

Application of experimental design-based assisted history matching for uncertainty quantification in radioactive waste repositories

Integrity of Nuclear Waste Repository Systems – Cross-Scale System Understanding and Analysis

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Bundesministerium
für Bildung
und Forschung

HELMHOLTZ

RESEARCH FOR GRAND CHALLENGES

OpenGeoSys

OPEN-SOURCE MULTI-PHYSICS

Internet – 04.05.2020

Safety assessment \Rightarrow **Probabilistic integrity analysis** \Rightarrow **UQ/SA**

- ▶ safety needs to be 'guaranteed' for $\approx 10^6$ a
- ▶ large spatial extends
- ▶ processes on many different scales need to be considered

\Rightarrow large epistemic uncertainties

Modelling of Underlying Physical Processes

Thermo-Hydro-Mechanical-Chemical and Biological Models

- ▶ host rocks: rock salt, crystalline, clay rock
- ▶ in deterministic FE models
- ▶ of THM/C(B) processes
- ▶ uncertainties: parameter and model

⇒ **OpenGeoSys**
OPEN-SOURCE MULTI-PHYSICS

Heat transport

$$c\rho \frac{\partial T}{\partial t} = -\nabla \cdot (-K\nabla T + \sum_{\beta} h_{\beta} \vec{F}_{\beta}^{\kappa}) + q$$

Thermodynamics

Mechanics

Deformation

$$\nabla \cdot \vec{\sigma} - \rho \vec{g} = 0$$

$$\nabla \cdot (\sigma - (S^L p^L + S^G p^G) \mathbf{I} - \beta_T \Delta T \mathbf{I}) + \rho \mathbf{g} = 0$$

Hydraulics

Fluid flow

$$\frac{\partial}{\partial t} \int_{V_n} M^{\kappa} dV_n = \int_{\Gamma_n} \vec{F}^{\kappa} \cdot \vec{n} d\Gamma_n + \int_{V_n} q^{\kappa} dV_n$$

$$M^{\kappa} = \Phi \sum_{\beta} \rho_{\beta} S_{\beta} X_{\beta}^{\kappa}$$

$$\vec{F}_{\beta}^{\kappa} = -\rho_{\beta} \frac{\vec{k} k_{r\beta}}{\mu_{\beta}} (\nabla P_{\beta} - \rho_{\beta} \vec{g})$$

$$\sum_{\beta} S_{\beta} = 1$$

Chemistry

Reactive transport

$$\vec{F}^{\kappa} = \sum_{\beta} (X_{\beta}^{\kappa} \vec{F}_{\beta}^{\kappa} + \rho_{\beta} \vec{D}_{\beta}^{\kappa} \nabla X_{\beta}^{\kappa})$$

$$\ln(K_{P,T}) = \frac{\Delta G_{P,T}^0}{RT}$$

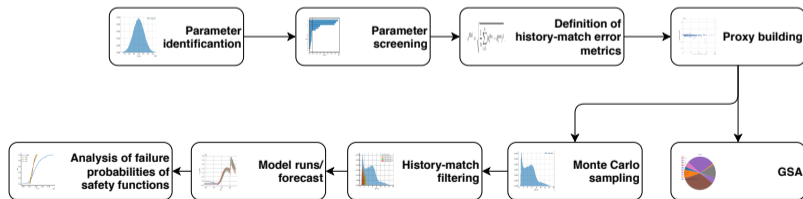
$$K_j = \frac{a_w^{\nu_{w,j}} \prod_i (\gamma_i C_i)^{\nu_{i,j}} \prod_m (a_m)^{\nu_{m,j}} \prod_g (f_g)^{\nu_{g,j}}}{\gamma_j C_j}$$

Source: Kolditz, Olaf, et al. "OpenGeoSys: an open-source initiative for numerical simulation of thermo-hydro-mechanical/chemical (THM/C) processes in porous media." *Environmental Earth Sciences* 67.2 (2012): 589-599.

DoE-based history matching

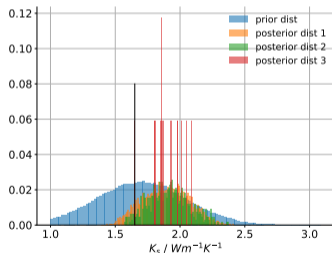
overview

- ▶ consideration of parameter and model uncertainties
- ▶ incorporates exp. data
- ▶ approach general and customizable
- ▶ global sensitivity can be studied on proxy model

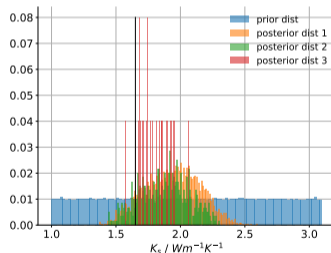


Impact of filter on different priors:

non-uniform prior



uniform prior



Uncertainty Quantification

UQ/SA of THMC models

- ▶ past effort has been mainly on "C"-part (parameter uncertainties in transport of radioactive nuclides)

We want a method that is/can deal with

- ▶ highly non-linear equations and couplings
- ▶ parameter and model uncertainties alike
- ▶ computationally feasible

Simplified analytical model

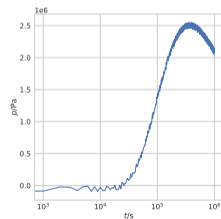
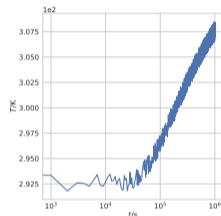
Consolidation around a point heat source

Simplified analytical model of one canister of rad. waste in inf. hom. medium for testing

Thermal consolidation around a point heat source in a fluid-saturated porous medium. Original publication: **Booker, J. R.; Savvidou, C. (1985), International Journal for Numerical and Analytical Methods in Geomechanics, 1985, 9. Jg., Nr. 2, S. 173-184.**

Correction: **Chaudhry, A. A.; Buchwald, J.; Kolditz, O. and Nagel, T. (2019), International Journal for Numerical and Analytical Methods in Geomechanics, 2019, <https://doi.org/10.1002/nag.2998>.**

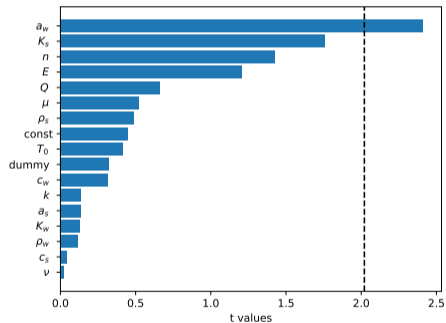
- ▶ includes THM coupling
- ▶ model used for synthetic exp. data generation + analysis



Sensitivity Screening

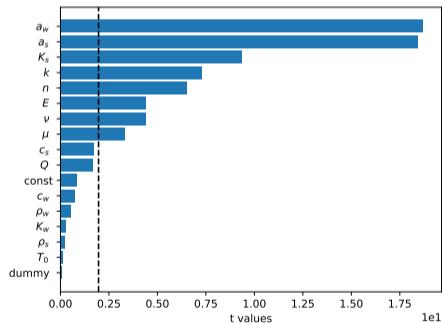
t-test

folded Plackett-Burman (32 samples):



F-Test: 0-Hypothesis confirmed
(prob ≈ 0.9)

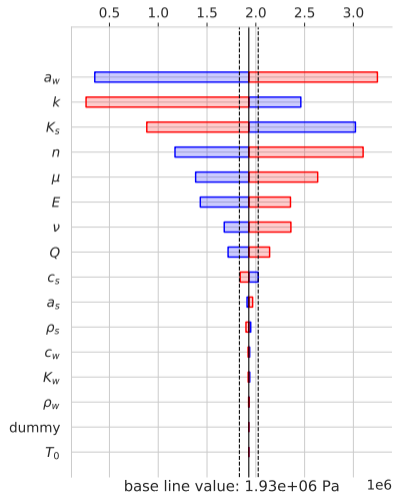
LHS 400 samples



0-Hypothesis rejected (prob $\approx 1.4e - 62$)

Sensitivity Screening

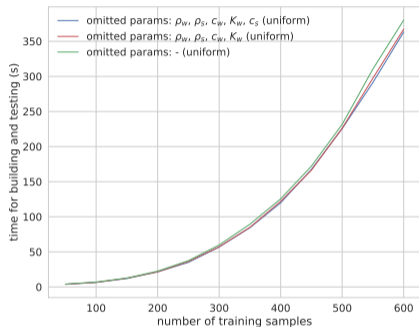
OVAT



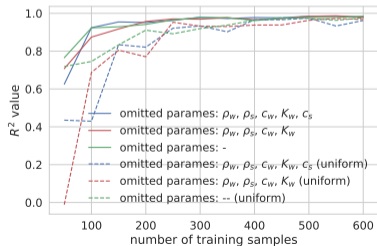
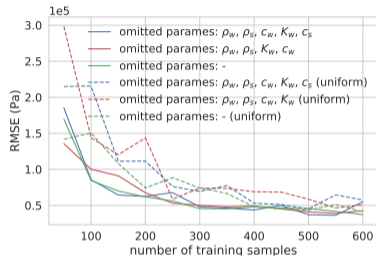
- ▶ Insignificant values: ρ_w , ρ_s , K_w and c_w confirmed by t-test with Latin-hypercube design
- ▶ however, idea is to throw away parameters before building design!
- ▶ what is the cost/gain of reducing uncertainty space?

Proxy Building

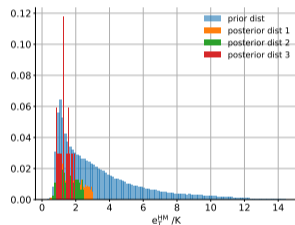
GP regression



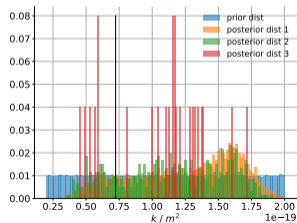
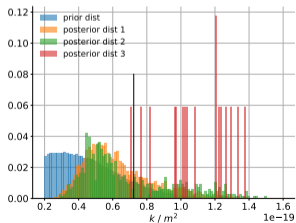
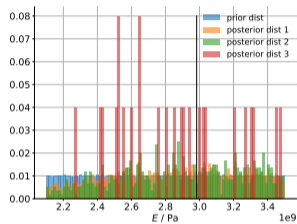
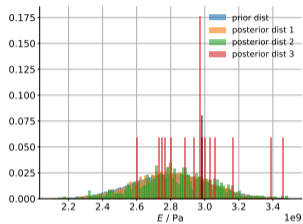
- ▶ neglecting parameters has nearly no influence
- ▶ proxy quality worse for all uniform sampling



- ▶ sampling on proxy
- ▶ sample size: 200 000
- ▶ HM: filtering with three test filters
- ▶ allows also for parameter estimation



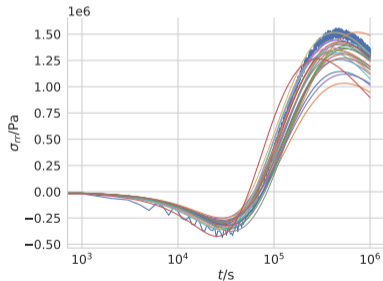
History Match Filtering2: Parameter estimation



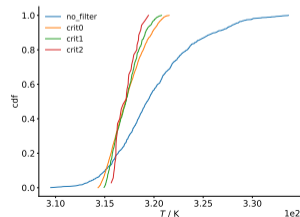
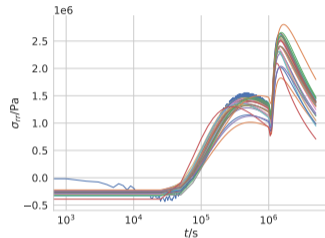
⇒ interactions?

- Real model runs with history match

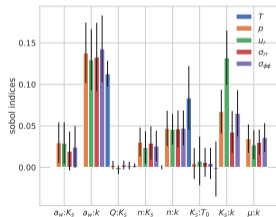
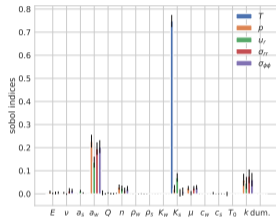
Ana for HM-match



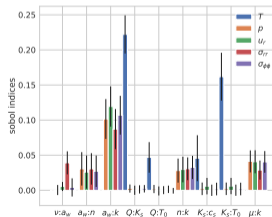
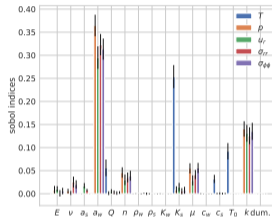
FE-run using OpenGeoSys for forecast with altered BC



S1/S2 based on prior bounds



S1/S2 based on posterior bounds



- ▶ Application of DoE based history-matching to THM model for purpose of UQ/SA in the field of radioactive waste management
- ▶ uncertainty space can be reduced by knowledge of a-priori distributions
- ▶ significant epistemic uncertainties in these systems are unavoidable
- ▶ however specific parameter distributions have only a minor influence on the output
- ▶ filter must be chosen with care
- ▶ filter effect is also significant for GSA

Outlook:

- ▶ application to real experiments already taking place at Mt. Terri URL site
- ▶ investigation of impact cross-scale heterogeneities