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Parameter-independent model reduction of transient groundwater flow models: Application to inverse problems

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ABSTRACT

A new methodology is proposed for the development of parameter-independent reduced models for transient groundwater flow models. The model reduction technique is based on Galerkin projection of a highly discretized model onto a subspace spanned by a small number of optimally chosen basis functions. We propose two greedy algorithms that iteratively select optimal parameter sets and snapshot times between the parameter space and the time domain in order to generate snapshots. The snapshots are used to build the Galerkin projection matrix, which covers the entire parameter space in the full model. We then apply the reduced subspace model to solve two inverse problems: a deterministic inverse problem and a Bayesian inverse problem with a Markov Chain Monte Carlo (MCMC) method. The proposed methodology is validated with a conceptual one-dimensional groundwater flow model. We then apply the methodology to a basin-scale, conceptual aquifer in the Oristano plain of Sardinia, Italy. Using the methodology, the full model governed by 29,197 ordinary differential equations is reduced by two to three orders of magnitude, resulting in a drastic reduction in computational requirements.

1. Introduction

Traditional inverse problems involve solving a weighted history matching optimization problem that yields a set of optimally selected parameters. The Bayesian inverse problem reformulates the solution by treating the parameters as random variables that are described by a posterior probability distribution. Markov Chain Monte Carlo (MCMC) methods are a powerful set of algorithms capable of exploring the probability space of the random variables used in the formulation of the Bayesian inverse problem. The MCMC simulation constructs a posterior distribution from samples generated by a proposal distribution. The samples are accepted or rejected to a Markov chain through the posterior density function and proposal density function evaluated at both the current step (previously accepted sample) and the proposed step (new sample). If the Markov chain is constructed correctly it should converge to a stationary distribution that represents the posterior distribution [1,2]. Shi et al. [3] evaluated for vadose zone modeling the confidence interval predictive performance of MCMC and compared with nonlinear regression. Their results indicated that MCMC produced better results and for small parameter dimensions was more computationally efficient. One method to lower the dimensionality of the parameter space is to parameterize it further with the Karhunen–Loueve expansion (KLE). Das et al. [4] applied MCMC with a KLE parameterization of saturated hydraulic conductivity fields for soil moisture problems.

One of the most commonly used MCMC methods for determining the acceptance of parameter samples is the Metropolis–Hastings (M–H) algorithm [5,6]. In the case of groundwater, and the focus of this paper's Bayesian inverse problem, the parameter of interest is the posterior probability distribution of hydraulic conductivity given historical water level data. This distribution can be used to quantify the uncertainty and assess its effects on model predictions [7]. A problem with solving the Bayesian inverse problem through M–H MCMC is that it requires a large number of sequential model simulations to characterize an unknown parameter's posterior probability distribution. There are parallel versions of MCMC, but they still require many sequential model simulations to construct the chains. As a result, Bayesian inversion for parameter estimation of a highly discretized groundwater simulation model can be computationally infeasible. Another alternative is to use a two-stage MCMC framework that relies on a surrogate model, composed of a coarser grid or simplified flow process, to first evaluate the acceptance of a proposed value before

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its acceptance is evaluated by the full model [8]. This can further be enhanced by using adaptive sparse-grids [9].

Model reduction based on the Galerkin projection is a technique that projects a high dimensional model characterized by ordinary differential equations (ODEs) onto a low dimensional subspace, spanned by a small number of optimally chosen basis functions (principal components) [10]. The application of model reduction to a confined, groundwater model has been shown to reduce the dimensionality by several orders of magnitude. A variety of papers have been written on model reduction techniques. Vermeulen et al. [11] applied proper orthogonal decomposition (POD) for model reduction to groundwater equations by collecting an ensemble of hydraulic head solutions, called snapshots, at specific times from the simulation and at a constant, reference pumping rate. Snapshots have to be taken for each reference extraction/injection well. Vermeulen et al. [11] then applied principal component analysis (PCA) to this ensemble to form a projection matrix that reduces the groundwater model. McPhee and Yeh [12] followed this methodology and demonstrated that a POD reduced model maintains its sensitivity of head with respect to pumping, enabling it to embed in a management optimization problem. Baú [13] increased the utility of POD by deriving a reduced model for each Monte Carlo realization of hydraulic conductivity to solve a stochastic, multi-objective, confined groundwater management problem.

In principle, the model reduction technique applies to linear systems, such as confined aquifers, because it uses the principle of superposition. Application to nonlinear systems is possible, but the reduced model error would be greater and may require significantly more basis functions to characterize the model [14]. Robinson et al. [15] and Li and Hu [16] applied POD model reduction to several synthetic one- and two-dimensional mass transport models without chemical reactions. Buchan et al. [17] solved for the population growth of free moving neutrons, an eigenvalue problem, in a nuclear reactor system. The eigenvalue problem was reformulated to create pseudo-time dependence that describes the snapshots used in their projection basis.

In general, the reduced model depends on the data used to construct the projection matrix. The data consists of snapshots generated from the original full model for a given set of model parameter values. Thus, the reduced model may be sensitive to changes in parameters. This causes problems when the reduced model is used for solving the inverse problem of parameter estimation.

Developing parameter-independent reduced models is a new area of active research. Vermeulen [18] applied a reduced model to an inverse problem by taking snapshot sets over a specific range of parameter combinations. The drawback of this procedure is that with a large number of parameters the combinations can get very large. Additionally, if the parameters move away from the specified range, the accuracy of the reduced model drops and a new set of snapshots is required. Lieberman et al. [19] proposed a greedy algorithm for the construction of a projection-based reduced model that reduces the parameter and state spaces for a steady state statistical inverse problem. A greedy algorithm solves a multi-stage optimization problem by combining the optimal solution obtained from each stage. At each stage, the algorithm selects the local optimum and moves on to the next stage. A solution to the original multi-stage optimization problem is built up stage by stage. In general, this greedy strategy does not guarantee global optimum, but in many instances yields a good approximation to the optimal solution. The advantages of the algorithm are its easy implementation and fast execution. The objective function proposed by Lieberman et al. [19] for the selection of the optimal parameter set maximized the error at steady state between the original full model and the reduced model. The parameter set that resulted from the optimization and its corresponding steady state solution were added to their respective projection matrices. The procedure was repeated until the specified error criterion was satisfied. Pasetto et al. [20] proposed an algorithm to reduce the computational burden associated with combinatorial search. The algorithm applied a greedy algorithm that searched over sets of parameter combinations and a snapshot selection strategy proposed by Siade et al. [21]. The greedy objective was evaluated using a scaled residual derived from the reduced model. This reduces the number of full model evaluations required for the determination of the principal components to be included in the reduced model.

In this study, we develop a new methodology for building the projection matrix for transient groundwater flow. Our proposed methodology is intended to work for linear, regional groundwater models where the zonation structure already has been determined; that is, the aquifer has been divided into a finite number of zones and each zone is characterized by a constant parameter (or parameters). The challenge of determining the optimum zonation structure of a random field by parameterization lies outside the scope of this paper.

This paper is organized into six sections. Section 1 is an introduction. Section 2 presents the governing equation for the confined aquifer and defines the notations. Section 3 discusses the deterministic inverse problem and the Bayesian inverse problem. Section 4 reviews the concept of projection-based model reduction and develops a parameter independent model reduction methodology. Section 5 applies the model reduction methodology to one- and two-dimensional test cases. Section 6 concludes the findings and discusses the results.

The proposed methodology constructs a projection matrix that covers the entire parameter space in the original full model and does not require taking new snapshots while solving the inverse problem. The projection matrix is assembled from snapshots generated iteratively by two greedy algorithms that select optimal parameter sets and snapshot times between the parameter space and the time domain. The proposed methodology is validated using a conceptual one-dimensional model that compares the result of a deterministic inverse problem with the empirical statistics from a Bayesian inverse problem. We then apply the methodology to a basin-scale, conceptual aquifer in the Oristano plain of Sardinia, Italy. Using the methodology, the full model is reduced by two to three orders of magnitude, resulting in a drastic reduction in computational requirements.

2. Confined groundwater modeling

The governing equation for confined, anisotropic, saturated groundwater flow can be expressed by the following parabolic partial differential equation [22,23]:

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial h}{\partial z}\right)\pm Q=S_S\frac{\partial h}{\partial t} \quad (1)$$

where h is the hydraulic head (L); K_x, K_y, K_z are the hydraulic conductivities (L/T) in the x, y, and z directions; S_S is the specific storage (L^{-1}); Q is a volumetric flux per unit volume in or out of the system (T^{-1}); and t is the time (T). Eq. (1) is subject to the following initial and boundary conditions:

$$h(x,y,z,t)=h_I(x,y,z),\quad (x,y,z)\in\Gamma_F,\ t=0$$
$$h(x,y,z,t)=h_D(x,y,z,t),\quad (x,y,z)\in\Gamma_D$$
$$K\frac{\partial h(x,y,z,t)}{\partial n}=q_N(x,y,z,t),\quad (x,y,z)\in\Gamma_N$$
$$\Gamma_D\cup\Gamma_N=\Gamma_B$$

where h_I is the initial condition, h_D is a specified Dirichlet boundary condition, q_N is a specified Neumann boundary condition, $\frac{\partial}{\partial n}$ is the normal derivative, Γ_F is the flow region, and Γ_B is the boundary