Reduced order modeling of the Newton formulation of MODFLOW to solve unconfined groundwater flow

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Abstract

Projection-based model reduction techniques have been shown to be very effective for reducing the computational burden of high-dimensional groundwater simulations, but only applied to confined groundwater flow. A new methodology is proposed that reduces the dimension of a discretized, transient, unconfined groundwater-flow model. This unconfined model reduction technique is based on Galerkin projection and the Newton formulation of MODFLOW. The method is implemented following the standard package design and code structure that MODFLOW employs for all its features. When the package is invoked within MODFLOW it can collect snapshots, produce a basis, construct the reduced model and propagate the reduced model forward in time. The new formulation accurately represents the water-table surface under a variety of nonlinear settings, such as intraborehole flow from a Multi-Node Well. The unconfined model reduction is applied to four test cases to illustrate its flexibility in handling

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nonlinear features. Several test cases are discussed to demonstrate the unconfined model reduction applicability. The final test case applies the new model reduction methodology to a scoping MODFLOW model of Santa Barbara, CA composed of 113,578 cells, which requires solving 113,578 equations per time step, and reduces it to 127 equations.

Keywords: Model reduction; Nonlinear Model Reduction; Proper orthogonal decomposition; Unconfined Groundwater Flow; MODFLOW

1 Introduction

Understanding groundwater resources is enhanced through the application of mathematical models that simulate the dynamics of an aquifer system. Conducting advanced analyses such as optimization of pumping schedules under different scenarios requires a large number of simulations. Such analyses are intractable for complex, highly-discretized models with large computational requirements. Reducing the computational burden associated with these simulation models provides the opportunity to perform more advanced analyses on a wider spectrum of groundwater management problems.

Projection-based model reduction techniques via the Galerkin method have been shown to be very effective for reducing the computational burden of large-scale, linear, groundwater simulations [1,2,3,4]. This type of model reduction involves construction of a basis spanned by solutions, referred to as snapshots, from the original simulation model. To form the basis, selected snapshots are collected as a snapshot set and analyzed with Proper Orthogonal Decomposition (POD). POD is a statistical pattern analysis technique that extracts a low-dimensional basis from a high-dimensional process, such as the snapshot set [5]. The discrete form of POD is identical to singular value decomposition where the POD basis, which is the

Galerkin projection matrix, are the left singular vectors and the proper orthogonal modes are the right singular vectors [6,7]. POD has also been referred to as Principal Component Analysis [8], Karhunen-Loève Expansion [9], and Empirical Orthogonal Functions [10,2]. The selection of the snapshots that compose the snapshot set is an area of active research, but not the focus of this paper. For more detailed information regarding snapshot selection see Boyce and Yeh [4] and Siade et al. [11].

Currently, most model reduction applications are applied to a linear, confined, groundwater model and demonstrate a reduction in dimensionality by several orders of magnitude. Vermeulen et al. [1] applied model reduction to the confined, groundwater-flow equation by collecting from a simulation model a snapshot set of simulated hydraulic heads at a constant, reference pumping rate. Vermeulen et al. [1] then applied principal component analysis (PCA) to the snapshot set to generate the basis used by the Galerkin method to derive the reduced model. McPhee and Yeh [2] followed this methodology and demonstrated that a reduced model maintains its sensitivity of hydraulic head with respect to pumping, enabling it to embed in a management optimization problem. Baú [12] increased the utility of POD model reduction by deriving a set of reduced models for each Monte Carlo realization of hydraulic conductivity to solve a stochastic, multi-objective, confined groundwater management problem.

In theory, the Galerkin projection model reduction technique only applies to linear systems, such as confined aquifers. Application to nonlinear systems is possible, but the reduced model's error is greater and may require significantly more basis functions (snapshots) to characterize the model [13]. The basis functions derived from POD can be thought of as tangent spaces that approximate the nonlinear system [5]. Robinson et al. [14] and Li and Hu [15] applied POD model reduction to several synthetic one- and two-dimensional mass-transport models without

chemical reactions. Buchan et al. [16] 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. With these nonlinear examples there has been limited application of model reduction to the nonlinear, unconfined groundwater flow equations.

Simulating unconfined groundwater flow is an essential part of groundwater modeling projects. MODFLOW [17] and its variants are one of the most popular groundwater modeling software packages available that solve the confined and unconfined equations. MODFLOW is designed as a series of independent modular pieces called packages. To solve the governing equations, MODFLOW uses a three-dimensional, block-centered finite difference scheme to discretize the model domain and implicit finite differencing to discretize time. The nonlinear system of equations is solved using the Picard method. To improve stability of solving the MODFLOW unconfined flow equations the Newton method has been shown to be a useful alternative to the Picard method [18,19]. This led to the development of the Newton formulation of MODFLOW, MODFLOW-NWT [20], which expands upon previous work with upstream weighting for determining horizontal intercell conductance, conductance smoothing functions, and a Newton solver. The two main packages for the Newton formulation of MODFLOW are the flow package Upstream weighting (UPW) and solver package Newton Solver (NWT). Conductance is MODFLOW's finite difference representation of hydraulic conductivity between two modeled grid cells and is derived from Darcy's Law and finite differences. While the Newton solver is more stable than the Picard method, it requires solving for the inverse of the nonsymmetric, Jacobian matrix for each Newton step (inner iteration).

Solving unconfined models with a high discretization through the Newton method can become computationally intractable due the difficulty of solving for the inverse of the nonsymmetric Jacobian. To reduce the computational burden, and thus the simulation runtime, we propose an approach that combines the Newton formulation of MODFLOW [20] with projection-based model reduction. This approach is implemented following the standard package design and code structure that MODFLOW employs for all its features. The source code modifications are implemented within a recent release of MODFLOW called MODFLOW One-Water Hydrologic Flow Model (MF-OWHM) [21]. The model-reduction package initially collects snapshots from a MF-OWHM simulation and converts them to a basis. Once the basis is constructed, the package performs a reduced model simulation by intercepting the NWT package where it solves for the inverse of the Jacobian. The reduced model uses Galerkin projection to form a reduced dimension Jacobian, solves for the inverse of the reduced Jacobian, and then calculates the Newton step.

2 Groundwater-flow modeling

2.1 Discretized groundwater-flow modeling

Darcy's Law is combined with the continuity equation to derive the governing equation for anisotropic, saturated groundwater flow. The resulting confined and unconfined groundwater flow equations are the following [19,22,23]:

$$\nabla \cdot (K \nabla h) \pm Q = S_s \frac{\partial h}{\partial t} \quad (1)$$

$$\nabla \cdot (Kh \nabla h) \pm Q = S_y \frac{\partial h}{\partial t} \quad (2)$$

where $\nabla \cdot$ is the divergence operator, ∇ is the gradient operator, K is the hydraulic conductivity tensor [L/T], h is the hydraulic head [L], Q is a volumetric flux per unit volume in or out of the system [T⁻¹], S_s is the specific storage [L⁻¹], t is the time [T], and S_y is the specific yield [-].

Within a three-dimensional groundwater system, Eq. 1 applies to regions under confined conditions (fully saturated model layers) and Eq. 2 applies to regions under unconfined conditions (not fully saturated model layers). During the course of a model simulation a particular model cell can switch from confined (Eq. 1) to unconfined (Eq. 2) conditions and vice-versa. For unconfined conditions the additional h variable, representing the saturated thickness, makes the equation nonlinear and acts as an upper boundary condition created by the water table.

Applying a spatial discretization to Eqns. 1 and 2 through a differencing scheme (e.g. finite differences or finite elements) yields a system of nonlinear ordinary differential equations (ODEs) of the form

$$Ah + f = B \frac{dh}{dt} \quad (3)$$

where $h \in \mathbb{R}^n$ is a vector of hydraulic heads at each nodal location; $A \in \mathbb{R}^{n \times n}$ is a nonlinear stiffness matrix, which contains spatial information about hydraulic conductivity and is a function of h (i.e. the saturated thickness) for model cells that are under unconfined conditions;

$B \in \mathbb{R}^{n \times n}$ is the mass matrix; and $f \in \mathbb{R}^n$ is a vector containing all Dirichlet, Neumann and part of the Cauchy boundary conditions. To solve for the time derivative an implicit difference scheme is applied to the time derivative to form the following system of nonlinear equations:

$$(B - \Delta t A)h^{t+1} = Bh^t + \Delta t f \quad (4)$$

where t is the time step index and $\Delta t = t^{t+1} - t^t$ is the time step that propagates the model forward to a new time. Nonlinearity arises because matrix A is a function of h for layers that are not fully saturated.

2.2 Newton formulation of the groundwater-flow equation

The Newton formulation, as described in Niswonger et al. [20] and Painter et al. [18], rearranges Eq. 4 into the following:

$$(B - \Delta t A^i) h^{t+1,i} - B h^t - \Delta t f = R^i \quad (5)$$

$$J^i \Delta h = R^i \quad (6)$$

$$J^i h^{t+1,i+1} = R^i + J^i h^{t+1,i} \quad (7)$$

where i is the Newton step index, A^i is the stiffness matrix evaluated at $h^{t+1,i}$, $h^{t+1,i}$ is the head at the i^{th} Newton step for the $t + 1^{\text{th}}$ time step, $R^i \in \mathbb{R}^n$ is the residual that results from an estimate of $h^{t+1,i}$, J^i is the Jacobian matrix defined as $J^i = \partial R^i / \partial h^{t+1,i} \in \mathbb{R}^{n \times n}$, and $\Delta h = h^{t+1,i+1} - h^{t+1,i}$. The Newton procedure then iteratively solves for $h^{t+1,i+1}$ until $R^i \rightarrow 0$.

The original MODFLOW approach removes dewatered cells from the finite difference equations and treats them as a no-flow boundary. A cell is dewatered when its hydraulic head (h) fall below its bottom elevation. Unlike the original version of MODFLOW, dewatered model cells are not removed in the Newton formulation of MODFLOW. Due to this design, the reduced model must reproduce the results from all the model cells, including the dewatered ones.

3 Model reduction via POD and the Galerkin projection for the Newton formulation of groundwater-flow

3.1 The Galerkin projection matrix

Projection-based model reduction proceeds by projecting a discretized groundwater-flow model, $h \in \mathbb{R}^n$, onto a reduced model subspace of $h_r \in \mathbb{R}^r$, where $r \ll n$. For this to occur, it is assumed that the hydraulic head, h , can be mapped linearly onto the reduced space, h_r , by some orthonormal matrix, $P \in \mathbb{R}^{n \times r}$, which contains information about the discretized groundwater-flow model's solutions in time [1,4]:

$$h = Ph_r \quad (8)$$

The vectors in the P matrix are sometimes referred to as the POD basis, spatial basis functions, empirical orthogonal functions, or principal vectors [4,8,9,10].

The matrix P is derived from a time series of solutions, h^{t_k} , called snapshots, that are collected from the groundwater-flow model under a constant/reference forcing (e.g. pumping well) taken at specific simulation times, t_k . A set of snapshots must be taken for each linearly independent forcing term in the groundwater-flow model. For example, if a model has two extraction wells that have no linear relation between them, then two sets of snapshots must be taken. If there are any linear relationships (e.g. Well A = 2 × Well B), then a single set of snapshots can be taken at that relationship. All the sets of snapshots are then combined to form the final snapshot set:

$$\begin{aligned} S^j &= [h^{t_1}, h^{t_2}, h^{t_3}, \dots, h^{t_k}] \quad \forall j = 1, 2, \dots, \text{NSET} \\ S &= [S^1, S^2, \dots, S^{\text{NSET}}] \in \mathbb{R}^{n \times m} \end{aligned} \quad (9)$$

where S^j is a set of snapshots collected for the j^{th} linearly independent forcing and is composed of k snapshots, NSET is the total number of linearly independent forcings, and S is the final snapshot set containing m snapshots.

For each snapshot set, S^j , the number of snapshots, k , and their specific solution time, t_k , are problem-dependent. Both the number of snapshots and specific solution times do not have to be the same for each snapshot set, S^j . From the literature and empirical tests using this study's methodology, each snapshot set, S^j , should be composed of snapshots that have 10 to 50 exponentially distributed values of t_k from the initial condition to quasi-steady state with the forcing set to a constant value and then another 10 to 50 snapshots with no forcing to adequately capture the model's nonlinear response and recovery. For simplicity, a set of exponentially distributed snapshots times are selected by visually examining the model output. For a more systematic approach to estimate the optimal number of snapshots, see Boyce and Yeh [4].

The snapshots from Eq. 9 form a basis that, when made orthonormal, derives the Galerkin projection operator. This operator is the same matrix as the linear map, P , defined in Eq. 8. The orthonormalization of the snapshots, S , is performed by POD, which for the discrete case is the Singular Value Decomposition (SVD) [24,25]:

$$S = U\Sigma V^T = \sum_{i=1}^{\text{rank}(S)} \sigma_i u_i v_i^T \Rightarrow P = U \quad (10)$$

where $\text{rank}(S)$ is the minimum between the number of linearly independent columns or rows in S , σ_i are the singular values that are ordered from largest to smallest, Σ is a diagonal matrix with singular values along the diagonal, $U = [u_1, u_2, \dots]$ are the left singular vectors that comprise the POD basis set equal to P , and $V = [v_1, v_2, \dots]$ are the right singular vectors that represent the proper orthogonal modes. For the test cases presented in Sections 4 and 5 the SVD is performed with the LAPACK library [26].

Without knowledge of the optimal choice for snapshots, the singular values can serve as weights to distinguish the left singular vectors, subsequently referred to as POD basis vectors,

207 that contribute the most amount of information to the projection operator P . This is
 208 accomplished by solving for r in the following relationship:

$$\begin{aligned} & \min r \\ \text{Subject to } & \frac{\sum_{i=1}^r \sigma_i}{\sum_{i=1}^{\text{rank}(S)} \sigma_i} \times 100\% \geq \text{PE} \end{aligned} \quad (11)$$

210 where PE is a user-specified minimum required percent energy contribution of the sum of the r
 211 largest singular values. Typical values for PE range from 99% to 99.99%, where smaller values
 212 lead to fewer basis vectors at a cost of less accurate reduced model results. Once r has been
 213 established, the final truncated POD basis is $P = [u_1, u_2, \dots, u_r]$, which defines the dimension of
 214 the reduced model, h_r (Eq. 8). This process of removing insignificant basis vectors is called
 215 singular-value truncation; if S is symmetric, then it is also called principal component analysis.

216 There are two methods that can improve the selection of basis vectors before applying SVD
 217 to construct the POD basis. The first method involves normalizing each column in S (i.e., each
 218 snapshot) by dividing it by its respective L^2 norm. Normalization produces a better spread of
 219 singular values by removing any issues of scale from the snapshots. The second method is to
 220 mean center and redefine S as follows:

$$\begin{aligned} \bar{h} &= \frac{1}{m} [S \mathbf{1}_m] \\ S &:= S - \bar{h} \mathbf{1}_m^T \end{aligned} \quad (12)$$

222 where $\mathbf{1}_m$ is a column vector of m ones, $\bar{h} \in \mathbb{R}^n$ contains the mean for each row in S . If the
 223 snapshots are mean centered, then Eq. 8 must be adjusted to include the missing information
 224 from the POD basis (P), i.e.,

$$h = Ph_r + \bar{h} \quad (13)$$

The advantage of mean centering is that it removes all time-invariant effects from the snapshots and can stabilize problems that may arise from boundary conditions. If both normalization and mean centering are required, it is important to first apply the mean centering and then normalize the redefined S to preserve the relationship defined in Eq. 13. For most situations the reduced form of the Newton formulation of MODFLOW (Section 3.2) produces the most accurate reduced models with both mean centering and normalization. Of the two improvements, our test cases indicate that mean centering has the greatest effect on improving accuracy and normalization only results in a minor improvement.

3.2 The Galerkin projection and the Newton formulation of MODFLOW

The Newton formulation of MODFLOW [20] is projected onto a reduced space via the Galerkin projection and a substitution that makes the system of equations dimensionally correct. The Galerkin projection involves pre-multiplying Eq. 7 by the transpose of the POD basis (P^T). The resulting system of equations now requires one of two possible substitutions to make it dimensionally correct. If mean centering is not applied, then substituting in $h^{t+1,i+1} = Ph_r^{t+1,i+1}$ is required to form Eq. 14. If there is mean centering, then substitute $h^{t+1,i+1} = Ph_r^{t+1,i+1} + \bar{h}$ to form Eq. 15.

$$P^T J^i P h_r^{t+1,i+1} = P^T [R^i + J^i h^{t+1,i}] \quad (14)$$

$$P^T J^i P h_r^{t+1,i+1} = P^T [R^i + J^i h^{t+1,i} - J^i \bar{h}] \quad (15)$$

Let $J_r^i = P^T J^i P \in \mathbb{R}^{r \times r}$ and $b_r^i = P^T [R^i + J^i h^{t+1,i}] \in \mathbb{R}^r$, or if there is mean centering,

$b_r^i = P^T [R^i + J^i h^{t+1,i} - J^i \bar{h}] \in \mathbb{R}^r$, then Eqns. 14 and 15 are then transformed to:

$$J_r^i h_r^{t+1,i+1} = b_r^i \quad (16)$$

Eq. 16 is subsequently referred to as the reduced model and Eq. 7 as the full model. The reduced model only requires the solution of r equations for each Newton step compared to the full model's n equations. After solving for $h_r^{t+1,i+1}$ for one Newton step either Eq. 8 (no mean centering) or Eq. 13 (mean centering) provide a means of obtaining $h^{t+1,i+1}$. For the reduced model to be efficient, it is necessary that $r \ll n$.

4 Two-dimensional synthetic, vertical test cases

A synthetic, unconfined, two-dimensional (2D), vertical groundwater-flow model is constructed in MF-OWHM [21] to demonstrate the application of model reduction to the Newton formulation of MODFLOW. The modeled domain contains 500 simulated cells with a total length (column direction) of 10 km and depth of 50 m. The model's top and bottom elevations are set to 0 m and -50 m, respectively. The initial condition is set to a uniform water level of -2 m to force an unconfined condition. The model discretization consists of five, 10 m-thick, convertible layers, one 100 m-wide row, and one-hundred, 100 m-long columns. A convertible layer in MF-OWHM uses, where appropriate, the confined (Eq. 1) and unconfined (Eq. 2) equations. The domain is divided into two zones with columns 1 through 40 and columns 41 through 100 having horizontal hydraulic conductivity values of 5 m/d and 15 m/d, respectively. The vertical hydraulic conductivity is set to be one-tenth that of the horizontal. The entire model domain has a specific yield (S_y) of 0.3 and specific storage (S_s) of $1E-5 \text{ m}^{-1}$. Using the aforementioned properties we evaluate two different test cases using different stresses and boundary conditions.

4.1 Three wells and fixed head boundary condition

Fig. 1: Two-dimensional, vertical test case, TC1, with three wells (WEL) and time-variant specified-head (CHD) boundary conditions.

The first test case, TC1, applies model reduction to a 2D groundwater-flow model that uses MODFLOW's well (WEL) and time-variant specified-head (CHD) packages (Fig. 1). The WEL package simulates pumping into or out of the model and CHD applies a time varying fixed-head boundary condition [23]. The three WEL locations are at Layer 2, Column 51; Layer 4, Column 21; and Layer 5, Column 51 (Fig. 1) and are subsequently identified only by their layer. All model cells that are specified with the CHD package are set to a constant value of -2 m to maintain unconfined conditions throughout the simulation.

Three sets of 90 snapshots are collected ($NSET = 3$) to construct the reduced model. Each snapshot set, j , is taken with one of the wells set to a pumping rate of $400 \text{ m}^3/\text{d}$ for 50,000 days, the quasi-steady state time, followed by 50,000 days of recovery (no pumping). Taking snapshots for each well allows their values to vary independently within the reduced model. The distribution of snapshot times, t_k , are shown in Fig. 2, where the 46th snapshot is the first one taken without pumping to record the model's recovery. The three sets of 90 snapshots are combined to form $S \in \mathbb{R}^{500 \times 270}$, which is subsequently mean centered and normalized. Using a PE of 99.99% results in a final POD basis composed of 61 vectors. This basis then reduces the Newton method's system of equations (Eq. 7) from 500 equations to 61 (Eq. 16). Further reduction could have been achieved if it was assumed that two or more of the wells pumped at the same rate. Then their snapshots could have been combined, resulting in a smaller final basis.

Fig. 2: Distribution of snapshot times. The first 45 are taken with pumping and the remainder without.

The simulation time frame used to compare the full and reduced models is 3,000 days with pumping followed by 3,000 days of recovery with a time step of 10 days. The pumping rate is set to 1,000 m³/d for each well to illustrate that the reduced model is independent of the pumping rate that was used for the snapshots (i.e., 400 m³/d).

To evaluate the reduced model's accuracy the following equations are defined:

$$\begin{aligned} \text{MAE} &= (1/N) \sum_{i=1}^N |h_i - (Ph_r)_i| \\ \text{RMSE} &= \sqrt{(1/N) \sum_{i=1}^N (h_i - (Ph_r)_i)^2} \\ \text{NRMSE} &= 100\% \times \text{RMSE} / (h_{\max} - h_{\min}) \end{aligned} \quad (17)$$

where MAE is the mean absolute error, RMSE is the root mean squared error, NRMSE is the normalized root mean squared error, N is total the number of model cells, i is the model cell index (e.g., row 1, column 1, layer 1 has index of 1), and $h_{\max}$ and $h_{\min}$ are the maximum and minimum head values across all model cells, respectively. The NRMSE weights the RMSE by the spread of information to provide a method of comparing accuracy of different models. The largest value of NRMSE from all the time steps is 0.075%. Fig. 3 presents a histogram of the MAE calculated at each time step and an error exceedance curve of the RMSE for TC1. The MAE errors are clustered around 0.007 m (Fig. 3, left) with the largest values being 0.015 m.

The reduced model replicates the full model with all the errors less than 0.02 m. The error exceedance curve demonstrates that the RMSE is very small with a 5% chance of being 0.016 m or greater. In addition, the full and reduced models' cumulative percent mass balance errors at the end of the simulation are 0% and 0.39%, respectively.

Fig. 3: TC1 (left) histogram of the mean absolute errors from all time steps and (right) exceedance curve of the RMSE. Note that the units are in mm.

The water table is calculated as the hydraulic head of the upper most model cells that are not dewatered. Fig. 4 presents the simulated water-table elevation for the full and reduced models at select times during the 6,000 day simulation. In the figure the model cells that are above the water table have hydraulic heads below their bottom cell elevation; conversely cells below the water table have hydraulic heads above their top elevation. During the first 3,000 days of simulation (Fig. 4, left) the pumping well removes water causing the water table to decline below layers 1, 2, and 3 within most of the model domain. This illustrates that despite multiple layers being dewatered, the reduced model accurately represents the full model. During the next 3,000 days (Fig. 4, right) there is no pumping and the reduced model still accurately reproduces the nonlinear recovery of the water table.

Unique to the Newton formulation of MODFLOW is that a WEL model cell simulates loss of production due to dewatering by reducing the pumping rate as a function of saturation in the

pumping cell. The pumping wells located in layers 2 and 4 (Fig. 1) undergo this reduction in rate during the first 3,000 days of pumping (Figure 5). Due to dewatering of the cell, the well located at layer 2 completely stops production after 850 days. The reduced model follows the same trend and visually matches the full model's reduction in pumping as illustrated in Figure 5.

Fig. 4: Two-dimensional test case, TC1, simulated water-table elevation during the first 3,000 days of pumping (left) and the next 3,000 days of recovery (right) at select times for the full and reduced models. Note that MAE and NRMSE are calculated from the simulated head at all 500 model cells.

Figure 5: Two-dimensional test case, TC1, full and reduced model's loss of pump capacity due to drawdown.

4.2 One multi-node well and a general head boundary condition

Fig. 6: Two-dimensional test case, TC2, with one multi-node well with two screened intervals (MNW2) and general head boundary conditions (GHB).

The second test case, TC2, applies model reduction to a two-dimensional model that uses MODFLOW's revised Multi-Node Well (MNW2) [27,28] and the General-Head Boundary (GHB) packages, shown in Fig. 6. The MNW2 package [28] simulates wells that extend over more than one model cell and is a more realistic representation of a groundwater pumping well than the WEL package. The MNW2 package calculates the head level within the well; its possible production rate is based on a desired flow rate and allows for intraborehole flow (i.e., flow within the well itself). When there is no desired flow rate specified, an MNW2 well can transmit water between layers via intraborehole flow. The location of the MNW2 well is at column 51 with a screened interval from -10 m to -20m and -40 m to -50 m (layers 2 and 5, respectively, in Fig. 6). The MNW2 well in TC2 has the losstype set to "skin" [28], a radius of 0.15 m (inner radius), a skin radius of 0.2 m (outer radius). The hydraulic conductivity of the skin material is 1.5 m/d.

The GHB package simulates head-dependent flux boundaries by allowing water to flow into or out of the system based on the water level and a user-specified conductance. For TC2, the GHB boundary head (Bhead) is set to -2 m and the conductance assigned to columns 1 and 100 is calculated such that it represents the model grid's hydraulic conductivity.

To construct the reduced model, one set of 90 snapshots is collected (NSET = 1). The first 45 snapshots are taken with the MNW2 well set to a desired pumping rate (Qdes) of 400 m³/d for

50,000 days -- the quasi-steady state time, to capture the response to MNW2 pumping. After the quasi-steady state is reached, 45 more snapshots are taken over 50,000 days with the MNW2 well's desired pumping rate set to 0 m³/d to capture the recovery from pumping and any associated intraborehole flow. The distribution of snapshot times, t_k , are the same as used in TC1 (Fig. 2). The TC2 snapshots from the MNW2 well are then mean centered and normalized. Using a PE of 99.99% results in a final POD basis composed of 22 vectors for reducing the Jacobian. The TC2 basis is smaller than the TC1 basis because the former is able to exploit the fact that the nodes within the MNW2 well are related while the latter assumes no relationship between the three wells.

Like TC1, the simulation timeframe used to compare the full and reduced models is progressed with a 10-day time step and composed of 3,000 days of pumping at a desired rate (Q_{des}) of 1,000 m³/d followed by 3,000 days of recovery at a desired rate (Q_{des}) of 0 m³/d. At the end of this timeframe the full and reduced models both have a 0% cumulative percent mass balance errors. The MAE and RMSE results from the full and reduced models are summarized in Fig. 7. The reduced model accurately represents the full model with all MAE's being less than 0.018 m and the largest NRMSE across all time steps is 0.135%. The exceedance curve increases slightly compared to TC1 with a 5% chance of being 0.021 m or greater. The errors are slightly greater than TC1 because there are more nonlinear features that the reduced model must represent and the reduced model dimension is smaller. This increase is nominal considering the overall accuracy of the reduced model and that the full model dimension is reduced by 96%.

Fig. 7: TC2 (left) histogram of the mean absolute errors from all time steps and (right) exceedance curve of the RMSE. Note that the units are in mm.

The simulated water-table elevation for the full and reduced models at selected times is presented in Fig. 8. The water table is accurately represented by the reduced model despite dewatering layers 1, 2, and 3 and an MNW2 well extracting water from layers 2 and 5 (Fig. 8). MNW2 determines the flow rate at each screen location based on a calculated well water level (hwell) relative to the head in layers 2 and 5 as it attempts to meet the desired pumping rate. Fig. 9 shows the full and reduced model's simulated well water level and screen flow rates. During the first 3,000 days, the pumping rate of 1,000 m³/d lowers the well water level (Fig. 9, top). When layer 2 dewateres at the well site (Time: ~1,500 days; Fig. 9, left) the screen's flow rate lowers to zero and the layer 5 screen increases to meet the desired rate. This nonlinear response is visually identical between the full and reduced models. For the 3,000 days of recovery (Time: 3,000 to 6,000 days; Fig. 9, right) the desired flow rate is set to zero; however, intraborehole flow may still occur. Water from layer 5 flows into the well bore and travels into layer 2 (Fig. 9, right). The reduced model does not visually match this nonlinear response, but the differences are negligible considering the scale of the flow rates, with the largest deviations no more than 0.06 m³/d.

Fig. 8: TC2 simulated water-table elevation during the first 3,000 days of pumping (left) and the next 3,000 days of recovery (right) at select times for the full and reduced models. Note that MAE and NRMSE are calculated from the simulated head at all 500 model cells.

Fig. 9: TC2 full and reduced model's simulated well water level (top) and screen flow rate with (left) and without pumping (right). The MNW2 screen flow rate is positive when flow is out of the layer and into well. Note the center and right parts are on different scales.

4 Three-dimensional test cases

Two synthetic, unconfined, three-dimensional (3D) groundwater-flow models are evaluated with the proposed model reduction methodology. The first 3D test case (TC3) is similar to TC1

and TC2, except a third dimension is added as well as other MODFLOW packages. The second 3D test case (TC4) is a complex-refinement of a scoping groundwater-flow simulation of Santa Barbara, CA [29]. This model is partially calibrated and only constructed to illustrate model reduction for the presented scenario.

4.1 Test Case 3: Synthetic model with multiple packages

Fig. 10: Plan overview of test case 3 (TC3).

The third test case, TC3, is a synthetic, three-dimensional, unconfined groundwater-flow model that incorporates multiple MODFLOW packages. The model is composed of 5 layers, 100 rows and 100 columns for a total of 50,000 simulated cells. Each layer is 10 m thick with the model's top and bottom elevations set to 0 m and -50 m, respectively. The length of each row and column is 100 m. The horizontal domain of TC3 is presented in Fig. 10. The initial condition is set to -2 m for the entire model domain. The domain is divided into two zones with columns 1 through 40 (Zone 1) and columns 41 through 100 (Zone 2) having a horizontal hydraulic of 5

427 m/d and 15 m/d, respectively, with no horizontal anisotropy. The vertical hydraulic conductivity
428 is set to one-tenth of the horizontal. The entire domain has a $S_y=0.3$ and $S_s=1E-5 \text{ m}^{-1}$.

429 TC3 is bounded by two GHB conditions located along columns 1 and 100, across all rows
430 and layers, and has a boundary head of -2 m and conductance calculated to represent a hydraulic
431 conductivity of 5 m/d and 15 m/d, respectively. Within the domain there are two recharge fields
432 and a drain field simulated using the recharge (RCH) and drain (DRN) packages, respectively
433 (Fig. 10). The recharge fields distribute a specified flux over the top of the model and are located
434 in the upper left (columns 11 to 30) and upper right (columns 11 to 30) of the model and have a
435 recharge flux of 0.1 mm/d. Note that since the Newton formulation does not allow cells to
436 deactivate when dewatered, a dewatered upper layer cell will receive the recharge and then
437 transmit it downward towards the upper-most saturated layer. The drain field is located between
438 columns 21 and 30, has a drain elevation set to -5 m, and the hydraulic conductance of the
439 interface between the aquifer and the drain is $100 \text{ m}^2/\text{d}$. Drains only remove water from the
440 model when the water table elevation is greater than -5 m.

441 A fault line is simulated using a horizontal flow barrier (HFB) [30] that is between two
442 columns. There is a break and shift in the barrier near a river to allow groundwater flow through
443 and to simulate a shifted and washed-out barrier. The barrier is located across all layers and is
444 either between columns 37 and 38 or between columns 39 and 40. The barrier has a thickness of
445 5 m and a hydraulic conductivity of 0.001 m/d. Running parallel to the barrier is a river (RIV
446 package) that crosses it near its break and then runs parallel again. The riverbed bottom elevation
447 (Rbot) is -2 m and the head of the river (Stage) is set to 1 m. The riverbed hydraulic conductivity
448 is 0.25 m/d and 0.5 m/d for Zones 1 and 2, respectively.

Water is extracted from the groundwater system by seven wells (WEL) and one multi-node well with two screens (MNW2). The well field represents four wells that always pump at the same rate and are located at layer 4 and along column 80. The left-most well is located at layer 4, row 26 and column 21, and the remaining two wells in Fig. 10 pump at the same rate and are located at layers 2 and 5 at row 71 and column 51. The location of the MNW2 well is at row 26 and column 65 with a screened interval from -20 m to -30 m and -40 m to -50 m (layers 3 and 5, respectively). The MNW2 well uses the “skin” losstype, has a radius of 0.1 m (inner radius), and a skin radius of 0.25 m (outer radius). The hydraulic conductivity of the skin material is 0.5 m/d.

To construct the reduced model, six sets of snapshots are collected ($NSET = 6$) from MNW2, WEL, RIV, and RCH for a total of 460 snapshots. For MNW2 and WEL there are 45 snapshots, exponentially distributed in time, taken while pumping is active for 50,000 days (quasi-steady state time), and then 45 more snapshots are taken for 22,500 days of recovery (no pumping). Since the well field always pumps at the same rate, it only requires one set of snapshots to represent the four wells. For both RCH and RIV there are 50 snapshots, exponentially distributed in time, taken for over 50,000 days. The snapshot set (S) is mean centered and normalized; SVD is then applied to obtain the singular values and POD basis. The magnitude of each singular value and its corresponding percent energy is presented in Fig. 11. This illustrates that there is a good spread of information among the chosen snapshots. Even with a good spread of singular values the PE indicates a rapid increase to 99.9% around the 60th singular value. To demonstrate an extreme reduction, a PE of 99% is selected, which results in a POD basis composed of 28 vectors. The lower PE still produces acceptable errors with the extreme reduction of the Jacobian dimension by 99.9% and Eq. 16 from 50,000 equations to 28 equations.

Fig. 11: Percent Energy (left y-axis) and Singular values (right y-axis) from applying SVD to the 460 snapshots taken from TC3.

To compare the full and reduced models, a simulation timeframe of 3,000 days is divided into 20 150-day, stress periods with a time step of 2 days. Water is extracted from the domain from the wells during the odd-numbered stress periods (e.g. 1, 3, etc.) and there is no pumping during the even-numbered stress periods (MNW2 may still have intraborehole flow). For all stress periods the GHB, DRN, RCH, and RIV remain at non-zero values. At the end of the simulation the full and reduced models' cumulative percent mass balance errors are 0% and 0.6%, respectively. The largest NRMSE across all time steps is 3.5%. The error results from the full and reduced models are summarized in Fig. 12. The histogram and RMSE exceedance curve is compiled by computing the MAE and RMSE from the reduced and full models for each time step of the simulation. The mean average errors are acceptable considering the level of reduction demonstrated in TC3. The exceedance curve has a 5% chance of being 0.212 m or greater, which is about an order of magnitude greater than the 5% from TC1 and TC2. This increase is expected since the number of cells in TC3 is an order of magnitude greater than TC1 and TC2.

Fig. 12: TC3 (left) histogram of the mean absolute errors from all time steps and (right) exceedance curve of the RMSE.

Assuming that errors propagate from previous time steps, the results of the final time step should be the least accurate. Fig. 13 is a contour plot of the water-table elevation at the last pumping stress period (2,850 days) and the last recovery stress period (3,000 days), which occur at times 1,425 and 1,500 days, respectively. The reduced model matches the full model with the contours in general agreement of each other (Fig. 13). By splitting the calculation the MAE and NRMSE for only the time steps with pumping (Fig. 13, top) and those with recovery (Fig. 13, bottom) shows that the reduced model is slightly more accurate during pumping. These associated errors for pumping and recovery are a MAE of 0.108 m and 0.116 m, respectively, and NRMSE of 0.62% and 2.4%, respectively. The larger error metrics during the recovery time steps is most likely the result of selected snapshots not adequately representing the recovery of the model or information that was related to the recovery is removed by using a PE of 99% (a higher PE would include more information from the snapshots).

Fig. 13: TC3 comparison between the full (left) and reduced (right) model's water table elevation at the last pumping stress period at 2850 days (top) and the last recovery stress period at 3000 days (bottom).

Fig. 14 presents the pumping from the MNW2 well in TC3 for the full and reduced models. Since the desired pumping rate (Q_{des}) is non-zero for the odd stress periods, the head in the well rapidly drops due to pumping. During the even stress periods there is no pumping and the well water level in the MNW2 well (Fig. 14, left) recovers as water seeps in from the two screened layers. During the course of an odd stress period (pumping) the net flow rate from the layer 3 screen starts to drop as the head in the well lowers. Consequently the layer 5 screen's net rate increases to meet the desired pumping rate. The reduced model does not exactly reproduce these nonlinear responses; however, the differences are negligible and the overall trend matches.

Fig. 14: TC3 full and reduced model's (left) MNW2 well water level and (center and right) MNW2 screen flow rate where there is positive is flow out of the layer and into the well.

4.2 Three-dimensional test case (TC4) of Santa Barbara groundwater-flow model

Fig. 15: Overview of the Santa Barbara Model, TC4.

In order to present our method's applicability to a “real-world” problem, we developed a scoping groundwater-flow model based on the published model of the Santa Barbara groundwater basin [29], located in Santa Barbara, CA, Fig. 15. The original model input files are designed for MODFLOW-88 [31]. To apply model reduction the flow and solver input files are converted to the UPW/NWT input files, and the remainder of the packages updated for simulation with MF-OWHM. This model has been partially calibrated and is constructed to illustrate the applicability of model reduction for the presented test case.

The Santa Barbara model, now referred to as TC4, is composed of 56 layers, 58 rows, 152 columns and has 113,578 active model cells. The first layer follows the land topography with a maximum and minimum elevation of 179 m mean sea level (msl) and -4 m msl, respectively. Each model layer has an average thickness of 6 m and the deepest model cell bottom has an elevation of -340 m msl. The row and column lengths are a constant value of 76 m. The TC4 domain (Fig. 15) contains six mapped fault lines that are represented as horizontal flow barriers (HFB). Mountain-front recharge along the northeast boundary is represented by the recharge package (RCH). In the southeast region there is a drain network (DRN) that removes water from the groundwater system. The rivers located in the active model domain are simulated using the RIV package. The ocean boundary is represented as a freshwater equivalent head using the GHB package and the remainder of the model boundary is no-flow. The cell-wise hydraulic conductivity data is developed by compiling drillers' log data, electrical-resistivity data, and geologic maps to derive a semi-continuous hydraulic conductivity value for every model cell. Seven production wells are simulated with the WEL package and have screening intervals that span across multiple layers. Unlike MNW2, the well package cannot accommodate pumping spread across multiple model cells directly. Instead, multiple WEL cells are required to represent a well's screened intervals. The total pumping from a well is distributed across the multiple WEL cells according to the cell's hydraulic-conductivity value. Due to this limitation the seven production well sites (Fig. 15) are represented by 114 WEL cells.

To construct the reduced model eight sets of snapshots, exponentially distributed in time, are collected ($NSET = 8$). To capture the model's unpumped dynamics, one set of 28 snapshots is collected, without pumping but with RCH, RIV, GHB, and DRN, spanning from 0.1 days to 5,000 days (near the initial condition to quasi-steady state time). The next seven sets of snapshots

contain 19 exponentially distributed snapshots from 0.03 days to 1,323 days (near the pumping quasi-steady state) with one of the seven wells set to a constant pumping rate. The combined snapshot sets are mean centered, normalized and then SVD is applied to obtain the POD basis. The associated errors from different POD basis dimensions are then evaluated using the TC4 scenario.

The accuracy of the reduced model is compared with the full model during a 2-year simulation with monthly pumping changes (24 stress periods). Each stress period is equal to the days in a month (e.g. 31, 28, 31 days) with four time steps per stress period and beginning in January. During the first year, the pumping rate for the seven wells increases from a small rate to a maximum rate from stress period 1 to 9 and then decreases to zero from 10 to 12. The pumping rates are different across the seven wells with the smallest stress period 1 rate being $178 \text{ m}^3/\text{d}$ and largest stress period 9 rate being $4,823 \text{ m}^3/\text{d}$. The second year repeats the same pumping schedule that is applied to the first.

For this synthetic scenario, the full and reduced models are evaluated at 99%, 99.9%, and 99.99% PE, which results in a POD basis composed of 86, 127, and 147 vectors, respectively. The three different bases derive reduced models with different levels of accuracy. At the end of the simulation the full and 99%, 99.9%, and 99.99% PE reduced models have a cumulative percent mass balance errors of 0.1%, 2.9%, 1.9%, and 1.88%, respectively. Fig. 16 presents the snapshot set's singular values and their corresponding PE values along with the associated errors for the three aforementioned PE values. The largest NRMSE across all time steps for the three PE values is 0.16%, 0.13%, and 0.13%, respectively. There is a direct correlation with the accuracy loss by lowering the PE below 99.99%. As would be expected, smaller values of PE have the benefit of a smaller POD basis, but at a loss in accuracy. This is not necessarily true for

577 larger values of PE ($>99.99\%$) due to the fact that eventually basis vectors will be included that
578 contribute nearly zero information to the reduced model. This is demonstrated by (Fig. 16) the
579 large improvement in the reduced model's MAE histogram and exceedance curves between PE
580 values of 99% and 99.9%, but a negligible improvement from PE values of 99.9% to 99.99%. In
581 fact, the RMSE for PE values of 99.9% and 99.99% are nearly identical (Fig. 16).

Fig. 16: TC4 snapshot set's singular values and corresponding percent energy (top) and the error between the full and reduced models at different percent energies (PE).

Since there is little improvement beyond a PE of 99.9% the subsequent discussion and analysis are from this PE value, which results in a POD basis composed of 127 basis vectors. This POD basis then reduces the model derived from TC4 from 113,578 equations (Eq. 7) to 127 (Eq. 16), reducing the dimension by 99.9%. Fig. 17 presents four hydrographs from the full and reduced models at well locations specified as A, B, C and D in Fig. 15. Only the well sites' upper-most (Top WEL cell) and lower-most (Bottom WEL cell) WEL cells are presented in the hydrographs. Due to the three-dimensional nature of this highly heterogeneous model, the Top WEL Cell does not necessarily have a higher hydraulic head. Many factors can cause this effect, such as having the Top WEL Cell being surrounded by lower hydraulic conductivity cells than those that surround the Bottom WEL Cell. The reduced model precisely represents the full model at each location through both the pumping and recovery of TC4.

Fig. 17: TC4's full and reduced models' simulated hydrographs at the four production wells identified as A, B, C and D in Fig. 15.

The simulated water table at the end of the two-year scenario is presented in Fig. 18. The simulated water-table elevation varies from -1.3 m msl to 133.5 m msl (Fig. 18). The effect of the fault lines (Fig. 18) is easily identified by the sharp contrasts in water-table elevation (Fig. 18). The drain network (Fig. 18) is also apparent from the lowered water-table elevation. At the scale of Fig. 18, visually, the simulated water tables for the full and reduced models are

indistinguishable. This is quite significant considering the original model requires the solution of 113,578 equations for each Newton step compared to the reduced model's 127 equations.

Fig. 18: TC4's full (top) and reduced (bottom) models' water table elevation at the end of the two year scenario.

4.3 Quantification of CPU time savings

It is difficult to quantify improvement in CPU time due to many factors that affect overall simulation time. For example, the reduced model's system of equations are solved by using the LAPACK's General Matrix LU decomposition with partial pivoting and row interchanges (DGESV) [26], while the NWT package includes a choice of two highly optimized solvers specifically designed for its matrix structure. The current implementation is also undertaken in a way to ensure that the computer code performs as expected with minimal code refactoring for speed purposes. What is common between the full and reduced models is that they are compiled with the Intel Visual Fortran Composer XE 2013 SP1 for single thread execution and run on a Dell Precision M6700 with Windows 7, 32GB RAM, a Samsung 840PRO SSD hard drive, and Intel Core i7-3840QM processor at 2.8 GHz. With the aforementioned computer the CPU time

required for completion of the full and reduced models for TC3 are 24.3 minutes and 7.6 minutes, respectively. For TC4 the CPU times are 33.5 minutes and 6 minutes, respectively. For this initial investigation of unconfined model reduction, there is a significant savings in CPU time. Further improvement is possible through better identification of snapshots and optimized solvers.

5 Discussions and Conclusion

This paper describes a novel method for applying projection-based model reduction to unconfined groundwater-flow systems and applies it to four test cases. The POD basis is derived from taking snapshots from the original, full model and applying singular value decomposition to identify the dominant proper orthogonal modes. This POD basis is applied through the Galerkin projection to the Jacobian in the Newton formulation of MODFLOW. This results in a significant reduction in the dimensionality of the Jacobian for transient, unconfined groundwater-flow models. This method is not limited to the unconfined groundwater flow and can be applied to a groundwater system that is strictly confined (Eq. 1). In fact, the model reduction of the four test cases were originally validated using only the confined equation (Eq. 1), before their evaluation with the unconfined equations (Eq. 1 and 2).

The four test case examples illustrate that the reduced model can replicate the full model under a variety of scenarios and maintain a small mass balance error. TC1 and TC2 demonstrate that the reduced model replicates the original model when multiple MODFLOW layers are dewatered. TC2 and TC3 incorporate an MNW2 well to increase the complexity. The reduced model verifies that not only for the simulated water table; it also closely matches the simulated well head level and intraborehole flows. TC3 and TC4 produce reduced models that simulate

three-dimensional groundwater flow in a heterogeneous system. TC4 is a more complicated case where the 113,578 model cells with spatially varying horizontal hydraulic conductivity, vertical hydraulic conductivity, and specific storage. In each of the test cases, the dimensionality reduction is at least an order of magnitude, resulting in faster simulation runs.

Snapshot selection does affect the reduced model's fidelity to the full model. Poorly selected snapshots result in a poor basis and consequently a reduced model that does not accurately reflect the full one. In this case, the best reduced models are developed from exponentially distributed snapshot times starting just after the initial condition to steady state under a constant forcing. For certain nonlinear problems the reduced model is further improved by continuing to take snapshots with the forcing turned off in order to capture the dynamics of the nonlinear recovery. This is especially important for multi-node wells in order to capture the intraborehole flows under no pumping. Another improvement, which was not needed for the presented test cases, is to collect snapshots at different constant rates (e.g. two snapshot sets for one well, but at different rates). Taking two sets at different rates makes the set less sensitive to the actual snapshot times, though generally this results in larger-dimensional reduced models. After the snapshots are collected, applying mean centering to the final set greatly improves the reduced model and is recommended for the presented model reduction formulation. An important area for future research and expansion is for an automatic or optimal decision tree for the selection of snapshots.

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756

757 **Figure Captions**

758 Fig. 1: Two-dimensional, vertical test case, TC1, with three wells (WEL) and time-variant specified-head
759 (CHD) boundary conditions.

760 Fig. 2: Distribution of snapshot times. The first 45 are taken with pumping and the remainder without.

761 Fig. 3: TC1 (left) histogram of the mean absolute errors from all time steps and (right) exceedance curve
762 of the RMSE. Note that the units are in mm.

763 Fig. 4: Two-dimensional test case, TC1, simulated water-table elevation during the first 3,000 days of
764 pumping (left) and the next 3,000 days of recovery (right) at select times for the full and reduced models.
765 Note that MAE and NRMSE are calculated from the simulated head at all 500 model cells.

766 Figure 5: Two-dimensional test case, TC1, full and reduced model's loss of pump capacity due to
767 drawdown.

768 Fig. 6: Two-dimensional test case, TC2, with one multi-node well with two screened intervals (MNW2)
769 and general head boundary conditions (GHB).

770 Fig. 7: TC2 (left) histogram of the mean absolute errors from all time steps and (right) exceedance curve
771 of the RMSE. Note that the units are in mm.

772 Fig. 8: TC2 simulated water-table elevation during the first 3,000 days of pumping (left) and the next
773 3,000 days of recovery (right) at select times for the full and reduced models. Note that MAE and
774 NRMSE are calculated from the simulated head at all 500 model cells.

775 Fig. 9: TC2 full and reduced model's simulated well water level (top) and screen flow rate with (left) and
776 without pumping (right). The MNW2 screen flow rate is positive when flow is out of the layer and into
777 well. Note the center and right parts are on different scales.

778 Fig. 10: Plan overview of test case 3 (TC3).

779 Fig. 11: Percent Energy (left y-axis) and Singular values (right y-axis) from applying SVD to the 460
780 snapshots taken from TC3.

781 Fig. 12: TC3 (left) histogram of the mean absolute errors from all time steps and (right) exceedance curve
782 of the RMSE.

783 Fig. 13: TC3 comparison between the full (left) and reduced (right) model's water table elevation at the
784 last pumping stress period at 2850 days (top) and the last recovery stress period at 3000 days (bottom).

785 Fig. 14: TC3 full and reduced model's (left) MNW2 well water level and (center and right) MNW2 screen
786 flow rate where there is positive is flow out of the layer and into the well.

787 Fig. 15: Overview of the Santa Barbara Model, TC4.

788 Fig. 16: TC4 snapshot set's singular values and corresponding percent energy (top) and the error between
789 the full and reduced models at different percent energies (PE).

790 Fig. 17: TC4's full and reduced models' simulated hydrographs at the four production wells identified as
791 A, B, C and D in Fig. 15.

792 Fig. 18: TC4's full (top) and reduced (bottom) models' water table elevation at the end of the two year
793 scenario.

794