Chemical and morphological uncertainty quantification by auto-weighted Bayesian Physics-Informed Neural Networks for reactive two-scale porous media at the pore scale

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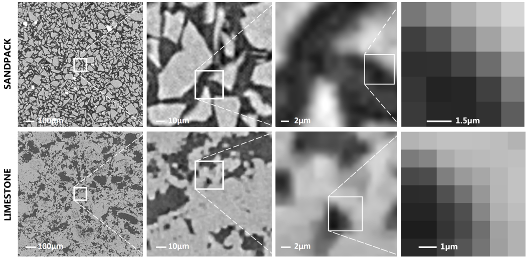
Summary

Table of contents:

X-ray μCT uncertainties in Digital Rock Physics

- **Micrometric reactive processes** in porous media
- X-ray **micro-tomography scans** up to the voxel scale
- μCT **unresolved features**
- Dynamical μCT: mineral reactivity assessment



- Pore-scale reactive models & DNS
- 3D Pore space geometry
- **Morphological uncertainties**
- Wide range of kinetic parameters

Reliability of model inputs & reactive parameters ?

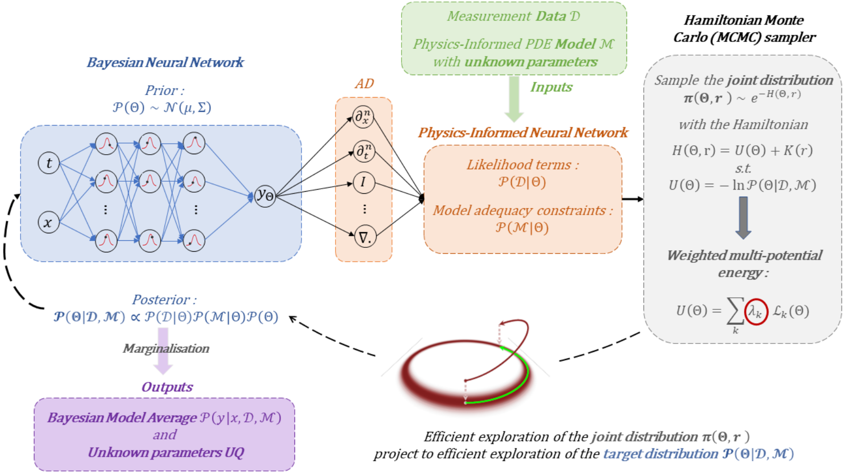
↓

Uncertainty Quantification

Quantify the imaging **uncertainties on the micro-scale properties.**
Improve the **reliability of reactive pore-scale modeling** and numerical simulations.
Manage their **impact on the macro-scale properties.**

Bayesian Physics-Informed Neural Networks

General formalism using Hamiltonian Monte Carlo (HMC) sampler



M. Betancourt, *A Conceptual Introduction to Hamiltonian Monte Carlo* (2018)

L. Yang, X. Meng and G.E. Karniadakis, *B-PINNs: Bayesian physics-informed neural networks for forward and inverse PDE problems with noisy data*, J. Comput. Phys. (2021)

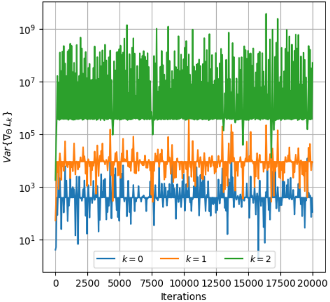
BPINNs failures modes

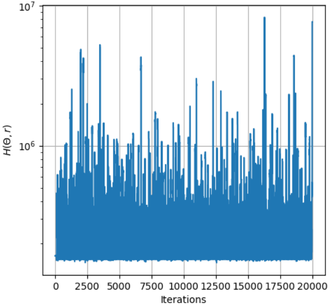
Uniform weights generates **instabilities** for **multi-scale, multi-objective** inference problems

Sobolev training benchmark at derivative order $\boldsymbol{K}$

- $\mathcal{D} = \{(x_i, u_i), i = 1 \dots N_d\}$ with $u_i = u_\theta(x_i) + \xi_i$ and $\xi \sim \mathcal{N}(0, \sigma_0^2 I)$

$$H(\theta, r) = \underbrace{\sum_{k=0}^{K} \left[\frac{\lambda_k}{2\sigma_k^2} \| D_x^k u_\theta - D_x^k u \|^2 \right]}_{\text{Loglikelihood}} + \underbrace{\frac{\lambda_{K+1}}{2\sigma_{K+1}^2} \|\theta\|^2}_{\text{LogPrior}} + \underbrace{\frac{1}{2} \|r\|^2}_{K(r)}$$



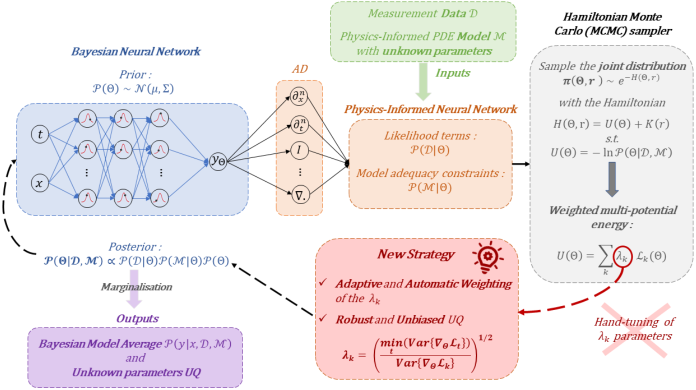


Uniform weights strategy $\Rightarrow$ Non conservative Hamiltonian

A novel Adaptive-Weighted HMC strategy

Complex multi-objective and multi-scale potential $U(\Theta)$

Question : How to set the weights λ_k to provide balanced condition between the objective terms ?



- **Dirichlet Weighting** finite adaptive steps in the HMC
- **Faster convergence** of B-PINNs
- Enhanced **stability** and **accuracy**
- **Automatic adjustment** of the weights w.r.t noise and task sensitivity
- **Robust** uncertainty quantification

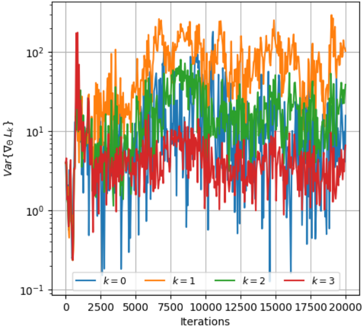
S. Perez, S. Maddu, I.F. Sbalzarini, P. Poncet, *Adaptive weighting of Bayesian Physics-Informed Neural Networks for multitask and multiscale forward and inverse problems*, Under review since 19-03-2023
ArXiv preprint: https://doi.org/10.48550/arXiv.2302.12697

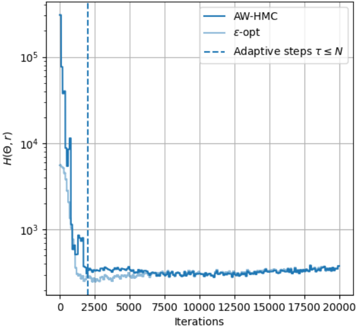
Adaptive-Weighted HMC for Sobolev benchmark

Balanced sampling toward an efficient exploration of the Pareto front

Sobolev training benchmark at derivative order ***K***

$$H(\theta, r) = \underbrace{\sum_{k=0}^{K} \left[\frac{\lambda_k}{2\sigma_k^2} \|D_x^k u_\theta - D_x^k u\|^2 \right]}_{\text{Loglikelihood}} + \underbrace{\frac{\lambda_{K+1}}{2\sigma_{K+1}^2} \|\theta\|^2}_{\text{LogPrior}} + \underbrace{\frac{1}{2}\|r\|^2}_{K(r)}$$



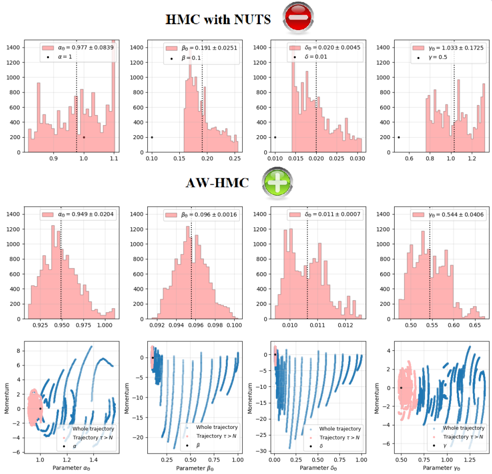


Dirichlet weighting strategy $\Rightarrow$ Conservative Hamiltonian

AW-HMC validations and comparisons

Benchmark on data-driven inverse problems

- Comparisons with classical HMC and NUTS formulations
- **Multi-scale** Lokta-Volterra inverse problem
  - **uninformative priors** on the inverse parameters scaling
- Bayesian inference of incompressible stenotic flow:
  - **unknown noise distributions**, potentially heteroscedastic
  - **unknown model adequacy**
- Stenotic flow inverse problem:
  - **latent field recovery**
  - Reynolds uncertainty quantification



S. Perez, S. Maddu, I.F. Sbalzarini, P. Poncet, *Adaptive weighting of Bayesian Physics-Informed Neural Networks for multitask and multiscale forward and inverse problems*, Under review since 19-03-2023
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Reactive Inverse Problem in pore-scale imaging

Two-scale porosity model and data-driven imaging context

Can we bring local descriptions of a material by the observation of its dissolution ?

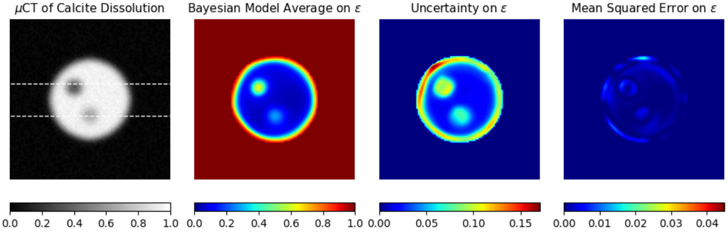
- Dynamical process $\Rightarrow$ Add information on initial state μCT scan ($\boldsymbol{Im}_{|t=0}$)
- Bayesian inference on calcite dissolution : $CaCO_3(s) + H^+ \rightleftharpoons Ca^{2+} + HCO_3{}^-$
- **Morphological uncertainty quantification** (UQ) on the micro-porosity field ε
- **Model chemical parameters UQ** $\Rightarrow$ $Da^*_{II} = K_{H^+} A_s \gamma_{H^+} T$ and $D^*_m = D_m T / L^2$
- **Dissolution dominant hypothesis** $Pe^* << 1$
- **Latent field** C_{H^+} and **μCT uncertainties** s.t $Im = 1 - \varepsilon_\Theta + \xi$ with $\xi \sim \mathcal{N}(0, \sigma^2 I)$
- **Physical model adequacy constraint**, given υ the solid molar volume and $\varepsilon = 1 - \upsilon C_{CaCo_3}$

$$
\begin{cases}
-\nabla.(2D(u)) + L^2 \kappa_0^{-1} \dfrac{(1-\varepsilon)^2}{\varepsilon^2} u = \varepsilon(f - \nabla p) \\
\dfrac{\partial C_{H^+}}{\partial t^*} + Pe^* \nabla.(\varepsilon^{-1} u C_{H^+}) - D^*_m \nabla.(\varepsilon^{\beta+1} \nabla \varepsilon^{-1} C_{H^+}) + Da^*_{II} C_{H^+} \mathbb{1}_{\{(1-\varepsilon)>0\}} = 0 \\
\dfrac{1}{C_0 \upsilon} \dfrac{\partial \varepsilon}{\partial t^*} = Da^*_{II} C_{H^+} \mathbb{1}_{\{(1-\varepsilon)>0\}} \\
+ \text{ initial and boundary conditions, along with } \mathrm{div} u = 0
\end{cases}
$$

Reactive Inverse Problem in pore-scale imaging

Bayesian UQ on the porosity field ε and reactive parameter inference

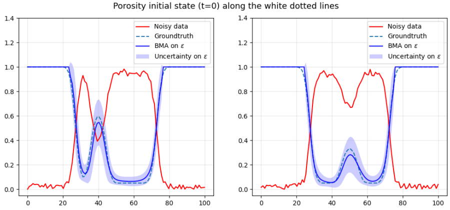
Application to 2D+T synthetic μCT data of calcite dissolution with **strong unknown noise**

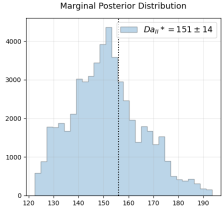


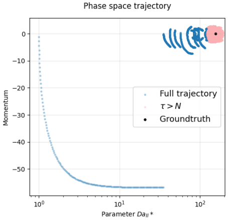
Posterior range of physical Damköhler:

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

$$= \mathbf{6.14 \pm 4.02}$$







Robust Bayesian Uncertainty Quantification for reactive inverse problem in pore-scale imaging

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Conclusion and prospects

- Develop a **novel methodology** for **automatic adaptive weighting** of BPINNs
- **Robust Bayesian inference** in the context of **multi-objective** and **multi-scale** data-driven problems...
- ... with **unknown noise** distributions and **unknown model adequacy**

- Application to **reactive inverse problem in pore-scale imaging**
- Quantify **morphological uncertainty** on ε micro-porosity through a dynamical process
- Image based identification and **UQ of the kinetic parameters**
- Extension to real μCT dissolution scans

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