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Prediction using Numerical Simulations, A Bayesian Framework for Uncertainty Quantification and its Statistical Challenge

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Abstract

Uncertainty quantification is essential in using numerical models for prediction. While many works focused on how the uncertainty of the inputs propagate to the outputs, the modeling errors of the numerical model were often overlooked. In our Bayesian framework, modeling errors play an essential role and were assessed through studying numerical solution errors. The main ideas and key concepts will be illustrated through an oil reservoir case study. In this study, inference on the input has to be made from the output. Bayesian analysis is adopted to handle this inverse problem, then combine it with the forward simulation for prediction. The solution error models were established based on the scale-up solutions and fine-grid solutions. As the central piece of our framework, the robustness of these error models is fundamental. In addition to the oil reservoir computer codes, we will also discuss the modelling of solution error of shock wave physics. Although the framework itself is simple, there is many statistical challenges which include optimal dimension of the error model, trade-off between sample size and the solution accuracy. These challenges are also discussed.

1 Introduction

One purpose of building complicated numerical models is to forecast outcomes of complex systems such as climate change, hydrocarbon reservoir production, contamination of groundwater and shock wave physics. However, a scientific prediction must be coupled with a good uncertainty assessment. Recently, uncertainty quantification (UQ) of numerical models has drawn significantly increased attention from several international scientific communities as well as government agencies.

The uncertainty of a numerical simulation comes from

three different sources, the errors in the physical model, the errors in the numerical model, and the uncertainty on the input parameters of the model.

The uncertainty on the input parameters includes the result of the difficulty in measuring corresponding parameters in the physical system. For example, the permeability and porosity of a petroleum reservoir could not be accurately measured with today's technology. In numerical simulation, uncertainty of the input parameters of a model gives rise to uncertainty regarding its output. This propagation of uncertainty from input to the output has been the main focus of UQ research. A variety of sophisticated statistical and probability methods have been developed and some have been implemented into software packages[6]. In addition, sensitivity analysis has also been applied to this aspect of UQ inference[18].

The error of a numerical model comprise solution errors and modelling errors. The solution errors are the result of a finite accuracy approximation to the governing equations describing continuum phenomenon. The modelling errors could be due to approximations in the equations and the physics they represent. Incorrect choice of the physical models give rise to the errors in the physics model. For example, a fault lies in an oil reservoir but is not represented in the model. Assessing both type of modelling errors is often referred to as model validation[5, 14], which is arguably the most important and most challenging component in UQ. This has to be done through systematic comparison between experimental and observational data, and comparison among competing models.

We have proposed a Bayesian framework for UQ inference[12, 13, 4, 8]. Our focus is distinct from the other UQ research in several aspects. First, our approach is motivated by petroleum engineering applications in which important parameters of the petroleum reservoir are not directly observable and have to be inferred through an *inverse problem*. Similar situations exist in many other applications

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including shock wave physics. Second, practically the inverse problem can be solved only with *coarse grid simulations* on a large ensemble sampled in the parameter space. Therefore, solution errors plays a big role in the uncertainty quantification.

We believe that different UQ approaches complement each other and each provides a unique view on some aspects of this challenging problem. Together they provide a complete picture. In this paper, we will discuss first a Bayesian Framework for UQ inference, then three statistical aspects in our UQ approach:

1. probability models of the solution errors, which is at the core of our approach;
2. partition of uncertainty to all substeps, which provide guidelines for improving prediction accuracy;
3. efficient sampling of ensembles.

2 A Bayesian UQ inference Framework

Our Bayesian UQ inference includes two equally important steps. The first is the *inverse problem*. In this step, the uncertainty of the model parameters that are not directly observable, are reduced using other observations. This is achieved by running forward simulations on an ensemble sampled from the parameter space, then assign posterior probabilities to each element of the ensemble. The better a solution matched up with the observations, the parameter setting used for this solution receives higher probability. The posterior probability is assigned with Bayes' formula,

$$P(m|\mathcal{O}) = \frac{P(\mathcal{O}|m)p(m)}{\int_{\mathcal{M}} P(\mathcal{O}|m)p(m)} \quad (1)$$

where \mathcal{M} and m represent the entire ensemble and one of its elements. The factor $P(\mathcal{O}|m)$ is the likelihood which measures how the observed data \mathcal{O} matches with the solution of m . The factor $P(m)$ is the prior probability on the ensemble which is often set to be flat. However, the ensemble can be sampled from a probability distribution that reflects the current knowledge on the parameter space. Using (1), the ensemble is refined in the sense that the probability concentrates on a small fraction of its elements and the remaining majority have only negligible probabilities. Figure 1 illustrates this idea through an oil reservoir model studied in Devolder et al.[4]. The top of the figure are 500 solutions of the entire ensemble sampled from a random field describing the geology of an oil reservoir. The bottom shows only those solutions that better match with observed history data. This inverse step is often referred to as "calibration" or "history matching" by other authors[16, 15]. However, it differs from "calibration" of the traditional sense. Traditional calibration finds a single parameter setting that best matches

the observed data. In this inverse step, the parameter space is only "confined" by the observations but never reduce to a point mass. A reality of this step is that the forward simulation have to be done on relatively coarse grids because one can not afford fine grid solutions on the entire ensemble.

The second step in our UQ inference is the *forward step*, in which the numerical simulation extends to the future only on the refined ensemble. Note that the ensemble can now be replaced by a subensemble, i.e. an one that with less elements, numerical simulations can be done on finer grids than in the inverse step. The posterior distribution of the prediction is a product of the probability distribution of the ensemble and the probability distribution of the simulation error. This posterior distribution fully characterize the prediction and its uncertainty, and provides confidence intervals for the prediction.

In the core of our UQ inference framework is a probability model for numerical simulation errors which produces the likelihood $p(\mathcal{O}|m)$ in (1). Without an appropriate understanding of these errors, the inverse step will be ill fated. One would have no meaningful way to assess how the observed data matches with the numerical solutions, ending up with either "under calibrated" model, giving overly pessimistic uncertainty assessment, or "over calibrated" model, giving overly optimistic uncertainty assessment.

A similar Bayesian approach has been proposed and applied by others to petroleum engineering applications[2, 17, 15, 1]. In these works, the numerical error is often replaced by an "observational" error, which is then postulated with little scientific basis. In the next session we will provide a scientific basis for the error models and likelihoods being used in the analysis.

3 Probability Model of Solution Errors

The inverse step in our Bayesian UQ inference relies on a probability model to calculate the likelihood $p(\mathcal{O}|m)$ in (1). Ideally, this probability model should account for the solution errors, the modelling errors and the observational errors. Among the three, modelling error is the most difficult to be assessed. One needs to compare results from physical experiments with numerical solutions, which can only be done under limited controllable experimental conditions and are very expensive[5]. A number of authors has proposed and applied a similar Bayesian inference framework to quantify uncertainties of numerical simulation predictions [15, 17, 2, 16, 3, 1]. Although the importance of such a probability error model are fully recognized, they either use subjective models "elicited by experts"[3], or disregard it completely but focus on statistical modelling of the output [16]. In general, the likelihood $p(\mathcal{O}|m)$ is obtained using postulated error models without further justification.

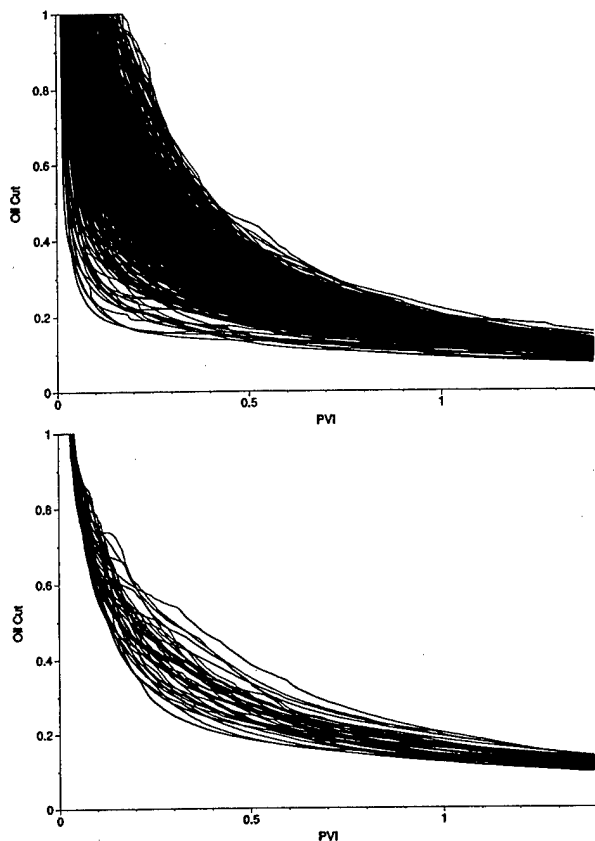


Figure 1. A full ensemble and a refined ensemble after "history matching"

Our approach to build such a probability error model is based on observation errors and solution errors. The latter can be observed by comparing the numerical solutions to more accurate numerical solutions. We think that in many applications it is the only practical way to make physically meaningful and objective assessment of the simulation error. Theoretically, the simulation error can be evaluated by comparing the simulation results with observed data. However, this is only possible when the values of all physical parameters describing the real system are well known. For complex systems, such cases rarely exist. For example, obtaining the exact geology parameters of an oil reservoir is practically impossible. Additionally, in our UQ inference framework, a large ensemble from the parameter space is sampled for the inverse problem, and numerical solutions are obtained for each parameter settings in the ensemble. For complex systems, the simulations on the entire ensemble has to be done on coarse grid due to constraints on the computational resource. The use of the coarse grid solution will make the solution errors account for a large pro-

portion of the total simulation error. This situation will remain true even as the computing power improves in the future, because the complexity of future numerical model will increase in the same pace as the computing power allows. However, one can afford to do both the coarse grid and the fine grid solutions on a small sample of the parameter spaces to evaluate the solution errors.

Since fine grid solutions are resource consuming, the error models have to be constructed from a sample with limited size. This has two implications. First, although the output is often high dimensional, error models must be simple and effective with low dimensionality. Second, uncertainty due to the finite sample size has to be assessed. Both issues have to be thoroughly studied. In our previous work[9], the effect of finite sample size can be handled by the Wishart distribution for Gaussian error models. However, the complexity of the error models is determined in ad hoc manners. Two questions should be answered:

- What is the optimal choice of the error model dimensionality and how can the dimension reduction be achieved?
- Is the Gaussian error models robust when the Gaussian assumption is violated?

Regarding the second question, the effect of finite sample size could be studied using re-sampling methods, when the error is non-Gaussian.

4 Transferrable Error Models in Shock Wave Physics

As discussed above, brutal force computing is needed to establish quality error models. Such brutal force may not always available for the most complicated problem and may not allowed in situations that require quick analysis. Therefore, it is very important to study the *transferability* of error models from relatively elementary problems to complex problems. The errors in a complex system can be viewed as composition of errors arising from repeated, but elementary processes. One of our ideas is to first develop the error models in a simple context then transferred to a related but more complex context. Because the simple models will be transferred across a series of related contexts, they can be used without reparameterization once verified. This idea, however, must be developed, refined and validated before it can be used.

We have test this idea in 1D shock wave physics models[7]. Shock waves are localized structures, and lie on surfaces in 3D. The interactions, i.e. crossing with one another or with fluid or material surfaces occur on lines, and the bifurcations, or modification of the interaction structures occur at isolated points in space, moving along curves in

space-time. These idealized structures are solved by shock Hugoniot and their interactions are given by solutions of Riemann problems and shock polars. Since Riemann problems and shock polars are basic ingredients in more complex shock wave physics problems, their errors can be used to build error models of those complex systems. Several idealized shock wave interaction problems were studied.

We start with a statistical approximation of the error in a given Riemann problem R_0 using multinomial expansion associated with initial waves and errors located inside its domain of dependence. For a 1D shock wave interaction problem, think of the solution as being primarily composed of localized waves, interacting through Riemann problems and generating outgoing waves, that further interact in the same manner. Each wave w is described by a vector ν_w that records its strength, location in state space, speed and starting location and time, and the errors or uncertainty associated with these quantities. The interaction of waves generates a planar (1D space and time) graph, the vertices of which are the Riemann problems and the bonds are the traveling waves, between Riemann problem interactions. Starting from a given Riemann problem (vertex) or wave (bond), we can trace backward and determine its domain of dependence. Call this graph \mathcal{G} .

For each Riemann problem, we consider three types of vertices, corresponding to the constant, linear and bilinear terms in the multinomial approximation of solution and error terms. See [7] for details. The linear terms allow a simple propagation law,

$$S_L = \int w(t=0)d\omega, \quad (2)$$

where $w(t=0)$ is a vector representing the strength of the time zero wave and its error or uncertainty, evaluated at the beginning of the path ω , and S_L is the purely linear propagation contribution to a final time error. The path space integral $d\omega$ is taken over all paths progressing in time order through \mathcal{G} from the initial time to the final vertex, with each term weighted by the appropriate linear factors from the formula for the approximate solution of the Riemann problems transversed. This path space representation makes evident the point that the solution S_L is that of a multiple (linear) scattering problem.

The amplitude S at the final time (vertex of \mathcal{G}) can similarly be thought of as a solution of a nonlinear multiple scattering problem, leading to a representation in terms of multipath integrals. Let $\mathcal{V} = \mathcal{V}(\mathcal{G})$ be the set of vertices of \mathcal{G} , and let $\mathcal{B} \subset \mathcal{V}$ be a subset of \mathcal{V} where constant or bilinear terms occur. The total amplitude S will then be a sum over terms S_B indexed by \mathcal{B} . For each $v \in \mathcal{B}$, let \mathcal{I}_v be the interaction coefficient obtained for basic Riemann problems.

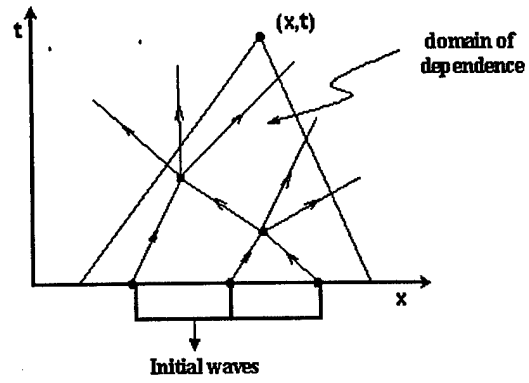


Figure 2. The solution and its errors at the point (x, t) can be obtained by “adding up” the solution and errors for the waves within the domain of dependence

We write

$$S = \sum_{\mathcal{B} \subset \mathcal{V}(\mathcal{G})} S_B = \sum_{\mathcal{B} \subset \mathcal{V}(\mathcal{G})} \int \prod_{v \in \mathcal{B}} \mathcal{I}_v d\omega_B. \quad (3)$$

Here $d\omega_B$ is a multipath integral over all multipaths. The multipath propagator $d\omega_B$ is a product of the individual propagators ω for each single path, as in (2). The summation in (3) can be understood schematically as the sum over all events within the domain of dependence of the evaluation point (x, t) at the vertex of \mathcal{G} . See Fig. 2.

The composition law (3) has been validated on several idealized composite interaction problems. It shows some promise of developing transferable error model for less idealized problems. More detailed modelling on the errors need to be done for more accurate error models.

5 Decomposition of the Uncertainty

Once a framework to quantify the uncertainty of prediction has been established, it is important to know the contribution of each component in the prediction uncertainty. Knowing the relative importance of each components will help us in improving the accuracy of a prediction.

The uncertainty of a prediction under our Bayesian framework arises from the following sources:

- forward simulation errors in the forward step
- uncertainty of the geology
- the sparsity of the observed real data
- forward simulation error in the inverse problem

- limited size of the ensemble in the inverse problem
- inadequacy of the error model resulted from limited sample size in the inverse problem

A breakup of total uncertainty to individual sources will provide guidelines for optimal distribution of resources to improve prediction accuracy. For example, should additional research effort be spend to develop more accurate numerical models or more advanced measuring systems for better observations; should the inverse problem be done using a large ensemble with coarse solutions or a smaller ensemble with finer solutions.

We have developed some statistical methods for partition of prediction uncertainty with an idealized oil reservoir model[11]. The idealized Darcy and Buckley-Leverett equations

$$\begin{aligned} v &= -K\Lambda\nabla p; & \nabla \cdot v &= 0 \\ s_t + v \cdot \nabla f &= 0 \end{aligned}$$

are solved for a total seepage velocity v and oil saturation s . Here $K = K(x, z)$ is the random total permeability, Λ the relative transmissivity and f the fractional flux. See also [8, 10] for a more detailed specification of the simulations. We model the real problem by selecting a particular geology K_{i_0} as the "correct" one. We assume that the actual geology is not observed and only the oil cut (oil to water ratio) $s(t)$ until present time T_0 is observed. The goal is to predict the future oil production $\int_{T_0}^{\text{final time}} s(t)dt$. To apply our Bayesian UQ framework, simulations are performed on an ensemble with varied viscosity ratio v and permeability fields K to observe the oil cut $s_i(t)$, as shown in the top graph of Figure 1. The solution error models are based on difference of arrival time between the fine grid solution and coarse grid solution. Its degree of freedom are reduced to five, the breakthrough time and the incremental elapsed time at oil cut levels of 0.8, 0.6, 0.4, and 0.2. That is $\Delta(t_l) = t(S_l) - t(S_{l-1})$, where

$$t(S_l) = \sup_t \{s(t) \geq S_l\}, \quad (4)$$

and $S_l = 1 - 0.2 \cdot l$, $0 \leq l \leq N$, and $\Delta(S_0) = t(S_0)$. Thus, the errors to be modelled are $e(S_l) = \Delta_f(S_l) - \Delta_c(S_l)$, where Δ_f and Δ_c represents the fine and coarse grid solution.

Here we briefly describe a method to partition the total uncertainty into four different components. For details, see [11]. First, we approximate σ_{geo}^2 , uncertainty inherited from uncertainty of the geology and due to insufficient observed data, by the following method. The posterior is determined by fine grid solutions, using the windowing method, while the future is also simulated using the fine grid. We average the prediction errors over an ensemble to estimate σ_{geo}^2 .

Then we obtain an estimate of σ_{inv}^2 by RMS difference between σ_{geo}^2 and the prediction errors of using coarse grid solution for the *inverse step* and fine grid for the *forward step*. Subsequently, we obtain an estimate of σ_{fwd}^2 by RMS difference between $\sigma_{\text{geo}}^2 + \sigma_{\text{inv}}^2$ and the prediction errors of using coarse grid solution for both inverse and forward steps. Finally, we obtain σ_{stat}^2 by RMS difference between $\sigma_{\text{geo}}^2 + \sigma_{\text{inv}}^2 + \sigma_{\text{fwd}}^2$ and the prediction errors of using coarse grid solution for both steps and a statistical approximation of the error model.

We found that σ_{geo}^2 dominates the other three components and σ_{stat}^2 contributes a little. This suggests that the inverse step does not sufficiently reduce the uncertainty on the geology because of the sparsity of the observed data. The observed data does not contain enough information for the inverse inference on the parameter space. Therefore, within the model assumptions used in the present study, efforts should be made to either gather more on the geology itself or collect other information that lead to better inference on the geology, if one would like to significantly improve the accuracy in prediction. On the other hand, a more adequate probability error models does not result much improvement on the prediction but it is the cheapest to do. We also found that solution errors in the forward step contribution more than the solution errors in the inverse step. This suggests use fine grid simulation in the forward step and coarse grid solution in the inverse step.

Although we developed the method on an oil reservoir model, they should be applicable to any applications that fit into our UQ inference frameworks. Of course, the relative importance of each components will not remain the same. Methods to further decompose σ_{geo}^2 and σ_{inv}^2 will be developed in the future. Formal statistical inferences will also be developed for estimation of each components. Based on the reliable methods for partition, one could study the necessary size and solution accuracy for the ensemble, and the necessary complexity and sample size for the error model.

6 Sampling Methods of Ensembles

In the inverse step of our UQ inference framework, an ensemble is sampled from the parameter space and their solutions are matched with the observed data. The quality of the ensemble is an important factor in the final prediction uncertainty. If all elements in the ensemble are far from the real parameters of the physical system, then the prediction is doomed to be poor. However, given a fixed amount of computational resources, deeper sampling in the parameter space is only possible with solutions on coarser grid. A challenge in our UQ framework is to find the delicate balance between the size of the ensemble and the quality of the solutions.

In our previous works, the ensembles are obtained us-

ing simple random sampling methods from a random field. It is conceptually simple but may not be the most efficient. Other sampling methods and their combinations deserve further investigation. Latin hypercube sampling generates ensembles that spread more evenly in the parameter space. Experimental design methods could also be used to refine the parameter space for more effective sampling, which might be necessary for large system with a lot of parameters. In real application, some directly information on the parameter space might be obtained. For example, some rock sample are obtained for an oil reservoir. In those cases, sampling methods that obtain samples consistent with those information need to be developed. Another alternative is to directly sample from the posterior using Markov Chain Monte Carlo method, as proposed by Oliver et al.[17, 2]. However, using MCMC methods alone might be too slow for large problems. But all of these choices need to be carefully compared and anyone of them might be more efficient than others in some situations.

7 Conclusion

In this paper, we presented a Bayesian UQ framework for predictions using numerical models. What is essential to this framework is a probability model for the simulation errors. Our approach is to formulate the model based on solution errors. An important idea for build a robust error model is transferrability, which allows us to build error model of a complex problem from the error models of its simpler components. Another challenge for error models, which are build based on finite samples, is to determine its dimensionality. Methods to partition the the total uncertainty into several components is also important. They provides foundations for optimal allocation of the resources to reduce the prediction uncertainty. Many works need to be done in these areas.

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