

Final Report on DOE Award DE-SC0004965. Bayesian Uncertainty Quantification in Predictions of Flows in Highly Heterogeneous Media and Its Applications to the CO2 Sequestration

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Abstract. In this proposal, we have worked on Bayesian uncertainty quantification for predictions of flows in highly heterogeneous media. The research in this proposal is broad and includes: prior modeling for heterogeneous permeability fields; effective parametrization of heterogeneous spatial priors; efficient ensemble-level solution techniques; efficient multiscale approximation techniques; study of the regularity of complex posterior distribution and the error estimates due to parameter reduction; efficient sampling techniques; applications to multi-phase flow and transport. We list our publications below and describe some of our main research activities. Our multi-disciplinary team includes experts from the areas of multiscale modeling, multilevel solvers, Bayesian statistics, spatial permeability modeling, and the application domain.

1 Prior Modeling Representation

Inference of complex heterogeneous rock properties from low-resolution dynamic flow measurements often leads to underdetermined nonlinear inverse problems that can have many non-unique solutions. The problem is usually regularized by reducing the number of unknown parameters and/or incorporating direct or indirect prior information. In subsurface flow modeling, structural connectivity in hydraulic properties plays a critical role in determining local and global flow and displacement processes. When reliable prior information about the structural connectivity of a formation is available it can be used to discourage implausible inversion solutions.

The goal of prior model representation in this project was to develop compact representation of complex fluvial channel facies under geologic uncertainty. This form of prior representation can then be used with appropriate dynamic data integration or conditional sampling techniques to reduce the initial geologic uncertainty. An example of such fluvial facies models and their uncertainty is shown in Figure 1. The figure shows 45x45 replicates of facies maps (out of 1000 such maps) with mainly 0, 45, and 90 degree orientations, from left to right, respectively. In some cases, the main uncertainty may be related to the shape and structure of these patterns, e.g., meandering, straight, or intersecting, etc. In this project, the uncertainty in both structure and orientation of the channels was considered and the results are reported in [20, 21, 25, 22, 23].

1.1 Sparse Representation of Complex Facies Connectivity

In this part of the project, we introduced a geologically-inspired conceptual framework, known as geologic dictionaries, for reconstructing complex subsurface physical properties from the flow data [22]. We evaluated the performance of this method under both reliable and highly uncertain prior knowledge and measurements.

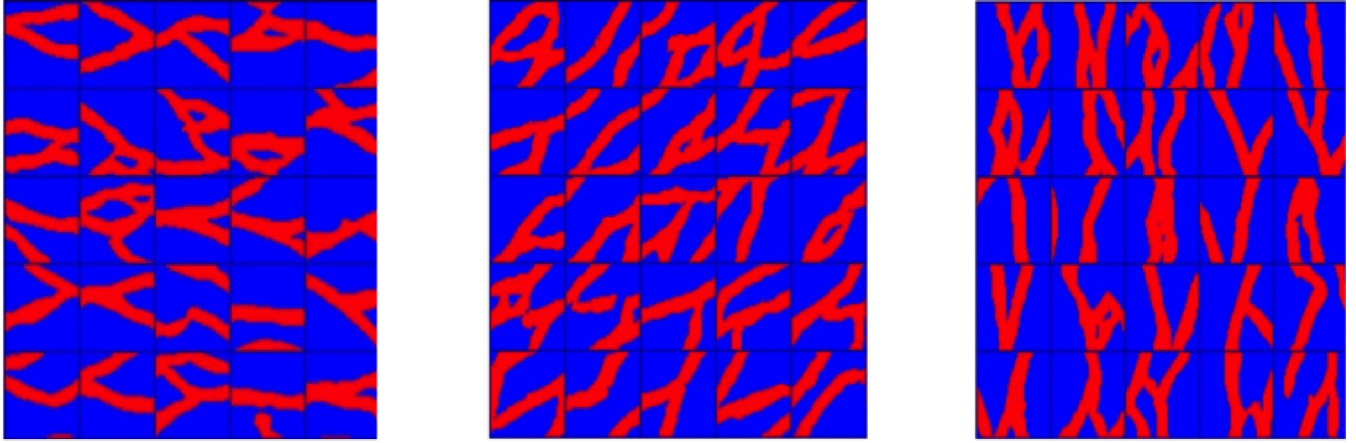


Figure 1: Sample channel facies maps for libraries with predominantly horizontal (left), diagonal (middle) and vertical (right) channel orientations.

We showed that the inversion results obtained with sparse geologic dictionaries that are learned from prior models are superior to classical parameterization methods, especially when estimation of complex heterogeneous subsurface hydraulic properties is considered. Learning methods were adapted to build, from a prior training library, specialized sparse geologic dictionaries that contain relevant structural elements (words) for constructing the solution of subsurface flow inverse problems. The key property of the constructed geologic dictionaries that is invoked during flow data integration is its sparsity; that is, we require that only a small subset of geologic dictionary elements be used for accurately approximating any prior model realizations in the training library. Using the sparsity property of the geologic dictionary, we developed inversion formulation to solve the nonlinear model calibration as a feature estimation problem. We illustrated the flexibility and effectiveness of the proposed method by applying it to a series of numerical experiments in multiphase flow systems and compared it with parameterization by truncated singular vectors.

1.2 Robustness of Sparse Representation to Prior Uncertainty

Using the introduced sparse geologic dictionaries, we extended the application of the approach under geologic uncertainty. In practice, the spatial connectivity in geologic systems has to be inferred from uncertain and incomplete sources of information, including qualitative geologic interpretations, formation type and outcrop maps, as well as scattered measurements (e.g., well core, log data, and seismic maps). Thus, the geologic continuity model that is used for generating prior models is likely to carry significant uncertainty. We investigated the performance of the proposed dictionary learning method under uncertain and incorrect prior continuity models and could show that, unlike the conventional reduced-order parameterization methods such as truncated SVD, diverse geologic dictionaries are robust against uncertainty in the structural prior model [23]. This robustness is attributed to the selection property of the sparse reconstruction algorithm and the

connectivity exhibited by the dictionary elements. Under highly uncertain prior models, the reconstruction problem is reduced to identifying and combining relevant elements from a large and diverse geologic dictionary. The diversity of the dictionary further enhances solution sparsity since a large number of dictionary elements will have negligible contribution to the solution. Consequently, the inversion provides considerable flexibility to accommodate significant levels of variability (uncertainty) in prior geologic models.

1.3 Prior Model Identification through Dynamic Data Integration

Construction of predictive reservoir models invariably involves interpretation and interpolation between limited available data and adoption of imperfect modeling assumptions that introduce significant subjectivity and uncertainty into the modeling process. In particular, the uncertainty in the geologic continuity model can significantly degrade the quality of fluid displacement patterns and predictive modeling outcomes. This part addresses a standing challenge in flow model calibration under uncertainty in geologic continuity by developing an adaptive sparse representation formulation for prior model identification (PMI), [21]. To this end, we developed a flow-data-driven sparsity-promoting inversion to discriminate against distinct prior geologic continuity models. Realizations from each geologic continuity model were used to generate sparse geologic dictionaries that compactly represent models from each respective prior. The inversion is formulated as a sparse reconstruction problem that uses the flow data to identify and linearly combine the relevant elements from the large and diverse set of geologic dictionary elements to reconstruct the solution. We develop an adaptive sparse reconstruction algorithm in which, at each iteration, the contribution of each dictionary to the solution is monitored to replace irrelevant elements with more geologically relevant elements to improve the solution quality. We used several numerical examples to illustrate the effectiveness of the proposed approach for model calibration under uncertainty in the prior geologic continuity model.

1.4 Continuous parametrization of channelized permeability features

In subsurface flow applications, structural connectivity in hydraulic properties plays a critical role in determining local and global flow and displacement processes. In [4], we consider multiscale re-parametrization for large-scale connectivity. In particular, using grid connectivity information, channelized prior models are constructed that honor features of initial geology. These priors can be used in conjunction with level set approaches, as described above, to honor dynamic and static data. The main idea of this parametrization is to consider eigenvalues and eigenvectors of the discrete flow equation that correspond to the initial prior geological model. Based on smallest eigenvalues, we identify important modes that represent the connectivity and the features within connected regions.

2 Posterior Distribution, Sampling, and Estimation

2.1 Posterior regularity

We have used Bayesian hierarchical models to integrate data from different sources that include dynamic data and static data such as permeability values at some distinct locations.

Our prior models can consist of log-Gaussian fields separated by interfaces, in general. One option is to assume that the interfaces are modeled using level set approaches that allow achieving smaller dimensional parametrization of the interfaces using the parametrization that corresponds to the velocity field which evolves the interface. The velocity field is assumed to be smooth as we are interested in smooth interfaces. We propose approaches to perform a dimension reduction in the velocity space and discuss how the parametrization of interfaces can be represented via the parametrization of the velocity field. As for level set approaches, we consider scalar random velocity fields that drive the interface either in the direction of fixed streamlines or in the direction that is normal to the interface [37, 28, 34, 7, 35]. As for parametrization within facies, Karhunen-Loeve (K-L) based techniques are applied offline to achieve a small dimensional parameter space. We also consider the parametrization of log-Gaussian fields when the correlation lengths are not fixed. In this case, we propose an interpolation based K-L [28] that allows pre-computing eigenvectors of a few K-L representations and using them in constructing realizations from log-Gaussian field. This way, one avoids expensive K-L expansions every time correlation lengths are chosen. Such hierarchical representations allow flexibility in prior modeling. We have also studied the use of MARS in prior modeling as well as coarse-grid permeability fields that are used for conditioning [28].

We have worked on investigating the regularity of the posterior measure, where we estimate the error in the posterior measure due to the truncation of the prior space with respect to the parameters representing the facies and the distribution within facies. Our techniques are general and can be used with various other parameterization. The parametrization of the prior is achieved by truncation of spectral expansions and it is important to understand the effects of such truncations on the posterior measure. In this regard, we show that the expectation of a smooth function, with respect to the full posterior and the reduced posterior that is defined on the reduced parameter space, can be bounded by the error of the parameter reduction in the prior space. This is important because it allows determining the dimension of the prior space that is needed given an error tolerance. We also show that the constants in our estimates are independent of the dimension of the parameter space, and thus our reduced parametrization techniques can be applied to fine-scale problems. This is done in [34, 28].

3 Bayesian sampling

It is important to have efficient sampling techniques to sample the posterior measure and assess the uncertainties in the predictions. Our approaches exploit efficient Markov chain Monte Carlo (MCMC) methods. Because each proposal requires a forward solve, MCMC approaches, if implemented directly, are prohibitively expensive. We consider multi-stage MCMC methods where various coarse-scale models are used in the first stage of Metropolis-Hastings criteria to avoid expensive forward simulations that result to rejected samples.

The first stage screens bad proposals with the help of inexpensive forward runs. We study the use of mixed multiscale finite element methods and other approximate models that are constructed statistically [28, 34, 7]. Based on apriori offline calculations, we develop error models between coarse (approximate) and fine simulations. These error models are constructed based on various statistical tools and used in multi stage MCMC approaches where approximate models are first run to decide whether or not to run fine-scale models. This allows us to avoid expensive fine-scale calculations when they are not needed. The numerical results are presented for both two-dimensional and three-dimensional examples [28, 34, 7]. We have also studied SAMC and DASAMC approaches in [33] where more advanced sampling methods are implemented. We show that, using these methods, we can avoid the problem of being trapped in the local minima. Moreover, we have generalized these methods to two-stage and used coarse-grid models to speed-up the simulations.

We have considered a design of efficient emulators in [30, 29, 28]. In particular, we develop an emulator based approach where the Bayesian multivariate adaptive splines (BMARS) has been used to model unknown functions of the model input. We consider discrete cosine transformation (DCT) for dimension reduction of the input field. The estimation is carried out using trans dimensional Markov chain Monte Carlo. Numerical results are presented by analyzing simulated as well as real data for reservoir characterization in [30, 28].

We have applied our methods to complex 2D and 3D reservoirs [36, 35], where we showed that, using the proposed methods, one can accurately reconstruct the channel boundaries.

3.1 Sparse Randomized Maximum Likelihood for Practical Uncertainty Quantification

Randomized Likelihood Approach has been frequently used in reservoir simulations. We have studied the application of Randomized Likelihood Approach. We formulated an approximate sampling approach to quantify solution uncertainty in a sparse model representation framework [20]. Given the uncertainty in describing subsurface properties, even after integration of the dynamic data, we were motivated to develop a practical sparse Bayesian inversion approach to enable uncertainty quantification. We use the concept of sparse geologic dictionaries in the previous parts to compactly represent uncertain subsurface properties and develop a practical sparse Bayesian method for effective data integration and uncertainty quantification. Since the multi-Gaussian assumption that is widely used in classical probabilistic inverse theory is not appropriate for representing sparse prior models, we adopted the Laplace (or double exponential) probability distribution to represent sparse parameters. However, combining Laplace priors with the frequently used Gaussian likelihood functions leads to neither a Laplace nor a Gaussian posterior distribution, which complicates the analytical characterization of the posterior. In our formulation, we first expressed the form of the Maximum A-Posteriori (MAP) estimate for Laplace priors and then used the Monte-Carlo-based Randomize Maximum Likelihood (RML) method to generate approximate samples from the posterior distribution. The proposed Sparse RML (SpRML) approximate sampling approach can be used to assess the uncertainty in the calibrated model with a relatively modest computational complexity. We demonstrated the suitability and effectiveness of the SpRML formulation using a series of numerical experiments of two-phase and three-phase flow systems in petroleum reservoirs.

3.2 Ensemble level solvers

Markov chain Monte Carlo (MCMC) techniques will substantially benefit from ensemble level approaches, such as ensemble level multiscale methods or ensemble level preconditioners. In these ensemble-level approaches, coarse spaces are constructed for a portion of the ensemble or the entire ensemble that make the computations of the forward simulations inexpensive. For example, in ensemble level multiscale methods, multiscale basis functions are constructed such that they can be used to solve flow equations for many proposals within MCMC and thus speed-up the computations in the first stage of MCMC techniques. In ensemble level preconditioners, the same preconditioner is used to solve the flow equation for a number of proposals, and thus this helps reducing the computational cost substantially. In this regard, one has to make sure that the number of iterations is independent of the contrast in order to reduce the number of iterations in these repeated MCMC forward calculations. Because of channelized structures of subsurface properties, the construction of robust preconditioners is a challenging task. The number of iterations in the preconditioners depends on the contrast (the ratio of high and low permeabilities) and can be very large. Thus, it will require many iterations for iterative methods to converge. It is important for our applications to keep the number of iterations independent of the contrast because of large contrasts in permeabilities. We considered various robust multi-level preconditioners for channelized permeability fields. These works are reported in [33, 18], where special coarse spaces are constructed to guarantee that the number of iterations is independent of the contrast and the dimension of the coarse spaces needed for this effort is minimal. We have designed a special type of ensemble level preconditioners for channelized reservoirs in [33, 18]. We have shown that both coarse-grid approximations and ensemble level solvers are robust in the channelized environments.

3.3 Multilevel Monte Carlo methods and applications to multi-phase flow

Numerical homogenization is often used to upscale media properties. Due to small scales and large uncertainties at the finest scales, one needs to solve many local problems to compute effective properties. Local problems are solved in Representative Volume Element (RVE). RVE computations can, in general, be expensive as one needs to resolve fine-scale features within local regions. The use of smaller RVEs provides an advantage in simulations at the cost of lower accuracy. However, when performing Monte Carlo simulations, one can run many such RVE problems and reduce the error while running fewer large size RVE problems. This constitutes the main idea of our application of multilevel Monte Carlo methods (MLMC). In MLMC, we run various numbers of RVE problems in regions of different sizes. In particular, the number of RVE problems in Monte Carlo simulations is chosen in the following way. Fewer samples with large RVE sizes are run, while many samples with small RVE sizes are performed. Furthermore, these results are combined in computing the expectation of the quantity of interest, e.g., two-point correlation function of upscaled conductivity. Our results show that one can achieve improvement using MLMC while keeping the amount of the computation the same. The proposed methods provide an inexpensive way of computing macroscopic statistics of effective permeability without sacrificing the accuracy. We also consider the computation of the effective solution and propose a variation of MLMC - weighted MLMC. The main idea of weighted MLMC is to compose the different RVE computations with weights in addition to the fact that these computations use

different number of samples in MC. We show that this is essential in the computations of effective solutions.

We have considered multilevel Monte Carlo methods for two-phase immiscible flow and transport in random multiscale media. We employ ensemble level multiscale methods where a number of realizations are selected and furthermore used to construct multiscale basis functions for the whole ensemble (or a part of the ensemble). These computations are done off-line and these basis functions are used to solve the forward problem on a coarse grid that provides a substantial speed-up in two-phase flow computations. If, for example, ten realizations are selected for constructing ensemble level multiscale basis functions, then there are 10 basis functions per coarse-grid element. In many cases, one needs many realizations to construct ensemble level multiscale basis functions to achieve high accuracy. As a result, the forward computations can be expensive on a coarse grid because each coarse grid region is represented with many basis functions. To speed-up these computations, multilevel Monte Carlo methods are employed where we use a different number of realizations for the construction of ensemble level basis functions. For forward simulations, we run many more simulations with a small number of basis functions, and fewer simulations with a large number of basis functions. Combining these results in a MLMC framework, we show that one can obtain 6-7 times more accurate results if MLMC is used. This summarizes the works [15, 16, 24]. Efendiev co-advised the student, C. Kronsbein, who worked on multi-level Monte Carlo methods. In addition, this research is continued in the thesis of Xiaosi Tan [32, 17]

3.4 Multiscale approximations of the solutions and applications

Multiscale approximation for the solution of stochastic PDEs has been studied in the project. In particular, our goal has been to construct a hierarchical approximation for the solution such that it can be used in multilevel MCMC or multilevel MC. These hierarchical approximations can be constructed such that one can estimate associated errors. The main idea of these hierarchical approximations is the use of multiscale basis functions. In [31, 6, 11, 12, 16, 10, 9], we developed and investigated several of such algorithms based on Generalized Multiscale Finite Element framework. In these works, we study how to use the ideas from sparsity and ensemble level approximations to construct multiscale basis functions across the ensemble.

4 Other activities

We (Datta-Gupta, Efendiev, and Mallick) have organized a workshop on uncertainty quantification (February 24-25, 2011). The funding for the workshop came from the Institute for Applied Mathematics and Computational Sciences (IAMCS) and the web site is at <http://isc.tamu.edu/events/inverseuq>. In this workshop, we brought some well-known experts from uncertainty quantification (mostly for subsurface related applications). The workshop participants addressed some challenging issues in the area of uncertainty quantification. These issues include: efficient data assimilation techniques; robust and accurate model reduction techniques; constructing and assessing the statistical accuracy of emulators; implementation of these methods on today's computer architectures. All these areas were relevant to our joint project. Another workshop that Efendiev has organized are on Multiscale Modeling, Advanced Discretization Techniques, and Simulation of Wave Propagation where P. Vassilevski has participated and gave an invited talk. B. Mallick has organized a

session in SIAM UQ where Efendiev participated and gave a talk. Mallick and Efendiev organized a small workshop on UQ at KAUST in May 2012.

A number of graduate students supported by this collaborative grant finished their Ph.D. theses. A. Mondal (Statistics) successfully completed his Ph.D. thesis in May 2011 (chair: Mallick; co-chair: Efendiev; a committee member: Datta-Gupta) and currently is an Assistant Professor in Case Western University, after his successful career in the oil industry, where he developed novel emulators. Eric Bhark (Petroleum Engineering) (chair: Datta-Gupta; co-chair: Jafarpour; committee: Efendiev) has successfully finished his Ph.D. thesis in May 2011 and joined oil industry. Jia Wei (Mathematics) has successfully graduated in 2012 (chair: Efendiev; co-chair: Datta-Gupta) and worked on uncertainty quantification for subsurface flow and transport. Her thesis is “Reduced order model and uncertainty quantification for stochastic porous media flows”. She investigated regularity of the posterior measure and proposed several efficient parameterization and sampling techniques. Jiang Xie (Petroleum Engineering) has successfully graduated in 2012 (chair: Datta-Gupta; co-chair: Efendiev). His thesis is “Applications of Level Set and Fast Marching Methods in Reservoir Characterization” and he worked on applications of level set approaches in re-parameterization of permeability fields and dynamic data inversion. Jiang Xie has joined to oil company. Seul-ki Kang (Mathematics) graduated in 2012 ([19]) (chair: Efendiev). Her thesis work was on uncertainty quantification for Richards’ equations, where she applied the methods developed in the project for studying the flow in groundwater applications. Xiaosi Tan (Mathematics) graduated in 2015 ([32]) (chair: Efendiev). Her thesis investigated various approaches for uncertainty quantification using multiscale and multilevel approaches. She has started her graduate studies in 2009. Currently, she is a postdoc in Petroleum Engineering. Jun Ren (Mathematics) graduated in 2015 (chair: Efendiev) and worked on developing multiscale methods for parameter-dependent problems, [31]. He has started her Ph.D. studies in 2009 and, currently, is working in the industry.

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