

# On Uncertainty Quantification in Hydrogeology and Hydrogeophysics

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## Abstract

Recent advances in sensor technologies, field methodologies, numerical modeling, and inversion approaches have contributed to unprecedented imaging of hydrogeological properties and detailed predictions at multiple temporal and spatial scales. Nevertheless, imaging results and predictions will always remain imprecise, which calls for appropriate uncertainty quantification (UQ). In this paper, we outline selected methodological developments together with pioneering UQ applications in hydrogeology and hydrogeophysics. The applied mathematics and statistics literature is not easy to penetrate and this review aims at helping hydrogeologists and hydrogeophysicists to identify suitable approaches for UQ that can be applied and further developed to their specific needs. To bypass the tremendous computational costs associated with forward UQ based on full-physics simulations, we discuss proxy-modeling strategies and multi-resolution (Multi-level Monte Carlo) methods. We consider Bayesian inversion for non-linear and non-Gaussian state-space problems and discuss how Sequential Monte Carlo may become a practical alternative. We also describe

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strategies to account for forward modeling errors in Bayesian inversion. Finally, we consider hydrogeophysical inversion, where petrophysical uncertainty is often ignored leading to overconfident parameter estimation. The high parameter and data dimensions encountered in hydrogeological and geophysical problems make UQ a complicated and important challenge that has only been partially addressed to date.

*Keywords:* Uncertainty quantification, hydrogeology, hydrogeophysics, inversion, proxy models, modeling errors, petrophysics

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## 1. Introduction

The subsurface environment is highly heterogeneous and non-linear coupled processes take place at multiple spatial and temporal scales. Valuable information about subsurface structures and processes can be obtained from borehole  
5 measurements, outcrops, laboratory analysis of field samples, and from geophysical and hydrogeological experiments; however, this information is largely incomplete. It is critical that basic scientific studies and management decisions for increasingly complex engineering challenges (e.g., enhanced geothermal systems, carbon capture and storage, nuclear waste repositories, aquifer storage  
10 and recovery, remediation of contaminated sites) account for this incompleteness in our system understanding. This enables us to consider the full range of possible future outcomes, to base scientific findings on solid grounds and to target future investigations. Nevertheless, uncertainty quantification (UQ) is highly challenging because it attempts to quantify what we do not know. For  
15 example, it is extremely difficult to properly describe prior information about a hydrogeological system, to accurately quantify complex error characteristics in our data, and to quantify model errors caused by incomplete physical, chemical, and biological theories.

Eloquent arguments have been put forward to explain why numerical models  
20 in the Earth Sciences cannot be validated [1, 2]. These arguments are based on Popperian viewpoints [3] and on the recognition that natural subsurface systems

are open and inherently under-sampled. This implies that UQ in the Earth Sciences can never be considered to be complete. Instead, it should be viewed as a partial assessment that is valid for a given set of prior assumptions, hypotheses, and simplifications. With this in mind, UQ in terms of probability distributions, often characterized in terms of probability density functions (pdfs), can still greatly help to make informed decisions regarding, for example, strategies for mitigating the effects of climate change, how to best exploit natural resources, how to minimize exposure to environmental pollutants, and how to protect environmental goods such as clean groundwater.

This review focuses on UQ in hydrogeology and hydrogeophysics. Using the term UQ, we refer both to (i) the forward UQ problem, namely how to characterize the distribution of output variables of interest (e.g., to determine the risk of contamination in a water supply well) given a distribution of input variables (e.g., subsurface material properties); and (ii) the solution of the Bayesian inverse UQ problem, whereby prior knowledge is merged with (noisy) observational data and numerical modeling in order to obtain a posterior distribution for the input variables. Note that it is beyond the scope of this work to make an exhaustive review of UQ or to present all existing and potential applications in hydrogeology and hydrogeophysics. Rather, we try to connect a number of recent methodological advances in UQ with selected contemporary challenges in hydrogeology and hydrogeophysics. The mathematical development and the description of the methods are kept to a minimum and ample references are provided for further reading. We emphasize general methods that do not necessarily rely upon linearizations or Gaussian assumptions. The price to pay for this generality is a substantial increase in computational cost, which is reflected by the fact that more approximate approaches are presently favoured (e.g., Ensemble Kalman filters [4], quasi-static linear inversion [5]). Clearly, these approximate methods are not only used because they are comparatively fast, but also because they have shown to produce useful and robust results in a wide range of application areas.

After introducing the main concepts and notations (section 2), we discuss

the definition of prior distributions for spatially distributed parameter fields (section 3.1). This is followed by a discussion on the role of proxy models in forward UQ (section 3.2), after which we present how Multi-Level Monte Carlo and related techniques can be used within forward UQ to propagate prior uncertainties into quantities of interest (section 3.3). Next, we consider the Bayesian inverse problem where we examine likelihood functions (section 4.1) and discuss sampling approaches with an emphasis on particle methods (section 4.2). This is followed by an outlook towards how to best account for model errors (section 5.1) and petrophysical-relationship uncertainty in hydrogeophysical inversions (section 5.2).

## 2. Main concepts and notations

In hydrogeology, it is often desirable to predict and characterize uncertainties on Quantities of Interest (QoI) given a set of inputs described by a multivariate parameter  $\mathbf{u}$ . Depending on the problem,  $\mathbf{u}$  may refer to a vector, a field, a more general function, or combinations thereof; here, without loss of generality, we use the “field” as a generic term to denote  $\mathbf{u}$ . As an example,  $\mathbf{u}$  may represent a permeability field and a contaminant source region, and the QoI may be the contaminant concentration in a water supply well at some future time. In this case, the forward model that links the two would typically be a numerical solver of the advection-dispersion equation for some set of (possibly uncertain) boundary and initial conditions. Herein,  $\mathbf{u}$  is treated either as a discretized (finite-dimensional) or continuous (infinite-dimensional) object. This distinction might seem superfluous at first because discretization is always needed at some stage when dealing with numerical forward models; however, considering an infinite-dimensional formalism can be highly relevant as discussed later.

A given QoI, denoted by  $\mathbf{Q}$ , is a function of the output from the considered *solution map* (in practice, the output of a numerical simulator), formalized as a deterministic function  $\mathcal{R} : \mathbf{u} \mapsto \mathcal{R}(\mathbf{u})$  that is generally non-linear. Here, we use  $\mathcal{Q}$  for the function mapping  $\mathbf{u}$  to  $\mathbf{Q}$ . This function can be formulated as  $\tilde{\mathcal{Q}} \circ \mathcal{R}$

for some function  $\tilde{\mathcal{Q}}$  as  $\mathbf{Q}$  is assumed to depend on  $\mathbf{u}$  solely via  $\mathcal{R}(\mathbf{u})$  so that  $\mathbf{Q} = \mathcal{Q}(\mathbf{u}) = \tilde{\mathcal{Q}}(\mathcal{R}(\mathbf{u}))$ .

In essence, the probabilistic approach to forward UQ consists of endowing  
85 the considered set of  $\mathbf{u}$ 's with a probability distribution  $\mu_0$ , and propagating this distribution to  $\mathbf{Q}$  by using uncertainty-propagation techniques. The standard means of doing this, referred to as the basic Monte-Carlo method, consists of drawing a sample  $\{\mathbf{u}_1, \dots, \mathbf{u}_N\}$  from  $\mu_0$ , calculating the corresponding sample  $\{\mathcal{Q}(\mathbf{u}_1), \dots, \mathcal{Q}(\mathbf{u}_N)\}$ , and empirically approximating expectations of functions  
90 of  $\mathbf{Q}$  under the discrete probability distribution  $\frac{1}{N} \sum_{i=1}^N \delta_{\mathcal{Q}(\mathbf{u}_i)}$ .

Practical and theoretical work over the past decade has focused on how to best account for imperfect numerical modeling (see section 3.2), for instance via error models, and how to take advantage of multiple numerical models with different levels of fidelity and computation times (see section 3.3). Overall, propa-  
95 gating uncertainties in the inputs, accounting for imperfect numerical modeling, and addressing real-world problems using statistical procedures and numerical models are broadly considered as part of *uncertainty propagation* or *forward UQ*.

Inverse problems have played an important role in applied mathematics for  
100 more than a century and are of crucial importance in hydrogeology (e.g., [6, 7, 8]) and geophysics (e.g., [9, 10, 11]). The starting point when solving an inverse problem is to write the relation linking observed data  $\mathbf{y}$  to model parameters  $\mathbf{u}$

$$\mathbf{y} = \mathcal{G}(\mathbf{u}) + \epsilon, \quad (1)$$

where the *forward map*  $\mathcal{G} : \mathbf{u} \mapsto \mathcal{G}(\mathbf{u})$  can be viewed as the combination of a *solution map*  $\mathcal{R}$  and an *observation map*  $\mathcal{O}$  that returns  $n \geq 1$  functionals of  
105  $\mathcal{R}(\mathbf{u})$  (typically linear forms, such as point-wise evaluations at specific locations and/or times), and  $\epsilon$  typically stands for observational noise. In simpler terms,  $\mathcal{O}$  extracts from the output of the solution map the information that is needed to calculate the forward responses  $\mathcal{G}(\mathbf{u}) = \mathcal{O}(\mathcal{R}(\mathbf{u}))$ , that are to be compared with the observed data  $\mathbf{y}$ .

110 For example,  $\mathbf{u}$  may stand for lithological properties of an aquifer, with

$\mathcal{R}$  returning the space-time evolution of contaminant concentration within this aquifer. The corresponding  $\mathcal{O}$  could indicate concentrations at specific well locations and times, and the inverse problem would then consist of recovering the unknown lithology from noisy measurements  $\mathbf{y}$  at these locations. In practice,  
115  $\mathcal{G}$  is the best possible numerical prediction of an experiment, but it is never a perfect map in a strict mathematical sense. This implies that virtually all  $\mathcal{G}$ 's in the geosciences could be considered as proxy models (see section 3.2) and we use  $\mathcal{G}$  herein when referring to high-fidelity forward simulations. While we do not explicitly consider  $\epsilon$  terms that incorporate model errors at this stage, the  
120 topic is implicitly tackled in forthcoming sections on likelihood functions and error modeling.

The inherent inaccuracies of forward solvers  $\mathcal{G}$  have two origins. First, geological and physical heterogeneity are present at all scales, but numerical forward solvers can only handle heterogeneity up to a given spatial (e.g., model cell size)  
125 or spectral (e.g., truncation of spherical harmonics) resolution. The impact of limited resolution on simulation results depends strongly on the physics involved. For example, predicted gravimetric or groundwater-level responses will be comparatively insensitive, whereas seismic or ground penetrating radar (GPR) full-waveform modeling or tracer transport simulation results may be highly sensi-  
130 tive [12]. Second, considerable simplifications of the underlying physics are often made, even when using the most advanced simulation algorithms. The needed simplifications and their impacts are strongly problem dependent. For instance, gravimetric modeling can be performed using physical descriptions that are highly accurate, whereas GPR forward modeling typically does not account for  
135 the well-known frequency-dependence of subsurface electrical properties or the finite sizes of transmitter and receiver antennas [13]. Furthermore, the accuracy of  $\mathcal{G}$  for a given physical description and model domain depends also on the numerical schemes (e.g., in time) and equation solvers (e.g., iterative, direct) employed. Despite these simplifications, evaluating  $\mathcal{G}(\mathbf{u})$  (i.e., solving the for-  
140 ward problem) often leads to significant computing times (e.g., [14, 15]), which limits the number of forward simulations that can be practically considered.

In hydrogeology and geophysics,  $\mathbf{u}$  is generally high-dimensional,  $\mathcal{G}$  is costly to evaluate and non-linear, and the size of  $\mathbf{y}$  is limited by data acquisition constraints. Bayesian inversion (the inverse UQ problem) provides a framework to make inferences on  $\mathbf{u}$  from observations  $\mathbf{y}$  by formulating and inferring the posterior distribution  $\mu^{\mathbf{y}}$ . Since analytical derivations of posterior distributions are generally intractable, Bayesian inverse problems call for Markov chain Monte Carlo (MCMC) and related sampling procedures (see section 4.2). Below, we first focus on the topic of defining the prior  $\mu_0$  (i.e., a probabilistic description of model parameter values and their relations before considering the observed data); an essential component both in uncertainty propagation (forward UQ) and Bayesian inversion (inverse UQ).

### 3. Prior distributions and forward UQ

#### 3.1. Prior distributions on parameter fields

Defining a prior distribution,  $\mu_0$ , for a spatial parameter field  $\mathbf{u}$  is a challenging task. Since the advent of geostatistics, and notably the seminal works of Krige [16] and Matheron [17], a central approach underlying the prediction of spatially distributed variables has been to view the true but unknown field of interest as one realization of a random field (i.e., a random process with multivariate index space). In basic versions of kriging, no distributional assumptions on the field were made beyond the existence of moments. However, the Gaussian assumption delivers a way to express the simple-kriging equations in terms of conditional expectation and variance, thus allowing for conditional simulations [18, 19]. With time, this initial Gaussian model was further developed to account for positivity (e.g., with log-Gaussian fields) and other constraints [20, 21]. Connections between kriging, Gaussian random fields, and Bayesian inference have been made notably in [22, 23, 24, 25, 11, 26]. This has led to a number of developments, for instance, hierarchical models that include distributions on hyperparameters describing Gaussian process models [27, 28]. Throughout the paper, we use the notions of random processes and fields exchangeably. Note

also that the Gaussian-random-field terminology is equivalent to what is often referred to as *multi-Gaussian* in the geosciences.

In mathematics, Gaussian-related priors have been recently revived through their omnipresence in the blossoming field of UQ. Due to their favorable properties and well developed mathematical theory, Gaussian random fields, or equivalently Gaussian measures on function spaces [29], have been extensively used in the study of stochastic partial differential equations (PDEs) [30, 31] and PDEs with random coefficients (e.g., [32]). Recent contributions to the stochastic PDE approach to Gaussian-random-field modelling have highlighted its ability to cope with large data sets and to encode non-stationarity in a powerful way [33, 34, 35, 36]. Also, theoretical aspects of infinite-dimensional Bayesian inverse problems with Gaussian-random-field priors have been investigated [37, 38, 39], where  $\mu_0$  is specified in terms of random series  $\mathbf{u} = \phi_0 + \sum_{j=1}^{+\infty} u_j \phi_j$ , with  $\phi_j$  denoting functions in a Banach space (i.e., a complete normed vector space) and  $u_j$  Gaussian random coefficients. Non-Gaussian extensions (e.g., for uniformly distributed  $u_j$ 's) have also been considered [40, 41, 42].

The impact of non-Gaussian property fields on stochastic forward simulations have been investigated (e.g., [43]) with results illustrating that covariances are insufficient to characterize geologically realistic subsurface properties. To address this, multiple-point statistics (MPS) simulation has arisen as a new paradigm that has deeply influenced modern geostatistics [44, 45, 46, 47, 48]. Connections between MPS and Markov random fields [49, 50], texture synthesis developed for computer graphics purposes [51], and universal kriging [52] have been investigated. [53] studied the ability of MPS to reproduce statistical properties of a random field by averaging over a large number of MPS realizations obtained from a single training image. Exact statistical recovery was only shown to be possible when the training image was an ‘infinitely’ large realization of a stationary and ergodic random field (i.e., statistical properties do not change in space and statistics can be recovered from one realization). The influence of Gaussian-random-field and training-image-based priors on the solution of geophysical inverse problems was examined in [54]. It was found that complex



prior information not only enhances the geological realism of posterior model realizations, but also renders the inference problem easier and faster to solve compared to the case of non-constraining priors. In field applications, the main challenge in applying MPS is how to obtain representative training images. For recent reviews on geologically realistic prior model definitions and inversion, we refer to [55, 56].

The process of choosing realistic and implementable prior distributions is a crucial yet rarely addressed topic that is often restricted to mean and covariance selection for Gaussian random fields or training image definition in MPS. In all instances, choices must be made that may dramatically influence forward UQ and the posterior distributions obtained through Bayesian inversion. Already for the Gaussian case, designing the covariance function (kernel) is a delicate task that implies a range of assumptions on the physical attributes for which one is inverting. For instance, the choice of a specific family of covariance function automatically defines the spatial regularity (smoothness class) of each realization drawn from the prior distribution and, hence, from the posterior distribution as well (see [57] for results in the Gaussian case and beyond). The impact of the prior is clearly shown in [54] who inverted the same synthetic data set using different prior models (Fig. 1). It is seen that the spatial statistics are largely determined by the prior model, while regions of predominantly high- or low velocities are determined by the data used in the inversion.

### 3.2. Proxy models for forward UQ

Proxy or surrogate models are often used when the full or high-fidelity forward response is too expensive to be systematically used in computations. They are commonly employed when a large number of forward simulations are required for UQ or sensitivity analysis applications. Proxy models can be grouped into two broad categories: lower-fidelity models and metamodels. Lower-fidelity proxies are typically physically-based; however, they contain less detail and therefore offer a less accurate, but cheaper-to-run, means of computing forward responses than their high-fidelity counterparts. Model simplifications are gen-

erally made by (i) considering only some of the physics involved, either through approximations or by explicitly ignoring particular elements (e.g., [58]); (ii) reducing the numerical accuracy of the forward model response by, for example, coarsening the spatial discretization (e.g., [59]) or using model-order-reduction (MOR) approaches (e.g., [60]). In contrast, metamodels are usually not linked to the physics of the problem at hand. Instead, they are based on data-driven approximations of the forward model response using a relatively small number of high-fidelity simulation outputs. Methods that fall into the latter category notably include response surface modeling (RSM) (e.g., [61]), polynomial chaos expansion (PCE) (e.g., [62]), artificial neural networks (e.g., [63]), radial basis functions (e.g., [64]), and Gaussian process (GP) models [65, 66].

Hydrogeology has seen significant use of proxy models for forward UQ and sensitivity analysis. Being physically-based, lower-fidelity models have the advantage over metamodels in that they may better emulate the original response in unexplored regions of the input parameter space and are generally less susceptible to problems in high parameter dimensions (e.g., [67]). In this regard, [68, 69] employ simplified-physics proxies for subsurface flow and transport together with distance and kernel methods (e.g., [70]) in order to select, from a large number of permeability fields, a small subset of representative fields upon which to run high-fidelity forward simulations.

In terms of metamodels, many studies have focused on the application of PCE-based methods to hydrogeological problems (e.g., [71, 72]). Basically, a PCE represents the response of a complex system by a polynomial expansion with respect to the input random variables. When using PCEs, polynomials must be chosen that form an orthogonal basis with respect to the assumed probability distribution of input random variables. An important advantage of PCE over other metamodels is that it delivers polynomial approximations that are fast to evaluate and can lead to closed-form expressions (e.g., for Sobol' sensitivity indices) provided that the orthogonal polynomial basis functions are chosen accordingly [73]. Initial work was limited to low-dimensional problems because of the marked increase in the required number of PCE terms with the number

of input parameters. However, recent applications involving sparse grids and truncated spectral expansions of the input random fields report successes with problems involving hundreds of model parameters. Nevertheless, the effectiveness of PCE techniques deteriorates when dealing with input random fields that are rough and/or have short correlation lengths. Hydrogeological applications of metamodeling with Gaussian process models include [74] that considered a hydrogeological transport problem. Here, the use of Gaussian process models were shown to outperform boosting regression trees and linear regression on most considered outputs. Another example is [75], in which a Gaussian process model incorporating proxy simulations and distance information was proposed for a sequential inversion problem where the candidate inputs were generated using MPS simulation.

### 3.3. Forward UQ with Multi-level Monte Carlo

Consider the forward problem of reliably computing the expectation of some quantity of interest  $\mathbf{Q}$  involving the solution of the forward model,  $\mathbf{Q} = \mathcal{Q}(\mathbf{u})$ , where  $\mathbf{u}$  is assumed random with prior distribution  $\mu_0$  (hence  $\mathbf{Q}$  is a random variable). Examples of QoIs could be tracer breakthrough curves or contaminant concentrations for an assumed prior distribution of lithological properties (e.g., porosity, permeability). In practice, approximations of  $\mathcal{Q}(\mathbf{u})$  can only be obtained by numerical simulations that inevitably require discretization or physical simplifications (see section 2). We denote by  $\mathcal{Q}_\ell(\mathbf{u})$  any such numerical solution, where  $\ell$  denotes the resolution level. The latter may refer to the spatial grid discretization and/or time step increments used in the forward simulator, or any other type of model simplification.

In recent years, the so-called *Multi Level Monte Carlo* (MLMC) method has been established as a computationally efficient sampling method that builds upon the classical Monte Carlo technique. It was first proposed in [76] for applications in parametric integration, and then extended to weak approximations of stochastic differential equations in [77] together with a full complexity analysis. The idea behind MLMC is to introduce multiple levels  $\ell = 0, \dots, L$  of increasing

resolution (accuracy) with corresponding numerical solutions  $\mathbf{Q}_0 = \mathcal{Q}_0(\mathbf{u})$ ,  $\mathbf{Q}_1 = \mathcal{Q}_1(\mathbf{u})$ ,  $\dots$ ,  $\mathbf{Q}_L = \mathcal{Q}_L(\mathbf{u})$ . While a classical Monte-Carlo approach would simply approximate the expected value of  $\mathbf{Q}_L$  on a sufficiently high-resolution level  $L$  using an ensemble-average over a sample of independent realizations from  $\mu_0$ , the MLMC method relies upon the simple observation that, by linearity of expectation,

$$\mathbf{E}[\mathbf{Q}] \approx \mathbf{E}[\mathbf{Q}_L] = \sum_{\ell=1}^L \mathbf{E}[\mathbf{Q}_\ell - \mathbf{Q}_{\ell-1}] + \mathbf{E}[\mathbf{Q}_0], \quad (2)$$

and computes each expectation in the sum by *statistically independent* Monte-Carlo sampling. Thanks to independence, the overall variance of the MLMC estimator is given by the sum of the variances of each Monte Carlo estimator. If  $\mathbf{Q}_\ell$  converges to a limit value as the resolution level  $\ell$  increases, the variance of  $(\mathbf{Q}_\ell - \mathbf{Q}_{\ell-1})$  will be progressively smaller as  $\ell$  increases. Dramatic computational savings can thus be obtained by approximating the quantities  $\mathbf{E}[\mathbf{Q}_\ell - \mathbf{Q}_{\ell-1}]$  with smaller sample sizes at higher, and computationally more costly, resolution levels.

The application of MLMC methods to forward UQ problems involving PDE models with random parameters has been investigated from the mathematical point of view [78, 79, 80, 81, 82, 83]. Recent work [84, 85, 86, 87, 88] has also explored the possibility of replacing the Monte-Carlo sampler on each level by other formulas, such as sparse polynomial or quasi-Monte-Carlo quadrature. *Multi-Index Monte Carlo* is a generalization of MLMC that was recently proposed [89] to accommodate and treat independently multiple resolution parameters; potentially, this leads to substantial improvements over MLMC. This idea has been extended to sparse polynomial quadratures [88, 90].

Despite recent efforts, performing accurate forward UQ analyses for high-dimensional hydrogeological and geophysical problems remains a challenging task and further advances are needed with respect to the above-mentioned methods to have a strong impact on applications. Indeed, in hydrogeology, the use of MLMC has been so far limited [91, 92, 93, 94]. For example, [94] considered water flooding of an initially saturated oil reservoir characterized

by a Gaussian-random-field prior describing the logarithm of permeability. Using different quantities of interest and a pre-defined approximation error, they investigated the performance of MC, MLMC with a grid hierarchy of five levels, and an alternative MLMC approach based on a solver hierarchy using fast streamline-based and full reservoir-simulator predictions. With  $\mathbf{Q}$  representing the mean saturation field at a given time, they found that MLMC with grid hierarchy and with solver hierarchy were 28.7 and 3.3 times faster than MC, respectively (Fig. 2). The authors argue that the solver-based hierarchy might be more practical when boundary conditions cannot be accurately defined with a coarse mesh. Combinations of MLMC techniques and metamodels based on sparse-grid PCE approximations have also been proposed [95] to further accelerate the computation of expectations in forward UQ problems with rough input permeability fields.

#### 4. Bayesian inversion

It is well understood [96] that inverse problems are ill-posed unless the search space is drastically restricted. Standard deterministic inversion approaches proceed by penalizing a measure of model structure (e.g., relying on gradients, curvatures, or deviations from a reference model), thereby leading to a unique “regularized” solution. Deterministic approaches are popular because of their simplicity and the efficiency of the associated numerical methods. Although obtaining a unique solution is appealing, these methods do not provide a reliable assessment of uncertainty.

For a finite set of model parameters, a general formulation of the inverse problem is found in the work of [97], wherein the solution of the problem is described as the conjunction of two states of information: (i) a density function describing the prior information about the system, including both the outputs of measurement instruments (i.e., the data) and prior assumptions about model parameter values; and (ii) a density function describing theoretical relationships between model parameters and data. This framework, which naturally accounts

for forward modeling errors, makes it possible to solve the majority of non-linear inverse problems provided that appropriate density functions and the necessary computing resources are available.

Here we focus on the case when  $\mathcal{G}$  is deterministic and we follow a classical *Bayesian* approach, which is extendable to infinite-dimensional model parameter spaces. This approach consists in combining a prior probability distribution  $\mu_0$  of  $\mathbf{u}$  with observed data in order to obtain the *posterior distribution*,  $\mu^{\mathbf{y}}$ . In  $d$ -dimensional cases where  $\mu_0$  and the probability distribution  $\nu_0$  of the error term  $\epsilon$  have probability densities  $\rho_0$  and  $\rho$  with respect to some given measures (e.g., Lebesgue measures on  $\mathbb{R}^\ell$  with  $\ell = d, n$ , respectively), one denotes by *likelihood* the function  $\mathbf{u} \mapsto L(\mathbf{u}; \mathbf{y}) := \rho(\mathbf{y} - \mathcal{G}(\mathbf{u}))$ . Note that the likelihood is also often noted  $L(\mathbf{u}|\mathbf{y})$ , but should generally not be confused with the conditional density of  $\mathbf{u}$  knowing  $\mathbf{y}$ . Assuming further that  $Z := \int_{\mathbf{R}^d} \rho(\mathbf{y} - \mathcal{G}(\mathbf{u}))\rho_0(\mathbf{u})d\mathbf{u} > 0$  then  $\mu^{\mathbf{y}}$  has the *posterior* density (Bayes' theorem)

$$\rho^{\mathbf{y}}(\mathbf{u}) = \frac{1}{Z}\rho(\mathbf{y} - \mathcal{G}(\mathbf{u}))\rho_0(\mathbf{u}) = \frac{1}{Z}L(\mathbf{u}; \mathbf{y})\rho_0(\mathbf{u}), \quad (3)$$

as recalled in [42] and generalized to the infinite-dimensional case as follows. Provided that the translate of  $\nu_0$  by  $\mathcal{G}(\mathbf{u})$ ,  $\nu_{\mathbf{u}}$ , possesses a density  $\frac{d\nu_{\mathbf{u}}}{d\nu_0}(\mathbf{y}) = \exp(-\Phi(\mathbf{u}; \mathbf{y}))$  with respect to  $\nu_0$  for some function  $\Phi$  referred to as *potential*, and assuming that  $Z := \int \exp(-\Phi(\mathbf{u}; \mathbf{y}))d\mu_0(\mathbf{u}) > 0$ , then the posterior distribution  $\mu^{\mathbf{y}}$  possesses a density with respect to  $\mu_0$  with:

$$\frac{d\mu^{\mathbf{y}}}{d\mu_0}(\mathbf{u}) = \frac{1}{Z}\exp(-\Phi(\mathbf{u}; \mathbf{y})). \quad (4)$$

In other words, the posterior distribution can be obtained from the prior distribution via reweighting. Following [42], in the case where  $\nu_0 = \mathcal{N}(0, \Gamma)$  for some  $n \times n$  invertible covariance matrix  $\Gamma$ , the potential function is

$$\Phi(\mathbf{u}; \mathbf{y}) = \frac{1}{2}\|\Gamma^{-1/2}(\mathbf{y} - \mathcal{G}(\mathbf{u}))\|_{R^n}^2 - \frac{1}{2}\|\Gamma^{-1/2}\mathbf{y}\|_{R^n}^2. \quad (5)$$

Analytical formulations for density values and more particularly density ratios make it possible to apply the Metropolis-Hastings algorithm and to generalize it to infinite-dimensional settings. Quoting [42], it is expected that “formulating

the theory and algorithms on the underlying infinite dimensional space [...] enables constructing algorithms which perform well under mesh refinement, since they are inherently well-defined in infinite dimensions.”

#### 4.1. Likelihoods in geoscientific inverse problems

Two important components that must be specified before inferring the posterior distribution  $\mu^{\mathcal{Y}}$  are the forward map  $\mathcal{G}$  and the noise distribution  $\nu_0$ , which together determine the likelihood function  $L(\cdot; \mathbf{y})$  for the finite-dimensional case and/or the potential function  $\Phi(\cdot; \mathbf{y})$  for the infinite-dimensional case. These functions are used to evaluate how likely a given model realization is given the observed data and its noise characteristics. To allow for a large number of forward simulations (as needed for inverse-problem solving), it is often necessary to favor computational speed and make concessions in terms of simulation accuracy. The appropriate trade-off between time-consuming high-fidelity simulations and many fast, but approximate, solutions is problem dependent. Optimal determination of this trade-off is an important topic that we do not treat herein. Presently, the vast majority of Bayesian inversion studies in the geosciences implicitly assume that forward simulators are perfect and hence that modeling errors are negligible (i.e., only observational errors are considered). When acknowledged, the modeling errors are usually considered to be part of  $\nu_0$  [98]. Alternative approaches exist and formal ways to account for proxy errors are discussed in section 5.1. The latter often proceed by an adaptation of the likelihood function by correcting proxy simulations with an error model in order to obtain error-corrected simulations with a quality similar to that of high-fidelity simulations (Fig. 3). There has been limited use of MLMC techniques in Bayesian inversion. The works [99, 100] have combined the multilevel idea with Metropolis-Hastings-type MCMC and, very recently, [101] applied the multilevel idea to Langevin dynamics to sample from a given distribution. An alternative approach to compute posterior expectations of QoIs, which does not resort to MCMC sampling but rather relies on standard MLMC or Quasi-Monte-Carlo integration, was proposed in [102].

Observational errors are most often treated as independent and identically distributed (iid) random variables with zero mean. These errors are typically considered to stem from Gaussian or Laplace distributions, partly because the corresponding likelihood functions have simple forms that are easy to manipulate. More advanced likelihood descriptions have been proposed. For example, [103] introduced and inverted for parameters describing a likelihood function with residual errors that are heteroscedastic and non-Gaussian with varying degrees of kurtosis and skewness. Hierarchical Bayes includes approaches in which parameters describing the likelihood function are considered uncertain. It can be a very powerful approach to relax assumptions about parameter values describing the likelihood function, but it still requires a certain class of noise model to be selected for which the corresponding parameters are inferred. It is common to account for the combined effects of model and data errors in the likelihood function. For instance, [104] estimated hierarchical autoregressive error models that enable efficient handling of correlated errors at low computational costs (e.g., no need to invert the covariance matrix or compute its determinant in order to evaluate the likelihood function). In [105], the authors estimated a correlated error model and used it in the likelihood function to account for errors related to local heterogeneities close to GPR antennas. Using crosshole GPR data, [98] demonstrated how to practically sample a model-error distribution, which was found to be well described by a correlated multivariate Gaussian distribution. They demonstrated severe bias in the inferred posterior distributions when modeling errors were ignored.

#### 4.2. Sampling: Markov chain Monte Carlo and particle filters

When performing Bayesian inference for complex statistical models, it is necessary to approximate numerically the resulting posterior distribution as it is typically intractable to compute analytically. For more than half a century, much effort has been placed on deriving sampling schemes for posterior distributions by relying on *Markov chain Monte Carlo* (MCMC) methods (see [106] and [107] for comprehensive reviews of the literature and [56] for the specific



case of informed spatial priors). These schemes generally consist of sequential perturbations to candidate inputs  $\mathbf{u}$  followed by either acceptance or rejection of the proposed perturbations with a probability that involves the likelihood ratio between the new and the old  $\mathbf{u}$  and their prior probability ratio. Standard algorithms such as the Metropolis-Hastings algorithm and the Gibbs sampler have become very popular but they can be highly inefficient if the proposal distributions are not well-chosen and/or if the target (posterior) distribution exhibits complex patterns of dependence. A substantial research effort has thus been placed on making MCMC approaches more efficient, for instance, via parallel tempering [108], population MCMC [109] and/or through derivative-based perturbations with Metropolis-adjusted Langevin algorithms and Hamiltonian MCMC [110]. In infinite-dimensional settings, adaptations of MCMC schemes have been touched upon, notably in [111], and the links between performance and the spectral gap that controls the rate of exponential decay to  $\mu^{\mathcal{Y}}$  have been established in [112].

MCMC methods for Bayesian inverse problems are suitable when we are interested in inferring parameters, for example, a hidden (unobserved) static random field from data. However, there is also a wealth of data assimilation problems in hydrogeological and geophysical applications that can be recast as statistical inference problems for non-linear and non-Gaussian state-space models [113, 4, 114, 115, 116, 117], with some of the published methods (e.g., [118, 119]) being applicable to complex prior information (e.g., MPS). We discuss below sampling techniques that have been developed in this context. These methods do not make any distributional assumptions on the prior distribution, but we highlight that it still remains to be investigated how they would perform within a MPS context.

Formally, a state-space model is defined by a discrete-time  $\mathbf{R}^{n_x}$ -valued hidden Markov process  $(X_t)_{t \geq 1}$  such that  $X_1 \sim p_{\theta}(\cdot)$  and  $X_t | (X_{t-1} = \mathbf{x}) \sim f_{\theta}(\cdot | \mathbf{x})$  for  $t \geq 2$  and we collect  $\mathbf{R}^{n_y}$ -valued observations  $(Y_t)_{t \geq 1}$  which are conditionally independent given  $(X_t)_{t \geq 1}$  and distributed according to  $Y_t | (X_t = \mathbf{x}) \sim g_{\theta}(\cdot | \mathbf{x})$ . For example, if we assume that  $Y_t = \phi(X_t) + \epsilon_t$  where  $\epsilon_t$  is a mul-

tivariate standard normal noise then  $g(y|x)$  is the multivariate normal density of argument  $y$ , mean  $\phi(x)$  and identity covariance. Here  $\theta \in \Theta$  denotes the parameters of the model. In the case of a static random field to be inferred,   
470  $\theta = \mathbf{u}$ . When  $\theta$  is known, inference about  $(X_t)_{t \geq 1}$  is referred to as state estimation. On-line inference (filtering) refers to sequential assimilation of the data as they become available. In batch/off-line inference (smoothing), the estimated states are also affected by the data acquired at later times. When  $\theta$  also needs to be estimated/calibrated from observations, this is referred to as parameter   
475 estimation and it can also be performed either on-line or off-line. In hydrogeology,  $Y_t$  could represent salinity measurements within a coastal aquifer at some specific time,  $X_t$  the corresponding salinity distribution throughout the same aquifer, and  $\theta$  an unknown hydraulic conductivity distribution and boundary conditions.

480 Standard MCMC methods can be used in this context, but it is often difficult to build efficient algorithms. In many fields such as computer vision, econometrics and robotics, particle methods, also known as Sequential Monte Carlo (SMC) methods, have emerged as the most successful class of techniques to address state estimation problems as they are easy to implement, suitable   
485 for both filtering and smoothing, admit parallel implementation and additionally provide asymptotically consistent state estimates. In its most generic form, SMC consists of initiating particles from an importance distribution at time zero, resampling them to ensure that they have the same weight, using the state associated with each particle to run a forward solver and analyze the   
490 resulting particle weight, and resampling until the particles at the new time have the same weight [120]. On- and off-line parameter estimation procedures building upon these state-estimation procedures have also been proposed; see [121] for a recent comprehensive review. An illustration of hydrogeophysical fully-coupled inversion using a particle filter [114] is given in Figure 4. Other   
495 low-dimensional applications to hydrogeological and hydrogeophysical problems include [113, 122, 123, 115].

Nevertheless, SMC methods have not yet become prominent in hydrogeol-

ogy. This is because  $X_t$  often corresponds to a high-dimensional spatial field and the variance of SMC state estimates is typically exponential in the state dimension  $n_X$  where routinely  $n_X > 10^3$ . This problem is often referred to in the literature as the *curse of dimensionality* for particle methods [124]. Hence, practitioners rely on alternative approximation techniques such as the Ensemble Kalman filter (EnKF) [4, 116, 117]. Empirically, the EnKF scales much better with  $n_X$  than particle methods, but relies on potentially crude Gaussian approximations of the posterior distributions of interest. A non-standard particle method known as the equivalent weights particle filter has also been proposed and has shown empirical success in addressing high-dimensional data assimilation problems [125]. However, it does not provide consistent state estimates and it is unclear how to control the error introduced by this scheme. The need for novel particle methods that can scale to high-dimensional settings has been recognized and there is a fast emerging literature addressing these problems in data assimilation and statistics [126, 127, 128, 129]. A detailed theoretical analysis of such a scheme has been proposed in [130] where it was shown rigourously that it can overcome the curse of dimensionality. These methods provide asymptotically biased state and parameter estimates, the bias being controlled under suitable regularity assumptions, or consistent estimates whose mean square errors go to zero at a slower rate than the usual  $1/N$  Monte Carlo rate [130, 131]. The main idea behind these techniques is to ignore long-range dependencies when performing Bayes updates in a filtering procedure, an idea borrowed from the ensemble Kalman filter literature where it is referred to as localization [4]. The components of the state are partitioned into blocks and resampled using only the corresponding observations. Some of these methods are promising for high-dimensional hydrogeological and hydrogeophysical state and parameter estimation although several challenges remain to be addressed. First, these methods introduce a non-homogeneous bias amongst state component estimates, which is damaging as  $X_t$  often corresponds to a spatial field (e.g., salinity or soil moisture distribution) in hydrogeological applications [129]. Second, the smoothing and parameter estimation procedures developed in [131]

cannot be applied when only forward simulation of  $(X_t)_{t \geq 1}$  is feasible. Third,  
530 while consistent estimates can be obtained by scaling the size of the blocks with  
 $N$ , the resulting rate of convergence is low and new efficient approaches are  
required.

An alternative class of particle-based techniques that provides consistent  
state and parameter estimates in high-dimensional settings are off-line proce-  
535 dures which build on particle MCMC methods, a class of MCMC methods  
relying on particle proposals introduced in [118]. For example, [132] presented  
a modification of the conditional SMC algorithm of [118] which performs em-  
pirically significantly better in high-dimensional settings by introducing posi-  
tive correlation between particles [119]. [133] proposed a block Gibbs sampling  
540 scheme by updating the path of one state component at a time conditional on the  
other component paths. Although these techniques are not yet well-understood  
theoretically, they are highly promising. However, when they are used to per-  
form parameter estimation, they alternate between updating  $\theta$  conditional to  
 $(X_t)_{t \geq 1}$  and  $(X_t)_{t \geq 1}$  conditional to  $\theta$ . As the parameter and states are very often  
545 strongly correlated under the posterior distribution, this can result in an ineffi-  
cient scheme. Alternative techniques such as the particle marginal Metropolis-  
Hastings algorithm that update parameters and states simultaneously scale very  
poorly in a data-rich environment [118, 134] but various improved schemes have  
been recently proposed to mitigate these problems [135, 136].

## 550 5. Selected challenges

Below, we highlight two important topics for future research: namely, how to  
best account for modeling errors in hydrogeological Bayesian inversion (section  
5.1) and for petrophysical errors in hydrogeophysical inversion (section 5.2). We  
describe existing work in these domains and possible paths forward.

### 555 5.1. Accounting for modeling errors in Bayesian inverse problems

Proxy models (section 3.2) are increasingly used in Bayesian inference for  
geoscientific problems, where it is not uncommon to require millions of for-

ward model runs when dealing with high-dimensional parameter spaces. In [137, 138], for example, a 1D Richards equation is used to approximate 3D unsaturated flow when estimating soil hydraulic properties from time-lapse geophysical data. Coarsened discretization proxies are employed in [139, 140] for unsaturated parameter estimation and reservoir history matching, respectively. There has also been increasing recent use of PCE surrogates for Bayesian parameter estimation [141, 142, 143, 144, 145, 146]. It is critical that modeling errors arising from the use of proxy models are properly taken into account when solving Bayesian inverse problems; not doing so can easily lead to biased posterior parameter estimates that have little to no predictive value [147]. While the latter finding is now relatively well understood in hydrology and reservoir engineering (e.g., [148, 149, 150, 151, 140]), few workable approaches (see below) for dealing with modeling errors are yet in view. As mentioned previously, a formal and general inverse problem formulation that accounts for modeling errors (described by a probability density function) has existed for 35 years [97]. A practical challenge, however, is how to accurately quantify and efficiently account for this probability density function when dealing with high-dimensional parameter fields, large data sets, and highly non-linear physical processes.

In hydrogeology and geophysics, work to address modeling errors for high-dimensional and data-rich inverse problems includes (i) studies where the errors are assumed to be multivariate Gaussian distributed and the corresponding means and covariances are determined either empirically prior to inversion based on a small number of stochastic model-error realizations [98, 140] or during the inversion by means of sequential data assimilation [152, 153, 154]; and (ii) applications of the two-stage MCMC approach, whereby the proxy is employed as a first “filter” to improve the acceptance rate of parameter configurations that are tested using the high-fidelity forward model [155, 156, 157]. A key challenge with respect to (i) is that modeling errors in real-world non-linear problems may be strongly non-Gaussian with characteristics that vary significantly over the input parameter space, meaning that the underlying assumptions are too simple and cannot be easily fixed by, for example, consideration of a more appropriate

parametric distribution or formalized likelihood (e.g., [158, 103]). With regard  
 590 to (ii), there is limited computational savings because each posterior sample  
 acquired using two-stage MCMC must be tested with respect to the high-fidelity  
 forward model.

In the field of statistics, one of the most influential works on model error is  
 [159], whereby the discrepancy between the proxy and the high-fidelity simu-  
 595 lation model is described by a GP. The approach is flexible as the parameters  
 governing the GP are estimated as a part of the inversion procedure. Never-  
 theless, one issue with such an approach is that it is not guaranteed that the  
 inferred model parameters and error model can be used for predictive forward  
 modeling with different boundary conditions and forcing terms. Another key  
 600 concern in the context of geoscience applications is model dimensionality. The  
 vast majority of applications of [159] and its variants (e.g., [160, 161, 147, 162])  
 have focused on small numbers of data and low-dimensional parameter spaces.  
 In contrast, spatially-distributed inverse problems in hydrogeology and geo-  
 physics may involve hundreds or thousands of data, often measured over both  
 605 space and time and under different source conditions, and many thousands of  
 unknowns. Nevertheless, when solving inverse problems over spatial domains,  
 it is important to realize that the number of independent model parameters is  
 typically much smaller than the number of grid elements on which the model  
 realizations are mapped. This is indeed a major motivation for introducing  
 610 spatial priors (Gaussian-random-field or based on MPS) as they help to make  
 intractable inverse sampling problems tractable (see discussion in [56]).

In terms of practical applications, open questions include: (i) Can a GP  
 model be used to effectively represent model discrepancy in problems where  
 spatial and temporal correlations between model parameters and data are com-  
 615 plex, the statistical nature of the modeling errors changes significantly over the  
 input parameter space, and/or the model discrepancy is not smoothly vary-  
 ing? (ii) How can hydrogeological and geophysical data be transformed and/or  
 spatially organized to enable appropriate representation of modeling errors us-  
 ing a GP model? (iii) How computationally burdensome does the approach of

620 [159] become in high-dimensional data spaces, and how may this be alleviated? Work by [163] suggests that basis representations can be exploited to significantly reduce dimensionality and help in the latter regard. Promising recent research by [164] shows that a data-driven GP construction can be used for effective inference under modeling errors in a moderate-dimensional hydrological  
625 problem (Fig. 5). From a more theoretical point of view, mathematical properties of Kennedy and O’Hagan’s approach and variations thereof have been investigated in [165, 166], tackling in particular parameter identifiability and estimation issues.

One recent idea to account for model errors is that of [167], whereby modeling errors are accounted for by model parameters that are intrinsically un-  
630 certain. That is, each model parameter is described by a mean value and, for example, a standard deviation that is inferred as part of the inversion process. Another avenue to be explored is the question of whether we are best to focus on “correcting” the simulated data from proxy forward models to better fit the  
635 high-fidelity forward simulations, or whether we should aim to transform measured data into quantities that are more consistent with the proxy. A related approach involving the use of data summary statistics (i.e., using statistics of the data set instead of likelihood functions that are based on pair-wise comparisons of observed and simulated data) is employed in approximate Bayesian  
640 computation to address similar issues (e.g., [168, 169]). Finally, it is possible to ignore modeling error altogether when performing MCMC posterior inference using a proxy if one subsequently corrects the corresponding pseudo-posterior using importance sampling based on the high-fidelity forward model [170]. The advantage of this approach is that, unlike two-stage MCMC, the use of the  
645 high-fidelity forward model can be parallelized.

## 5.2. *Hydrogeophysics and uncertain petrophysical relationships*

Since the early 1990’s [171, 172, 173], hydrogeology has seen an ever-increasing use (and acceptance) of geophysics. Geophysics offers non-invasive imaging of lithology and monitoring of mass transfer without the need for borehole access

650 (even though such infrastructure is very helpful). It is well established that  
 geophysical data offer complementary information to traditional hydrogeologi-  
 cal data [174] (e.g., different sensitivity patterns and scales of investigation, no  
 need to inject or pump water and solutes in the subsurface). Currently, there is  
 a push towards so-called fully-coupled hydrogeological and geophysical modeling  
 655 and inversion aiming at seamless integration of hydrogeological and geophysical  
 data [175, 176]. In a fully-coupled approach, the hydrogeological model and  
 its predicted states define, together with a petrophysical relationship, the geo-  
 physical model. Discrepancies between associated geophysical forward model  
 predictions and observed data can then be used in the inversion to guide, possi-  
 660 bly together with hydrogeological data, the update of the hydrogeological model  
 parameters. This research field at the interface of hydrogeology and geophysics  
 is often referred to as hydrogeophysics. Despite its promise, petrophysical rela-  
 tionships that link geophysical properties with hydrogeological properties and  
 state variables are uncertain and we are not aware of hydrogeophysical inversion  
 665 studies that fully account for this uncertainty. By referring to hydrogeophysical  
 inversion, we exclude the extensive literature in hydrogeophysics on sequential  
 approaches in which geophysical models are first obtained by inversion before  
 these models are treated as “data” in a second stage to predict hydrological tar-  
 get variables given an uncertain petrophysical relationship and available hydro-  
 670 logical data [172, 177]. The risk for strong bias when applying such approaches is  
 well demonstrated [178]. Ignoring petrophysical uncertainty in hydrogeophysi-  
 cal inversion leads to overconfident predictions and the risk that hydrogeological  
 colleagues become disenchanted with geophysics [179]. In terms of methodology,  
 the petrophysical relationship is the only major difference in hydrogeophysical  
 675 inversion compared with classical hydrogeological inversion.

Before discussing the general non-linear case, we illustrate the strong im-  
 pact of petrophysical uncertainty by considering the simple synthetic case of a  
 linear forward model and a linear petrophysical relationship. For linear theory,  
 a Gaussian-random-field prior model, Gaussian noise and petrophysical errors,  
 680 one can propagate petrophysical uncertainties into the data covariance matrix



and rely on well-known analytical solutions for the posterior mean and standard deviation [11]. Figure 6a is the true porosity field. Assuming a total of 729 first-arrival ground-penetrating radar travel times acquired for various source and receiver positions at the left and right side of the model domain (contaminated with 0.5 ns of uncorrelated Gaussian noise) and a perfect petrophysical relationship (black line in 6e) leads to the mean porosity field in Figure 6b. The information content in the data is high and there is an important decrease in posterior porosity uncertainty (Fig. 6c) compared to the standard deviation of 0.04 in the prior model. Figure 6d confirms that the resulting data covariance matrix is the conventional diagonal matrix. When accounting for uncorrelated petrophysical errors with strong (correlation coefficient of 0.85; Fig. 6e) and moderately strong (correlation coefficient of 0.59; Fig. 6i) petrophysical relationships, we find that the resulting mean porosity field is smoother (Figs. 6f and 6j), and that the posterior standard deviations are larger (Figs. 6g and 6k) compared to the case of no petrophysical error. Importantly, the data covariance matrix that accounts for both data and petrophysical errors is no longer a diagonal matrix (Figs. 6h and 6i). Clearly, petrophysical uncertainty decreases the information content of the geophysical data for hydrogeological inference and broadens the likelihood function (for the true model, the noise-contaminated data have a log-likelihood of -508 when there is no petrophysical errors, -944 for the strong petrophysical relationship and -1259 for the moderately strong petrophysical relationship). The impact of petrophysical errors is even stronger when considering spatial correlations (not shown). Unfortunately, the inference problem is much more complicated for the general non-linear case as discussed below.

Geophysical data (e.g., electrical resistances, electromagnetic transfer functions, waveform recordings) are related to subsurface physical properties (e.g., electrical conductivity, seismic wave speeds). In most applications, these properties represent hidden variables  $\mathbf{v}$  of limited practical interest, while the underlying goals of geophysical surveys are often to infer state variables (e.g., temperature, pressure, water content, gas saturation) or lithological properties

(e.g., porosity, permeability) of, for example, aquifers. For conciseness, we refer to all such target variables and properties as  $\mathbf{u}$ . When forward solvers take the hidden variables  $\mathbf{v}$  rather than  $\mathbf{u}$  as input, for example, via a non-linear geophysical “forward map”  $\mathcal{G}_V : \mathbf{v} \mapsto \mathcal{G}_V(\mathbf{v})$ , some knowledge of the petrophysical (rock physics) relationships that link  $\mathbf{u}$  and  $\mathbf{v}$  is required to infer  $\mathbf{u}$  from geophysical observables  $\mathbf{y} = \mathcal{G}_V(\mathbf{v}) + \boldsymbol{\epsilon}$ . These relationships are typically non-linear, uncertain, and non-stationary [180]. A possible description of such a relationship is

$$\mathbf{v} = \mathcal{F}(\mathbf{u}) + \boldsymbol{\epsilon}_P, \quad (6)$$

where the residual  $\boldsymbol{\epsilon}_P$  may exhibit non-stationarity and spatial dependence. Spatial dependence of  $\boldsymbol{\epsilon}_P$  is expected because of the common simplifying assumption of constant petrophysical model parameters in hydrogeophysical inversions [181, 182]. In nature, the most appropriate petrophysical parameter values will be different for different lithologies, which suggests that the scales of spatial dependence correspond to those of geological bodies. An alternative is to infer for geological bodies with different petrophysical parameters, but this has its own problems in terms of non-uniqueness, assumptions of low variability within each lithological unit [6] and a much more non-linear inverse problem than for the continuous case. Assuming here for simplicity finite-dimensional settings with continuous distributions and denoting  $\rho_P$  the probability density of  $\boldsymbol{\epsilon}_P$ , we obtain a joint prior on  $(\mathbf{u}, \mathbf{v})$  with density

$$\rho_{joint,0}(\mathbf{u}, \mathbf{v}) = \rho(\mathbf{u})\rho_P(\mathbf{v} - \mathcal{F}(\mathbf{u})). \quad (7)$$

In geophysics, inference of the joint conditional distribution of  $(\mathbf{u}, \mathbf{v})$  given geophysical data  $\mathbf{y}$  is referred to as lithological tomography [183]. A recent tutorial [184] describes how to formulate Bayesian networks (using direct acyclic graphs) for arbitrarily complicated situations involving multiple data and parameter types, as well as a hierarchy of hidden variables. For simplicity, we focus our discussion on a single hidden variable  $\mathbf{v}$ . The standard approach (notably

advocated by [184]) for posterior simulations of  $\mathbf{u}$  consists in applying (varia-  
 tions of) the Metropolis-Hastings algorithm to  $(\mathbf{u}, \mathbf{v})$ , where at each iteration  
 740 the model perturbation consist in (i) drawing  $\mathbf{u}$ , and then (ii) drawing  $\mathbf{v}$  con-  
 ditionally on  $\mathbf{u}$ . Unfortunately, such a sampling strategy can be very inefficient  
 when confronted with high parameter dimensions, large data sets with small  
 errors  $\epsilon$ , and uncertain petrophysical relationships. The main reason for this  
 is that the likelihood  $L_V(\mathbf{v}; \mathbf{y}) = \rho(\mathbf{y} - \mathcal{G}_V(\mathbf{v}))$  is very peaked, which implies  
 745 that the geophysical data need to be fit in great detail even for cases when  
 petrophysical uncertainty is significant (see discussion surrounding Fig. 6).

As alternatives, we suggest two approaches to directly sample from  $\rho^{\mathbf{y}}(\mathbf{u})$   
 without needing to sample from  $\rho_{joint}^{\mathbf{y}}(\mathbf{u}, \mathbf{v})$ . The underlying motivation is to  
 take advantage of the uncertainty of petrophysical relationships and work di-  
 rectly with approximations of  $L_U(\mathbf{u}; \mathbf{y}) = \int L_V(\mathbf{v}; \mathbf{y}) \rho_P(\mathbf{v} - \mathcal{F}(\mathbf{u})) d\mathbf{v}$ , which is  
 750 expected to be less informative (i.e., less peaked) than  $L_V(\mathbf{v}; \mathbf{y})$ . These approxi-  
 mations are needed as there are generally no closed-form expressions to evaluate  
 $L_U(\mathbf{u}; \mathbf{y})$ .

The first approach builds on the pseudo-marginal MCMC method [185, 186]  
 755 and the recent correlated pseudo-marginal method [187]. These methods are  
 based on the remarkable property identified by [185] that a Metropolis-Hastings  
 algorithm that uses a non-negative unbiased estimate  $\tilde{L}_U(\mathbf{u}; \mathbf{y})$  of  $L_U(\mathbf{u}; \mathbf{y})$  will  
 sample the same target distribution as an ideal marginal Metropolis-Hastings  
 algorithm that uses  $L_U(\mathbf{u}; \mathbf{y})$ . Since the expression needed to evaluate  $L_U(\mathbf{u}; \mathbf{y})$   
 760 during MCMC sampling is unknown, it is convenient to estimate  $\tilde{L}_U(\mathbf{u}; \mathbf{y})$  by  
 Monte Carlo averaging of  $L_V(\cdot; \mathbf{y})$  over samples of  $\mathbf{v}$  conditional on  $\mathbf{u}$ . Clearly,  
 $L_V(\cdot; \mathbf{y})$  can be evaluated using standard likelihood expressions. The correlated  
 pseudo-marginal method improves on the pseudo-marginal MCMC method by  
 using correlated random samples to estimate the ratios between  $\tilde{L}_U(\cdot; \mathbf{y})$  val-  
 765 ues of the present and proposed models in the Metropolis-Hastings algorithm.  
 This leads to lower variance estimates of the ratios, which results in significant  
 performance improvements (e.g., two orders of magnitude).

The second approach relies on a linearized Gaussian approximation. A first-

order expansion of  $\mathcal{G}_V$  around  $\mathcal{F}(\mathbf{u})$  delivers

$$\mathcal{G}_V(\mathcal{F}(\mathbf{u}) + \boldsymbol{\epsilon}_P) \approx \mathcal{G}_V(\mathcal{F}(\mathbf{u})) + \langle \nabla \mathcal{G}_V(\mathcal{F}(\mathbf{u})), \boldsymbol{\epsilon}_P \rangle. \quad (8)$$

770 From there it is straightforward to derive the data covariance matrix of  $\mathbf{y}$  given  $\mathbf{u}$  by adding two distinct contributions: one related to the observational errors and the other one related to the petrophysical errors (after appropriate scaling with the Jacobian matrix). Assuming further Gaussian distributions for  $\boldsymbol{\epsilon}_P$  and  $\boldsymbol{\epsilon}$  leads to a completely determined Gaussian approximation for  $L_U$ . In  
775 essence, this is an extension of the linear analysis in Figure 6 to the weakly non-linear case. We expect this approach, which is similar to the so-called multivariate delta method [188], to be efficient when the Jacobian matrix is comparatively cheap to calculate. The accuracy of the method is expected to degrade with increasing non-linearity and degree of petrophysical uncertainty.

## 780 6. Concluding remarks

It is only recently that computational resources have enabled routine forward UQ and Bayesian sampling-based inversion for non-trivial problems involving high-parameter dimensions and complex prior distributions. In this review, we argue that (1) multi-resolution modeling using MLMC approaches is suitable  
785 for effective forward UQ given a distribution of material properties, while their role in inverse modeling remains to be explored; (2) general formulations of data assimilation problems based on particle methods (Sequential Monte Carlo) that are valid under strong non-linearity and non-Gaussianity are still underused in hydrogeology and geophysics and that more work is needed to enable accurate  
790 inference of posterior parameter distributions for such state-space models; (3) the use of low-fidelity (proxy) forward models are inevitable both for forward UQ and large-scale Bayesian inversion problems, while the question of how to quantify and efficiently account for modeling errors remains an important research topic; (4) that new approaches, such as the pseudo-marginal MCMC method,

795 are needed to effectively incorporate petrophysical uncertainty in hydrogeophys-  
ical inversion and, thereby, to allow for proper weighting of hydrogeological and  
geophysical data in joint inversions and to avoid overly optimistic UQ. The high  
dimensionality and data rich environments encountered in modern hydrogeology  
and geophysics, together with complex spatial parameter relations, call for ad-  
800 vanced mathematical and statistical methods that work well in high parameter  
and data dimensions. We hope that this review on selected topics on UQ will  
contribute in stimulating such research.

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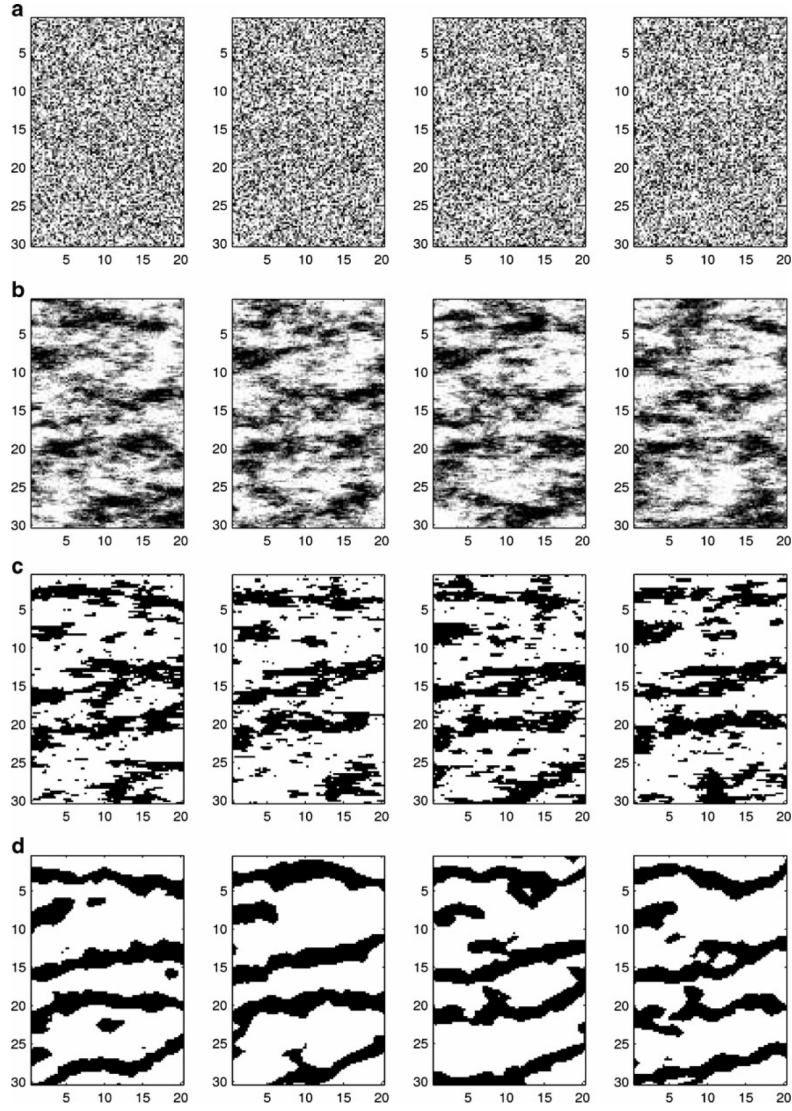


Figure 1: Sampled MCMC posterior realizations based on 800 crosshole first-arrival GPR travel times acquired between the left and the right sides of the model domain. The true subsurface structure (not shown) used to create the data in this synthetic example has channel-like features similar to those in (d). The other posterior realizations are based on: (a) a nugget prior model with the correct mean and variance; (b) a Gaussian-random-field prior model with the correct two-point statistics; and (c) the same Gaussian-random-field prior model truncated into a binary field with the correct facies proportions provide realizations that are largely incompatible with the true subsurface structure. From [54]

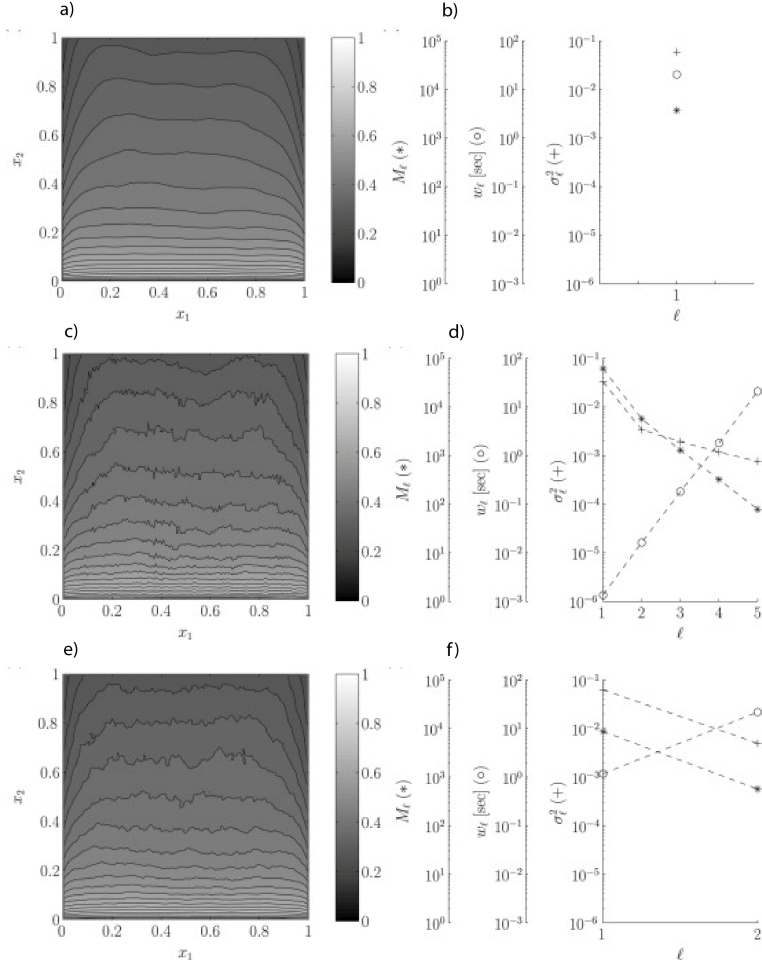


Figure 2: Considering water flooding of a saturated petroleum reservoir, [94] evaluated the performance of MLMC strategies. (a) MC estimation of the mean saturation field at time  $t$ ; and (b) plots showing the number of evaluations at each level,  $M_l$ , the computation time for one evaluation at each level,  $w_l$ , and the variance between levels,  $\sigma_l^2$ . Note that there is only one level for the MC case. Corresponding results for MLMC with (c-d) grid and (e-f) solver hierarchy. Note that the mean solutions in (a), (c) and (e) have the same numerical accuracy, while the computational times and the distributions across different levels vary strongly.

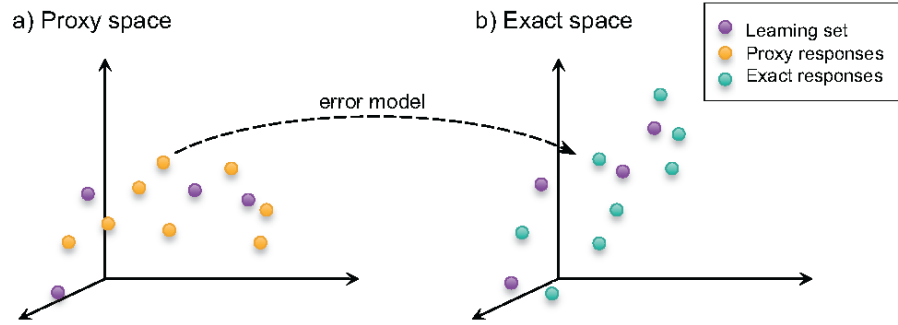


Figure 3: By considering a learning set of contaminant breakthrough curves consisting of proxy responses based on single-phase saline transport simulations “exact” responses obtained using a two-phase solver (purple dots in (a) and (b)), [58] used functional principal components analysis (FPCA) to develop an error model that allows proxy simulations (orange dots in (a)) to be mapped into “exact” responses (blue dots in (b)). Using a learning set based on 20 geostatistical realizations, they demonstrated for a fluvial aquifer with five distinct facies how error-corrected proxy modeling leads to error-corrected predictions that are similar (correlation coefficient of 0.97) to the full physics responses.

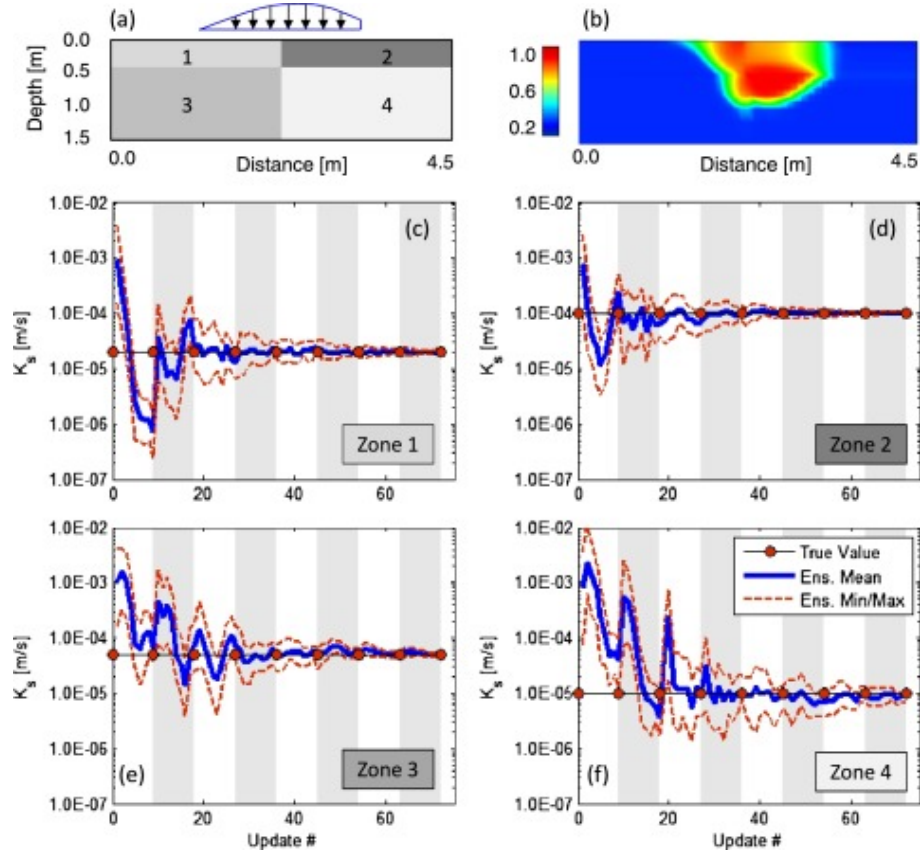


Figure 4: An iterated particle filter method was developed by [114] to infer the hydraulic conductivity of four zones of known geometry given geophysical data. (a) A synthetic infiltration experiment in the vadose zone led to a (b) water plume evolving over time that was sensed by electrical resistivity tomography data under the assumption of a known and perfect petrophysical relationship. (d-f) The inferred hydraulic conductivities converged to the true values.

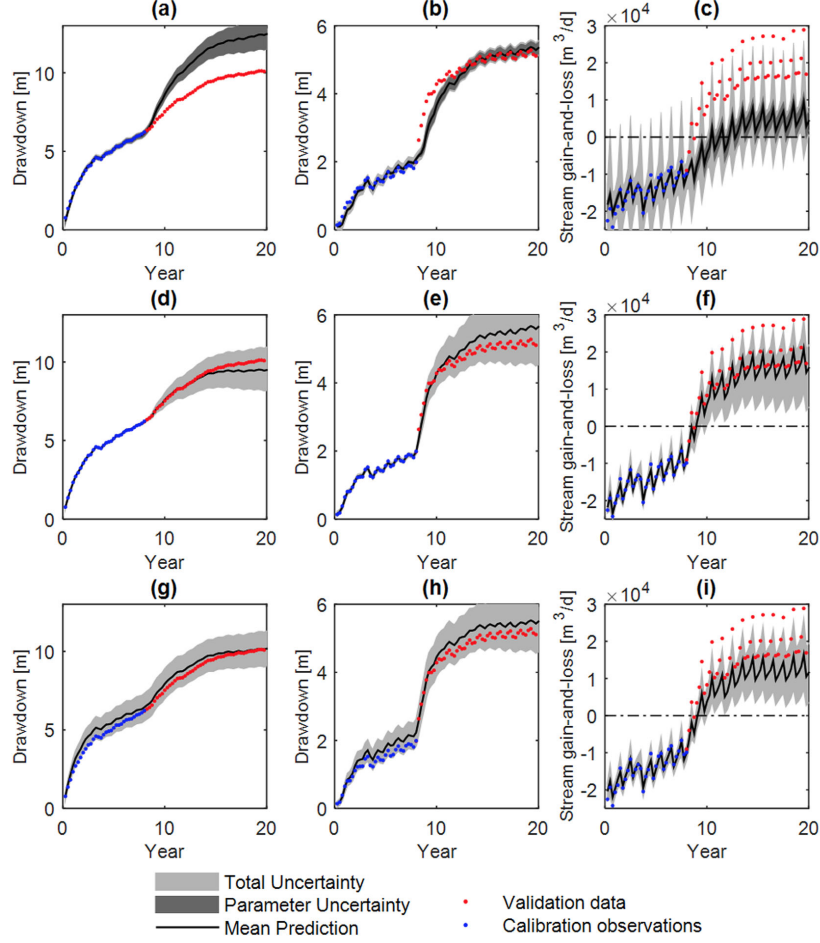


Figure 5: [164] considered a synthetic test example involving a “true” 2-D Gaussian hydraulic conductivity field in contact with a river. The inverse problem was parameterized in terms of 12 pilot points. Ignoring model errors caused by this smooth representation leads to biased predictions in terms of (a-b) drawdown at two locations and (c) river-groundwater exchange and unrealistically low uncertainty bounds. By inferring a Gaussian process model describing model errors during the calibration period, the authors obtained (d-f) significantly improved predictions and more realistic uncertainty bounds. Unfortunately, this approach lead to predictions that are unphysical (e.g., not honoring mass constraints). To circumvent this, they considered inversion with a data covariance matrix that include both the observational and the previously inferred model errors. (g-i) The corresponding predictions based on the resulting inversion model are physically-consistent and the bias is low.



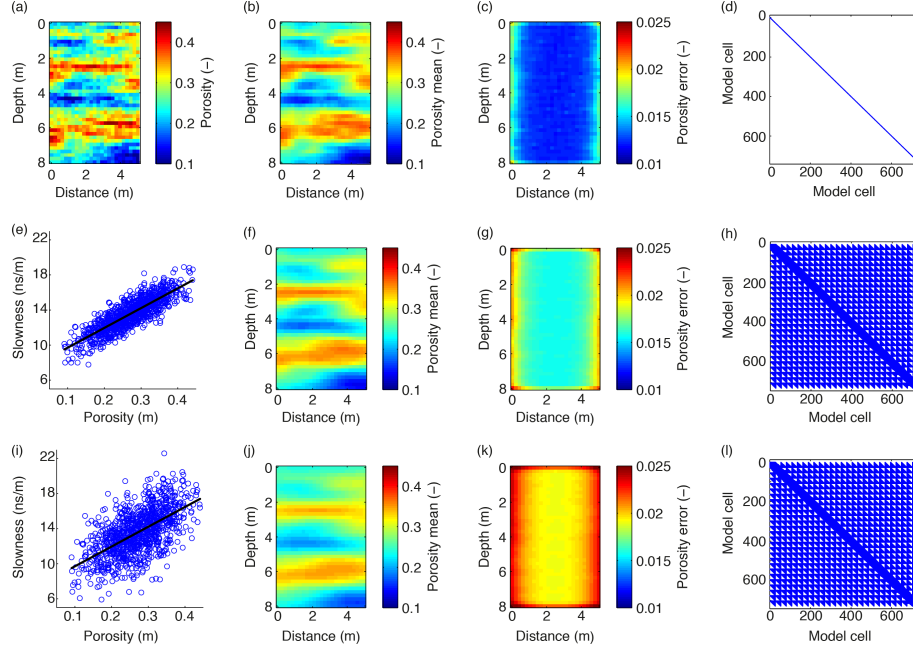


Figure 6: Synthetic example of porosity inference from crosshole GPR travel time data under assumptions of linear theory, a known Gaussian-random-field model, and uncorrelated data and petrophysical errors. (a) True porosity field, (b) inferred mean model, (c) standard deviation and (d) structure of the data covariance matrix under the assumption of a perfect petrophysical relationship (black line in (e)). (e) Strong petrophysical relationship and resulting (f) mean model, (g) standard deviation and (h) structure of the data covariance matrix. (j-l) corresponding results for a (i) rather strong petrophysical relationship.