INFERRING PRESSURE PROFILES FROM NEUTRON DATA THROUGH BAYESIAN CALIBRATION

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Summary: We propose employing Bayesian calibration to match observed neutron data with calculated moisture contents. Hereby the calibration effort aims at minimizing the uncertainty regarding the experimental boundary conditions, after which the model can be interrogated for pressure data. The proposed formulation explicitly accounts for image noise and model bias. The approach is illustrated for the case of evaporative drying in limestone.

1. INTRODUCTION

Dynamic imaging of fluid flow in porous media is of interest to a wide range of problems, ranging from the integrity of civil engineering structures, over the storage of CO_2 or natural gas in underground reservoirs, up to the safe storage of long-term nuclear waste. Hereby imaging methods can yield quantitative information on the phase distributions and the local saturation degree. Directly observing pressure is however not possible. Typically these are inferred based on a suitable model, in which the uncertain model parameters would be calibrated in order for the results to match the experimental data as closely as possible.

In this contribution we essentially propose a rigorous and automated framework for the calibration procedure, hereby removing the often laborious efforts to obtain a good fit between model and experiment. The proposed approach is based on Bayesian inference, and explicitly accounts for possible model bias and random errors, such as image noise. Furthermore the approach permits estimating uncertainties on the inferred quantities.

2. MODEL CALIBRATION FRAMEWORK

The adopted framework for model calibration is strongly rooted in the work of [1], which by itself is an adaptation of a framework initially proposed by [2]. In this approach, we assume that n observations y are made of a physical system ζ under conditions $\boldsymbol{x}_i$:

$$y(\boldsymbol{x}_i) = \zeta(\boldsymbol{x}_i) + \varepsilon(\boldsymbol{x}_i)$$

where ε describes the observation error and i an index ranging from 1 to n. The physical system can be modelled by means of a suitable simulator $\eta(\boldsymbol{x}_i, \boldsymbol{\theta})$, which generally depends on a number of (physical or non-physical) model parameters $\boldsymbol{\theta}$. Moreover, the model being an imperfect representation of reality, some bias $\delta(\boldsymbol{x}_i)$ cannot be disregarded. The response of the true physical system can thus be replaced by $\zeta(\boldsymbol{x}_i) = \eta(\boldsymbol{x}_i, \boldsymbol{\theta}) + \delta(\boldsymbol{x}_i)$, leading to:

$$y(\boldsymbol{x}_i) = \eta(\boldsymbol{x}_i, \boldsymbol{\theta}) + \delta(\boldsymbol{x}_i) + \varepsilon(\boldsymbol{x}_i)$$

or, the observations y correspond to simulations η made using model parameters $\boldsymbol{\theta}$ after correcting for model bias δ and observation errors ε. The objective of the approach proposed here is to statistically determine the most likely contribution of each of these terms based on a limited number of observations and simulation runs.

To that extent, each of the terms is represented in a stochastic sense. Observation errors can e.g. be represented by a Gaussian distribution with mean zero and a yet unknown variance σ_ε. Unlike observation errors, the bias term is probably not entirely random. Model bias can be considered as an (unknown) function which maps the calculation results on reality under given conditions. A probability distribution on functions (as opposed to values) is called a "stochastic process", and if the distribution is considered Gaussian, we speak of a Gaussian Process (or GP). GPs are fully described by a mean and a covariance function. Here we make the typical choice to adopt a zero mean and a squared exponential covariance function (see e.g. [1]). The zero mean is justified if all data are properly normalized

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prior to the calibration procedure. The covariance function is characterized by two (unknown) parameters, a length scale l_δ and a magnitude σ_δ and is sufficiently flexible to cover a large range of possible functions. Finally, the numerical model η can also be represented by a GP, characterized by a squared exponential covariance function with length scale l_η and magnitude σ_η. The statistical representation of the problem at hand thus adds the unknown variables σ_ε, σ_δ, σ_η, l_δ and l_η to the sought optimal parameters $\boldsymbol{\theta}$.

The unknown parameters can be determined using Bayes theorem, which reads:

$$\pi\left(\boldsymbol{\theta}, \sigma_\varepsilon, \sigma_\delta, \sigma_\eta, l_\delta, l_\eta \middle| y\right) \propto L\left(y \middle| \boldsymbol{\theta}, \sigma_\varepsilon, \sigma_\delta, \sigma_\eta, l_\delta, l_\eta\right) \times \pi(\boldsymbol{\theta}) \times \pi(\sigma_\varepsilon) \times \pi(\sigma_\delta) \times \pi\left(\sigma_\eta\right) \times \pi(l_\delta) \times \pi\left(l_\eta\right)$$

The left hand side term describes the probability distribution for all unknown parameters. This distribution is proportional to the product of the likelihood L with a number of prior distributions π. The likelihood simply yields the probability to obtain a result y with a given combination of parameters. The prior distributions give first estimates for these parameters. The Bayesian theorem can be explored with well-established iterative techniques such as Markov Chain Monte Carlo (MCMC). Since a distribution is obtained, we dispose of a quantitative measure for the uncertainty associated with the model parameters $\boldsymbol{\theta}$ (as well as for the other parameters).

3. APPLICATION TO NEUTRON DATA

The described framework is now employed to determine the unknown evaporative flux at the top surface of a limestone sample subjected to drying (see [3] for experimental details). Neutron radiographies are taken at given time intervals and post-processed with QNI [4] (Fig. 1a). Vertical moisture profiles are extracted, averaged over the middle third of the sample to reduce noise, and constitute the observations y (Fig. 1b, grey). Diffusion simulations are conducted using a 1D finite element code for 5 transfer coefficients ranging from 10^{-9} to 10^{-8} s/m. The MCMC solution yields a narrow distribution around 3.95×10^{-9} s/m. Simulated moisture profiles for this value are shown in Fig. 1b (black) and corresponding pressure profiles in Fig. 1c. MCMC calibration takes around 150 ms.

References

[1] Higdon, D., Gattiker, J., Williams, B., Rightley, M., 2008. Computer model calibration using high dimensional output, Journal of the American Statistical Association 103, 570-583.

[2] Kennedy, M. C., O'Hagan, A., 2001. Bayesian calibration of computer models, J. R. Stat. Soc. Ser. B Stat. Methodol. 63, 425–464.

[3] Derluyn, H., 2012. Salt transport and crystallization in porous limestone: neutron - X-ray imaging and poromechanical modelling, dissertation, ETH Zurich, Switzerland.

[4] Hassanein, R.K., 2006. Correction methods for the quantitative evaluation of thermal neutron tomography, dissertation, ETH Zurich, Switzerland.

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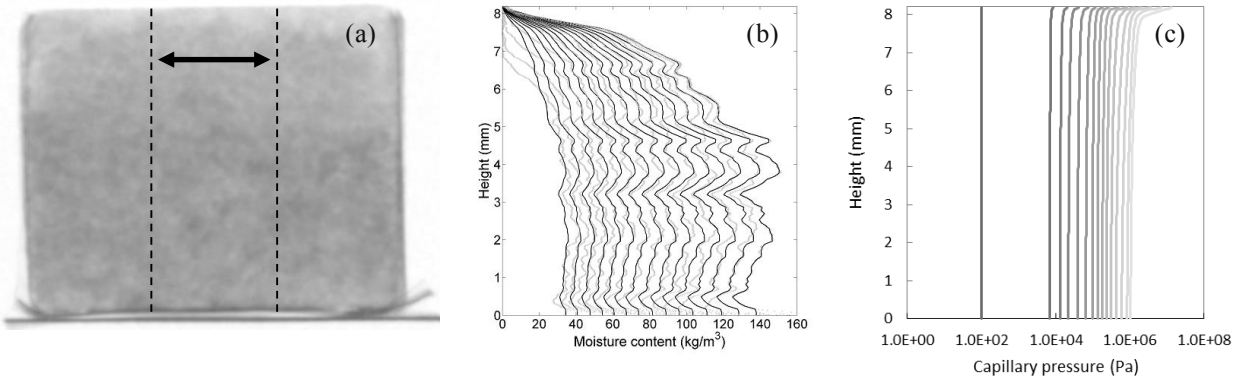

Figure 1: (a) neutron radiography in a limestone sample subjected to drying at t_0, (b) measured (grey) and simulated (black) moisture content profiles for different points in time, and (c) simulated pressure profile. Simulated profiles in (b) and (c) use the most likely transfer coefficient, as determined from MCMC.