Quantifying Uncertainty in Coupled-THM Integrity Analysis

Origins of Uncertainty – From Data to Models

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Inferring Uncertain Parameters

Uncertain parameters in repository safety assessment

Challenges of uncertain physical parameters[1] for THM simulation:

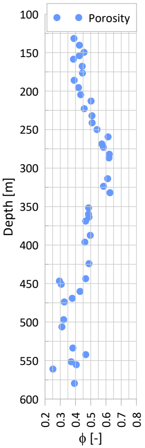
- observations of crucial input parameters often indirect, always noisy
- spatial variability, anisotropy ☞ **Poster Aqeel Chaudry**
- available data: often only best estimate,
  sometimes min, max, confidence interval
- original measurement values/conditions often not reported
- only independently determined values reported
- ☞ **Poster Sibylle Mayr**

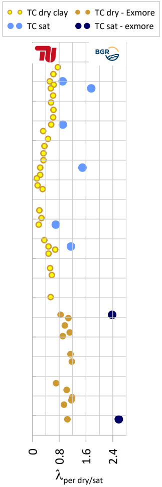
Parameter	Symbol/Unit	Min	Max	Mean	Std. Dev.	Distribution
Total thermal conductivity	$K/\mathrm{W\,m^{-1}\,K^{-1}}$	1.29	2.45	1.79	0.34	Truncated normal
Total specific heat capacity	$C/\mathrm{J\,kg^{-1}\,K^{-1}}$	774	1182	978	68	Normal
Total density	$\rho/\mathrm{kg\,m^{-3}}$	2420	2540	2480	30	Truncated normal
Young's modulus	E/Pa	$5.5 \cdot 10^{9}$	$20.1 \cdot 10^{9}$	$12.8 \cdot 10^{9}$	$3.7 \cdot 10^{9}$	Truncated normal
Volumetric thermal expansion coefficient of solid skeleton	$a_s/\mathrm{K^{-1}}$	$3 \cdot 10^{-5}$	$7.5 \cdot 10^{-5}$	$5.25 \cdot 10^{-5}$	–	Uniform
Intrinsic permeability	$k_s/\mathrm{m^2}$	$7.8 \cdot 10^{-21}$	$2.2 \cdot 10^{-19}$	$5.6 \cdot 10^{-20}$	$5.5 \cdot 10^{-20}$	Truncated normal
Poisson's ratio	$\nu/-$	0.2	0.4	0.3	–	Triangular
Porosity	$\phi/-$	0.097	0.185	0.15	0.0276	Truncated normal

[1] Aqeel Afzal Chaudhry, Jörg Buchwald, and Thomas Nagel. "Local and global spatio-temporal sensitivity analysis of thermal consolidation around a point heat source". In: *International Journal of Rock Mechanics and Mining Sciences* 139 (2021), p. 104662. DOI: 10.1016/j.ijrmms.2021.104662.

Inferring Uncertain Parameters

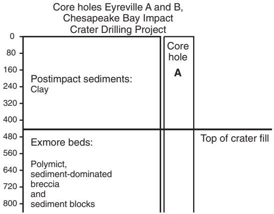
Case study: inferring thermal conductivity from observational data[2]





Depth observations of

- porosity ϕ
- thermal conductivity λ
- Saturated measurements of λ difficult to obtain.
  Best estimate of λ?
- temperature T



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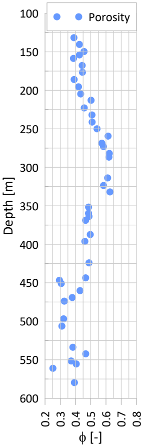

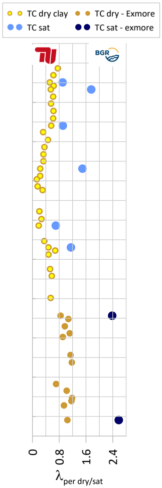

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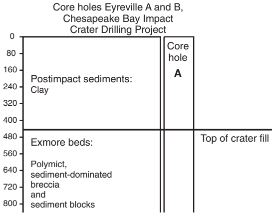

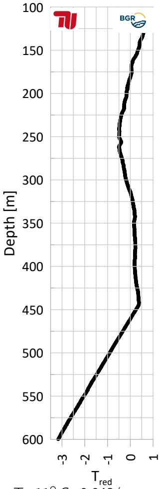

$= T - 11^\circ C - 0.048/m \times z$

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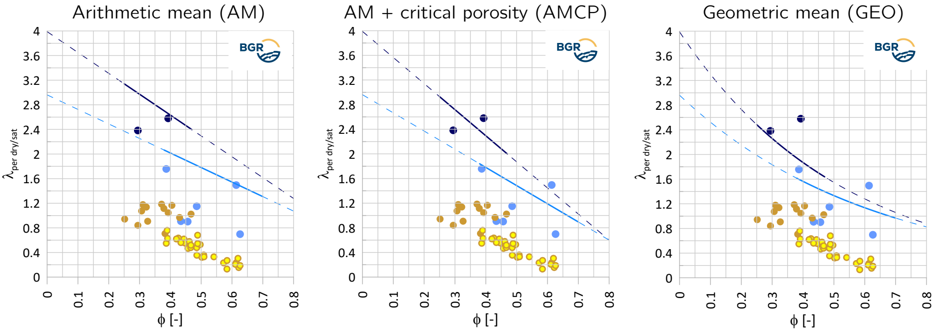
Inferring Uncertain Parameters

Case study: inferring thermal conductivity from observational data

Approach 1: Infer from porosity using mixing models and λ_S



$$\lambda_{\text{AM}} = \phi\lambda_F + (1-\phi)\lambda_S$$

$$\lambda_{\text{AMCP}} = \frac{\phi}{\phi_c}\lambda_F + \left(1 - \frac{\phi}{\phi_c}\right)\lambda_S$$

$$\lambda_{\text{GEO}} = \lambda_F^{\phi} \cdot \lambda_S^{1-\phi}$$

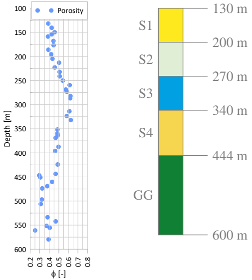
λ_F : fluid thermal conductivity

λ_S : solid thermal conductivity

ϕ_c : critical porosity (=0.8)

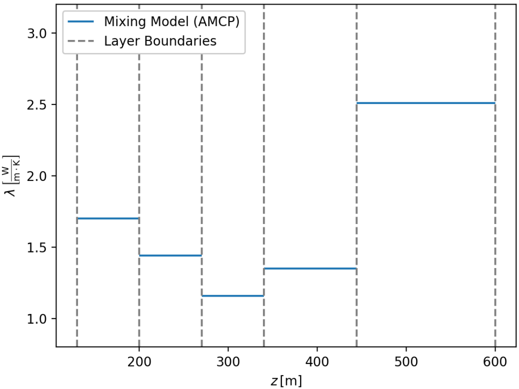
Inferring Uncertain Parameters

Case study: inferring thermal conductivity from observational data



number	abbr	name
0	S1	clay
1	S2	no name
2	S3	Calcareous clay - 1
3	S4	Calcareous clay - 2
4	GG	Exmore

- Determine layer boundaries from porosity observations, mineralogy
- Obtain best fit via mixing model (AMCP) and expert judgment using temperature data.



Inferring Uncertain Parameters

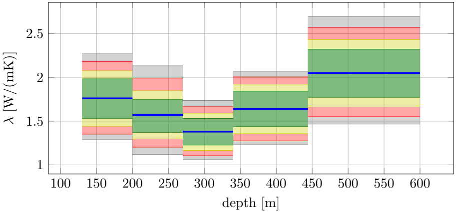
Case study: inferring thermal conductivity from observational data

Allow for uncertainty in ϕ, λ_S, λ_F, q: 5×10^6 uniform Monte Carlo samples

HA	porosity	arithmetic mixing (AM)		AM critical porosity		geometric mixing		heat flow
		λ_S	λ_F	λ_S	λ_F	λ_S	λ_F	
0	0.380 … 0.460	1.82 … 3.38		1.9 … 4.0		3.28 … 5.67		
1	0.425 … 0.605	1.82 … 3.38		1.9 … 4.0		3.28 … 5.67		
2	0.580 … 0.640	1.82 … 3.38	0.6	1.9 … 4.0	0.6	2.98 … 5.20	0.6	0.059..0.071
3	0.460 … 0.500	1.82 … 3.38		1.475 … 3.475		2.64 … 4.01		
4	0.300 … 0.400	1.981 … 3.679		2.989 … 4.989		3.13 … 3.98		

99th, 90th, 70th, 50th percentiles in each layer (AMCP)

Example: ☞ **Poster Thermobase**



Approach 2: Invert T measurements for λ (based on T_{top}, q_{bottom})

Fourier's law + conservation of energy
$\rightsquigarrow$ 1D boundary value problem relating $\lambda = \lambda(z)$ with $T = T(z)$

$$
\begin{aligned}
(\lambda T')' &= 0, \qquad z_0 < z < z_\infty, \\
T|_{z=z_0} &= T_0, \\
\lambda T'|_{z=z_\infty} &= q_\infty.
\end{aligned}
$$

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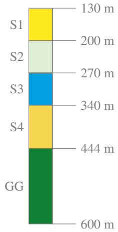
$$\begin{aligned} (\lambda T')' &= 0, \qquad z_0 < z < z_\infty, \\ T|_{z=z_0} &= T_0, \\ \lambda T'|_{z=z_\infty} &= q_\infty. \end{aligned}$$

Given temperature measurements $\{T(z_j)\}_{j=1}^n$, estimate λ (piecewise constant) by least squares (LS) minimization

$$\sum_{j=1}^n [T(z_j;\lambda) - T_j]^2 \to \min_\lambda,$$

Comparison with mixing model



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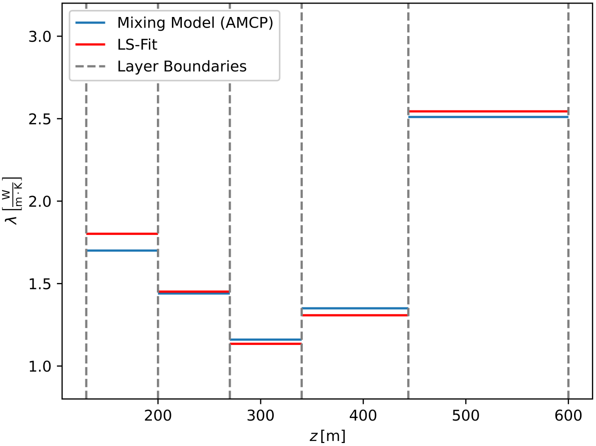


Modeling uncertainty via Bayesian inference

Procedure:

1. Prior: model uncertain $\lambda = \lambda(z)$ as random function drawn from a probability distribution μ_0 on $C[z_0, z_\infty]$.
2. Data: inform prior distribution by incorporating temperature measurements $\{T(z_j)\}_{j=1}^n$.
3. Posterior: model reduced uncertainty in λ due to measurements by conditional distribution $\mu = \mu_0 | \{T(z_j)\}_{j=1}^n$
4. Statistics: infer statements on λ from statistics of posterior distribution such as posterior mean

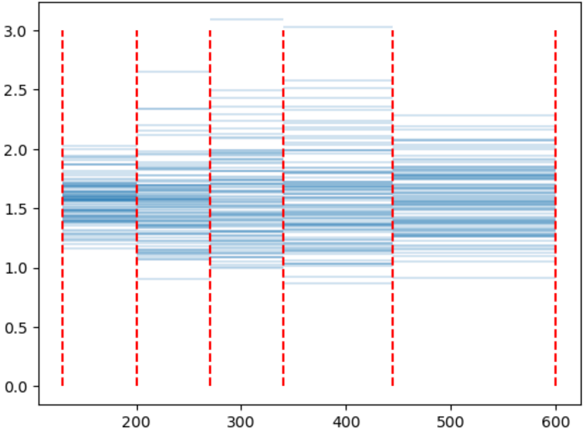
$$\overline{\lambda} := \mathbf{E}_{\lambda \sim \mu} [\lambda.]$$

Inferring Uncertain Parameters

Case study: inferring thermal conductivity from observational data

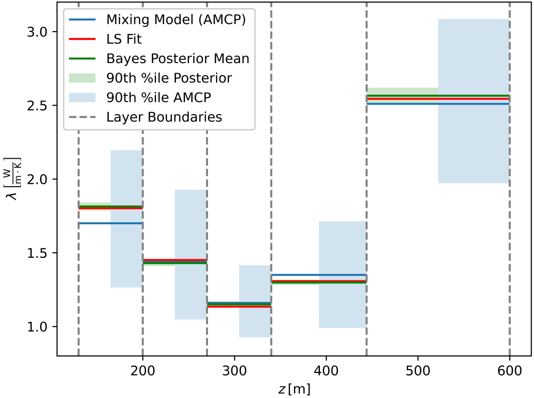
Modeling uncertainty via Bayesian inference

Prior distribution: Correlated Gaussians at layer centers



Modeling uncertainty via Bayesian inference

Comparison of layer-wise UQ approaches: variation of 5 layer values of λ

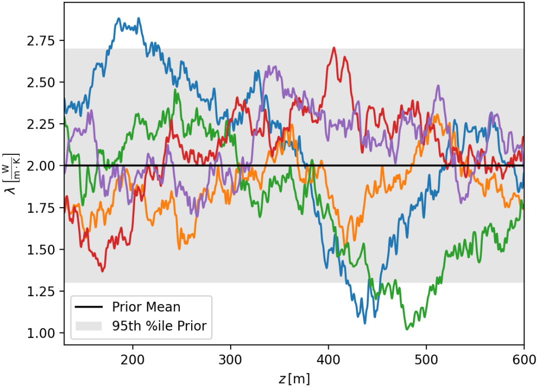


Inferring Uncertain Parameters

Case study: inferring thermal conductivity from observational data

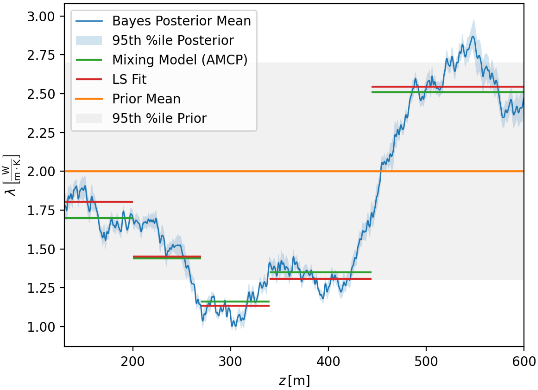
Bayesian inference in function space

Function space prior: Samples from Gaussian process on $[z_0, z_\infty]$
constant mean from data, correlation length 140 m



Bayesian inference in function space

Posterior distribution: Posterior mean and variability
prior with constant mean (no layer information)

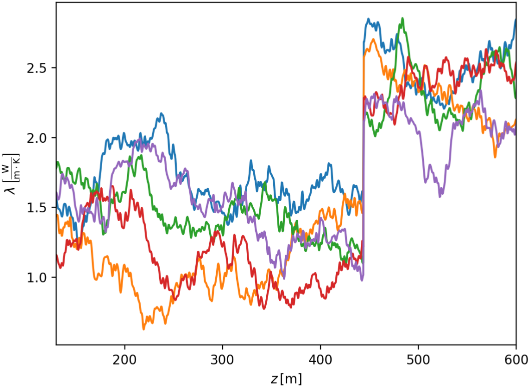


Inferring Uncertain Parameters

Case study: inferring thermal conductivity from observational data

Bayesian inference in function space

Prior distribution: Samples from Gaussian process on $[z_0, z_\infty]$
discontinuous mean at 1 layer boundary

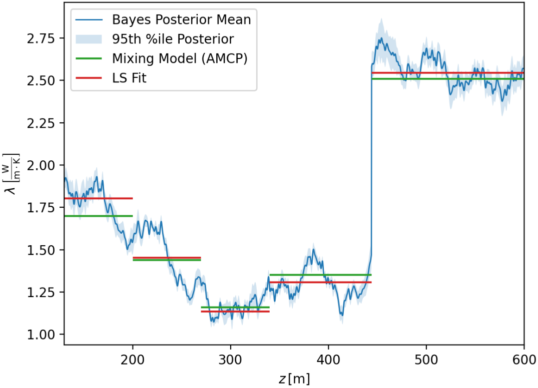


Inferring Uncertain Parameters

Case study: inferring thermal conductivity from observational data

Bayesian inference in function space

Posterior distribution: Posterior mean and variability
last layer jump in prior



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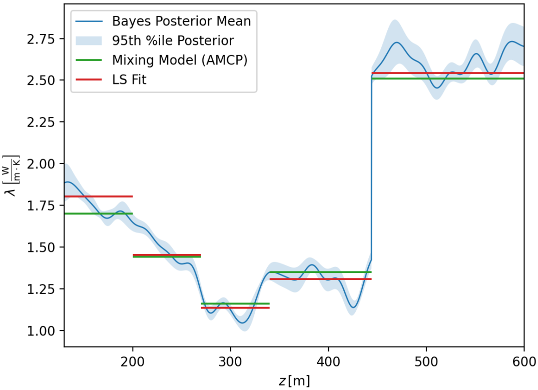
Bayesian inference in function space

Posterior distribution: Posterior mean and variability
low-dimensional state space (smoother realizations)

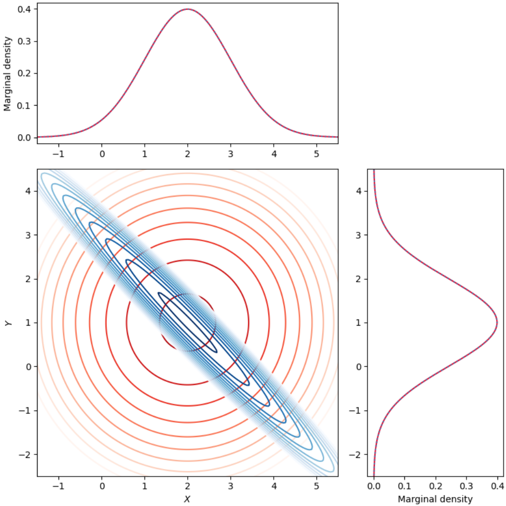


Outlook

Data-Free Inference (Berry et al., 2012)

Is it enough to model each parameter independently?

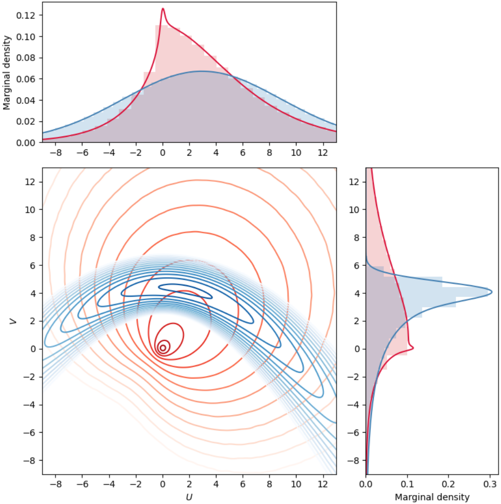
Two bivariate normals
with the same marginals.



Is it enough to model each parameter independently?

Their image distributions under mapping

$$\begin{bmatrix} X \\ Y \end{bmatrix} \mapsto \begin{bmatrix} X^2 - Y^2 \\ 2XY \end{bmatrix}$$



Conclusions / Ongoing Work

- Probabilistic assessment of parameter uncertainty
- Crucial for assessing variability of simulation inputs
- Combination of geological expertise and statistical computing[3]
- Model uncertainty in choice of mixing models

Ongoing:

- DFI to recover dependencies between uncertain parameters (allows reduction in parameter combinations)
- Neural networks for Bayesian posterior via conditional optimal transport

Save the date:
Frontiers of Uncertainty Quantification in Subsurface Environments
September 2026, TU Bergakademie Freiberg (GAMM AG UQ)

Thank you for your attention ☺.

[3] Sibylle I. Mayr et al. "Uncertainty-Guided Interpretation of Thermal Measurements in Sedimentary Units". In: *In preparation* (2025).

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