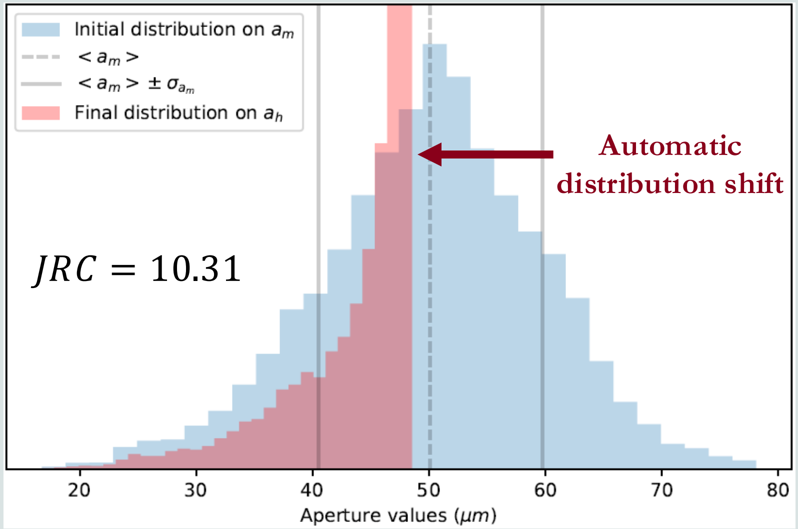
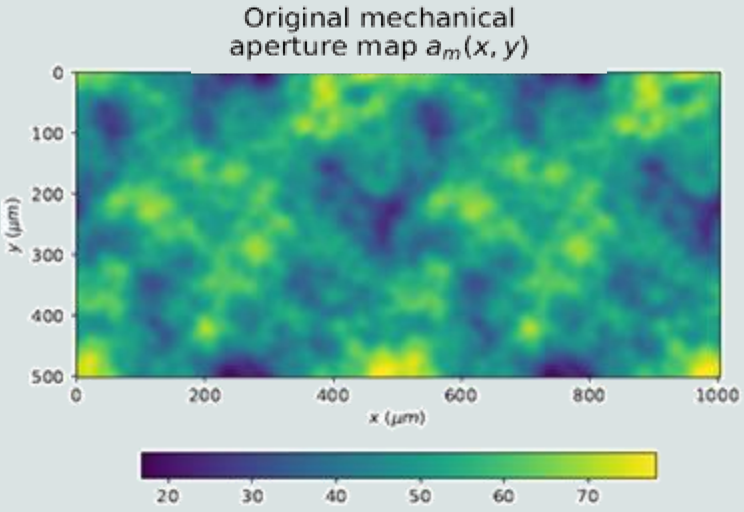


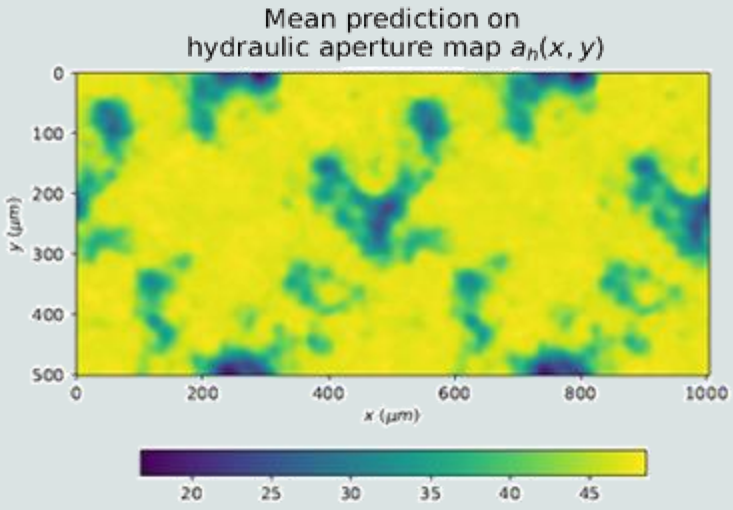
✓ **Adaptive correction given mechanical aperture maps**

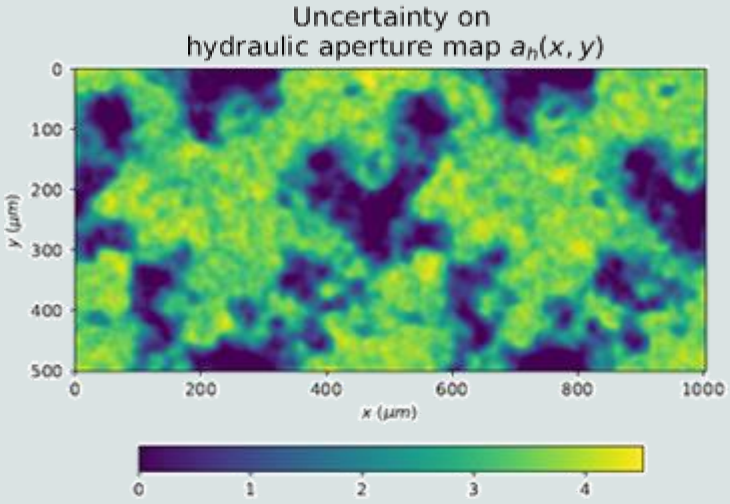
Data-based, Geometric & Local

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

Automatically account for roughness

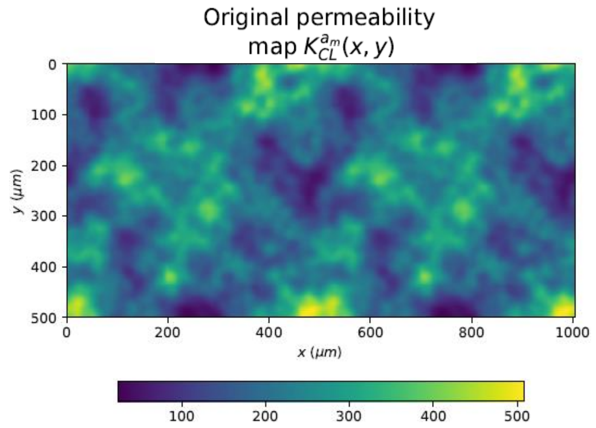






Uncertainty on Fault-Related Leakage

CORRECT MODEL MISSPECIFICATION ON HYDRAULIC CONDUCTIVITY

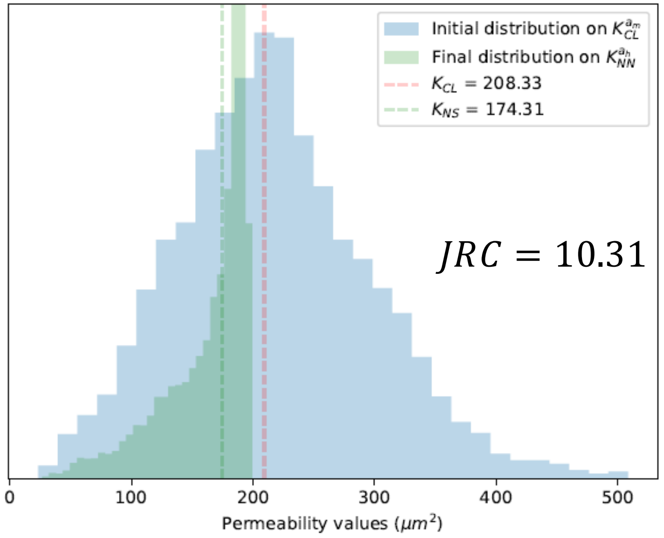


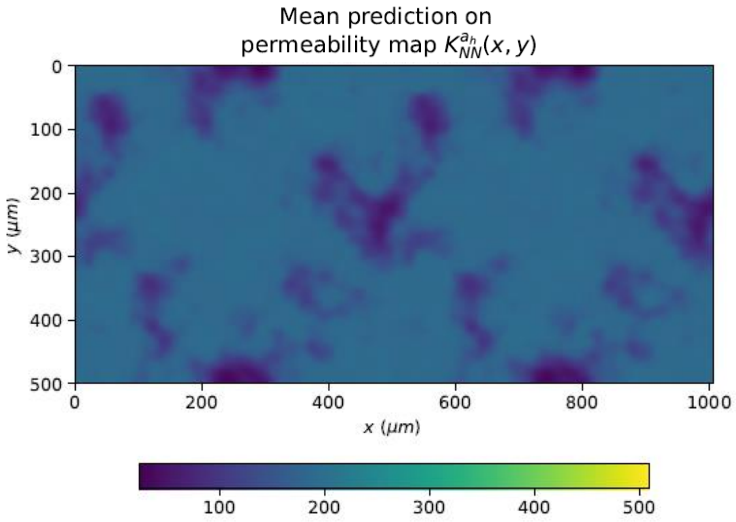
✓ **Uncertainties on fracture permeability**

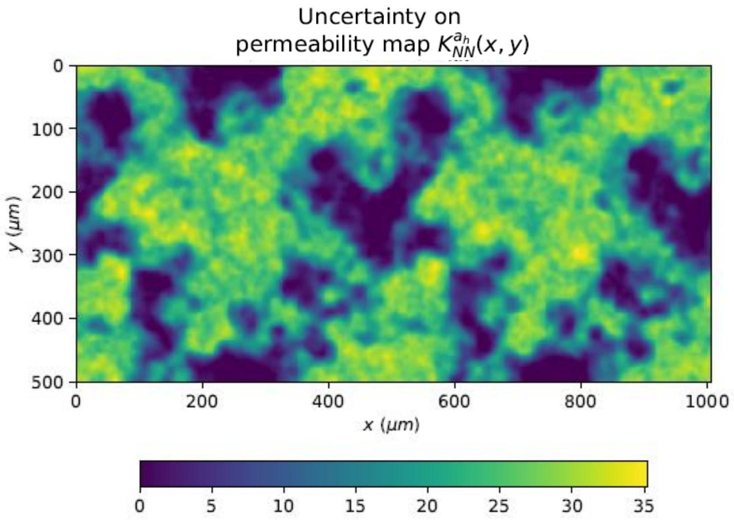
Automatically account for roughness

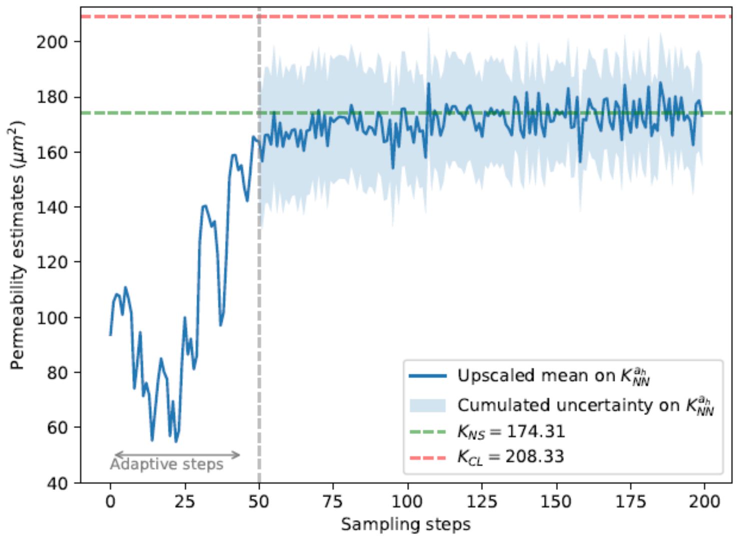
✓ **Infer local permeability field $K_{NN}^{a_h}(x,y)$**

Compatible with Stokes and Darcy upscaling









Uncertainty on Fault-Related Leakage

CORRECT MODEL MISSPECIFICATION ON HYDRAULIC CONDUCTIVITY

$< a_m >$ → Cubic Law; $a_m(x,y)$ → $\cancel{K_{CL}^{a_m}(x,y)}$ → Darcy; Ω^{3D} → (Navier) Stokes; $a_m(x,y)$ → Bayesian PINN

Increase Roughness ↓

Roughness JCR	Cubic Law K_{CL}	Darcy $K_D^{a_m}$	(Navier) Stokes K_{NS}	Bayesian PINN Mean on $K_{NN}^{a_h}$	Bayesian PINN 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]

$$\boxed{K_{CL} > K_D^{a_m} > K_{NS} \simeq K_{NN}^{a_h} \simeq K_D^{a_h}}$$

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

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

2D Darcy flow-based upscaling

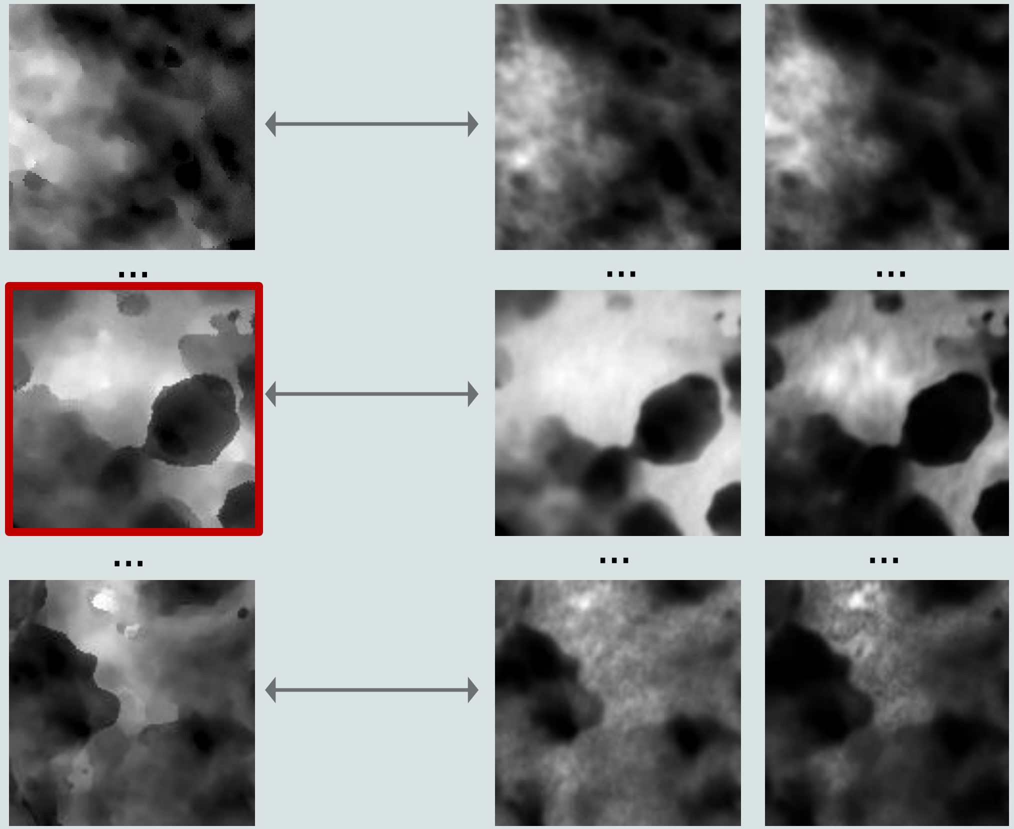
Propagation of uncertainties across scales

PROSPECTS AND ONGOING WORK

$a_m(x,y)$

$K_{NN}^{a_h}(x,y)$

Mean Uncertainty



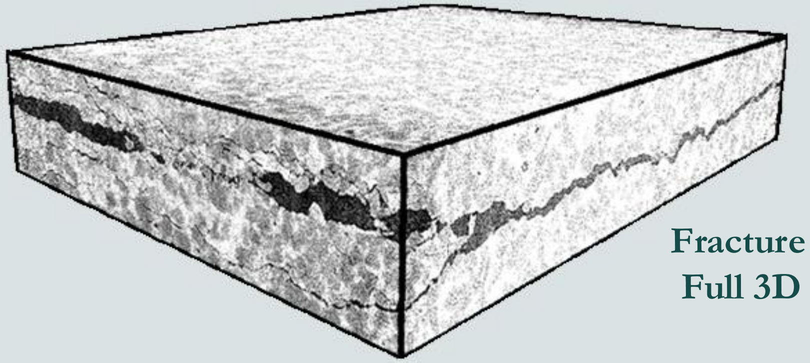
Ny = 128

Nx = 128

Representative Dataset with Multi-Output Mapping

Patterns identification

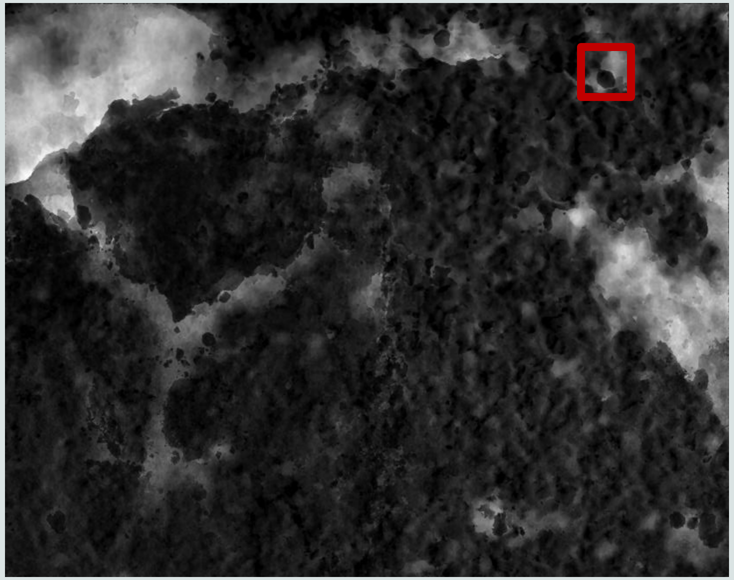
Generalization



Fracture (network)
Full 3D geometry

Nx = 1873

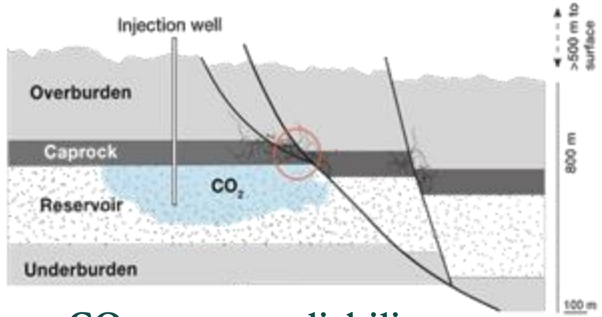
Ny = 1480



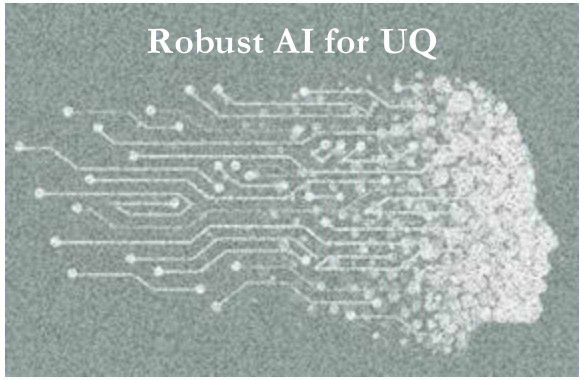
Mechanical Aperture map(s)

Flow direction

Conclusion



CO_2 storage reliability



AI-driven uncertainty quantification for reliable leakage risk assessment

- Correct **model misspecification**
- **Model calibration** – Prior Distributions ?
- **Data uncertainties**, noise & sparsity
- Learn from **models & experiments** at small scales
- **Propagation of uncertainties** at larger scales
- **Sensitivity Analyses** of fault leakage rates