Multi-physics Markov chain Monte Carlo methods for subsurface flows[☆]

V. Ginting^a, F. Pereira^{b,*}, A. Rahunanthan^c

^a*Department of Mathematics, University of Wyoming, Laramie, WY 82071, USA*

^b*Department of Mathematical Sciences, University of Texas at Dallas, Richardson, TX 75080, USA*

^c*Department of Mathematics and Statistics, University of Toledo, Toledo, OH 43606, USA*

Abstract

In CO₂ sequestration in deep saline aquifers, contaminant transport in subsurface, or oil or gas recovery, we often need to forecast flow patterns. In the flow forecasting, subsurface characterization is an important step. To characterize subsurface properties we establish a statistical description of the subsurface properties that are conditioned to existing dynamic (and static) data. We use a Markov Chain Monte Carlo (MCMC) algorithm in a Bayesian statistical description to reconstruct the spatial distribution of two important subsurface properties: rock permeability and porosity. The MCMC algorithm requires repeatedly solving a set of nonlinear partial differential equations describing displacement of fluids in porous media for different values of permeability and porosity. The time needed for the generation of a reliable MCMC chain using the algorithm can be too long to be practical for flow forecasting. In this paper we develop computationally fast and effective methods of generating MCMC chains in the Bayesian framework for the subsurface characterization. Our strategy consists of constructing a family of computationally inexpensive preconditioners based

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*Corresponding author

Email addresses: vginting@uwyo.edu (V. Ginting), 1fp140030@utdallas.edu (F. Pereira), arunasalam.rahunanthan@utoledo.edu (A. Rahunanthan)

on simpler physics as well as on surrogate models such that the number of fine-grid simulations is drastically reduced in the generation MCMC chains. We assess the quality of the proposed multi-physics MCMC methods by considering Monte Carlo simulations for forecasting oil production in an oil reservoir.

Keywords: MCMC, Porous media, Multi-physics, Multi-stage

1. Introduction

Scientifically correct models based on first principles, accurate numerical simulators and state-of-the-art computers are of utmost importance in producing reliable predictions of multiphase flows in the subsurface. However, uncertainty in the determination of subsurface properties, such as permeability and porosity, remains the main challenge that one has to overcome to produce accurate predictions.

The typical situation encountered in the investigation of problems such as CO₂ sequestration in saline aquifers, contamination of subsurface, or oil recovery is that there is very little data available to characterize subsurface properties. Only sparse data is available: at well locations permeability and porosity (static data) can be measured as well as well pressure values, production curves, and saturation or concentration values at monitoring wells (dynamic data) are usually available. Thus, the problem of determining permeability and porosity fields from available data is not well posed and a stochastic prediction methodology must be considered [23].

We are concerned with the development of a computationally fast and effective Bayesian framework for the characterization of porous media. To characterize subsurface properties we establish a statistical description of the subsurface properties that are conditioned to existing dynamic (and static) data. We use a Markov Chain Monte Carlo (MCMC) algorithm in a Bayesian statistical description to reconstruct the spatial distribution of rock permeability and porosity. In this context however, acceptance or rejection criterion in the MCMC algorithm requires the calculation of likelihood function that involves repeatedly solving

25 a set of nonlinear partial differential equations describing displacement of fluids
in porous media for different values of permeability and porosity. For each proposal
in the MCMC algorithm we compare measured data with its simulated
counterpart [27, 11, 7]. The time needed for the generation of a reliable MCMC
chain using the algorithm can be too long to be practical for the subsurface
30 characterization.

The search of computationally efficient MCMC methods has been attracting
the attention of several research groups. Fox and Nicholls [13] employed a
perturbation technique to identify proposals that are most likely rejected in the
posterior probability exploration. Oliver et al. [29] were perhaps among the first
35 to apply MCMC in the petroleum reservoir simulations to characterize uncertainty
in the permeability fields conditioned to the pressure data. The authors
in [15] improved the algorithm in [29] by proposing a blocking MCMC approach
in which each proposed member of the chain is different from the previous one
over an entire, relatively large, block of cells. This blocking scheme accelerates
40 the creation of the chain of realizations. Higdon et al. [24] presented a methodology
for improving the speed and efficiency of an MCMC by combining runs
on different scales. They introduced a coarse-scale to make the MCMC chain
run faster and better explore the posterior, and linked the coarse chain back to
the original fine-scale chain of interest. In [6] a two-stage MCMC algorithm was
45 presented for generating samples from an unnormalized posterior distribution in
which the evaluation of the posterior distribution is very difficult or computationally
demanding. The algorithm was applied to recovering resistor values in a
network from electrical measurements made at the boundary. Later in [11, 12],
the two-stage MCMC algorithm, which utilizes inexpensive coarse-scale models
50 to screen out detailed flow and transport simulations, was used to explore the
posterior distribution of the permeability field. In the first stage, a new proposal
is tested at the coarse-scale model. If the proposal passes the testing at
the coarse-scale model, then at the second stage the fine-scale simulation will be
run and this fine-scale run is computationally very expensive when compared
55 to the coarse-scale run. Vrugt et al. [32] developed a population-based MCMC

algorithm that allows for the exchange of information among multiple chains to enhance the efficiency of MCMC sampling. Kavetski et al. [26] and Kavetski and Kuczera [25] showed that some computational complexities can be removed by smoothing the objective function in parameter optimizations of hydrological model calibration in accelerating the Bayesian posterior sampling. A multiple-try MCMC algorithm [34] was designed for a hydrological and environmental simulation model by making better use of the information generated in a costly run of the model. The authors used multiple evaluations of the posterior density in the less computationally expensive subspace of error model parameters.

Furthermore, in the same spirit of two-stage procedures [6, 11, 12, 17], the authors introduced a multi-stage Bayesian prediction framework for subsurface flows in [20]. The authors described a predictive procedure in a Bayesian framework, which uses a single-phase flow model for characterization aiming at making prediction for a two-phase flow model. The quality of the characterization of the underlying formations was accessed through the prediction of future fluid flow production. They also considered parallelizing the generation of MCMC chains to speed-up the posterior exploration in [18, 21]. In [18] the authors addressed this issue using several parallel MCMC chains for flow prediction. In [21] the authors parallelized single MCMC chains using a prefetching technique implemented on GPUs and showed that the parallelization can make the Bayesian approach computationally tractable for subsurface characterization and prediction of porous media flows.

The original contribution of the present work is the introduction of the concept of multi-physics MCMC (MP-MCMC) methods. In our strategy a family of computationally inexpensive preconditioners is constructed based on simpler physics as well as on surrogate models such that the number of fine-grid simulations of the problem of interest is drastically reduced in the whole MCMC calculation. Moreover, we assess the quality of the characterization step by considering Monte Carlo simulations for prediction. We use partial (in time) data from production wells to characterize permeability and porosity fields. A set of accepted proposals is then sent to the numerical model to run the forward

problem and predict the remaining portion of measured production data by aggregating the solutions of the forward problem [22]. We refer to this prediction stage as the Monte-Carlo (MC) step of our Bayesian framework.

90 We focus on the development of MP-MCMC methods that may incorporate ad-hoc characterization procedures of use in engineering practice (for example, tracer tests and huff-puff procedures [1]) in a mathematically and computationally sound framework. We remark that frequently a *geological model* is constructed by geologists and geophysicists based on seismic information, well
 95 measurements, etc. The framework discussed here can take such models into account: we characterize a perturbation of such deterministic fields that allows us to match simulation results to existing dynamic data.

The development of MP-MCMC methods naturally refers to a hierarchy of models for porous media flows, from full compositional multiphase flow to the
 100 simple tracer flow problem. In order to explain our framework we will refer mainly to two-phase, immiscible, incompressible displacement and tracer flows.

This paper is organized as follows. We discuss the current state of practice for subsurface characterization in Section 2. In this section a parametrization of uncertainty using the Karhunen-Loève expansion [28, 33] for unknown permeability and porosity fields is discussed. The parametrization is followed by a
 105 discussion of MCMC sampling for quantifying uncertainty in both permeability and porosity fields. We then recall a two-stage MCMC algorithm that uses an upscaling of the characteristics of the subsurface on a fine-grid to a computationally quicker coarse-grid; the novel MP-MCMC reduces to this procedure as
 110 a particular case. In Section 3 we introduce a multi-physics MCMC algorithm for efficient and effective subsurface characterization. In the simulation studies in Section 4 we implement MCMCs to predict the partial production curves in an oil reservoir and compare MCMC algorithms. Section 5 contains our conclusions that support our proposed multi-physics MCMC algorithm for reliable
 115 characterization and prediction of porous media flows.

2. Current state of practice

2.1. Physical and mathematical modeling

We consider a heterogeneous oil reservoir which is confined in a domain Ω . The reservoir contains an injection and two production wells. Water is discharged at the injection well to displace the trapped oil towards the production wells (see Fig. 1). The dynamics of the movement of the fluids in the reservoir is categorized as an immiscible two-phase system with water and oil (denoted by w and o , respectively) that is incompressible. Capillary pressure is not included in the model. To further simplify the model, we assume a gravity-free environment with no sources or sinks, and water and oil fill the pore space. The injection and production wells are modeled through boundary conditions.

Fig. 1: Permeability (in logarithmic scale) and porosity distribution of the reference field on the left and right, respectively. Closed and open circles denote the location of injection and production wells, respectively.

Darcy's law with a statement of conservation of mass allow us to write the governing equations of the flow as

$$\nabla \cdot \mathbf{u} = 0, \quad \text{where} \quad \mathbf{u} = -\lambda(s)k(\mathbf{x})\nabla p, \quad (1)$$

and

$$\phi(\mathbf{x})\frac{\partial s}{\partial t} + \nabla \cdot (f(s)\mathbf{u}) = 0, \quad (2)$$

where $\mathbf{u}$ is the Darcy velocity, s is the water saturation, k is the absolute permeability and ϕ is the porosity. The total mobility $\lambda(s)$ and the flux function $f(s)$ are respectively given by

$$\lambda(s) = \frac{k_{rw}}{\mu_w} + \frac{k_{ro}}{\mu_o}, \quad f(s) = \frac{k_{rw}(s)/\mu_w}{\lambda(s)}, \quad (3)$$

where k_{rj} , $j = w, o$, is the relative permeability of the phase j [5].

We sample rock permeability and porosity of the oil reservoir using partial fractional flow data. For each production boundary the fractional flow $F(t)$ is defined as the fraction of oil in the produced fluid, which depends on dimensionless time t (in PVI):

$$F(t) = 1 - \frac{\int_{\partial\Omega_{\text{out}}} u_n f(s) \, dl}{\int_{\partial\Omega_{\text{out}}} u_n \, dl}, \quad (4)$$

and

$$\text{PVI} = \int_0^T V_p^{-1} \int_{\partial\Omega_{\text{in}}} u_n \, dl \, d\tau, \quad (5)$$

where $\partial\Omega_{\text{out}}$ ($\partial\Omega_{\text{in}}$) denotes outflow (inflow) boundary, u_n is normal velocity field, V_p is the total pore-volume of the reservoir, and T denotes the time taken

for injection of water.

The pressure and saturation equations, (1) and (2), are coupled together by the Darcy velocity $\mathbf{u}$ and water saturation s . For a better computational efficiency in solving these equations, we employ an operator splitting technique (see for example [9, 2, 3]). This technique allows us to use very larger time steps for solving (1) than the time steps for solving (2), which are governed by the CFL condition. We thus introduce a variable time step Δt_s for the saturation calculation, and a longer time step Δt_p for the pressure calculation. The pressure and thus the Darcy velocity are approximated at times $t^m = m\Delta t_p$, where $m = 0, 1, \dots$; the saturation is approximated at times $t^{m,k} = t^m + \sum_{i=1}^k (\Delta t_s)_i$ for $t^m < t^{m,k} \leq t^{m+1}$. We specify the water saturation at $t = 0$. We refer the reader to [30, 31] for further discussion on the numerical schemes used in solving the forward problem possibly taking advantage of GPU hardware for high performance computing.

Fig. 2: Decay of eigenvalues for the Gaussian covariance with $L_x = L_y = 0.1$ and $\sigma_Y^2 = 4$.

2.2. Parametrization of uncertainty

145 In this subsection we discuss Karhunen-Loève (KL) expansion [28, 33] to reduce dimension of uncertainty space for permeability and porosity. This reduction technique has been applied within a Bayesian statistical framework in [11, 17, 18, 20, 19, 21]. Here we reproduce the technique for the sake of completeness of the discussion.

We assume that permeability distribution is log-normal [8]. This simplification leads to $\log[k(\mathbf{x}, \omega)] = Y^k(\mathbf{x}, \omega)$, where $\mathbf{x}$ represents spatial location, and ω introduces randomness. The $Y^k(\mathbf{x}, \omega)$ represents a field with a Gaussian covariance function. Here we assume a covariance of the form

$$R(\mathbf{x}_1, \mathbf{x}_2) = \sigma_Y^2 \exp\left(-\frac{1}{2}|\mathbf{L}^{-1}(\mathbf{x}_1 - \mathbf{x}_2)|^2\right), \quad (6)$$

where, $\mathbf{L} = \text{diag}(L_x, L_y)$ with the correlation lengths L_x and L_y in x - and y -direction, respectively, and $\sigma_Y^2 = E[(Y^k)^2]$, and $|\cdot|^2 = \langle \cdot, \cdot \rangle$ is the usual norm induced by the Euclidean inner product. We assume $Y^k(\mathbf{x}, \omega) \in L^2(\Omega)$ with a probability of one and $E[Y^k(\mathbf{x})] = 0$. This leads to the Karhunen-Loève expansion

$$Y^k(\mathbf{x}, \omega) = \sum_{i=1}^{\infty} \sqrt{\lambda_i} \theta_i^k(\omega) \varphi_i(\mathbf{x}), \quad (7)$$

where φ_i and λ_i satisfy

$$\int_{\Omega} R(\mathbf{x}_1, \mathbf{x}_2) \varphi_i(\mathbf{x}_2) d\mathbf{x}_2 = \lambda_i \varphi_i(\mathbf{x}_1), \quad i = 1, 2, \dots, \quad (8)$$

150 where $\lambda_i = E[(Y_i^k)^2] > 0$.

We remark that instead of (6) one could use other covariance functions. For example, one could assume

$$R(\mathbf{x}_1, \mathbf{x}_2) = \sigma_Y^2 \exp\left(-\frac{1}{2} |\mathbf{L}^{-1}(\mathbf{x}_1 - \mathbf{x}_2)|^{(1+\delta)}\right), \quad (9)$$

for some $0 \leq \delta \leq 1$. When $\delta = 1$, we get the covariance function in (6). The eigenvalues decay for $\delta = 1$ is faster than the eigenvalues decay for $0 \leq \delta < 1$ [14]. Therefore, we must add more terms in the truncated KL expansion (10) for $0 \leq \delta < 1$. This, in turn, will increase the parameter space dimension.

155 The larger the parameter space dimension, the more expensive the sampling of permeability and porosity becomes.

The L^2 basis functions $\varphi_i(\mathbf{x})$ in (8) are deterministic and resolve the spatial dependence of the permeability field and in particular its correlation structure. The scalar random variables θ_i^k represent uncertainty in permeability. We order the eigenvalues $\{\lambda_i\}_{i=1}^{\infty}$ in the KL expansion (7) (i.e., $\lambda_1 \geq \lambda_2 \geq \dots$). This permits us to keep the leading order terms (quantified by the magnitude of λ_i), which capture most of the energy of the stochastic process $Y^k(\mathbf{x}, \omega)$. For a N_k -term KL expansion we write

$$Y_{N_k}^k = \sum_{i=1}^{N_k} \sqrt{\lambda_i} \theta_i^k \varphi_i. \quad (10)$$

In Fig. 2 we show a decay of eigenvalues for the Gaussian covariance (6) with $L_x = L_y = 0.1$ and $\sigma_Y^2 = 4$. In this case we can sample $Y^k(\mathbf{x}, \omega)$ from the truncated KL expansion (7) with 80 eigenvalues.

We now focus on the KL expansion for porosity. Let us assume that both spatial correlation structures for permeability and porosity are similar. This enables us to employ the same Karhunen-Loève basis functions (8). Following the same reduction technique for the permeability field, we use a N_{ϕ} -term KL

expansion

$$Y_{N_\phi}^\phi(\mathbf{x}, \omega) = \sum_{i=1}^{N_\phi} \sqrt{\lambda_i} \theta_i^\phi(\omega) \varphi_i(\mathbf{x}). \quad (11)$$

The porosity values should fall between $\phi_{\min}$ and $\phi_{\max}$, where $\phi_{\min}$ and $\phi_{\max}$ are the lower and upper limits of the porosity distribution of subsurface. Therefore, we define the porosity as

$$\phi(\mathbf{x}) = \frac{\phi_{\min} + \phi_{\max} e^{Y_{N_\phi}^\phi}}{1 + e^{Y_{N_\phi}^\phi}}, \quad \phi_{\min} \text{ and } \phi_{\max} \in (0, 1). \quad (12)$$

160 For simplicity, we here assume that both permeability and porosity fields share a similar correlation structure. However, one could use a correlation structure of porosity different from that of permeability, and use the same Bayesian framework for characterizing permeability and porosity fields.

2.3. Bayesian inference

In this subsection we introduce a Bayesian framework to sample the permeability and porosity fields conditioned on measured production data F_m . We sample from the conditional distribution $P(\boldsymbol{\psi}|F_m)$. The $\boldsymbol{\psi}$ represents the field generated by the vectors $\boldsymbol{\theta}^k$ and $\boldsymbol{\theta}^\phi$, which contain the random coefficients in the KL expansions (10) and (11), respectively. i.e., $\boldsymbol{\psi} = [\boldsymbol{\theta}^k \ \boldsymbol{\theta}^\phi]$. With Bayes' theorem we can write

$$P(\boldsymbol{\psi}|F_m) \propto P(F_m|\boldsymbol{\psi})P(\boldsymbol{\psi}), \quad (13)$$

where $P(F_m|\boldsymbol{\psi})$ represents the likelihood function (that requires the forward solution of the two-phase flow) and $P(\boldsymbol{\psi})$ is the prior distribution of $\boldsymbol{\psi}$. We assume that the likelihood function follows a Gaussian distribution [12]

$$P(F_m|\boldsymbol{\psi}) \propto \exp\left(-\langle F_m - F_\psi, \Sigma(F_m - F_\psi) \rangle\right), \quad (14)$$

where F_ψ represents simulated production data that is obtained by solving the forward problem with known permeability k and porosity ϕ , in other words with known $\boldsymbol{\psi}$, and Σ is the covariance matrix representing the measurement errors. $\Sigma = I/2\sigma_F^2$, where I is the identity matrix and σ_F^2 is the precision associated

with the measurement F_m and numerical solution F_ψ . We denote the posterior distribution by $\pi(\psi|F_m)$. Combining (13) and (14) we get

$$\pi(\psi|F_m) \propto \exp\left(-\langle F_m - F_\psi, \Sigma(F_m - F_\psi) \rangle\right) P(\psi). \quad (15)$$

165 In the previous section we indicated that both permeability and porosity fields share a similar correlation structure. This correlation structure sharing does not imply that the fields are statistically correlated. Therefore, to avoid using an ad-hoc correlation between porosity and permeability, we assume that θ^k and θ^ϕ are independent of each other.

170 2.3.1. Markov chain Monte Carlo method

We now discuss the standard Metropolis-Hasting MCMC algorithm for exploring the posterior distribution for the underlying field. In this algorithm we rely on the construction of a Markov chain with an equilibrium distribution equal to the posterior distribution of interest. At each iteration, $\psi = [\theta^k \ \theta^\phi]$ is 175 drawn from an instrumental distribution $q(\psi|\psi_{j-1})$, where ψ_{j-1} is the previous state/iteration in the chain. It is then proceeded by solving the forward problem to get F_ψ which in turn is used in the calculation of (14). The likelihood values along with the prior information are the basis for the decision making of either to reject or accept ψ . See Algorithm 1 for a detailed procedure.

180 2.3.2. Two-stage Markov chain Monte Carlo method

We discuss a two-stage MCMC algorithm that aims at reducing computational cost on proposals that are most likely rejected after the fine-scale simulation. The detailed algorithm was described in [6] for recovering resistor values in a electrical network, and for characterization of subsurface in [11]. We explain 185 the main idea of the algorithm in the context of our problem of interest. We introduce a screening process to compare the measured production curves against inexpensive simulated production curves obtained on a coarse-grid. In the coarse-grid simulation we solve the equations (1) and (2) on the coarse-grid whose discretization is done in a similar fashion as in the fine-scale simulation.

Algorithm 1 Single-stage MCMC

Given the covariance function R , generate KLE parametrization $\{\lambda_n, \varphi_n\}_{n=1}^N$

Set initial state $\boldsymbol{\psi}_0 = [\boldsymbol{\theta}_0^k \ \boldsymbol{\theta}_0^\phi]$

for $j = 1$ to M_{mcmc} **do**

(1) At state $\boldsymbol{\psi}_{j-1}$ generate $\boldsymbol{\psi} = [\boldsymbol{\theta}^k \ \boldsymbol{\theta}^\phi]$ from $q(\boldsymbol{\psi}|\boldsymbol{\psi}_{j-1})$

(2) With $\boldsymbol{\psi}$ compute k and ϕ using KLE and solve the forward problem on the fine-scale to get F_ψ

(3) Accept $\boldsymbol{\psi}$ with probability

$$\text{Pr} = \alpha(\boldsymbol{\psi}_{j-1}, \boldsymbol{\psi}) = \min \left(1, \frac{q(\boldsymbol{\psi}_{j-1}|\boldsymbol{\psi})P(\boldsymbol{\psi}|F_m)}{q(\boldsymbol{\psi}|\boldsymbol{\psi}_{j-1})P(\boldsymbol{\psi}_{j-1}|F_m)} \right),$$

i.e., $\boldsymbol{\psi}_j = \boldsymbol{\psi}$ with probability Pr or $\boldsymbol{\psi}_j = \boldsymbol{\psi}_{j-1}$ with probability $1 - \text{Pr}$

end for

190 For the coarse-grid simulation we need to know the permeability and porosity distributions on the coarse-grid. However, we have the distributions of permeability and porosity on the fine-grid. Therefore, the permeability and porosity information should carefully be transferred on the coarse-grid. For transferring the information, we use an upscaling procedure such that effective permeability and porosity fields on the coarse-grid produce a similar average response as that of the fine-grid problem locally. As described in [10, 22] we find the effective permeability on the coarse-grid cells. We then solve (1) on the coarse-grid with $\bar{k}$ replacing k to get the upscaled Darcy's velocity. In a similar way, we solve (2) on the coarse-grid with an upscaled porosity. The upscaled porosity of a coarse-grid cell is computed by taking the arithmetic average over all fine-grid cells in the coarse-grid cell [4]. See Algorithm 2.

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3. Development of the multi-physics Markov chain Monte Carlo method (MP-MCMC)

In this section we develop a new effective algorithm for the characterization of the subsurface. For the discussion below we focus on multiphase flows in rigid

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Algorithm 2 Two-stage MCMC

Given the covariance function R , generate KLE parametrization $\{\lambda_n, \varphi_n\}_{n=1}^N$

Set initial state $\psi_0 = [\theta_0^k \ \theta_0^\phi]$

for $j = 1$ to M_{mcmc} **do**

(1) At ψ_{j-1} generate $\psi = [\theta^k \ \theta^\phi]$ from $q(\psi|\psi_{j-1})$

(2) With ψ compute k and ϕ using KLE and solve the forward problem on a coarse-scale to get F_ψ^c

(3) Accept ψ with probability

$$\alpha_c(\psi_{j-1}, \psi) = \min \left(1, \frac{q(\psi_{j-1}|\psi)P_c(\psi|F_m)}{q(\psi|\psi_{j-1})P_c(\psi_{j-1}|F_m)} \right)$$

if (ψ rejected) **then**

Set $\psi_j = \psi_{j-1}$ and go to the beginning of *for* loop

else

Use ψ in the fine-scale simulation to get F_ψ^f

Accept ψ with probability

$$\alpha_f(\psi_{j-1}, \psi) = \min \left(1, \frac{P_f(\psi|F_m)P_c(\psi_{j-1}|F_m)}{P_f(\psi_{j-1}|F_m)P_c(\psi|F_m)} \right)$$

if (ψ rejected) **then**

Set $\psi_j = \psi_{j-1}$

else

Set $\psi_j = \psi$

end if

end if

end for

porous media and take advantage of the fact that fluid flow problems in porous media with increasing complexity share the same coefficients (e.g., permeability and porosity fields) in the governing systems of partial differential equations. The overall framework would also be applicable to multiphase flows coupled
210 with geomechanical rock deformation that will be addressed elsewhere. Typical characterization procedures of reservoir engineering (such as tracer tests) are combined in a multi-stage, multi-physics Bayesian framework that reduces drastically the computational cost of the classical Metropolis-Hastings MCMC algorithms when applied to porous media flow problems. Distinct applications
215 might need different combination of preconditioners such that the available data is properly used to inform the simulation models.

Motivated by the single-physics two-stage MCMC algorithm [11] we present an algorithm for MP-MCMCs. The algorithm takes into account a family (N_d) of physically-based auxiliary flow problems, production data and posterior dis-
220 tributions. We denote the flow problems, measured production data, and posterior distributions by $\{FP_i^*\}_{i=1}^{N_d}$, $\{F_{m,i}^*\}_{i=1}^{N_d}$, and $\{\pi_i^*(\psi|F_{m,i}^*)\}_{i=1}^{N_d}$, respectively. Here we want to make predictions for FP (the flow problem of interest). The MP-MCMC algorithm is outlined in Algorithm 3.

Algorithm 3 Multi-physics MCMC

Given the covariance function R , generate KLE parametrization $\{\lambda_n, \varphi_n\}_{n=1}^N$

Set initial state $\psi_0 = [\theta_0^k \ \theta_0^\phi]$

for $j = 1$ to M_{mcmc} **do**

(A) At state ψ_{j-1} generate $\psi = [\theta^k \ \theta^\phi]$ from $q(\psi|\psi_{j-1})$

(B) Set $Q_0(\psi|\psi_{j-1}) = q(\psi|\psi_{j-1})$

for $i = 1$ to N_d **do**

(1) With ψ solve the forward problem FP_i^* to get F_i^*

(2) Accept ψ with probability α_i , where

$$\alpha_i = \min \left(1, \frac{Q_{i-1}(\psi_{j-1}|\psi)\pi_i^*(\psi|F_{m,i}^*)}{Q_{i-1}(\psi|\psi_{j-1})\pi_i^*(\psi_{j-1}|F_{m,i}^*)} \right)$$

if (ψ rejected) **then**

Set $\psi_j = \psi_{j-1}$ and go to the beginning of j -for loop

end if

end for

(C) With ψ solve the fine-scale forward problem FP to get F_f

(D) Accept ψ with probability α_f , where

$$\alpha_f = \min \left(1, \frac{Q_{N_d}(\psi_{j-1}|\psi)\pi(\psi|F_{m,f})}{Q_{N_d}(\psi|\psi_{j-1})\pi(\psi_{j-1}|F_{m,f})} \right)$$

if (ψ rejected) **then**

Set $\psi_j = \psi_{j-1}$

else

Set $\psi_j = \psi$

end if

end for

In the algorithm $Q_i(\cdot | \cdot)$ is an effective instrumental distribution. The effective instrumental distribution is given by [16]

$$\begin{aligned} Q_i(\psi|\psi_{j-1}) &= \alpha_i(\psi_{j-1}, \psi) Q_{i-1}(\psi|\psi_{j-1}) \\ &\quad + \left(1 - \int \alpha_i(\psi_{j-1}, \psi) Q_{i-1}(\psi|\psi_{j-1}) d\psi \right) \delta_{\psi_{j-1}}(\psi), \end{aligned}$$

where $i = 1, \dots, N_d$. As in [11] it can be shown that

$$\frac{Q_i(\psi_{j-1}|\psi)}{Q_i(\psi|\psi_{j-1})} = \frac{\pi_i^*(\psi_{j-1}|F_{m,i}^*)}{\pi_i^*(\psi|F_{m,i}^*)}. \quad (16)$$

Then α_i in Algorithm 3 can be written as

$$\alpha_i = \min \left(1, \frac{\pi_{i-1}^*(\psi_{j-1}|F_{m,i}^*)\pi_i^*(\psi|F_{m,i}^*)}{\pi_{i-1}^*(\psi|F_{m,i}^*)\pi_i^*(\psi_{j-1}|F_{m,i}^*)} \right), \quad (17)$$

where π_i^* s can be computed using (15).

225 4. Simulation studies

As an indication of the feasibility of our proposed developments we present numerical results of single- and multi-physics MCMCs. We inject tracer or water in a reservoir with the well configuration described in Fig. 1. If the injected fluid is tracer, we will have a single-phase flow problem. We will have a two-phase
230 flow problem if we inject water. For our simulation study we considered synthetic measured tracer data (single-phase flow data) until 1.0 PVI and synthetic measured oil production data (two-phase flow data) until 0.4 PVI. See Fig. 3. The break through time of a reservoir often reveals very valuable information about reservoir heterogeneity. Therefore, the PVI values for dimensionless time
235 t were selected such that the break through occurs before 1.0 PVI and 0.4 PVI for single- and two-phase flows, respectively. These $F(t)$ curves were obtained by running the flow simulator on the reference field. In the following discussion we refer the standard Metropolis-Hastings MCMC algorithm as single-stage MCMC and we abbreviate this as SMCMC.

240 We now consider the following two cases for multi-stage, single-physics MCMCs. For these MCMCs we use a two-phase flow model with measured data until 0.4 PVI. The first case SP-2S denotes the two-stage MCMC, where we use a grid of 32×32 for filtering. In the second case SP-3S we have two coarse-grids 32×32 and 64×64 for filtering. In Table 1 we show results for these single-physics
245 MCMCs. Clearly a considerable increase in the acceptance rates is observed by adding an extra computationally relatively inexpensive level to the two-stage procedure described above.

Fig. 3: Synthetic measured data for single- and two-phase flows.

grid	σ_F^2	no. of acc. proposals and acc. rate		
		SMCMC	SP-2S	SP-3S
32×32	8×10^{-4}	—	8304 (42%)	8762 (44%)
64×64	4×10^{-4}	—	—	5978 (68%)
128×128	1×10^{-4}	4026 (20%)	3373 (41%)	3212 (54%)

Table 1: A comparison of accepted proposals out of 20000 proposals for single-physics MCMCs.

grid	σ_F^2	no. of acc. proposals and acc. rate		
		MP-1P2P	MP-1P1P2P	MP-1P2P2P
32×32 (tracer)	8×10^{-4}	—	9037 (45%)	10151 (51%)
32×32 (2-phase)	4×10^{-4}	—	—	6494 (64%)
128×128 (tracer)	4×10^{-4}	9107 (46%)	7065 (78%)	—
128×128 (2-phase)	1×10^{-4}	3033 (33%)	2251 (32%)	2607 (40%)

Table 2: A comparison of accepted proposals out of 20000 proposals for multi-physics MCMCs.

Next we consider multi-stage, two physics MCMCs. In the MCMCs, we

Fig. 4: A correlation study of two-stage MCMCs: On the left SP-2S and on the right MP-1P2P.

use tracer data until 1.0 PVI for preconditioning with two-phase flow being the
 250 problem of interest. Here we consider three cases. In the first case MP-1P2P we
 use tracer flow until 1.0 PVI on a 32×32 grid as the filtering step. MP-1P1P2P
 denotes a three-stage multi-physics MCMC with tracer flow until 1.0 PVI on
 32×32 and 128×128 grids for screening out proposals. In the third case MP-
 1P2P2P we use tracer flow until 1.0 PVI for the first stage on a grid 32×32 , and
 255 two-phase flow until 0.4 PVI for the second stage on the same grid 32×32 . In
 all the cases we run two-phase simulation on a fine-grid of 128×128 in the final
 stage. Again, computationally very inexpensive filtering stages based on tracer
 tests (that require only one elliptic solution) are quite efficient as they produce
 acceptance rates comparable to those of more expensive upscaled two-phase
 260 filtering stages (see Table 2).

In line with the discussion of the two-stage procedure [11] we remark that the
 preconditioners are chosen according to the following criteria: (1) They should
 be computationally very inexpensive; (2) They do not need to be very accurate;
 and (3) In a multi-stage procedure the errors in two successive steps should show
 265 correlation (for several realizations). In the design of our MP-MCMCs we used
 the most inexpensive preconditioners in the earlier stages of our procedures, such
 that we reduce the number of runs associated with more expensive simulations,
 or the fine grid runs of interest. Fig. 4 and Fig. 5 display the error correlations
 for two-stage and three-stage MCMCs investigated here, respectively, for 1000

Fig. 5: A correlation study of three-stage MCMCs: From top to bottom SP-3S, MP-1P1P2P, and MP-1P2P2P, respectively.

270 realizations. To plot error correlations we ran the numerical simulator without
 any MCMC algorithms. In these plots we show the errors defined by $\|F_m - F_\psi\|^2$
 in (14). For example, the plot on the right in Fig. 4 was plotted by considering
 the first and second stage errors in the MP-1P2P approach. In the first stage
 the single-phase flow problem was solved and the error was computed for each
 275 realization by comparing with the synthetic measured single-phase flow data.
 We solved the two-phase flow problem in the second stage and the simulated two-
 phase flow data was compared with the synthetic measured two-phase flow data.
 Clearly all successive stages show correlation. Moreover, our preconditioners are
 relatively inexpensive because they refer to simpler physics and/or coarser mesh
 280 problems.

Fig. 6: A set of accepted fields for single-physics MCMCs: Permeability (in logarithmic scale) and porosity distribution on the left and right, respectively. Closed and open circles denote the location of injection and production wells, respectively. Top to bottom, SMC, SP-2S, and SP-3S were used for characterization, respectively.

Fig. 7: A set of accepted fields for multi-physics MCMCs: Permeability (in logarithmic scale) and porosity distribution on the left and right, respectively. Closed and open circles denote the location of injection and production wells, respectively. Top to bottom, MP-1P2P, MP-1P1P2P, and MP-1P2P2P were used for characterization, respectively.

Fig. 8: Prediction using single- and multi-physics MCMCs: Vertical line separates measurement and prediction data. Top to bottom 4000, 8000, and 12000 proposals were used for prediction, respectively.

Now we discuss single- and multi-physics MCMCs for prediction. A set of accepted fields collected in Bayesian framework using single-physics MCMCs and multi-physics MCMCs is shown in Fig. 6 and Fig. 7, respectively. We run the numerical simulator on each accepted field until 1.4 PVI to produce the rest of the production curve for each production well. We then take a

weighted average of these production curves and we refer to this average as the prediction. In taking the average, 10% of the accepted proposals are thrown out as burn-in. For example, consider the prediction using 4000 proposals in the case of SMC MC in Fig. 8. We have 805 accepted proposals out of 4000
290 proposals. After throwing out 10% of the accepted proposals as burn-in, we have 725 accepted proposals for the prediction. If the i th accepted proposal remains w_i times as the present state in the MCMC chain, a weight of w_i will be assigned to the i th accepted proposal in taking the weighted average. As shown in Fig. 8 when we considered a fixed number of proposals for the
295 prediction in our problem of interest, the predictions using standard Metropolis-Hastings MCMC and multi-physics MCMCs are more reliable than those using single-physics MCMCs. It highlights that the convergence rates of standard Metropolis-Hastings MCMC and multi-physics MCMCs are better than those of single-physics MCMCs. However, the standard MCMC is computationally
300 more expensive than the multi-physics MCMCs.

5. Conclusion

We developed computationally fast and effective methods of generating MCMC chains in a Bayesian framework for subsurface characterization. We constructed a family of computationally inexpensive preconditioners based on simpler physics
305 and we drastically reduced the number of fine-grid simulations in proposed multi-physics MCMCs.

We considered prediction in an oil reservoir to assess the quality of the proposed MCMCs. We used a two-phase flow model to describe the movement of fluid in porous media. In subsurface characterization we explored samples in
310 single- and multi-physics MCMCs in a Bayesian framework to collect probable candidates for the underlying subsurface. In the characterization the MCMC algorithm accepts or rejects fields conditioned to measured partial oil production curves. In the multi-physics MCMCs we used tracer (single-phase) flow model on coarse-grids to screen out proposals before running expensive fine-grid, two-

315 phase flow simulations. The accepted fields in the characterization step were
used to simulate the rest of production curves. By aggregating the rest of
simulated production curves we predicted the production in each MCMC. Our
results provide an indication that the multi-physics MCMCs are efficient and
effective for subsurface characterization and prediction of porous media flows.

320 One could use a huff-puff technique as a screening step in the proposed
multi-physics MCMC framework. The huff-puff technique consists of injecting
and producing the same fluid for a short period of time. This strategy could
enable for a better characterization of the reservoir near wells. The authors
intend to study this case in the proposed multi-physics MCMC framework in
325 the near future.

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