DEVELOPMENT AND APPLICATION OF REDUCED-ORDER
MODELING PROCEDURES FOR RESERVOIR SIMULATION

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Abstract

Subsurface flow modeling is essential for understanding and managing many energy-related processes, including oil production and the geological storage of carbon dioxide. Some applications, particularly those involving optimization of field performance, are very demanding computationally due to the large number of flow simulations that must be performed and the typically large dimension of the simulation models. In this work, reduced-order modeling (ROM) techniques are developed for subsurface flow modeling and applied to reduce the simulation time of subsurface flow models. The two ROM procedures considered are proper orthogonal decomposition (POD) and trajectory piecewise linearization (TPWL).

Proper orthogonal decomposition is a commonly used ROM technique that can be applied for nonlinear problems. In the POD procedure a full (high-fidelity) simulation is run, solution snapshots for the pressure and saturation states are stored, and singular value decomposition (SVD) is performed on the resulting data matrix. This provides a reduced basis which is used to project the solution into a low-dimensional subspace. Using this basis, we need only solve for a reduced set of unknowns. We extend the standard POD approach by incorporating a clustering technique and a missing point estimation (MPE) procedure. These act to reduce the number of columns and rows in the basis matrix. The ROM procedure is implemented into Stanford’s general purpose research simulator (GPRS). Extensive flow simulations involving water injection into a geologically complex 3D oil reservoir model containing 60,000 grid blocks are performed. The numerical solutions demonstrate that the POD-based ROM procedure can accurately reproduce the reference simulations over a reasonable range of control settings and provide speedups of up to an order of magnitude when compared with the high-fidelity model simulated using an optimized solver.

In an attempt to achieve significantly greater speedups, a trajectory piecewise linearization (TPWL) procedure for the reduced-order modeling of two-phase flow in subsurface formations is formulated. The method represents new pressure and saturation states using
linear expansions around states previously simulated and saved during a series of preprocessing training runs. The linearized representation is projected into a low-dimensional space, with the projection matrix constructed using the reduced POD basis. The TPWL method is applied to heterogeneous reservoir models and extensive test simulations are performed. It is shown that the TPWL approach provides accurate results when the controls (bottom hole pressures of the production wells) applied in test simulations are within the general range of the controls employed in the training runs, even though the well pressure schedules for the test runs can differ significantly from those of the training simulations. Runtime speedups using the procedure are very significant - a factor of 2 – 3 orders of magnitude (depending on model size and whether or not mass balance error is computed at every time step) for the cases considered.

Finally, the TPWL representations are used in several optimizations involving the determination of optimal bottom hole pressures for producer wells. Three different geological models are considered. Both gradient-based and generalized pattern search optimization algorithms are considered for one model; for the other two models only the gradient-based algorithm is applied. Results for optimized net present value (NPV) using TPWL are shown to be in consistently close agreement with that computed using high-fidelity simulations. Most significantly, when the optimal well settings obtained using TPWL are applied in high-fidelity models, the resulting NPVs are within 0.7% of the values determined using the high-fidelity simulations. Additionally, the TPWL procedure is applied to a computationally demanding multiobjective optimization problem, for which the Pareto front is determined. Limited high-fidelity simulations demonstrate the accuracy and applicability of TPWL for this challenging problem.
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Chapter 1

Introduction and Literature Review

Reservoir simulation is an indispensable tool for the management of hydrocarbon reservoirs. It is used for understanding flow and recovery processes, for sensitivity and uncertainty assessments, to predict reservoir performance under different operating conditions, and for optimizing reservoir performance.

Optimization and uncertainty assessment require time consuming computations. The number of flow simulations that must be performed can be very significant. For example, using gradient-based (numerical finite-difference) optimization algorithms, this number can be several hundred, while with evolutionary algorithms it can be several thousand. Additionally, the detailed three-dimensional reservoir simulation models can be very complex, as they may contain several hundred thousand cells, two or more unknowns per grid block, multisegmented wells, regions of local grid refinement, etc. Thus the computational requirements can be substantial even for a single evaluation of the simulation model. Therefore it is very useful to reduce computational demands to enable the practical application of reservoir simulation for optimization and uncertainty assessment.

This issue can be addressed in a variety of manners. Possible solutions include the use of parallel computing, in which many simulations are performed simultaneously, or upscaling (coarsening) of the reservoir model. In this work we apply another approach, namely reduced-order modeling.
CHAPTER 1. INTRODUCTION AND LITERATURE REVIEW

1.1 Literature Review

1.1.1 General Overview of Reduced-Order Modeling Procedures

Reduced-order modeling is the transformation of high-dimensional models into meaningful representations of reduced dimensionality. Ideally, the reduced-order model should have a dimension that approaches the minimum number of parameters necessary to explain the system dynamics.

Reduced-order modeling has been applied in diverse areas for simulation, classification, visualization, and compression of high-dimensional data. Its use for subsurface flow is relatively new, and for reservoir simulation only a few applications have been presented. Descriptions of the major classes of reduced-order modeling methods, with extensive references, are presented by Antoulas and Sorensen [3] and Rewieński [56]. Our overview below follows these reviews.

Many of the existing reduced-order modeling (ROM) algorithms were developed for linear systems. The three most widely used methods are based on Krylov subspace, balanced truncation and proper orthogonal decomposition (POD) techniques. All of those approaches are projection methods, which project the high-dimensional state space of the original model into a low-dimensional subspace. We now briefly discuss these three approaches, first within the context of linear problems and then for nonlinear cases.

Given a linear system of equations $Ax = b$, the order-$r$ Krylov subspace ($K_r$) is given by the subspace spanned by the images of $b$ under the first $r$ powers of $A$ starting from $A^0 = I$, that is, $K_r = \text{span}(b, Ab, A^2b, \ldots, A^{r-1}b)$ [10, 24]. Krylov-based methods find the eigenvalues of large sparse matrices or solve large linear systems of equations without performing matrix-matrix operations, but rather through matrix-vector multiplication. Starting with a vector $b$ the vector $Ab$ is computed, then this vector is multiplied by $A$ to find $A^2b$, and so on. However, because the vectors tend very quickly to become almost linearly dependent, Krylov-based methods commonly contain an orthogonalization scheme, such as Lanczos iteration for Hermitian matrices or Arnoldi iteration for more general matrices [39]. The resulting orthogonalized set of vectors constitutes the reduced-order basis.

Krylov-based methods provide algorithms for generating reduced bases that can approximate the original simulation model around a specified frequency or collection of frequency points. Krylov subspace algorithms are able to preserve stability (the tendency of a variable
of a system to remain within defined and recognizable limits despite the impact of disturbances) and passivity (a property that guarantees the system does not produce energy) [38], making them suitable for reduction of large-scale systems. Some applications include circuit simulation [10, 55, 63], micromachined devices [55, 71], wireless systems [38], power systems [24], and magnetic devices [52]. The advantages of Krylov-based methods are robustness and low numerical cost, however its limitation is that the resulting reduced-order model has no guaranteed error bound.

Balanced truncation is a model reduction method for linear systems that takes account of both the inputs and outputs of the system to determine which states to retain in the reduced-state representation [14, 57, 74]. Consider a linear system $dx/dt = Ax + Bu$ and $y = Cx$ where $u(t) \in \mathbb{R}^m$ is a vector containing $m$ external forcing inputs, $y(t) \in \mathbb{R}^p$ is a vector of outputs, and $x(t) \in \mathbb{R}^n$ is the state vector. The matrices $A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times m}$, and $C \in \mathbb{R}^{p \times n}$ have constant coefficients evaluated at steady-state conditions. The controllability and observability gramians are matrices defined as:

$$W_c = \int_0^\infty e^{At}BB^*e^{A^*t}dt, \quad W_o = \int_0^\infty e^{A^*t}C^*Ce^{At}dt,$$

where $*$ denotes Hermitian matrices [62] (for real matrices the Hermitian is equivalent to the transpose). The $n \times n$ matrices $W_c$ and $W_o$ describe the controllable and observable subspaces of the linear system and are usually computed by solving the Lyapunov equations $AW_c + W_cA^* + BB^* = 0$ and $A^*W_o + W_oA + C^*C = 0$. The controllable subspace is the set of states that can be obtained with zero initial state and a given input $u(t)$, while the observable subspace contains the states which as initial conditions could produce a certain output $y(t)$ with no external input. The largest eigenvalues of the controllability and observability gramians describe the most controllable and observable states in the system, respectively [14].

A balanced realization of the system is obtained by changing to coordinates in which the controllability and observability gramians are diagonal and equal. The following procedure was proposed by Rowley [57]. First a change of coordinates is applied as $W_c \mapsto T^{-1}W_c(T^{-1})^*$ and $W_o \mapsto T^*W_oT$, where $T$ is a balancing transformation. Then the transformed gramians are computed as $W_c \mapsto T^{-1}W_c(T^{-1})^* = W_o \mapsto T^*W_oT = \Sigma = \text{diag}(\sigma_1, \ldots, \sigma_n)$. 
The diagonal elements $\sigma_1 \geq \ldots \geq \sigma_n \geq 0$ are the Hankel singular values of the system. A reduced-order basis given by the balancing transformation $T$ will always exist as long as the system is both controllable and observable. The transformation is found by computing the eigenvectors of the product $W_c W_o$. Finally, the least controllable and observable states, which have little effect on the input-output behavior, are truncated.

In contrast to Krylov-based methods, truncated balancing realization (TBR) techniques have provable error bounds for the ROM and guarantee that the stability of the original system is preserved in the reduced-order model. A limitation is the computational complexity, which is $O(n^3)$, required to solve the Lyapunov equations. TBR techniques have been applied for single-phase flow reservoir models by Zandvliet [74] and proposed by Markovic et al. [45] and Heijn et al. [37] for two-phase flow models. Bui-Thanh and Willcox [14] and Rowley [57] applied TBR to fluid dynamics problems.

Proper orthogonal decomposition (POD) was first proposed by Lumley [44] to identify coherent structures in dynamical systems. POD is described as an orthogonal linear transformation that transforms a set of data to a new coordinate system such that the greatest variance lies in the first coordinate, the second greatest variance in the second coordinate, and so on. The POD procedure characterizes the relevant states of a model by a set of orthonormal basis functions which correspond to the leading eigenvectors of a covariance matrix constructed from a set of computed solutions. These computed solutions are generated using high-fidelity (high-dimension) “training” simulations and are referred to as snapshots. The method of snapshots or strobes was introduced by Sirovich [61] as a manner to efficiently identify the POD basis functions for large systems. The basis functions can also be generated more efficiently through a singular value decomposition (SVD) of the snapshot matrix.

POD allows the representation of the state space of the model using only the first few (most relevant or highest energy) basis functions. The reduced-order model is obtained by projecting the original governing equations onto the POD basis functions, enabling a significant reduction in the number of unknowns that must be computed. The basis formed is optimum in the sense that it minimizes the error between the original data (snapshots from the high-fidelity model) and the reconstructed data for any given number of basis functions. POD is the same as principal component analysis, or PCA. It is also referred to as a discrete Karhunen-Loève (K-L) transform.
An advantage of POD is the relatively low cost required to generate a reduced-order basis from the snapshot set. A drawback is that the appropriate choice of controls used in the training runs is not obvious. This is an issue because the ROM may be unable to provide adequate accuracy for controls far from those used in the training runs.

Reduced-order modeling is well established for constructing macromodels (the term macromodel refers to the reduced-order representation) for linear time invariant (LTI) systems of the form \( \frac{dx}{dt} = Ax + Bu \) and \( y = Cx \) as introduced above. For such linear systems the matrices \( A, B \) and \( C \) are not updated and the resulting reduced-order model is fixed in time. Consequently, meaningful reductions in computational requirements can be expected. For nonlinear systems, however, these matrices are not fixed and must be updated. This is the case in many application areas. For example, in reservoir simulation, nonlinearities appear because relative permeabilities are nonlinear functions of saturation, and densities and rock compressibility are functions of pressure. In contrast to linear models, the reduced-order model cannot technically be pre-computed in this case, but must be updated constantly because the parameters change in time. Reconstruction of the ROM is computationally demanding and leads to procedures that may require as much computation as the original (high-fidelity) model. Thus, the use of ROMs for nonlinear systems is a challenge, though a number of approaches have been developed to address this issue. We now discuss some of these procedures.

One such technique for the reduced-order modeling of nonlinear systems is based on linearized or polynomial expansion of the nonlinearity and application of Krylov-based projection methods [26, 51]. A limitation of these approaches is that the reduced-order model is valid only around the initial operating point of the nonlinear system, which limits the application of the ROM to weakly nonlinear systems and limited input disturbances.

Balanced truncation was also applied for nonlinear systems. Condon and Ivanov [29] proposed a new approach to construct empirical controllability and observability gramians. They reported that the method is successful if the state-space of the nonlinear solution is well defined. However this is not the case for all nonlinear systems and the method is thus applicable for systems in which the nonlinearities are not too severe.

Proper orthogonal decomposition is probably the most popular method for the reduced-order modeling of nonlinear systems. Since the basis functions are computed from the snapshots (which are recorded from the actual simulation of the nonlinear model), the
POD-based ROM thus inherits the stability and some of the behavior of the original system [58]. In addition, the formulation can be improved through use of specialized techniques (discussed below) designed to improve the efficiency of the standard POD. For these reasons, POD will be used for the ROMs developed in this thesis.

The range of applications for POD is substantial. Zheng et al. [75] applied POD for modeling nonlinear reactor systems described by partial differential equations (PDEs). Meyer and Matthies [48] used POD on a nonlinear structural model of a horizontal axis wind turbine rotor blade. Bui-Thanh et al. [13] employed POD to reconstruct flow-fields from incomplete aerodynamic data sets, and Cao et al. [19] applied POD to model a large-scale upper ocean circulation in the tropic Pacific domain. POD has also been applied for subsurface flow problems [68, 66, 67, 37, 64, 46] as discussed in the next section.

We note that, even though the ROMs discussed above can be used for nonlinear problems, their performance generally degrades significantly relative to that for linear cases [56, 5]. To overcome these limitations Rewiński [56] developed a linearization method that approximates the nonlinear system with a weighted combination of linearized models generated and saved from training simulations of the system. This method will be discussed in detail in section 1.1.4.

1.1.2 POD for Subsurface Flow

There have been several applications of POD-based reduced-order modeling approaches to subsurface flow problems. Vermeulen et al. [68] applied POD for a heterogeneous aquifer model with 33,000 active nodes. The reduced-order model was designed to simulate the long-term effects of change in precipitation/evaporation and the effects of variable well production rate. The number of snapshots recorded from the training runs was minimized based on the fact that the model was linear and the individual states could be combined by superposition. Applying POD, a reduced-order model of dimension 16 was generated and a runtime speedup of 625 was reported. This very large speedup is achieved because this is a linear time invariant model, for which ROM procedures can be expected to provide substantial speedups.

The implementation of POD for inverse modeling of groundwater flow was reported by Vermeulen and Heemink [66, 67]. Reduced-order modeling was applied to the groundwater flow formulation and to the adjoint equations used to compute the gradients of an objective function. The method was applied for an aquifer model containing 34,000 grid blocks.
in which the transmissibility between regions was to be estimated. The accuracy of the estimated parameters computed using the reduced model was very good compared with the values found using the high-fidelity model. In this case, in contrast to the runtime speedup of 625 reported in [68], the speedup was less than a factor of 2 relative to the high-fidelity model. This large difference in runtime speedups was due to the formulation of the reduced adjoint method, which required that a particular variable be updated using the high-fidelity model.

Reduced-order modeling for nonlinear two-phase (oil-water) subsurface flow has also been addressed [37, 64, 46]. van Doren et al. [64] developed an adjoint-based optimal control methodology for waterflooding. Proper orthogonal decomposition was used to compute reduced-order models for both the forward model and the adjoint system. They successfully applied their procedure to optimize the net present value (NPV) of a heterogeneous two-dimensional model containing 2,025 grid blocks and two horizontal wells, one producer and one injector, both divided into 45 independently controlled segments. POD reduced the number of unknowns from 4,050 in the high-fidelity model to 20 – 100 in the ROMs. Runtime speedups for the forward simulations were only about a factor of 1.5, however. The speedups achieved for the overall optimization process were even more modest due to the need for some amount of high-fidelity computation (see section 1.1.5 for further discussion). This illustrates the challenges inherent in the use of POD for problems with significant nonlinearity.

Markovinović and Jansen [46] proposed the use of POD to accelerate the iterative linear solver used for the full (high-fidelity) model. Thus, in their procedure, the ROM was used in conjunction with the full model. The authors considered complex models (e.g., a three-dimensional model containing 93,500 grid blocks) and achieved up to a factor of 3 in speedup. This method, however, requires that the full system be simulated along with the ROM and it also requires that the reduced-order basis be updated during the course of the simulation. Further, it is to be expected that the impact of the ROM (and thus the degree of speedup) would be less if a highly optimized linear solver was used for the high-fidelity problem.

The developments cited above are promising in that they demonstrate the application of POD procedures to subsurface flow problems. Previous work does not, however, demonstrate the application of ROM techniques for practical nonlinear multiphase flow cases (involving highly heterogeneous geological characterizations containing, e.g., $10^4 - 10^5$ grid...
blocks) in which reduced-order models can be used in place of full high-fidelity reservoir flow simulations. In addition, there does not appear to have been any implementation of ROM procedures into general purpose subsurface flow simulators.

The limited speedups achieved in previous POD-based ROMs for two-phase flow can be better understood by considering the computations required for a reservoir model with $N_c$ grid blocks, which corresponds to $2N_c$ unknowns (oil pressure and water saturation for all grid blocks). Suppose that by applying proper orthogonal decomposition a reduced-order model of dimension $\ell$ can be formed, with $\ell << 2N_c$. The POD procedure works at the level of the linear solver, reducing the sparse $2N_c \times 2N_c$ linear system to a full $\ell \times \ell$ system. The solver time is thus reduced substantially. Computational requirements for other operations, by contrast, such as the construction of the Jacobian matrix (which must be performed at each iteration of every time step), are not reduced at all through the use of the standard POD technique. Also, after a new Jacobian matrix ($J$) is constructed it must be projected into the reduced-order space using a reduced-order basis $\Phi$. Specifically, the reduced Jacobian ($J_r$) is computed as $J_r = \Phi^T J \Phi$, and these matrix multiplications are computationally demanding. Thus, the construction of both $J$ and $J_r$ is computationally costly. In the next section we describe some improvements to the standard POD procedure that enable better performance for nonlinear problems.

1.1.3 Enhanced POD

Two approaches within the context of POD – a clustering technique to optimize the snapshots for the eigen-decomposition problem, which acts to reduce the number of POD basis vectors needed, and a missing point estimation (MPE) procedure to reduce the dimension of the POD basis vectors – have been developed previously [16, 35, 5, 4, 8, 7, 6]. These procedures have not been applied within the context of subsurface flow modeling. We now discuss these approaches, as we will later apply them for reservoir simulation.

Clustering

The snapshots generated from training runs are used for the construction of the reduced-order basis matrix. In our approach the snapshots are simply the states computed at each time step of the high-fidelity training runs. One concern that arises is that the snapshots depend on the controls used in the training run (this is discussed in section 2.2). Another
issue is that, in state space, the distribution of snapshots can be far from uniform, meaning that in some regions of the state space the snapshots are concentrated while in other regions they are sparsely distributed. The irregular distribution of snapshots can bias the resulting reduced basis.

Burkardt et al. [16] introduced centroidal Voronoi tessellation (CVT) to generate a reduced-order basis from the generators of a CVT of snapshots. CVT is also known as k-means clustering and the generators of a CVT of snapshots are the centroids of the clusters formed from the snapshot set. In our approach we apply the k-means clustering technique to reduce the number of recorded snapshots, which are not in general uniformly distributed in the state space, into a smaller number of centroids that are more regularly distributed.

The clustering of snapshots has a twofold benefit. First, it provides a more uniform distribution of snapshots in state space, which enables the construction of a reduced-order basis with a smaller number of basis functions (columns of $\Phi$). Second, the SVD of the data matrix can be performed more efficiently. This second advantage is not a major benefit for the cases considered in this thesis, but it could be important if a very large number of snapshots are recorded.

**Missing Point Estimation**

Astrid [5] introduced the method of missing point estimation (MPE) to improve the computational efficiency of the reduced-order model. This approach was motivated by the Gappy-POD approach developed for image reconstruction, introduced by Everson and Sirovich [32]. The MPE methodology seeks to reduce the computational cost of updating the matrices required by the reduced-order model (i.e., $J_r$). This reduction is based on the assumption that the reduced-order basis $\Phi$ can be constructed using information from only a portion of the spatial domain rather than from the entire spatial domain.

Within the context of POD applied to reservoir simulation, MPE can be used to accelerate the construction of the Jacobian matrix $J$ and the reduced Jacobian matrix $J_r = \Phi^T J \Phi$, which must be formed at each iteration of every time step. Specifically, rather than using information from all $N_c$ grid blocks of the reservoir model, MPE allows us to use information from $n_m$ selected grid blocks, where $n_m < N_c$. Grid block selection is achieved with awareness of the fact that $\Phi$ should be an orthonormal basis, meaning that the condition number of $\Phi^T \Phi$ should be very close to 1. Then, applying different procedures, rows of $\Phi$
are eliminated (each row of $\Phi$ corresponds to a specific grid block), such that the condition number of $\Phi^T\Phi$ stays close to 1 (Astrid [5]).

Missing point estimation has been applied previously for different nonlinear problems. In the original development of MPE, Astrid [5] implemented the method within a reduced-order model constructed with POD to simulate the temperature distribution in a glass melt feeder. The high-fidelity model contained 7,128 cells. A reduced-order model constructed using the standard POD provided a runtime speedup of 3.2 while using POD-MPE with 465 cells selected the speedup increased to 8.5. Another application of POD with MPE was presented by Astrid [8] for a nonlinear heat conduction model used to compute the temperature distribution on a thin plate. Compared with the original full-order model a speedup of 10 was obtained using the standard POD and 200 when POD-MPE was applied with 200 grid blocks selected (the full model contained 1,452 grid blocks).

1.1.4 Trajectory Piecewise Linearization

Even using the enhanced POD procedures (clustering and MPE) described above, there are still some inherent limitations in the achievable speedup. This is because the required number of rows of $\Phi$ would still be expected to be a reasonable fraction of $2N_c$. In addition, a full implementation of MPE requires modifications throughout the simulator; e.g., in the Jacobian construction code.

Some of these limitations are addressed by the trajectory piecewise linearization approach (TPWL) introduced by Rewieński [56]. In this methodology a nonlinear system is represented as a weighted combination of piecewise linear systems and each linear system is projected into a low-dimensional space using Krylov subspaces or other ROM procedure. A key feature of the TPWL method is that during subsequent simulations it linearizes around one or more states selected from a large collection of snapshots. New states are represented in terms of piecewise linear expansions around previously simulated (and saved) states and Jacobian matrices as:

$$g(x^{n+1}, u^{n+1}) = g(x^i, u^i) + \left( \frac{\partial g}{\partial x} \right)_i (x^{n+1} - x^i) + \left( \frac{\partial g}{\partial u} \right)_i (u^{n+1} - u^i) + \ldots,$$

where $g$ is the residual we seek to drive to zero, $x^{n+1}$ is the new state we wish to determine, $u^{n+1}$ is the new set of controls (which are specified), and both $(\partial g/\partial x)_i$ and $(\partial g/\partial u)_i$ are (saved) matrices evaluated at $(x^i, u^i)$.
Very high degrees of computational efficiency are achieved because all of these computations are performed in reduced space. Rewieński [56] applied the TPWL technique to compute the sinusoidal steady state for a nonlinear transmission line circuit model containing 1,500 unknowns. He used 21 linearization states and generated a reduced-order model of dimension 30. The runtime speedup of the TPWL model compared with the full-order nonlinear model was 1,150. The error on the harmonics of the sinusoidal steady state using the reduced-order TPWL representation varied between 0.4% and 13.5%, depending on the harmonic analyzed, when compared with the high-fidelity model.

TPWL has also been successfully applied in other areas. Gratton and Willcox [34] employed TPWL for a computational fluid dynamics problem involving flow through an actively controlled supersonic diffuser. Proper orthogonal decomposition was used to project the linearized model with 11,703 states to a reduced-order space of 110 states. Their results showed that the TPWL reduced-order model provided a speedup of a factor of 1,440 compared to the high-fidelity nonlinear model. The authors reported accurate results when a sufficient number of basis functions was used, though they stated that the error increased when the reduced-order model was used for simulations outside the range of controls used in the training simulations.

Yang and Shen [71] developed a nonlinear heat-transfer ROM based on TPWL and Krylov subspaces. This technique was applied to simulate steady-state and transient models. The errors between the high-fidelity and reduced-order models were less than 0.5% and the runtime speedup was about two orders of magnitude.

A modified version of the TPWL method was developed and applied by Vasilyev et al. [65] to generate reduced-order models of nonlinear biomedical micro-electromechanical systems (BioMEMS). In their approach the Krylov subspace method for linear reduction was replaced by the truncated balanced realization (TBR) method. They showed that the proposed methodology improved the reduced-order model accuracy relative to Krylov-subspace methods, though speedups were not reported. Additional applications of TPWL were presented by Tiwary and Rutenbar [63] and Dong and Roychowdhlury [30] for modeling electronic circuits. TPWL does not appear to have been considered for oil reservoir simulation or for any closely related subsurface flow application. Thus it will be of interest to assess TPWL for this application area.
1.1.5 Optimization of Reservoir Performance

Computational optimization can be applied for many oil field problems. Our specific interest here is for optimization of waterflooding. This is important for wells under surface control and for smart wells equipped with downhole inflow control valves. In either case optimization is performed to determine the settings for the well controls such that an objective function (cumulative oil production or net present value) is maximized.

The optimized well controls can be determined using gradient-based algorithms, with gradients computed either numerically (using finite differences) or by solving adjoint equations. The benefit of using optimization algorithms with numerical gradients is that an existing reservoir simulator with advanced capabilities can be used directly. Such an approach was used by Yeten et al. [72, 73] in their optimization of downhole valve settings. Aitokhuehi and Durlofsky [1] extended this approach for combined history matching and smart well optimization. However, this is a computationally demanding methodology that requires many function evaluations as the number of control valves and/or the number of setting updates increase. The total number of simulation runs required to computed the numerical gradient is given by one plus the number of control variables.

As indicated above, optimization procedures that require only objective function evaluations (and which treat the simulator as a black box) are useful in many cases, though they tend to require many forward simulations. Gradient-based methods with gradients determined through solution of adjoint equations represent a much more efficient alternative. Some of the first adjoint-based optimizations for oil reservoir problems were presented by Ramirez [53]. Brouwer and Jansen [12] and Sarma et al. [59] recently implemented adjoint-based production optimization procedures. These approaches involve detailed coupling with the reservoir simulator and thus require access to the source code.

In recent work Reynolds and coworkers [70] compared the performance of three optimization algorithms for production optimization. The algorithms considered were an adjoint method, a simultaneous perturbation stochastic approximation (SPSA) in which all parameters are perturbed stochastically, and an ensemble Kalman filter (EnKF). The results showed that the gradient-based algorithm was the most efficient, requiring many fewer iterations than the SPSA and EnKF algorithms. Another application of the ensemble Kalman filter for closed-loop production optimization was presented by Chen et al. [27].

Genetic algorithms are another class of techniques that can be used for production optimization. Those methods are theoretically able to find the global optimum of the
objective function with a sufficiently large number of simulations runs, though an unrealistic number of runs may be required. Relatively few applications of genetic algorithms for production optimization have been presented. Almeida et al. [2] applied a genetic algorithm to optimize downhole valve settings for smart wells. They used a small synthetic reservoir model with a conventional production well and a smart injection well equipped with three control valves. For this very idealized system, 120 simulations were required to increase the NPV by 4.6%.

Optimization with Reduced-Order Models

Because optimization procedures often require many forward simulations, they are a natural application area for ROMs. The high computational cost required to simulate microelectromechanical systems (MEMS) when transient dynamic effects are included motivated Han et al. [36] to apply a ROM procedure using Krylov subspaces to optimize MEMS devices. A commercial general-purpose gradient-based optimization software (“DOT”) and an in-house model order reduction tool were used. The ROM was applied to a micro-accelerometer model used in automotive airbags. The model consisted of 2,197 nodes with 3 degrees of freedom per node, giving a total of 6,591 degrees of freedom. Two ROMs, one of dimension 5 and another of dimension 30, were employed for the optimizations. Compared with the high-fidelity simulation model, both reduced-order models resulted in only small errors. Runtime speedups of 5 and 20 were reported for the ROMs of dimension 30 and 5, respectively. These low speedups are due to the optimization procedure used, in which the high-fidelity model must be updated with the optimized design variables until a convergence criterion is reached.

As discussed in section 1.1.2, van Doren et al. [64] implemented reduced-order simulation and adjoint models using POD for waterflood optimization. After using the reduced-order forward and adjoint models to find the optimized controls, a high-fidelity simulation was performed to check the solution accuracy. Then, if required, a new reduced-order basis \( \Phi \) was constructed, and the process repeated until convergence of the net present value with the full-order model was achieved. The speedups observed for these computations were modest, with CPU time reduced by only about 35%. This is due in part to the need for some amount of high-fidelity computation.
1.2 Scope of this Work

The development of reduced-order modeling procedures has received significant attention in recent years. However, relatively few studies have been conducted to investigate the application of these approaches for reservoir flow simulation. This dissertation is mainly devoted to furthering the development and application of ROM methods for subsurface flow problems. Though the target application here is oil reservoir simulation, our findings are also relevant to other closely related areas such as aquifer management and the geological storage of carbon dioxide. We also study the use of reduced-order models for production optimization. To accomplish this we develop a technique that couples trajectory piecewise linearization (TPWL) with proper orthogonal decomposition (POD). The resulting model will be shown to achieve runtime speedups of 2–3 orders of magnitude in the optimization computation.

The specific goals of this dissertation are:

• to further the development and application of POD-based methods for subsurface flow problems. Specifically, by incorporating new reduced-order modeling procedures developed within other application areas, we aim to apply these approaches to more realistic reservoir simulation models and to achieve better computational performance. The specific techniques to be incorporated in the standard POD include the clustering [16] and missing point estimation [5] procedures described in section 1.1.3

• to incorporate our developments into a general purpose flow simulator [17, 41], so they can eventually be used for a wider variety of flow problems.

• to develop and apply TPWL procedures for subsurface flow modeling. Toward this end we formulate a TPWL representation for oil-water flow.

• to evaluate the performance of the enhanced POD and TPWL-POD techniques for challenging nonlinear subsurface flow problems. Our examples involve highly heterogeneous geological models and nonlinear relative permeability curves.

• to apply the new TPWL-POD technique for single and multiobjective optimization problems involving complex three-dimensional reservoir models and to compare the optimization results with those using high-fidelity simulation models.
1.3 Dissertation Outline

This dissertation proceeds as follows. In Chapter 2, reduced-order modeling (ROM) techniques are applied to complex large-scale subsurface flow models. Starting with a high-fidelity training simulation, snapshots are recorded for the oil pressure and water saturation states. Then, an eigen-decomposition (SVD) is performed on both states to compute the basis matrix \( \Phi \) used to project the high-dimensional system into a low-dimensional subspace. To improve the performance of the reduced-order model, a clustering technique is introduced to reduce the number of columns of \( \Phi \) and a missing point estimation (MPE) approach is applied to remove selected rows of \( \Phi \). The reduced-order modeling procedure, which includes proper orthogonal decomposition (POD), clustering and MPE, was implemented into Stanford’s general purpose research simulator [17, 41].

The POD-based methodology is then tested for simulations involving waterflood for a geologically complex three-dimensional oil reservoir model containing 60,000 grid blocks. The performance of the various techniques (standard POD, clustering and MPE) is assessed in terms of their ability to reproduce high-fidelity simulation results for the training run and also for test simulations with different well schedules. The results demonstrate that the ROM procedure can accurately reproduce the reference high-fidelity simulations. Runtime speedups of up to an order of magnitude are observed relative to the high-fidelity model simulated using an optimized solver. Speedups will be significantly less, however, if the relative permeability curves are highly nonlinear or if there is a large density difference between the oil and water phases.

The work presented in Chapter 2 was published in the International Journal for Numerical Methods in Engineering [22]. Dr. Pallav Sarma contributed to this work, primarily by implementing the ROM procedure in Stanford’s general purpose research simulator (GPRS), and is a co-author of the journal publication.

Although the ROM presented in Chapter 2 can provide reductions in simulation time, more substantial runtime speedups may be required for optimization problems. In Chapter 3 the trajectory piecewise linearization (TPWL) procedure for the reduced-order modeling of two-phase flow in subsurface formations is developed and applied. The linearization of the governing equations for reservoir flow is described in detail and two approaches for constructing a reduced-order TPWL representation are provided. In the first step of the TPWL methodology, a small number (3–4) of training simulations is performed and, in
addition to the pressure and saturation states needed for the POD procedure, Jacobian matrices are also recorded. The construction of the basis matrix $\Phi$ is accomplished using POD (the same approach described in Chapter 2 is applied). Using this $\Phi$, the linearized model is projected into a low-dimensional space. The preprocessing overhead required for the training runs and to project the recorded states and Jacobian matrices into the low-dimensional space is roughly comparable to 6–8 high-fidelity simulations.

The TPWL model is then applied to two reservoir models containing 24,000 and 79,200 grid blocks and characterized by heterogeneous permeability descriptions. Based on extensive test simulations for both models it is shown that the TPWL approach provides accurate results when the controls (bottom hole pressures of the production wells in this case) applied in test simulations are within the general range of the controls applied in the training runs, even though the well pressure schedules for the test runs can differ significantly from those of the training runs. A key finding is that this new TPWL-POD methodology can provide runtime speedups between two and three orders of magnitude. Thus it appears to be well suited for use in optimization problems. The work presented in Chapter 3 has been submitted for publication to the *Journal of Computational Physics*.

In Chapter 4 we evaluate the performance of the TPWL representation for production optimization problems involving waterflood in heterogeneous reservoir models. Using the two reservoir models described in Chapter 3 and another model with 20,400 grid blocks, single-objective optimizations are performed using the TPWL representation and the high-fidelity simulation model and the results compared.

Production optimization is performed for the 20,400 grid-block model using both gradient-based and generalized pattern search algorithms [21]. In these optimizations the bottom hole pressures (BHPs) of four production wells at six different times (24 control variables) are determined such that the net present value is maximized. Utilizing only the gradient-based algorithm, similar optimizations are also performed for the other two models described in Chapter 3. Although slightly different BHP control schedules are computed by the optimizations with the TPWL representation as compared to those using the high-fidelity model, results for the optimized NPV using the high-fidelity model with the controls determined using TPWL are shown to be in consistently close agreement with those computed using high-fidelity simulations. Runtime speedups using the TPWL representation of between 450 and 2,000 are observed.
1.3. DISSERTATION OUTLINE

The TPWL procedure is applied to a computationally demanding multiobjective optimization problem with 48 control variables, for which the Pareto front is determined. Limited high-fidelity simulations demonstrate the accuracy and applicability of TPWL for this optimization. This multiobjective optimization is extremely demanding computationally; i.e., it would require more than two months of CPU time using the high-fidelity model. Using TPWL, the full optimization is accomplished in 3.3 hours. The work appearing in Chapter 4 has been presented in two papers [21, 20].

Finally, in Chapter 5, we present detailed conclusions and recommendations for future research in the development of efficient reduced-order models for reservoir flow simulation.
Chapter 2

Reduced-Order Modeling of Subsurface Flow Using Proper Orthogonal Decomposition

In this chapter we further the development and application of POD methods for subsurface flow problems. We begin by describing the equations and the standard finite volume discretization for two-phase flow. We then discuss the POD-based reduced-order modeling technique. This includes a description of the clustering and missing point estimation procedures and a description of the implementation of POD into an existing general purpose simulator. Then, in section 2.2, we present results for a number of cases involving a simulation model of a geologically complex reservoir containing 60,000 grid blocks. Different specifications for the time-varying bottom hole pressures of the production wells are considered. These results demonstrate the robustness and computational speedup of the POD techniques for realistic cases. Additional findings and a discussion of some of the limitations of the POD procedures are presented in section 2.3.

2.1 Modeling Procedure

In this section we describe the governing equations, the discretized system, and the proper orthogonal decomposition procedure for oil-water flows.
2.1.1 Oil-Water Flow Equations and Discretization

Subsurface flow models are derived by combining mass conservation equations with the multiphase version of Darcy’s law. For the oil-water case considered here, there is no mass transfer between phases; i.e., the oil component resides only in the oil phase and the water component only in the water phase. Then, for each component/phase \( j \) (with \( j = o \) denoting oil and \( j = w \) water), we have:

\[
\nabla \cdot \left[ \lambda_j k \left( \nabla p_j - \rho_j g \nabla D \right) \right] = \frac{\partial}{\partial t} \left( \phi \frac{S_j}{B_j} \right) + \tilde{q}_j^w, \tag{2.1}
\]

where \( k \) is the absolute permeability (assumed to be a diagonal tensor), \( \lambda_j = k_{rj} / (\mu_j B_j) \) is the phase mobility, \( k_{rj} \) is the relative permeability to phase \( j \), \( \mu_j \) is the phase viscosity, \( B_j \) is the formation volume factor for phase \( j \) (defined below), \( p_j \) is phase pressure, \( \rho_j \) is the phase density, \( g \) is gravitational acceleration, \( D \) is depth, \( t \) is time, \( \phi \) is porosity (void fraction of the rock), \( S_j \) is saturation and \( \tilde{q}_j^w \) is the source/sink term. All terms are of units \( 1/\text{time} \). The formation volume factor is defined as the ratio of the volume of phase \( j \) at reservoir conditions to the phase volume at reference (stock tank) conditions. Designating the reference density of phase \( j \) as \( \rho_0^j \), it follows that \( B_j = \rho_0^j / \rho(p) \). In the case of incompressible flow, density does not vary with pressure and \( B_j = 1 \). The general two-phase flow description is completed through the saturation constraint (\( S_o + S_w = 1 \)) and by specifying a capillary pressure relationship; i.e., \( p_c(S_w) = p_o - p_w \), which relates the phase pressures.

The two-phase flow description entails four equations and four unknowns (\( p_o, p_w, S_o, S_w \)). We select \( p_o \) and \( S_w \) as primary unknowns. Once these are computed, \( p_w \) and \( S_o \) can be readily determined from the capillary pressure relationship and saturation constraint.

We now briefly discuss the finite volume representation for Eq. 2.1 (see [9] or [33] for more details). Figure 2.1 shows a portion of a one-dimensional grid. For simplicity, here we neglect capillary pressure (so \( p_o = p_w \)), treat horizontal flow in the \( x \)-direction (for which \( \nabla D = 0 \)), and assume the grid block dimensions (\( \Delta x, \Delta y, \Delta z \)) are constant. We consider fully implicit discretizations. For this case the discretized form for the flow terms (left hand side of Eq. 2.1) is

\[
\frac{\partial}{\partial x} \left[ k \lambda_j \left( \frac{\partial p_j}{\partial x} \right) \right] \approx \left\{ (T_j)_{i-1/2}^{n+1} \left[ p_i^{n+1} - p_{i-1}^{n+1} \right] + (T_j)_{i+1/2}^{n+1} \left[ p_{i+1}^{n+1} - p_i^{n+1} \right] \right\} \frac{1}{V}, \tag{2.2}
\]
where subscript \( j \) indicates phase and \( i \) designates grid block, superscript \( n + 1 \) specifies the next time step, and \( V = \Delta x \Delta y \Delta z \) is the volume of grid block \( i \). The transmissibility \( (T_j)^{n+1}_{i-1/2} \) relates flow in phase \( j \) to the difference in pressure between grid blocks \( i - 1 \) and \( i \) and is given by:

\[
(T_j)^{n+1}_{i-1/2} = \left( \frac{k A}{\Delta x} \right)_{i-1/2} \left( \frac{k_{rj}}{B_j \mu_j} \right)^{n+1}_{i-1/2},
\]

Figure 2.1: Portion of a one-dimensional grid

The first term on the right hand side of Eq. 2.1 represents mass accumulation and is represented discretely as:

\[
\frac{\partial}{\partial t} \left( \phi S_j B_j \right) \approx \frac{1}{\Delta t} \left[ \left( \phi S_j B_j \right)^{n+1} - \left( \phi S_j B_j \right)^n \right],
\]

where \( \Delta t \) is the time interval. For incompressible systems \( \phi \) is constant and \( B_j = 1 \), in which case Eq. 2.4 reduces to:

\[
\frac{\partial}{\partial t} \left( \phi S_j B_j \right) \approx \frac{\phi}{\Delta t} \left[ (S_j)^{n+1} - (S_j)^n \right].
\]

The second term on the right hand side of Eq. 2.1 represents the source/sink term. In reservoir simulation, the sources and sinks correspond to wells which are modeled using a well equation:

\[
(q_j^w)^{n+1}_i = \left( q_j^w \right)^{n+1}_i V = W_i (\lambda_j)^{n+1}_i (p_i^{n+1} - p_i^{w}),
\]

where subscript \( j \) indicates phase and \( i \) designates grid block, superscript \( n + 1 \) specifies the next time step, and \( V = \Delta x \Delta y \Delta z \) is the volume of grid block \( i \). The transmissibility \( (T_j)^{n+1}_{i-1/2} \) relates flow in phase \( j \) to the difference in pressure between grid blocks \( i - 1 \) and \( i \) and is given by:

\[
(T_j)^{n+1}_{i-1/2} = \left( \frac{k A}{\Delta x} \right)_{i-1/2} \left( \frac{k_{rj}}{B_j \mu_j} \right)^{n+1}_{i-1/2},
\]

where \( A = \Delta y \Delta z \) is the area of the common face between blocks \( i - 1 \) and \( i \). The transmissibility \( (T_j)^{n+1}_{i+1/2} \) is defined analogously. The flow terms can be seen to introduce nonlinearity into the system as \( (T_j)^{n+1}_{i+1/2} \) are functions of pressure and saturation and multiply terms involving pressure. In Eq. 2.3, \( k_{i-1/2} \) is computed as the harmonic average of \( k_{i-1} \) and \( k_{i} \), and \( (k_{rj}/(B_j \mu_j))^{n+1}_{i-1/2} \) is upwinded depending on the flow direction of phase \( j \).
where \((q_j^w)_{i,j}^{n+1}\) is the volumetric flow rate of phase \(j\) from block \(i\) into the well (or vice versa) at time \(n + 1\), \(p_i^n\) is grid block pressure at \(n + 1\), \(p_w^w\) is the wellbore pressure for well \(w\) in grid block \(i\), and \(W_i\) is the well index. For a vertical well that fully penetrates block \(i\), \(W_i\) is given by [50]:

\[
W_i = \left[ \frac{2\pi k \Delta z}{\ln \left( \frac{r_0}{r_w} \right)} \right]_i,
\]

where \(r_w\) is the wellbore radius and \(r_0 = 0.2\Delta x\). See [50] for expressions for \(W_i\) for more general cases. Note that, if a well is operating under bottom hole pressure (BHP) control, this is represented in the simulation model by specifying \(p_w^w\) in Eq. 2.6.

For the discretized models, we consider logically Cartesian systems (meaning blocks follow a logical \(i, j, k\) ordering) containing a total of \(N_c\) grid blocks. The state vector \(x\) contains the two primary unknowns:

\[
x = \begin{bmatrix} (p_o)_1, (S_w)_1, (p_o)_2, (S_w)_2, \ldots, (p_o)_{N_c-1}, (S_w)_{N_c-1}, (p_o)_{N_c}, (S_w)_{N_c} \end{bmatrix}^T.
\]  

Introducing the discretizations presented in Eqs. 2.2 through 2.7, the discretized fully implicit version of Eq. 2.1 for incompressible systems (Eq. 2.5) can be expressed as [9]:

\[
g = T^{n+1}x^{n+1} - D^{n+1}(x^{n+1} - x^n) - Q^{n+1} = 0,
\]  

where \(g\) is the residual vector we seek to drive to zero, \(T\) is a block pentadiagonal matrix for two-dimensional grids and a block heptadiagonal matrix for three-dimensional grids, \(D\) is a block diagonal matrix, and \(Q\) represents the source/sink terms. The time level is designated by the superscript \(n\) or \(n + 1\). The \(T^{n+1}x^{n+1}\) term represents transport (flow) effects while the \(D^{n+1}(x^{n+1} - x^n)\) term represents accumulation. The matrices \(T, D\) and \(Q\) depend on \(x\) and must be updated at each iteration of every time step. See [9] for further details.

Eq. 2.9 represents a nonlinear set of algebraic equations and is solved by applying Newton’s method to drive \(g\) to zero:

\[
J\delta = -g,
\]  

where \(J\) is the Jacobian matrix given by \(J_{ij} = \partial g_i / \partial x_j\) and \(\delta_i = x_i^{n+1,v+1} - x_i^{n+1,v}\) with \(v\) and \(v + 1\) indicating iteration level.
2.1. MODELING PROCEDURE

2.1.2 Proper Orthogonal Decomposition

In order to generate a POD reduced-order basis, a simulation of the full flow model must first be performed and the states of the system saved. These states, represented by ‘snapshots,’ comprise solutions for \( p_o \) and \( S_w \) for all \( N_c \) grid blocks at particular times. We denote as \( X_p \) and \( X_S \) the matrices which represent the system states for \( p_o \) and \( S_w \) (from here on designated simply as \( p \) and \( S \)), respectively:

\[
X_p = [x_1^p, x_2^p, \cdots, x_S^p], \quad X_S = [x_1^S, x_2^S, \cdots, x_S^S].
\]

Each column of these matrices contains the solution of the system for a specific simulation time (these solutions are designed \( x_i^p \) and \( x_i^S \), where \( i \) indicates the snapshot number). The pressure states are normalized by computing \( x_i^p = (p_i - p_{\text{min}})/(p_{\text{max}} - p_{\text{min}}) \), where \( p_i \) is the simulated grid block pressure and \( p_{\text{max}} \) and \( p_{\text{min}} \) are the maximum and minimum pressures encountered during the high-fidelity flow simulation. A similar normalization is applied to the saturation states.

The basic POD procedure we employ is well established and is discussed in a variety of publications (e.g., \([61, 25]\)). The development in this section follows the work of van Doren et al. \([64]\). As in their approach, we apply the ROM procedure separately for the pressure and saturation states. This is appropriate because the two variables are governed by distinct physics (as can be readily demonstrated by manipulating Eq. 2.1 into pressure and saturation equations; see \([33, 9]\) for details). After the snapshots are obtained, the mean of the snapshots is computed (Eq. 2.11) and the data matrices \( \bar{X}_p \) and \( \bar{X}_S \) are determined by subtracting the mean from each snapshot (Eq. 2.12):

\[
\bar{x}_p = \frac{1}{S} \sum_{i=1}^{S} x_i^p, \quad \bar{x}_S = \frac{1}{S} \sum_{i=1}^{S} x_i^S, \quad (2.11)
\]

\[
\bar{X}_p = [x_1^p - \bar{x}_p, x_2^p - \bar{x}_p, \cdots, x_S^p - \bar{x}_p]_{N_c \times S},
\]

\[
\bar{X}_S = [x_1^S - \bar{x}_S, x_2^S - \bar{x}_S, \cdots, x_S^S - \bar{x}_S]_{N_c \times S}. \quad (2.12)
\]

The following procedure is performed for both \( \bar{X}_p \) and \( \bar{X}_S \). We describe it using \( \bar{X} \), where \( \bar{X} \) designates either \( \bar{X}_p \) or \( \bar{X}_S \). A covariance matrix \( C \) is determined by applying the method of snapshots \([61]\)

\[
C = \bar{X}^T \bar{X}, \quad (2.13)
\]
from which the following eigen-decomposition problem is solved:

\[ C \Psi = \lambda \Psi, \]  
(2.14)

where \( \Psi \) represents the eigenvectors and \( \lambda \) the eigenvalues of \( C \), respectively. We do not actually perform an eigen-decomposition of Eq. 2.14 but rather a singular value decomposition (SVD). Alternatively, we can perform SVD directly on \( \hat{X} \), which is an efficient way of obtaining the eigen-decomposition of the covariance matrix given by Eq. 2.13. The singular values \( (\sigma_i) \) of \( \hat{X} \) are related to eigenvalues \( (\lambda_i) \) of \( \hat{X}^T \hat{X} \) via \( \sigma_i = \lambda_i^{1/2} \).

The POD basis functions are then given by a linear combination of the snapshots [61]:

\[ \Phi = \hat{X} \Psi. \]  
(2.15)

In this context, the term “energy” is used to refer to the magnitude of the eigenvalue associated with each eigenvector. By arranging the eigenvalues in decreasing order, this energy can be used to selectively retain eigenvectors, meaning those eigenvectors possessing small amounts of energy can be removed. The energy in the first \( \ell \) eigenvectors is given by:

\[ E_\ell = \sum_{i=1}^\ell \lambda_i, \]  
(2.16)

where \( \lambda_i \) represents the energy of each eigenvector and \( E_\ell = \sum_{i=1}^S \lambda_i \). The number of basis functions retained for the pressure unknown, designated \( \ell_p \), is simply the number of eigenvalues necessary to provide a specified fraction of \( E_\ell \). The number of basis functions for the saturation unknown, \( \ell_s \), is determined analogously.

Following application of Eq. 2.16, the basis matrix \( \Phi \) will contain only \( \ell \) columns, where \( \ell = \ell_p + \ell_s \). We refer to this reduced \( \Phi \) matrix as \( \Phi_\ell \). Now, the reduced state vector, designated \( z \), can be related to the full oil pressure and water saturation states \( x \) as follows:

\[ x \simeq \Phi_\ell z + \bar{x}. \]  
(2.17)

As indicated above, for an oil-water system two basis matrices will be created, \( \Phi_{\ell_p} \) and \( \Phi_{\ell_s} \) for the oil pressure and water saturation states, respectively. Combining both matrices, Eq. 2.17 can be represented in matrix form as:
where $\mathbf{x}$ is of dimension $2N_c$, $\Phi_\ell$ is a $2N_c \times (\ell_p + \ell_s)$ matrix, $\mathbf{z}$ has dimension $\ell_p + \ell_s$, and $\bar{\mathbf{x}}$ is of dimension $2N_c$. The benefits of the method are achieved because $\ell_p + \ell_s \ll 2N_c$; i.e., the dimension of $\mathbf{z}$ is much less than that of $\mathbf{x}$.

An important aspect of the reduced-order modeling process is the generation of snapshots (see, e.g., Burkdardt [16]). The information embodied in the snapshots is used to compute the POD basis and therefore impacts strongly the ability of the reduced-order basis to represent the states of the system. The predictive capabilities of the model are important because our target application is production optimization. This means that we require the ROM to be predictive for a variety of different flow scenarios, and these scenarios are not known at the time the snapshots are generated.

We will not consider the issue of snapshot selection in detail in this work. Rather, we apply a simple heuristic approach for snapshot generation that appears to perform adequately for current purposes. We note, however, that detailed treatments exist for snapshot selection that could be investigated in future work. For example, Kunisch and Volkwein [43] developed the optimality system proper orthogonal decomposition (OS-POD) which addresses the problem of un-modeled dynamics, as occurs when the optimum solution is considerably different from the training simulation. Bui-Thanh et al. [15] presented an alternate procedure that employs a greedy algorithm for the selection of snapshots in high-dimensional space.
2.1.3 Reduced-Order Oil-Water Reservoir Model

Our intent is now to introduce the reduced state $z$ into the discretized flow equations. This will allow us to solve for only $\ell_p + \ell_s$ unknowns rather than $2N_c$ unknowns. By inserting Eq. 2.17 into the discrete model (Eq. 2.9) we obtain:

$$ g = T^{n+1}(\Phi_{\ell}z^{n+1} + \bar{x}) - D^{n+1}\Phi_{\ell}(z^{n+1} - z^n) - Q^{n+1}. \tag{2.19} $$

Premultiplying Eq. 2.19 by $\Phi_{\ell}^T$, the reduced form of the residual equation is given by:

$$ g_r = \Phi_{\ell}^Tg = \Phi_{\ell}^T\Phi_{\ell}z^{n+1} + \bar{x}) - \Phi_{\ell}^TD^{n+1}\Phi_{\ell}(z^{n+1} - z^n) - \Phi_{\ell}^TQ^{n+1}, \tag{2.20} $$

where the reduced residual $g_r$ has dimension $\ell = \ell_p + \ell_s$ rather than $2N_c$.

To apply Newton’s method to the reduced representation, we start with $J\delta = -g_r$, express $\delta \cong \Phi_{\ell}\delta_r$, where $(\delta_r)_i = z_i^{n+1,v+1} - z_i^{n+1,v}$, and premultiply both sides by $\Phi_{\ell}$. This gives:

$$ J_r\delta_r = -g_r, \tag{2.21} $$

where

$$ J_r = \Phi_{\ell}^TJ\Phi_{\ell}. \tag{2.22} $$

The reduced Jacobian $J_r$ has dimensions $\ell \times \ell$, in contrast to the $2N_c \times 2N_c$ dimensions of the original Jacobian. However, the heptadiagonal matrix structure of the original Jacobian (for three-dimensional systems) is lost, and $J_r$ is in general a full matrix.

Although the reduced system of equations is of much lower dimension than the full system, the procedure described above still requires the construction of the full-order Jacobian and residual at every iteration in order to form $J_r$ and $g_r$. Thus the speedup resulting from this procedure will be somewhat limited. An alternate approach that does not require the construction of the full $J$ and $g$ will be discussed in section 2.1.5.

2.1.4 Clustering Snapshots

The POD basis is optimal in the sense that it captures the most information on average from a set of snapshots [54]. Specifically, under some technical assumptions, given a snapshot set, for any number of basis functions POD minimizes the average of the square distance
between the centered snapshots \((x^i - \bar{x})\) and the projections \(\Phi_\ell z^i\):

\[
E_p = \frac{1}{S} \sum_{i=1}^{S} \| x^i - \bar{x} - \Phi_\ell z^i \|^2,
\]

where \(E_p\) is the quantity minimized.

In our application, the snapshots are simply the states computed at each time step (or every \(n^{th}\) time step, with \(n\) an integer) of the full-order model. This means that, depending on the time stepping strategy employed in the simulation of the full-order model, the snapshots may not be evenly distributed in state space. In other words, snapshots might be concentrated in relatively small fractions of state space, and this may bias the resulting \(\Phi_\ell\) by overweighting certain regions of state space. Thus, although \(E_p\) in Eq. 2.23 is still minimized, this minimization is based on a set of snapshots that is not as representative of the overall state space as it could be.

We address this issue by clustering the snapshots such that the cluster centroids are spaced approximately evenly in state space. By applying the POD procedure to the cluster centroids, we are then able to generate a slightly more accurate basis matrix. For this purpose we apply the k-means clustering procedure available in Matlab [47]. Our use of this clustering approach was motivated by the centroidal Voronoi tesselation (CVT) reduced-order modeling introduced by [16]. CVT reduced-order modeling also starts with a snapshot set, but instead of determining a POD basis from the snapshot set, a clustering technique is applied to determine the generators (cluster centroids) of a CVT of the snapshot set, and those generators are the reduced-order basis. Our approach also applies a clustering technique to the snapshot set, but instead of determining generators, the cluster centroids are used in the POD methodology.

Matlab’s [47] k-means procedure uses a two-stage iterative algorithm to minimize the sum of distances between snapshots and centroids summed over all \(C\) clusters. The initial cluster centroid positions are chosen by randomly selecting \(C\) snapshots from the original \(S\) snapshots. Each iteration of the first stage consists of simultaneously reassigning snapshots to their nearest cluster centroids, followed by recalculation of cluster centroids. In the second stage, snapshots are reassigned only if this reduces the sum of distances, after which cluster centroids are recomputed. The overall algorithm converges to a local minimum. By running it several times with random starting points, the optimization space is sampled more globally. The clustering is performed separately for the pressure and saturation snapshots.
Applying this procedure, $S$ snapshots are reduced to $C$ centroids. Then the POD procedure is applied to the $C$ centroids. In our implementation, in order to achieve a high degree of computational efficiency for this clustering, we have the option of performing most of the clustering computations in a reduced space. The resulting algorithm is very efficient so the clustering introduces negligible overhead. We note that this clustering procedure will also be useful if we have a very large number of snapshots, in which case performing the SVD of the full data matrix will be time consuming. This is not a significant issue here, however, as the number of snapshots is not excessive.

### 2.1.5 Missing Point Estimation

The key attribute of the basis matrix $\Phi_\ell$ is its ability to approximate the $2N_c$ states in the spatial domain using relatively few basis functions. However, the reduced-order modeling procedure still requires substantial computation because the reduced-order model is constructed from the full model [49, 11]. Specifically, as in a standard simulation, at each iteration of each time step we must first construct the full Jacobian matrix, after which the reduced Jacobian can be formed using Eq. 2.22. Both the initial construction of the full Jacobian and the formation of the reduced Jacobian via two matrix multiplications ($J_r = \Phi_\ell^T J \Phi_\ell$) are time consuming. We note that iterative linear solution techniques could be applied to solve Eq. 2.21 (here we use a direct method), in which case $J_r$ would not need to be constructed explicitly. We did not investigate iterative techniques here, though we note that the missing point estimation procedure described below should also improve their performance.

The missing point estimation (MPE) procedure was introduced by Astrid et al. [4, 8, 7]. This method represents the basis functions in terms of column vectors not of length $N_c$ (as in Eq. 2.18) but rather of length $N_m$, with $N_m < N_c$. This acts to reduce the size of $\Phi_\ell$ and can therefore lead to computational speedup. Astrid et al. applied MPE to a model of a glass melt feeder where the temperature distribution had to be controlled very precisely. In the following, we describe the use of MPE for our application.

The basis matrix $\Phi_\ell$ is an orthonormal basis, meaning that its columns are normal and mutually orthogonal. This means that the magnitude of each column is 1 and the condition number of $\Phi_\ell^T \Phi_\ell$ is also near 1 (i.e., $1 + \epsilon$, where $\epsilon \sim O(10^{-10})$). The condition number is computed as:

$$K(\Phi_\ell^T \Phi_\ell) = \frac{\lambda_{\max}(\Phi_\ell^T \Phi_\ell)}{\lambda_{\min}(\Phi_\ell^T \Phi_\ell)}.$$  (2.24)
2.1. MODELING PROCEDURE

where \( \lambda_{\text{max}}(\Phi_{\ell}^T \Phi_{\ell}) \) and \( \lambda_{\text{min}}(\Phi_{\ell}^T \Phi_{\ell}) \) are the maximum and minimum eigenvalues of \( \Phi_{\ell}^T \Phi_{\ell} \) respectively.

The idea behind the missing point estimation is to remove a number of rows of the \( \Phi_{\ell} \) basis matrix while allowing the condition number to increase only to a specified value. The new basis matrix will be designated \( \Phi_{\ell}^* \in \mathbb{R}^{N_m \times \ell} \), where \( N_m \) represents the number of grid blocks retained. Astrid [5] presented two different methods for grid block selection. The first method classifies the grid blocks by considering one block at a time and then computing \( e = \| \Gamma_{\ell}^T \Gamma_{\ell} - I \| \), where \( \Gamma_{\ell} \) represents the row of \( \Phi_{\ell} \) corresponding to the target block and \( I \) is the identity matrix. The blocks are then ordered and those corresponding to the smallest values of \( e \) are retained, with the condition number for the resulting \( \Phi_{\ell}^* \) computed using Eq. 2.24. This procedure is continued until a target condition number is reached.

As reported by Astrid [5], this method requires that a relatively large number of grid blocks be retained. To overcome this limitation Astrid implemented a greedy algorithm. This procedure applies the algorithm described above to select the first block. Then, all remaining \( (N_c - 1) \) blocks are considered one at a time and the block that gives the minimum condition number for the two-block system is retained. The procedure is repeated until the target condition number is reached. We found this method to perform reasonably well for small models but it is much too time consuming for application to large problems (e.g., for the 60,000 grid block example considered in section 2.2).

We achieved the greatest reduction in the number of rows of \( \Phi_{\ell} \) using a sequential QR decomposition (SQRD) approach. This approach was suggested by Y. Efendiev (private communication), who applied it for conditioning permeability fields generated using Karhunen-Loève expansions. This was done within the context of history matching reservoir models to production data using Markov chain Monte Carlo methods [31].

We implemented SQRD in Matlab and applied it to classify the grid blocks from the most important to the least important. For the pressure state, given \( \Phi_{\ell_p}^T \in \mathbb{R}^{\ell_p \times N_c} \), QR decomposition finds the \( \ell_p \) orthogonal vectors that correspond to the \( \ell_p \) greatest independent vectors of \( \Phi_{\ell_p}^T \) (a set of \( N_c \) vectors in \( \mathbb{R}^{\ell_p} \) is linearly dependent if \( N_c > \ell_p \)). This set of \( \ell_p \) vectors is then removed from \( \Phi_{\ell_p}^T \) and the process is repeated until all grid blocks are classified. The same procedure is applied for the saturation state.

We then apply the condition number criterion to construct a new basis matrix. The number of grid blocks to be added in each step is specified \( (N_b) \). Then, following the classification order, \( N_b \) grid blocks are selected for the pressure state \( (N_{b_p}) \) and \( N_b \) grid
blocks are selected for the saturation state \( N_{bs} \). The number of grid blocks added in each step \( k \) \( (N^k_b) \) is given by the union of \( N_{bp} \) and \( N_{bs} \), \( N^k_b = N_{bp} \cup N_{bs} \). Grid blocks (rows of \( \Phi^\ell \)) are added in this way until the target condition number for \( (\Phi^\ell)^T \Phi^\ell \) (which includes both pressure and saturation information) computed by Eq. 2.24 is reached. For the cases studied here the condition number that produced an appropriate balance between speedup and error was generally between 5 and 10.

### 2.1.6 Implementation in General Purpose Research Simulator

Stanford’s general purpose research simulator (GPRS), originally formulated by Cao [17] and recently enhanced and extended by Jiang [40, 41], has evolved into a modeling package containing many advanced capabilities and features. These include linkages to adjoint-based optimal control procedures [59, 60], advanced linear solvers [41, 18], and models for ‘smart wells,’ e.g., multibranched wells containing downhole sensors and inflow control devices [41]. All of the simulations presented in the following sections were performed using a new version of GPRS which is able to handle the basic POD procedure described above. The simulator also contains a partial implementation of MPE. We now briefly describe these implementations.

The ROM described previously can be separated into off-line (pre-processing) and in-line portions. The off-line portion, executed just once, contains all of the computations needed to construct the POD basis matrix. Figure 2.2 shows the flow chart for the off-line portion. This entails first running a training simulation and recording snapshot sets for pressure and saturation. Then, following the procedure given in section 2.1.4, the snapshots can be clustered, the basis functions generated (section 2.1.2) and the grid blocks selected by the MPE procedure (section 2.1.5).

The in-line portion of the ROM, integrated with the reservoir simulator, is depicted in Figure 2.3. This ROM can be applied for a variety of different simulation scenarios. The basis functions and selected grid blocks (if MPE is used), as determined from the off-line procedure, are inputs. Then, within the Newton loop, the standard Jacobian matrix and residual vector are generated, after which the reduced Jacobian and residual are formed using \( \Phi^\ell \) or \( \Phi^* \) if MPE is being used. Newton’s method is then applied to the reduced system of equations, after which the full state vector \( (x) \) is reconstructed using \( \Phi^\ell \) (note that \( \Phi^\ell \) rather than \( \Phi^* \) is used in this step even if MPE is applied). The model initialization and time stepping are exactly as in the standard simulator.
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Our current implementation of the missing point estimation in GPRS is restricted to code at the level of the linear solver. By this we mean that we use MPE to speed up the matrix multiplications ($\Phi^T \Phi$) and in the solution of the reduced-order system, but not elsewhere in the code. This is clearly suboptimal, as the full implementation of MPE would allow us to construct residual equations and Jacobian entries for only $N_m$ (rather than $N_c$) grid blocks. This full implementation would, however, require code modifications throughout GPRS, while the solver-level implementation leads to much more limited modifications. The reduced-order models generate small but full matrices. We therefore apply direct solution techniques for these linear systems.

In the following section, we will compare the performance and timing of the ROM to full GPRS simulations, so some discussion of the linear solvers applied in GPRS is appropriate. The linear system of equations arising in the full simulation model is very sparse. For this solution, GPRS employs the iterative generalized minimum residual (GMRES) solver along with various preconditioners. The constrained pressure residual (CPR) preconditioner [69, 18, 41, 42] is the most advanced option. This preconditioner is specially

![Figure 2.2: Flow chart for the off-line portion of the ROM](image)
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Figure 2.3: Flow chart for the in-line portion of the ROM
designed for the reservoir simulation equations (it takes full advantage of the elliptic character of the underlying pressure equation) and is therefore highly efficient. This high efficiency is due to a multistage procedure that uses in the first stage an algebraic multigrid (AMG) preconditioner to solve the pressure system and a local preconditioner in the second stage to solve the entire system. Most of our comparisons will be against full simulation models that use CPR, so we are comparing against what we believe to be (essentially) the best current procedure. More generic preconditioners, such as ILU(0), are also available within GPRS and will be considered.

2.2 Simulation Using Reduced-Order Modeling

We now illustrate the application of the POD-based procedure to a realistic reservoir simulation model. We will consider each component in turn (construction of the reduced basis, clustering, MPE) and then demonstrate the ability of the reduced model to provide accurate predictions for cases that differ from the initial training simulation. Simulation times and errors due to the various ROM procedures are quantified at the end of this section.

The simulation model, shown in Figure 2.4, is a portion of a very large geological model developed by Castro [23]. This model represents a fluvial channel system. Realistic permeability and porosity values were assigned to channel sands and to background ‘mud’ regions. The model is three-dimensional and contains a total of 60,000 grid blocks (with
\( n_x = 75, \ n_y = 100 \) and \( n_z = 8 \), where \( n_x, n_y \) and \( n_z \) designate the number of grid blocks in the corresponding coordinate direction). Five production wells and four water injection wells drive the flow.

Figure 2.5 shows the permeability in the \( x \)-direction for all 8 layers. A number of channelized geological features are clearly evident. The mean permeability and porosity are 2,600 mD and 0.26 respectively for the channels and 20 mD and 0.08 outside the channels. The production wells are completed in layers 1, 2 and 3 and the injector wells in layers 7 and 8.

Figure 2.5: Permeability in \( x \)-direction for all 8 layers

The initial saturations of oil and water are 0.85 and 0.15 respectively and the residual oil saturation is 0.30. The oil viscosity at standard conditions is 1.16 cp and the water viscosity is 0.325 cp. Capillary pressure is neglected and the fluid densities are set to be equal. The relative permeabilities for the oil and water phases are shown in Figure 2.6.

To extract the information needed to reproduce the behavior of the system, a full run (referred to as the training simulation) was performed. As indicated earlier, the conditions
2.2. SIMULATION USING REDUCED-ORDER MODELING

Figure 2.6: Relative permeability curves for the oil and water phases

applied for this training simulation impact the quality of the reduced basis, so they should be selected with care. Here we apply a heuristic procedure in which we vary the bottom hole pressures (BHPs) of the production wells randomly and independently over their expected ranges (between 3,500 and 4,500 psia). These BHPs are changed every 100 days and the resulting schedule is shown in Figure 2.7. The injection well BHPs are constant in time for each well, though the actual values vary from well to well (the BHPs for injectors 1 and 2 are 6500 psia, for injector 3 BHP is 7000 psia and for injector 4 BHP is 6000 psia). The maximum timestep allowed was 20 days and a total of 211 snapshots for the oil pressure and water saturation states were recorded.

Figure 2.7: Schedule for bottom hole pressures for the production wells
Applying the proper orthogonal decomposition approach provides the eigenvalue spectra for pressure and saturation shown in Figure 2.8. It is evident that the maximum eigenvalue for the pressure state is almost $10^3$ while the minimum approaches $10^{-16}$, which means that the pressure eigenvalues vary over around 19 orders of magnitude. For the water saturation state this variation is also substantial, about 18 orders of magnitude.

![Figure 2.8: Eigenvalue variation for pressure and saturation matrices](image)

We seek to form a basis such that the fraction of energy in the pressure state that we ignore is very low, around $10^{-6}$, and the fraction ignored in the saturation state is around $10^{-4}$. This requires that we retain the first 14 eigenvalues for the oil pressure state and the first 26 eigenvalues for the water saturation state. Therefore, the basis matrix $\Phi_\ell \in \mathbb{R}^{2N_c \times \ell}$, where $\ell = \ell_p + \ell_s$, has $14 + 26 = 40$ basis vectors. This means that, while the standard reservoir simulation model needs to solve Eq. 2.10 for $2N_c = 120,000$ unknowns, the reduced-order reservoir simulation model needs to solve Eq. 2.21 for only 40 unknowns.

We present the first six pressure and saturation basis functions for the first layer in Figures 2.9 and 2.10. The fraction of energy contained in each basis function is also indicated. These basis functions clearly reflect the locations of the wells and the pressure and saturation gradients, though it is otherwise difficult to attribute direct physical interpretation to their detailed shapes.

Implementing the clustering technique presented in section 2.1.4, the number of snapshots for each state is reduced from 211 to 50. Ignoring the same amounts of energy as before, the number of basis functions required for the oil pressure state decreases from 14 to 12, while for the water saturation state it decreases from 26 to 22. Thus the reduced-order reservoir simulation model now requires only 34 unknowns.
Applying the missing point estimation technique to the clustered snapshots and using the grid block selection procedure described in section 2.1.5, the grid blocks are ordered from the most important to the least important in terms of their impact on the condition number. Allowing the condition number to increase to 5, the number of grid blocks selected is $N_m = 19,441$. Figure 2.11 shows that the selected grid blocks (shown in black) are related to the wells and the high permeability channels, as indicated for layer 1, where the red circles indicate the location of the producer wells, the blue arrows the injector wells and the green contours regions of high permeability. The basis matrix, now of dimension $N_m \times 34$, can be applied to efficiently compute the reduced Jacobian appearing in Eq. 2.22. As indicated in section 2.1.6, the MPE procedure was implemented into GPRS only at the solver level. Thus the full benefits of this treatment will not be realized in the simulation.
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Figure 2.10: Six most important reduced-order basis functions for the water saturation state (layer 1)

(a) Energy: $8.79 \times 10^{-1}$  
(b) Energy: $9.03 \times 10^{-2}$  
(c) Energy: $1.70 \times 10^{-2}$  
(d) Energy: $4.52 \times 10^{-3}$  
(e) Energy: $2.87 \times 10^{-3}$  
(f) Energy: $1.84 \times 10^{-3}$

results presented below.

The ability of the reduced-order model to reproduce the training simulation will be tested using the three basis function matrices obtained above. The first matrix was generated using only proper orthogonal decomposition, $\Phi \in \mathbb{R}^{120,000 \times 40}$; the second matrix was generated using clustered snapshots and proper orthogonal decomposition, $\Phi \in \mathbb{R}^{120,000 \times 34}$; and the third was formed using clustered snapshots, proper orthogonal decomposition and missing point estimation, $\Phi^* \in \mathbb{R}^{38,882 \times 34}$.

Figures 2.12 through 2.16 display the oil and water flow rates for all production wells and Figures 2.17 through 2.20 show the injection rates for all injector wells using the three procedures. The total quantity of injected fluid is equal to 0.67 of the total pore volume of the system. However, because of the residual (nonflowing) oil and water fractions, this
corresponds to 1.22 mobile pore volumes of fluid. The reference oil and water flow rates from the training simulation (solid red line for oil and blue for water, labeled as GPRS/CPR in the figures) are very well reproduced using POD only (red circles for oil and blue for water), clustered snapshots + POD (solid red circles for oil and blue for water), and clustered snapshots + POD + MPE (light green dots for oil and light blue for water, labeled as Clusters/QR in the figures). The reference water injection rate from the training simulation (green line) are also well reproduced using POD (green circles), clustered snapshots + POD (solid green circles) and clustered snapshots + POD + MPE (light green dots). These results are very encouraging and indicate that the snapshot set and the basis contain sufficient information to reproduce the training simulation. We can also observe that the clustering approach enables a reduction in the size of the basis matrix without losing significant accuracy in the simulation results. We note that the use of POD only (without clustered snapshots) with 34 unknowns (the number used for the clustered snapshots + POD case) provided less accurate simulation results than those obtained using clustered snapshots + POD. This demonstrates the benefit of the clustering procedure. Finally, using fewer than
1/3 of the grid blocks, the MPE technique provides results that continue to agree with the training simulation. Errors for this and subsequent runs will be quantified in section 2.2.5.

Figure 2.12: Oil and water flow rates for production well 1 (training run)

Figure 2.13: Oil and water flow rates for production well 2 (training run)

We next consider two different flow scenarios to evaluate the predictive capability of the three ROMs.
Figure 2.14: Oil and water flow rates for production well 3 (training run)

Figure 2.15: Oil and water flow rates for production well 4 (training run)

Figure 2.16: Oil and water flow rates for production well 5 (training run)
Figure 2.17: Water flow rate for injection well 1 (training run)

Figure 2.18: Water flow rate for injection well 2 (training run)

Figure 2.19: Water flow rate for injection well 3 (training run)
2.2. SIMULATION USING REDUCED-ORDER MODELING

2.2.1 Prediction Using ROM - Schedule I

The schedule for the bottom hole pressures of the production wells is shown in Figure 2.21. The overall range (between 3,650 and 4,350 psia) is smaller than the range used in the training simulation. In this example the BHPs are changed every 200 days, while in the training simulation they were changed every 100 days. The injection well BHPs are the same as in the training simulation. The maximum timestep for this case was increased to 50 days.

Figures 2.22 through 2.26 show the oil and water flow rates for production wells using the three basis matrices. The flow rates from the high-fidelity (reference) solution (red line for oil and blue for water) are, in general, well reproduced using the three ROMs. Relatively small mismatches can be observed, however, in some of the results. The results for water injection rates for the injection wells, shown in Figures 2.27 through 2.30, demonstrate close agreement with the reference simulation, although some slight mismatches can be observed.
CHAPTER 2. ROM OF SUBSURFACE FLOW USING POD

Figure 2.21: Bottom hole pressure for the production wells using schedule I

Figure 2.22: Oil and water flow rates for production well 1 (schedule I)

Figure 2.23: Oil and water flow rates for production well 2 (schedule I)
2.2. SIMULATION USING REDUCED-ORDER MODELING

Figure 2.24: Oil and water flow rates for production well 3 (schedule I)

Figure 2.25: Oil and water flow rates for production well 4 (schedule I)

Figure 2.26: Oil and water flow rates for production well 5 (schedule I)
CHAPTER 2. ROM OF SUBSURFACE FLOW USING POD

Figure 2.27: Water flow rate for injection well 1 (schedule I)

Figure 2.28: Water flow rate for injection well 2 (schedule I)

Figure 2.29: Water flow rate for injection well 3 (schedule I)
2.2. SIMULATION USING REDUCED-ORDER MODELING

Figure 2.30: Water flow rate for injection well 4 (schedule I)

2.2.2 Prediction Using ROM - Schedule II

The schedule for the production well BHPs is shown in Figure 2.31. These BHPs are changed every 200 days, and the overall range, between 3,350 and 4,650 psia, is larger than the range used in the training simulation. The specifications for the injection wells are the same as in the previous cases.

Figures 2.32 through 2.36 show the oil and water flow rates for schedule II for the production wells using the three basis matrices. The flow rates from the high-fidelity solution are again reasonably well reproduced using the three ROMs, though some errors are evident. The results for water injection rates, shown in Figures 2.37 through 2.40, also demonstrate generally close agreement with the reference simulation. Taken in total, these results are encouraging as they demonstrate the ability of the ROM to provide flow results for scenarios that differ substantially from the training simulations. This is important if the ROM is to be used within the context of optimization.
CHAPTER 2. ROM OF SUBSURFACE FLOW USING POD

Figure 2.31: Bottom hole pressure for the producer wells using schedule II

Figure 2.32: Oil and water flow rates for production well 1 (schedule II)

Figure 2.33: Oil and water flow rates for production well 2 (schedule II)
2.2. SIMULATION USING REDUCED-ORDER MODELING

Figure 2.34: Oil and water flow rates for production well 3 (schedule II)

Figure 2.35: Oil and water flow rates for production well 4 (schedule II)

Figure 2.36: Oil and water flow rates for production well 5 (schedule II)
Figure 2.37: Water flow rate for injection well 1 (schedule II)

Figure 2.38: Water flow rate for injection well 2 (schedule II)

Figure 2.39: Water flow rate for injection well 3 (schedule II)
2.2. SIMULATION USING REDUCED-ORDER MODELING

2.2.3 Simulation Time Reduction with ROMs

The simulation times for the high-fidelity models and the three ROMs for the base case and schedules I and II are summarized in Figure 2.41. In the figure, the first set of bars refers to the base case, the second set to schedule I and the third set to schedule II. For each set the first bar represents the simulation time for the high-fidelity simulation using the fastest current solution procedure (GMRES solver with CPR preconditioner). The second, third and fourth bars in each set show the simulation times for the three reduced-order models (POD, clusters + POD, and clusters + POD + MPE, respectively). Additionally, for each bar the gray segment represents the time spent solving the linear system of equations and the black segment the time spent in all other computations (computing block properties, forming the residual vector and Jacobian matrix, etc.).

For the base case the first set of bars shows that the ROM with POD was able to reduce the simulation time by a factor of $\sim 2.9$. Applying the ROM with clusters + POD the simulation time was reduced by a factor of $\sim 3.3$. Further reduction, namely a factor of $\sim 5.9$, was obtained when the ROM with clusters + POD + MPE was employed. The speedups achieved using the various ROMs, though significant, are not dramatic. This is because our ROM procedures target only the solver. Thus, even if the ROM reduces the solver time to zero, we are still left with the remaining simulation computations. We note, however, that a full MPE implementation (which was not introduced here) would provide additional speedup. This is because, in contrast to the other reduced-order modeling
procedures, a full MPE implementation would also reduce the time required for residual and Jacobian construction.

The computation times for the schedule I and schedule II simulations are indicated (respectively) by the second and third sets of bars. For schedule I, the speedups resulting from the ROMs are greater than those observed for the base case (e.g., about a factor of 9.5 for clusters + POD + MPE). This is due in part to the ability of the ROMs to take larger timesteps than the high-fidelity model. Similar results were obtained using schedule II. As indicated by the third set of bars, the speedup for the clusters + POD + MPE reduced-order model was 9.8.

![Figure 2.41: Comparison of simulation time](image)

2.2.4 Comparison of ROMs with ILU(0) Preconditioner

As explained in section 2.1.6, the full-order simulations are performed using GPRS with the GMRES solver and the CPR preconditioner. This is a highly developed preconditioner that provides essentially the best available linear solution methodology for many reservoir simulation applications. Its inherent speed therefore limits the degree of speedup achievable using our algorithms.

It may also be appropriate, therefore, for us to evaluate speedups relative to a more generic solver. This is because, for many applications, a highly specialized solver plus preconditioner combination will not be available. For example, our current gradient-based production optimization algorithm, which requires the solution of an adjoint equation in conjunction with the simulation model, is not yet compatible with GMRES + CPR but
2.2. SIMULATION USING REDUCED-ORDER MODELING

instead uses ILU(0) as a preconditioner [59, 60]. Thus we now assess the speedup achieved by the ROM procedures relative to GMRES + ILU(0).

We consider the schedule I predictive scenario. The timings for GPRS using the ILU(0) and CPR preconditioners relative to the ROM (clusters + POD + MPE) are shown in Figure 2.42. Note that the time axis is logarithmic and the simulation time using preconditioner ILU(0) was normalized to 1. For this case, the preconditioner CPR provides a speedup of about 73 and the ROM (clusters + POD + MPE) a quite dramatic speedup of about a factor of 700 relative to GPRS with ILU(0). This is because, for the full (high-fidelity) simulation using GPRS with ILU(0), the solver requires almost all of the computation time, so our ROM procedure has substantial impact.

Figure 2.42: Comparison of simulation time for schedule I using full model with ILU(0) and CPR preconditioners and ROM

2.2.5 Quantification of Error Using ROMs

Errors arise from the ROM simulations for two main reasons. These are (1) we discard a large number of basis vectors which, although less important than the basis vectors retained, do carry some information, and (2) the ROM is in general applied to models that differ from the training simulation used to generate the reduced basis. It is therefore appropriate to quantify the ROM error for the various cases.

This error quantification could be accomplished in a variety of manners. Here we apply a simple procedure and focus on average error in oil and water (injected and produced) rates. For each production well m, at every simulated time step i, the oil production rate in the reference simulation \( Q_{o,full}^{m,i} \) and in each ROM simulation \( Q_{o,ROM}^{m,i} \) is computed.
Results from the ROMs are interpolated to provide rates at the times computed in the reference simulation (with care being taken to avoid interpolating across discontinuities in well BHP). The time-average error for each well, designated $E^m$, is then calculated as the average of the absolute differences, normalized by the time-average oil flow rate $Q_{o,\text{full}}^m$ for the well:

$$E^m = \frac{1}{n_t Q_{o,\text{full}}^m} \sum_{i=1}^{n_t} |Q_{o,\text{full}}^{m,i} - Q_{o,\text{ROM}}^{m,i}|,$$

(2.25)

where $n_t$ is the total number of time steps. The overall averaged error, designated $E$, is then given by:

$$E = \frac{1}{n_w} \sum_{m=1}^{n_w} E^m,$$

(2.26)

where $n_w$ is the number of production wells. The same procedure is applied for the water production and water injection rates.

Values for $E$ computed via Eq. 2.26 for the training simulation and the two schedules are presented in Tables 2.1, 2.2 and 2.3 for oil production, water production and water injection rates, respectively.

Table 2.1: Errors in the oil rate for the various ROMs

<table>
<thead>
<tr>
<th>ROM</th>
<th>Training</th>
<th>Schedule I</th>
<th>Schedule II</th>
</tr>
</thead>
<tbody>
<tr>
<td>POD</td>
<td>0.0164</td>
<td>0.0539</td>
<td>0.0453</td>
</tr>
<tr>
<td>Clusters + POD</td>
<td>0.0294</td>
<td>0.0492</td>
<td>0.0526</td>
</tr>
<tr>
<td>Clusters + POD + MPE</td>
<td>0.0424</td>
<td>0.0849</td>
<td>0.0761</td>
</tr>
</tbody>
</table>

Table 2.2: Errors in the water production rate for the various ROMs

<table>
<thead>
<tr>
<th>ROM</th>
<th>Training</th>
<th>Schedule I</th>
<th>Schedule II</th>
</tr>
</thead>
<tbody>
<tr>
<td>POD</td>
<td>0.0202</td>
<td>0.0911</td>
<td>0.0636</td>
</tr>
<tr>
<td>Clusters + POD</td>
<td>0.0406</td>
<td>0.0761</td>
<td>0.0707</td>
</tr>
<tr>
<td>Clusters + POD + MPE</td>
<td>0.0509</td>
<td>0.0734</td>
<td>0.0718</td>
</tr>
</tbody>
</table>

It is evident from the tables that the training simulation case results in the smallest errors for all of the ROMs for oil rate and water production rate; for water injection rate the training
and schedule I errors are the same for the clusters + POD + MPE model. Specifically, the errors for all models for the training case are less than 5.1% in all three tables. It is not surprising that reproduction of the training runs is generally the most accurate as the basis vectors were generated using snapshots from this case. For schedules I and II, errors in oil production rate vary from about 4.5% to 8.5% for the different models; for water production rate errors vary from about 6.4% to 9.1%, and for for water injection rate the errors vary from about 1.0% to 1.9%. Thus, for all simulations the errors in these injection and production rates are reasonable, less than 10% (when quantified in this way). We note that there is a tradeoff between speedup and accuracy, as further speedup could be achieved by decreasing the dimension of $\Phi$, though this will generally result in increased error. This effect will be quantified in the next section.

Another error that arises in reservoir simulation is mass balance error. The finite volume formulation is constructed to conserve mass, but mass balance errors can still appear as a result of nonzero tolerances in the linear and nonlinear (Newton) solution loops. Reservoir simulators typically compute global relative mass balance errors for each component (with the mass balance error normalized relative to the total mass originally in place). For the high-fidelity models, these mass balance errors are typically about $10^{-7}$. For the ROMs they are somewhat larger, up to $10^{-2}$, for example, when MPE is applied. The ROMs also do not guarantee that water saturation always remains between the physical limits of $S_{wc}$ (connate water saturation) and $1 - S_{or}$ (where $S_{or}$ is residual oil saturation). However, when saturation values outside of the physical range did occur, the violations were quite small (maximum of 0.001) and no special treatment was required.
2.3 Further Observations

In this section we consider the behavior of the reduced-order modeling procedure when (1) fewer basis vectors are used and (2) when the flow problem is more nonlinear or includes additional physics. These results are of interest because they indicate some of the limitations of the current ROM implementation and therefore suggest directions for future investigations.

We first assess the impact of retaining less energy (and thus fewer basis functions) in the pressure and saturation bases. As the number of basis functions is reduced, we expect to achieve a higher degree of speedup but also a loss of accuracy. Three different reduced-order bases are considered, each of which neglects different fractions of the energy. All three of these ROMs were generated using only POD (i.e., no clustering or MPE procedures were applied). For these runs the ROMs are applied to reproduce the base case (this is the same base case as was used in the examples in section 2.2).

The first ROM is the same as that used in section 2.2. As indicated in section 2.2, this basis ignores $10^{-6}$ of the energy in the pressure state and $10^{-4}$ of the energy in the saturation state. Thus 14 basis functions are used for pressure and 26 for saturation. The simulation time for this case is normalized to 1. The second ROM ignores a slightly larger fraction of the total energy: $5 \times 10^{-6}$ for the pressure state and $2.5 \times 10^{-4}$ for the saturation state. This ROM contains 11 basis functions for pressure and 20 for saturation. The simulation using this basis requires 0.74 as much time as the first ROM. The third ROM neglects a still larger fraction of the total energy: $5 \times 10^{-5}$ for pressure and $6 \times 10^{-4}$ for saturation. Only 8 basis functions are now used for pressure and 14 for saturation. The normalized simulation time for this ROM is 0.69.

The results for errors in oil production rate, water production rate and water injection rate using the three ROMs are summarized in Figure 2.43. Errors are computed using Eq. 2.26. It is evident that error increases as $\ell_p$ and $\ell_s$ decrease. This increase is relatively slight when $\ell = \ell_p + \ell_s$ decreases from 40 to 31, but the increase in error is large when $\ell$ is further decreased to 22. The results using the first and second ROMs are quite acceptable (errors for all quantities less than 0.1), though for the third ROM the errors increase appreciably (e.g., 0.60 for oil rate). This demonstrates that, even though a large fraction of energy (>0.999) may be captured by the basis, simulation accuracy can still be very sensitive to the number of basis functions used in $\Phi$. In our current implementation, the
appropriate $\ell_p$ and $\ell_s$ must be determined through numerical experimentation, as we do not yet have an accurate means for the a priori determination of the size of $\Phi$.

![Figure 2.43: Tradeoff between speedup and accuracy for the training simulation](image)

We next consider the impact of increased nonlinearity on the performance of the ROM. For the models considered, the key source of nonlinearity is the oil and water relative permeability curves. This nonlinearity can be adjusted through the so-called Corey exponents $a$ and $b$ in the relative permeability functions:

\begin{equation}
    k_{ro} = k_{ro}^0 \left( \frac{1 - S_w - S_{or}}{1 - S_{wc} - S_{or}} \right)^a, \tag{2.27}
\end{equation}

\begin{equation}
    k_{rw} = k_{rw}^0 \left( \frac{S_w - S_{wc}}{1 - S_{wc} - S_{or}} \right)^b. \tag{2.28}
\end{equation}

The original relative permeability curves, shown in Figure 2.6, were determined experimentally and were specified in tabular form. Expressed in the form of Eqs. 2.27 and 2.28, these curves correspond approximately to $a = 1.7$ and $b = 1.5$. We now consider curves with $a = 3$ and $b = 3$. These curves are plotted with the original curves in Figure 2.44. The other parameters used for the new curves are, with reference to Eqs. 2.27 and 2.28, $k_{ro}^0 = 1.0$, $k_{rw}^0 = 0.5$, $S_{wc} = 0.15$ and $S_{or} = 0.3$.

The training simulation with well BHPs described in section 2.2 was run using these more nonlinear relative permeability curves. The number of POD basis functions needed to reproduce the high-fidelity results with errors comparable to those presented in section 2.2.5 was then determined through numerical experimentation. The number of basis functions
required was 29 for pressure (as compared to 14 for the previous case) and 84 for saturation (as compared to 26 for the previous case). This basis neglects about the same amount of energy for the pressure state as the previous case, but for the saturation state it neglects only $10^{-5}$ of the total energy, as compared to $10^{-4}$ for the previous case. Due to the use of larger $\ell_p$ and $\ell_s$, the speedup using the ROM with the more nonlinear relative permeability curves is less than that achieved with the previous case. Specifically, in this case we achieve a very modest speedup of $\sim 1.3$, as compared to a speedup of $\sim 2.9$ using the original curves (though we note that more substantial speedups could be obtained through use of the clustering and MPE procedures). This demonstrates the impact of high degrees of nonlinearity on the ROM and the need for better treatments for such cases.

Another significant issue is the impact of gravitational effects on the performance of the ROM. The governing equations for a two-phase incompressible system can be written in terms of a pressure (flow) equation and a saturation (transport) equation:

\[
\nabla \cdot \mathbf{u}_t = -\tilde{q}_t, \tag{2.29}
\]

\[
\phi \frac{\partial S_w}{\partial t} + \nabla \cdot \mathbf{F} = -\tilde{q}_w, \tag{2.30}
\]

where $\mathbf{u}_t$ is the total Darcy velocity given by $\mathbf{u}_t = -\mathbf{k} \cdot [\lambda_t \nabla p + g (\lambda_w \rho_w + \lambda_o \rho_o) \mathbf{i}_z]$, with $\lambda_t = \lambda_w + \lambda_o$, $\mathbf{F} = f_w [\mathbf{u}_t - \mathbf{k} \cdot \mathbf{i}_z \lambda_o g (\rho_w - \rho_o)]$, where $f_w = \lambda_w / \lambda_t$ is the Buckley-Leverett fractional flow function, $\mathbf{i}_z$ is the unit vector in the $z$ direction, $\tilde{q}_t = \tilde{q}_o + \tilde{q}_w$, and all other quantities are as defined previously. Gravitational effects in the saturation equation can
be quantified through the density difference ($\Delta \rho$) between the oil and water phases (we note that a more complete quantification of this effect would be in terms of a dimensionless gravity number, though for current purposes the use of $\Delta \rho$ will suffice). The impact of gravitational effects on reduced-order models is here assessed by applying proper orthogonal decomposition to high-fidelity snapshots generated with varying $\Delta \rho$.

Results are displayed in Figure 2.45, where we present the variation in eigenvalues for the pressure and saturation states for models with $\Delta \rho = 0, 1, 5$ and $20$ lb/ft$^3$. For all of these runs the simulation time was 1,000 days and 170 snapshots were generated. It is apparent from the figure that the decay in the magnitudes of the eigenvalues is slower, for both pressure and saturation, with increasing $\Delta \rho$. In general, the slower the decay in the eigenvalues, the larger the number of basis functions that must be retained in the ROM. Thus we expect to observe decreasing computational efficiency using ROMs as $\Delta \rho$ is increased. Numerical experiments confirm this expectation.

![Figure 2.45: Eigenvalue variation for pressure and saturation for models with density differences](image)

In order to further assess the impact of gravitational effects, we consider a simpler model. Here we specify linear relative permeability curves ($k_{rw} = S_w$ and $k_{ro} = 1 - S_w$) and equal viscosities ($\mu_o = \mu_w = 1$ cp). For this case, when $\Delta \rho = 0$, the model is linear and pressure does not change in time (for the incompressible case). The reservoir model used here contains 20,400 cells and, like the model used in all other simulations in this chapter, is also extracted from the model developed by Castro [23]. See section 4.1 for further description of the reservoir model. Using this model the simulation time was 3,000 days and 190 snapshots were generated for the pressure and saturation states.
Figures 2.46 and 2.47 show the variation in eigenvalues for the pressure and saturation states, respectively, for models with \( \Delta \rho = 0, 1, 2, 5, 15 \) and 20 lb/ft\(^3\). It is apparent that with \( \Delta \rho = 0 \) only one basis function is needed for pressure. This is as expected since the pressure field does not change in time. Pressure does change in time for nonzero \( \Delta \rho \) and, as \( \Delta \rho \) increases, more basis functions are required to retain a specified fraction of the total energy (as was observed in Figure 2.45). The saturation equation is linear in this case for \( \Delta \rho = 0 \) though, because the solution still changes in time, more than one basis function is needed. The saturation equation becomes nonlinear for nonzero \( \Delta \rho \), and we observe flattening in the eigenvalue decay as \( \Delta \rho \) increases in Figure 2.47. There is a large difference in the shapes of the curves for \( \Delta \rho = 0 \) and \( \Delta \rho = 1 \).

The results presented in Figures 2.45, 2.46 and 2.47 suggest that the use of ROM procedures will be more challenging when significant density differences are present. At this point we cannot, however, determine whether this is because additional physics enters the problem or simply because the problem is now more nonlinear. A detailed assessment of this issue should be a topic for future work.

![Figure 2.46: Eigenvalue variation for pressure for 20,400-cell models with density differences](image)

There are many practical subsurface flow cases for which the relative permeability curves are not highly nonlinear and gravitational effects are small relative to viscous effects. For such cases, the ROM procedures applied here would be expected to be effective. However, for cases with highly nonlinear relative permeability curves and/or strong gravitational effects, further enhancements in our reduced-order modeling procedures will likely be required before they can be applied in practice. This may entail the use of new training procedures.
Figure 2.47: Eigenvalue variation for saturation for 20,400-cell models with density differences

or the use of techniques other than POD to construct the basis matrix. We have also observed a reduction in accuracy when the injector BHPs are varied over a wide range, so better treatments for that case will also be required.

In this chapter we developed and tested new POD-based ROM procedures for oil-water flow. For the class of problems considered, speedups of up to about a factor of 10 were observed. In the next chapter, we consider a different reduced-order modeling approach, which uses POD as one of its components, that is able to provide significantly greater runtime speedups.
Chapter 3

Trajectory Piecewise Linearization for Reservoir Simulation

Our goal in this chapter is to develop and apply a trajectory piecewise linearization (TPWL) procedure for subsurface flow problems. We first develop the linearized representation of the governing equations for oil-water flow. POD procedures and their use in conjunction with the linearized oil-water model are then described. Next, some implementation issues are discussed. We then present simulation results for two cases, involving heterogeneous reservoirs with 24,000 and 79,200 grid blocks. These computations demonstrate that the TPWL technique is able to provide accurate solutions for a variety of well BHP schedules with very significant speedups. Finally, some additional issues are discussed.

3.1 TPWL for Subsurface Flow

We consider the two-phase flow system presented in Chapter 2. The governing equations and discretizations are specified by Eqs. 2.1 – 2.7. The discrete system is given by Eq. 2.9, which we write here as:

\[ g(x^{n+1}, u^{n+1}) = F(x^{n+1}) + A(x^{n+1}, x^n) + Q(x^{n+1}, u^{n+1}) = 0, \]  

(3.1)

where \( g \) represents the residual vector, which we seek to drive to zero, \( x \) designates the system states (pressure and saturation), \( u \) indicates the system controls (well BHPs), and \( F, A \) and \( Q \) represent the convective, accumulation and source/sink terms, respectively.
See [9] for detailed expressions. Note that, in Chapter 2, we wrote \( F(x^{n+1}) = T^{n+1}x^{n+1} \) and \( A(x^{n+1}, x^n) = -D^{n+1}(x^{n+1} - x^n) \). The fully implicit system defined by Eq. 3.1 is nonlinear and is solved through application of Newton’s method, with the Jacobian matrix given by \( \partial g/\partial x \).

### 3.1.1 Linearization of Governing Equations

Linearized models can be constructed through use of a Taylor series expansion about a known state and set of controls, which we designate as \((x^i, u^i)\). These states are saved from a small number (e.g., 3–5) of preprocessing ‘training’ simulations [56]. Applying such an expansion to Eq. 3.1 gives:

\[
g(x^{n+1}, u^{n+1}) = g(x^i, u^i) + \left( \frac{\partial g}{\partial x} \right)_i (x^{n+1} - x^i) + \left( \frac{\partial g}{\partial u} \right)_i (u^{n+1} - u^i) + \ldots, \tag{3.2}
\]

where \( u^{n+1} \) is the new set of controls (which are specified), \( x^{n+1} \) is the new state we wish to determine, and both \( (\partial g/\partial x)_i \) and \( (\partial g/\partial u)_i \) are matrices evaluated at \((x^i, u^i)\). The necessary information associated with these matrices is saved along with the states during the training runs, though in a reduced form as described below.

Given the solution at time step \( n \) \((x^n)\), our goal is to represent \( x^{n+1} \) in the form of Eq. 3.2. We designate the saved state that is ‘closest’ to \( x^n \) as \( x^i \). There are various criteria for determining the closest saved state, and we will specify our particular approach below. It is then reasonable to assume that the closest saved state to \( x^{n+1} \) (the state we seek to determine) is \( x^{i+1} \), which is the saved state that follows \( x^i \).

We can now proceed with expansions of the form of Eq. 3.2 for each of the terms in Eq. 3.1. Expanding around \( x^{i+1} \), we have, for the convective effects

\[
F^{n+1} \approx F^{i+1} + \frac{\partial F^{i+1}}{\partial x^{i+1}}(x^{n+1} - x^{i+1}), \tag{3.3}
\]

where \( F^{n+1} = F(x^{n+1}) \) (and similarly for \( F^{i+1} \)) and \( \partial F^{i+1}/\partial x^{i+1} \) designates the flow term portion of the Jacobian matrix for the state \( x^{i+1} \). Note that the controls do not appear in the flow terms.

The accumulation term depends on the states at time levels \( n \) and \( n + 1 \). We thus expand around both \( x^{i+1} \) and \( x^i \), which gives:

\[
A(x^{n+1}, x^n) \approx A^{i+1}(x^{i+1}, x^i) + \frac{\partial A^{i+1}}{\partial x^{i+1}}(x^{n+1} - x^{i+1}) + \frac{\partial A^{i+1}}{\partial x^i}(x^n - x^i). \tag{3.4}
\]
From here on $\mathbf{A}^{i+1}(\mathbf{x}^{i+1}, \mathbf{x}')$ will be designated simply as $\mathbf{A}^{i+1}$.

The source/sink term $\mathbf{Q}$ depends on both $\mathbf{x}^{n+1}$ and the new controls $\mathbf{u}^{n+1}$. The source/sink term can thus be represented as

$$\mathbf{Q}(\mathbf{x}^{n+1}, \mathbf{u}^{n+1}) \approx \mathbf{Q}^{i+1}(\mathbf{x}^{i+1}, \mathbf{u}^{i+1}) + \frac{\partial \mathbf{Q}^{i+1}}{\partial \mathbf{x}^{i+1}}(\mathbf{x}^{n+1} - \mathbf{x}^{i+1}) + \frac{\partial \mathbf{Q}^{i+1}}{\partial \mathbf{u}^{i+1}}(\mathbf{u}^{n+1} - \mathbf{u}^{i+1}). \quad (3.5)$$

Recall that the controls in our case are the well bottom hole pressures, $p_w^i$. Because of the way in which the controls appear in the source term (Eq. 2.6), we can compute $\mathbf{Q}(\mathbf{x}^{i+1}, \mathbf{u}^{n+1})$ directly. In other words, this term is evaluated using the new controls $\mathbf{u}^{n+1}$ and not the controls $\mathbf{u}^{i+1}$ (which are the controls associated with the saved state $\mathbf{x}^{i+1}$). Thus we can write

$$\mathbf{Q}(\mathbf{x}^{n+1}, \mathbf{u}^{n+1}) \approx \mathbf{Q}(\mathbf{x}^{i+1}, \mathbf{u}^{n+1}) + \frac{\partial \mathbf{Q}^{i+1}}{\partial \mathbf{x}^{i+1}}(\mathbf{x}^{n+1} - \mathbf{x}^{i+1}). \quad (3.6)$$

This representation eliminates the need to save $\frac{\partial \mathbf{Q}^{i+1}}{\partial \mathbf{u}^{i+1}}$ from the training simulations.

Applying Eqs. 3.3, 3.4 and 3.6 into Eq. 3.1 we have:

$$\mathbf{g}(\mathbf{x}^{n+1}, \mathbf{u}^{n+1}) \approx \mathbf{F}^{i+1} + \mathbf{A}^{i+1} + \frac{\partial \mathbf{A}^{i+1}}{\partial \mathbf{x}^{i+1}}(\mathbf{x}^{n+1} - \mathbf{x}^{i+1}) + \mathbf{Q}(\mathbf{x}^{i+1}, \mathbf{u}^{n+1}) + \frac{\partial \mathbf{Q}^{i+1}}{\partial \mathbf{x}^{i+1}}(\mathbf{x}^{n+1} - \mathbf{x}^{i+1}). \quad (3.7)$$

Defining the Jacobian matrix as:

$$\mathbf{J}^{i+1} = \frac{\partial \mathbf{F}^{i+1}}{\partial \mathbf{x}^{i+1}} + \frac{\partial \mathbf{A}^{i+1}}{\partial \mathbf{x}^{i+1}} + \frac{\partial \mathbf{Q}^{i+1}}{\partial \mathbf{x}^{i+1}}, \quad (3.8)$$

enables us to express Eq. 3.7 more concisely

$$\mathbf{g}(\mathbf{x}^{n+1}, \mathbf{u}^{n+1}) \approx \mathbf{F}^{i+1} + \mathbf{A}^{i+1} + \frac{\partial \mathbf{A}^{i+1}}{\partial \mathbf{x}^{i}}(\mathbf{x}^{n} - \mathbf{x}^{i}) + \mathbf{Q}(\mathbf{x}^{i+1}, \mathbf{u}^{n+1}) + \mathbf{J}^{i+1}(\mathbf{x}^{n+1} - \mathbf{x}^{i+1}) = 0. \quad (3.9)$$

Now, setting the residual using the new controls at the new state to zero ($\mathbf{g}(\mathbf{x}^{n+1}, \mathbf{u}^{n+1}) = 0$), we arrive at a matrix equation that can be solved to determine $\mathbf{x}^{n+1}$:

$$\mathbf{J}^{i+1}(\mathbf{x}^{n+1} - \mathbf{x}^{i+1}) = - \left[ \mathbf{F}^{i+1} + \mathbf{A}^{i+1} + \frac{\partial \mathbf{A}^{i+1}}{\partial \mathbf{x}^{i}}(\mathbf{x}^{n} - \mathbf{x}^{i}) + \mathbf{Q}(\mathbf{x}^{i+1}, \mathbf{u}^{n+1}) \right]. \quad (3.10)$$
3.1.2 Construction of the POD Basis Matrix

Eq. 3.10 provides a representation for new states in terms of saved information, but it is not practical to use this equation in its current form. This is because $J^{i+1}$ and $\partial A^{i+1}/\partial x^i$ are, although sparse, of dimensions $2N_c \times 2N_c$, and the other terms in Eq. 3.10 are vectors of dimension $2N_c$ (recall that $N_c$ is the number of grid blocks in the high-fidelity model). We therefore proceed by applying proper orthogonal decomposition (POD) to construct an orthonormal basis that can be used to project the high-fidelity linearized model (Eq. 3.10) to a lower-dimensional representation. As shown in Chapter 2, POD can be applied directly to the general simulation equations to provide a reduced-order model (as was also done in [64, 22]). Here, by contrast, we apply POD in conjunction with the linearized representation. We note that most previous TPWL implementations [56, 71, 65, 63, 30] used Krylov techniques to construct the reduced-order basis, though POD was used by [34].

The basic POD procedure was presented in detail in section 2.1.2. Consistent with previous TPWL implementations [56, 71, 65, 63, 30, 34], in constructing the basis for the TPWL procedure, here we do not subtract the mean of the snapshots ($\bar{x}_p, \bar{x}_S$) when computing the data matrices $\hat{X}_p$ and $\hat{X}_S$. We also constructed the POD basis by subtracting the mean of the snapshots (as in Eq. 2.12), though we observed slightly less accurate TPWL results when proceeding in this manner. The basis matrix allows us to relate the high-dimensional state $x$ to a reduced state $z$; i.e.,

$$x \approx \Phi z,$$  \hspace{1cm} (3.11)

where $z$ is of dimension $\ell$. Because $\Phi$ is orthonormal, we also have $z = \Phi^T x$. The states $x^i_p$ and $x^i_S$ used to construct $\Phi$ are simply the snapshots saved during the 3–5 training runs.

3.1.3 TPWL Representation with POD Basis Matrix

We now use $\Phi$ to project Eq. 3.10 into a reduced space. Premultiplying both sides of Eq. 3.10 by $\Phi^T$ and representing $x$ as $\Phi z$ gives:

$$\Phi^T J^{i+1} \Phi(z^{n+1} - z^{i+1}) = -\Phi^T \left[ F^{i+1} + A^{i+1} + \frac{\partial A^{i+1}}{\partial x^i} \Phi(z^n - z^i) + Q(x^{i+1}, u^{n+1}) \right].$$  \hspace{1cm} (3.12)
This equation can be rewritten more concisely by defining:

\[ J_{i+1}^r = \Phi^T J_{i+1} \Phi, \quad (\partial A_{i+1}^r / \partial x_i) = \Phi^T (\partial A_{i+1} / \partial x_i) \Phi, \] (3.13)

\[ F_{i+1}^r = \Phi^T F_{i+1}, \quad A_{i+1}^r = \Phi^T A_{i+1}, \quad Q_r = \Phi^T Q_r. \] (3.14)

The resulting equation can be solved directly for \( z_{n+1} \), which gives

\[ z_{n+1} = z_{i+1} - (J_{r}^{i+1})^{-1} \left[ F_{r}^{i+1} + A_{r}^{i+1} + \left( \frac{\partial A^{i+1}}{\partial x} \right)_r (z^n - z^i) + Q_r (x^{i+1}, u_{n+1}) \right]. \] (3.15)

In Eq. 3.15, \( J_{r}^{i+1} \) and \( (\partial A^{i+1} / \partial x_i) \) are full matrices of dimension \( \ell \times \ell \) and the other terms are vectors of dimension \( \ell \). The matrices \((J_{r}^{i+1})^{-1}\) and \((\partial A^{i+1} / \partial x_i)\), and the vectors \( z_{i+1} \), \( F_{r}^{i+1} \) and \( A_{r}^{i+1} \) can be precomputed because they are constructed from the reduced basis \( \Phi \) and information saved during the training runs. The vector \( Q_r (x^{i+1}, u_{n+1}) \), by contrast, cannot be precomputed because it depends on the controls \( u_{n+1} \), which are not known when the training simulations are performed. This term can be efficiently computed, however, because high-fidelity information is required only for the small fraction of grid blocks that contain wells. After the well block entries to \( Q(x^{i+1}, u_{n+1}) \) are computed, this vector can be projected into the reduced space using \( Q_r (x^{i+1}, u_{n+1}) = \Phi_w^T Q(x^{i+1}, u_{n+1}) \), where \( \Phi_w^T \) includes only those rows of the basis matrix that correspond to grid blocks containing wells.

We implemented and tested the TPWL model defined by Eq. 3.15 for the case of incompressible flow (the simplifications that arise for the incompressible flow case will be indicated below) and observed a reasonable level of accuracy relative to reference high-fidelity simulations. We also implemented a variant of this approach and found it to perform slightly better (e.g., in limited tests, the error in produced water, as reported in the tables in the next section, differed by a factor of two for some cases). We now describe this alternate approach, which is the method used to generate the results presented in the next section.

The alternate TPWL representation proceeds by expressing

\[ x_{n+1} - x_{i+1} = (x_{n+1} - x^n) - (x_{i+1} - x^n). \] (3.16)

We then write:

\[ F_{n+1} \approx F_{i+1} + \frac{\partial F_{i+1}}{\partial x_{i+1}} (x_{n+1} - x^n) - \frac{\partial F_{i+1}}{\partial x_{i+1}} (x_{i+1} - x^n), \] (3.17)
\( A(x^{n+1}, x^n) \approx A^{i+1} + \frac{\partial A^{i+1}}{\partial x^{i+1}}(x^{n+1} - x^n) - \frac{\partial A^{i+1}}{\partial x^i}(x^{i+1} - x^i) \), (3.18)

\[ Q^{n+1}(x^{n+1}, u^{n+1}) \approx Q(x^{i+1}, u^{n+1}) + \frac{\partial Q^{i+1}}{\partial x^{i+1}}(x^{n+1} - x^n) - \frac{\partial Q^{i+1}}{\partial x^i}(x^{i+1} - x^i). \] (3.19)

Now, by noting that

\[ Q(x^{i+1}, u^{n+1}) - \left( \frac{\partial Q^{i+1}}{\partial x^{i+1}}(x^{i+1} - x^n) \right) \approx Q(x^n, u^{n+1}), \]

\[ Q^{n+1}(x^{n+1}, u^{n+1}) \approx Q(x^n, u^{n+1}) + \frac{\partial Q^{i+1}}{\partial x^{i+1}}(x^{n+1} - x^n). \] (3.20)

Applying Eqs. 3.17, 3.18, 3.20 and the Jacobian matrix \( J^{i+1} \) as given by Eq. 3.8 into the
residual equation (Eq. 3.1), we have:

\[ J^{i+1}(x^{n+1} - x^n) = - \left[ F^{i+1} - \frac{\partial F^{i+1}}{\partial x^{i+1}}(x^{i+1} - x^n) + A^{i+1} - \frac{\partial A^{i+1}}{\partial x^{i+1}}(x^{i+1} - x^n) \right. \]
\[ \left. + \frac{\partial A^{i+1}}{\partial x^i}(x^n - x^i) + Q(x^n, u^{n+1}) \right]. \] (3.21)

Premultiplying both sides of Eq. 3.21 by \( \Phi^T \) and writing \( x \approx \Phi z \), we arrive at the TPWL representation for \( z^{n+1} \):

\[ z^{n+1} = z^n - (J^{i+1})^{-1} \left[ F^{i+1} - \left( \frac{\partial F^{i+1}}{\partial x^{i+1}} \right)_r (z^{i+1} - z^n) + A^{i+1} - \left( \frac{\partial A^{i+1}}{\partial x^{i+1}} \right)_r (z^{i+1} - z^n) \right. \]
\[ \left. + \left( \frac{\partial A^{i+1}}{\partial x^i} \right)_r (z^n - z^i) + Q, (x^n, u^{n+1}) \right]. \] (3.22)

The actual TPWL implementation accomplished in this work is for the case of incompressible fluid and rock. For such systems, with reference to Eq. 2.5, the accumulation term becomes

\[ A(x^{n+1}, x^n) = D(x^{n+1} - x^n) \quad \text{and} \quad A(x^{i+1}, x^i) = D(x^{i+1} - x^i), \] (3.23)

which gives \( \frac{\partial A^{i+1}}{\partial x^{i+1}} = -\frac{\partial A^{i+1}}{\partial x^i} = D \). Here \( D \) is a constant matrix. Inserting
this representation of the accumulation term into Eq. 3.22 gives the TPWL model for
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incompressible systems:

\[ z^{n+1} = z^n - (J_r^{i+1})^{-1} \left[ F_r^{i+1} - \left( \frac{\partial F_r^{i+1}}{\partial x_r^{i+1}} \right) r (z^{i+1} - z^n) + Q_r(x^n, u^{n+1}) \right]. \] (3.24)

The reason why Eq. 3.24 provides slightly better accuracy than the incompressible version of Eq. 3.15 is not entirely clear. It may, however, be related to the different treatments of \( Q_r \) that appear in the two equations. Specifically, in developing Eq. 3.15, we express \( Q(x^{n+1}, u^{n+1}) \) in terms of an expansion around \( Q(x^{i+1}, u^{n+1}) \) (see Eq. 3.6), while for Eq. 3.24, we represent \( Q(x^{n+1}, u^{n+1}) \) using an expansion around \( Q(x^n, u^{n+1}) \) (Eq. 3.20). As it is often the case that \( x^{n+1} \) is closer to \( x^n \) than it is to \( x^{i+1} \), we would expect better overall accuracy for Eq. 3.24 than for Eq. 3.15.

3.1.4 Implementation Issues

We now comment briefly on some aspects of the numerical implementation. The high-fidelity simulations are all performed using Stanford’s general purpose research simulator, GPRS [17, 41]. The simulator was modified to output the states (snapshots) and Jacobian information from the training runs, as required by the TPWL procedure. The output files occupy substantial disk space, as the matrices for the high-fidelity model can be quite large. Following the simulation of 3–5 training runs, the reduced basis \( \Phi \) is constructed, the reduced matrices are generated, and the reduced Jacobian matrices are inverted. The computational requirements for constructing the basis and generating the required matrices are comparable to the time required to perform the training simulations. These operations are however now performed using Matlab [47], so it is likely that they can be accelerated.

The TPWL solution (Eq. 3.24) is implemented as a Matlab procedure. Our formulation generally avoids the need to perform any computations using the high-fidelity model. However, in the following section we do report on the mass balance error observed using TPWL for some cases. For such calculations, the high-fidelity model must be reconstructed (using \( x \approx \Phi z \)) and computations then performed using it. This will of course reduce the speedup achieved using TPWL.

The TPWL procedure represents new solutions, designated \( x^{n+1} \), in terms of expansions around saved solutions, designated \( x^{i+1} \). As described above, this requires that we first determine the ‘closest’ saved state \( x^i \) to the solution at the previous time step, \( x^n \). It would be time consuming if this determination was performed using high-fidelity states. Therefore,
we investigated various approaches for finding the closest state using only reduced state information. The best accuracy was achieved by determining the saved state that minimizes $|z_s^n - z_s^i|$, where $z_s^n = \Phi_s^T x_s^n$ and $z_s^i = \Phi_s^T x_s^i$ designate reduced saturation states. Inclusion of the reduced pressure states in this determination did not provide additional accuracy. This finding is reasonable because, during the course of the simulation, the global saturation changes more significantly and more abruptly than pressure (saturation is described by an essentially hyperbolic conservation equation, while pressure is determined from an elliptic solution for the incompressible case, as is evident from Eqs. 2.29 and 2.30), so the accuracy of the TPWL solution is more sensitive to the saturation state used in the expansion.

### 3.2 Simulation Results Using TPWL Procedure

In this section we apply the TPWL procedure to two reservoir models – one containing 24,000 grid blocks and the other containing 79,200 grid blocks. We consider the performance of the TPWL models for a variety of test runs.

#### 3.2.1 Reservoir Model 1

**Model Description**

This reservoir model, shown in Figure 3.1, is a modified portion of a channelized reservoir model presented in [28] (the full model is often referred to as SPE 10). The model is three-dimensional and contains 24,000 grid blocks (with $n_x = 60$, $n_y = 80$ and $n_z = 5$, where $n_x$, $n_y$ and $n_z$ designate the number of grid blocks in each direction). There are four production wells (designated P1–P4) and two water injection wells (designated I1 and I2).

Permeability is taken to be a diagonal tensor, with $k_x = k_y$. The mean $k_x$ is 418 mD and the mean porosity is 0.203. The vertical permeability ($k_z$) is prescribed as $k_z = 0.3k_x$ in the channels and $k_z = 10^{-3}k_x$ in the non-channel regions. The initial oil and water saturations are 0.8 and 0.2 respectively and the residual oil ($S_{or}$) and water ($S_{wr}$) saturations are 0.2. For oil we set $\rho_o = 45 \text{ lb/ft}^3$, $\mu_o = 3.0 \text{ cp}$; for water, $\rho_w = 60 \text{ lb/ft}^3$, $\mu_w = 0.5 \text{ cp}$. The system is incompressible and capillary pressure effects are neglected. The relative permeabilities for the oil and water phases are specified by Eqs. 2.27 and 2.28 with $k_{ro}^0 = k_{rw}^0 = 1$ and $a = b = 2$. 
Training Runs

The first step in the TPWL procedure is to perform a few training runs using the high-fidelity model to generate the states and Jacobian matrices (GPRS is used for these simulations). For this reservoir model four training simulations are performed. In all of these simulations the injection wells are prescribed to maintain constant bottom hole pressure (BHP) of 10,000 psia. This condition will be maintained in subsequent test runs (our focus here is on varying the production well BHPs). For the production wells, the BHPs are prescribed to follow schedules that are expected to represent approximately the operating conditions that will be encountered in subsequent simulations. We have not yet established a fully systematic approach for prescribing the training run BHPs, so we instead apply the following heuristic procedure.

In the first training simulation, the BHPs of all four production wells are kept constant at 1,000 psia. For the second training run, the BHPs are changed every 200 days, as indicated in Figure 3.2, such that the total flow rate (oil+water) of each production well is approximately the same and approximately constant in time for each 1,000 day interval. Specifically, over the first 1,000 days, the total flow rate per well is 2,000 stb/d (stock tank barrels per day), from 1,000 to 2,000 days it is 2,300 stb/d, from 2,000 to 3,000 days it is 2,700 stb/d, from 3,000 to 4,000 days it is 3,100 stb/d and from 4,000 to 5,000 days it is 3,300 stb/d. In the third training schedule, the BHPs of the production wells are varied...
every 200 days, randomly and independently, between 2,000 and 4,000 psia, as illustrated in Figure 3.3. For the fourth training simulation, the producer BHPs are again varied randomly, but this time between 1,000 and 3,000 psia as shown in Figure 3.4. Thus with the training runs we attempt to capture constant BHP behavior (training run 1), constant flow rate behavior (run 2) and more variable effects (runs 3 and 4). Other training sequences could of course be devised, though as we will see below this set of training runs generally results in accurate predictions in the subsequent test runs.

In the training runs, we simulated reservoir performance for a total of 5,000 days with a maximum time step of 30 days. From the four training runs 759 pressure and saturation snapshots and Jacobian matrices were recorded. The POD basis matrix was constructed following the approach described in section 2.1.2. We did not apply the clustering or missing point estimation procedures described in sections 2.1.4 and 2.1.5. The reduced basis $\Phi$ used for most of the runs in this section contains a total of 325 columns, 78 of which correspond to pressure states and 247 to saturation states.

We now assess the ability of the TPWL representation (Eq. 3.24) to reproduce results from the training simulations by applying the BHP schedules used for training simulation 2. Figure 3.5 presents the oil rates and Figure 3.6 shows the water rates for all production wells. Figure 3.7 depicts the injection rates for wells I1 and I2. We see from these figures that the TPWL results, depicted by circles, are in essentially perfect agreement with the reference high-fidelity (GPRS) solutions, depicted by solid curves.
3.2. SIMULATION RESULTS USING TPWL PROCEDURE

Figure 3.2: Producer BHP schedules for training run 2

Figure 3.3: Producer BHP schedules for training run 3

Figure 3.4: Producer BHP schedules for training run 4
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Figure 3.5: Oil rate for each production well for training run 2

Figure 3.6: Water rate for each production well for training run 2

Figure 3.7: Injection rate for each injection well for training run 2
Test Runs

We perform a total of eight test simulations using a variety of specifications for producer BHPs. Five tests (designated A–E) are performed with random schedules. In test A the production well BHPs vary from 2,000 to 3,000 psia, for test B from 1,500 to 3,500 psia, for test C from 1,000 to 4,000 psia, for test D from 500 to 4,500 psia, and for test E from 0 to 5,000 psia. Figure 3.8 presents the BHPs for the production wells for test A and Figure 3.9 shows the BHPs for test E. Note that the BHPs for tests A–C are within the range of the training runs, while those for tests D and E are outside of this range.

Another set of three tests (F–H) is performed by modifying the producer BHPs used in training run 2 by varying amounts. Figure 3.10 shows that for tests F and G the BHPs of production well P1 are consistently below the BHPs used in training run 2. On the other hand, for test H the BHPs are consistently above those used for training. The same is true for wells P2 and P3. For production well P4, which is the well with the highest flow rate, in tests F–H we prescribe BHPs below that of training run 2, as indicated in Figure 3.11 (test H entails the largest deviation from the training run and is therefore the most challenging for the TPWL model). Figure 3.12 presents the BHPs for all of the production wells in test F and Figure 3.13 depicts those for test H.

![Figure 3.8: Producer BHP schedules for test A](image-url)
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Figure 3.9: Producer BHP schedules for test E

Figure 3.10: Producer BHP schedules for training run 2 and tests F–H for well P1

Figure 3.11: Producer BHP schedules for training run 2 and tests F–H for well P4
3.2. SIMULATION RESULTS USING TPWL PROCEDURE

Figure 3.12: Test F: BHP schedules for all production wells

Figure 3.13: Test H: BHP schedules for all production wells
Error Measures

The accuracy of the TPWL simulations can be assessed both visually and by computing the average error, relative to the reference high-fidelity simulation, for the oil and water production rates and the water injection rate. We compute these errors as indicated in section 2.2.5. Rates from the TPWL simulation are interpolated to correspond to the simulation times in the high-fidelity simulation. We avoid interpolating across discontinuities in the well BHP. For each production well \( m \), at every simulated time step \( i \), the oil production rates in the high-fidelity simulation (\( Q_{o,hf}^{m,i} \)) and in the TPWL simulation (\( Q_{o,tpwl}^{m,i} \)) are computed. The time-average error for each well, designated \( E^m \), is calculated as the average of the absolute differences, normalized by the time-average oil flow rate \( \bar{Q}_{o,hf}^m \) for the well:

\[
E^m = \frac{1}{n_t \bar{Q}_{o,hf}^m} \sum_{i=1}^{n_t} |Q_{o,hf}^{m,i} - Q_{o,tpwl}^{m,i}|, \tag{3.25}
\]

where \( n_t \) is the total number of time steps. The overall average error, designated \( E \), is computing by averaging \( E^m \) over all wells, as shown in Eq. 2.26.

The material balance errors in the TPWL computations for the oil and water components are also of interest. These are computed as follows for the incompressible case considered here. For oil, at every time step \( i \), the volume of oil in place (\( V^i_o \)) and the cumulative production of oil (\( Q^i_o \)) are computed (note that this requires that we reconstruct the high-fidelity solution). The oil material balance error at time step \( i \) (\( \text{MBE}_o^i \)) is given by:

\[
\text{MBE}_o^i = \frac{V^0_o - (V^i_o + Q^i_o)}{V^0_o}, \tag{3.26}
\]

where \( V^0_o \) is the volume of oil in place at initial time. For the water component, the volume in place (\( V^i_w \)), the cumulative production (\( Q^i_w \)) and the cumulative injection (\( I^i_w \)) are similarly updated at each time step and the material balance error is computed as:

\[
\text{MBE}_w^i = \frac{V^0_w - (V^i_w + Q^i_w - I^i_w)}{V^0_w}, \tag{3.27}
\]

where \( V^0_w \) is the volume of water originally in place. The material balance errors reported below are the maximum \( \text{MBE}_o^i \) and \( \text{MBE}_w^i \) computed during the course of the TPWL simulation.
Model 1 Simulations

We now present results illustrating and quantifying the performance of TPWL for the test runs. Figures 3.14 – 3.17 demonstrate the accuracy of the TPWL model relative to the high-fidelity model for test C. The producer BHP schedules are shown in Figure 3.14. It is apparent that these well BHPs differ significantly from any of the training runs, though they are within the range of the training BHPs. Figure 3.15 presents the oil rates and Figure 3.16 shows the water rates for all production wells. Figure 3.17 depicts the injection rates for wells I1 and I2. It is evident from these figures that the TPWL results are in very close agreement with the reference high-fidelity (GPRS) solutions. Thus these results demonstrate the viability of the TPWL method for modeling subsurface flow.

Figure 3.14: Test C: BHP schedules for all production wells

Figure 3.15: Results for test C: Oil rate for each production well
Figure 3.16: Results for test C: Water rate for each production well

Figure 3.17: Results for test C: Injection rate for each injection well
We next consider test E. The TPWL model for test E would not be expected to be as accurate as in the previous case because the well BHPs vary over a larger range. In addition, these well BHPs are outside of the range of the training runs. Thus this is a challenging test case. Figure 3.18 presents the oil rates for all production wells. Although acceptable accuracy is achieved over most of the simulation, well P3 displays significant error in oil rate between 1,500 and 2,000 days. Figure 3.19 shows the water production rates, which are generally quite accurate. Figure 3.20 presents the injection rates for injection wells I1 and I2. Some error is evident for well I1 between 1,500 and 2,500 days, though the overall TPWL results are reasonable. This case illustrates that the TPWL model can lose accuracy if the test runs involve well settings (and thus states) that are outside the range of the training runs. However, the magnitude of the discrepancy between the TPWL model and the high-fidelity simulation is for the most part not excessive, suggesting that the TPWL model is reasonably robust.

![Figure 3.18: Results for test E: Oil rate for each production well](image)

The average oil and water production rate errors, the average water injection rate error, and the maximum material balance errors for oil and water, for tests A–E, are presented in Table 3.1. From the results in this table, it is evident that the errors in production and injection rates increase consistently as we proceed from test A to test E (thus test C represents in some sense an ‘average’ result). For the mass balance errors, there is not a monotonic increase as we proceed from test A to test E, though test E does provide the largest errors. The general level of the production and injection rate errors is relatively small, though we reiterate that they are average errors and significant instantaneous errors are observed in some cases (e.g., test E above).
Figure 3.19: Results for test E: Water rate for each production well

Figure 3.20: Results for test E: Injection rate for each injection well
3.2. SIMULATION RESULTS USING TPWL PROCEDURE

Table 3.1: Errors in TPWL solutions for tests A–E

<table>
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<th></th>
<th>Test A</th>
<th>Test B</th>
<th>Test C</th>
<th>Test D</th>
<th>Test E</th>
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<td>Water inj</td>
<td>0.0049</td>
<td>0.0072</td>
<td>0.0079</td>
<td>0.0190</td>
<td>0.0197</td>
</tr>
<tr>
<td>MBE oil</td>
<td>0.0014</td>
<td>0.0022</td>
<td>0.0020</td>
<td>0.0030</td>
<td>0.0034</td>
</tr>
<tr>
<td>MBE water</td>
<td>0.0031</td>
<td>0.0070</td>
<td>0.0051</td>
<td>0.0053</td>
<td>0.0388</td>
</tr>
</tbody>
</table>

We now consider the second set of test runs. Results for test G are shown in Figures 3.21 – 3.24. Figure 3.21 presents the BHP schedules prescribed for each production well, Figure 3.22 shows the oil rates and Figure 3.23 depicts the water rates. Figure 3.24 provides the injection rates for wells I1 and I2. For all of these results, the agreement between the TPWL and the high-fidelity models is quite close, though some discrepancy is evident in the I2 injection rate at the end of the run.

Figure 3.21: Test G: BHP schedules for all production wells

The average well rate errors and maximum material balance errors for tests F–H are presented in Table 3.2. Errors for test H are in all cases greater than those for test F, as would be expected, though test G errors do not always fall between these two. In any event, the errors in Table 3.2 are generally comparable in magnitude to those presented in Table 3.1 for tests A–E, again indicating the general level of accuracy and robustness of the TPWL model for this example.

The results above demonstrate that, for the case considered, the TPWL model is able
Figure 3.22: Results for test G: Oil rate for each production well

Figure 3.23: Results for test G: Water rate for each production well

Figure 3.24: Results for test G: Injection rate for each injection well
3.2. SIMULATION RESULTS USING TPWL PROCEDURE

Table 3.2: Errors in TPWL solutions for tests F–H

<table>
<thead>
<tr>
<th></th>
<th>Test F</th>
<th>Test G</th>
<th>Test H</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oil prod</td>
<td>0.0050</td>
<td>0.0081</td>
<td>0.0166</td>
</tr>
<tr>
<td>Water prod</td>
<td>0.0069</td>
<td>0.0201</td>
<td>0.0382</td>
</tr>
<tr>
<td>Water inj</td>
<td>0.0060</td>
<td>0.0158</td>
<td>0.0149</td>
</tr>
<tr>
<td>MBE oil</td>
<td>0.0016</td>
<td>0.0013</td>
<td>0.0027</td>
</tr>
<tr>
<td>MBE water</td>
<td>0.0122</td>
<td>0.0250</td>
<td>0.0189</td>
</tr>
</tbody>
</table>

to provide simulation results in reasonable agreement with high-fidelity simulations, particularly when the controls (producer BHPs in our case) are kept within the range of the training simulations. The computational requirements for the high-fidelity (GPRS) and TPWL simulations are, however, considerably different. The GPRS simulations require about 430 seconds of CPU time, while the TPWL runs consume only about 0.85 seconds if we do not compute the material balance errors at every time step. This represents a runtime speedup of about 500. If we compute the material balance errors at every time step, the TPWL computations require about 4 seconds, which reduces the runtime speedup to about a factor of 100. It is not necessary to compute the material balance errors at every time step, however, and if they are computed relatively infrequently (e.g., every 20 time steps), the additional computation will not be excessive.

Because the runtime speedups using TPWL are quite substantial, the major computational cost results from the training simulations and the preprocessing computations. The computational requirements for the preprocessing step depend to some extent on the number of columns ($\ell = \ell_p + \ell_s$) of the basis matrix $\Phi$. The size of $\Phi$ will also impact the speed of the TPWL simulations. Thus it is useful to assess the impact of $\ell_p$ and $\ell_s$ on the accuracy of the TPWL model. To quantify this effect, we now perform TPWL simulations for the four training runs and the eight test runs using different sized $\Phi$ matrices.

Figure 3.25 presents the average error for oil and water production rates and water injection rates using different numbers of basis functions. For these computations, we use prescribed percentages (from 20% to 100%) of the $\ell_p$ and $\ell_s$ used in the results presented above (recall that for those results $\ell_p = 78$, $\ell_s = 247$). From the figure, it is evident that TPWL maintains accuracy in oil and water production rates even with very small $\ell_p$ and $\ell_s$, though accuracy in water injection rate decreases rapidly for $\ell < 200$. Thus there appears
to be a minimum value of \( \ell \) that is required to maintain accuracy in the TPWL model. It is also worth noting that the accuracy of the TPWL model for the training runs in all cases exceeds that for the test runs, as would be expected.

![Figure 3.25: Errors in the TPWL simulations for different numbers of basis functions](image)

3.2.2 Reservoir Model 2

Model Description

We now consider a larger model in order to demonstrate the applicability of the TPWL representation for models approaching sizes encountered in practical reservoir simulation. Like the reservoir model used in the examples above, this system is derived from [28]. The model, again containing four production wells and two water injection wells, is of dimensions \( 60 \times 220 \times 6 \), for a total of 79,200 grid blocks (see Figure 3.26). All fluid properties are the same as those used previously except for the oil and water densities, which we prescribe as \( \rho_o = \rho_w = 55 \) lb/ft\(^3\). We take the fluid densities to be equal because, as shown in section 2.3, the underlying POD procedure requires a potentially large number of basis functions when significant density differences exist, and this can lead to precision issues in our Matlab implementation (see section 3.3 for further discussion). This was less of an issue in the previous example (where we did have a significant difference in densities) because the model contained fewer grid blocks and thus the required number of basis functions was not excessive.
### Training and Testing Runs

For this reservoir model we perform three training runs, all with the injection wells prescribed to operate at a constant bottom hole pressure of 8,000 psia. For the first training run the BHPs of the four production wells are held constant at 2,500 psia. In the second training run (Figure 3.27) the BHPs are updated every 200 days such that the total flow rate of each production well is constant at 2,000 stb/d. For the third training run (Figure 3.28) the BHPs are varied randomly and independently over a range of 1,000 to 4,000 psia. The training runs were simulated for 5,000 days with a maximum time step of 30 days. A total of 606 pressure and saturation snapshots and Jacobian matrices were recorded. The POD basis contains a total of 439 columns, 207 of which correspond to pressure and 232 to saturation.

We perform a total of five test simulations (designated I–M) using random producer well BHP schedules. In test I the production well BHPs range from 2,000 to 3,000 psia, for test J from 1,500 to 3,500 psia, for test K from 1,000 to 4,000 psia, for test L from 500 to 4,500 psia, and for test M from 0 to 5,000 psia.

### Model 2 Simulations

Figures 3.29 – 3.32 demonstrates the performance of the TPWL representation for test K. Figure 3.29 presents the BHP schedule for each production well, Figure 3.30 shows the oil
Figure 3.27: Producer BHP schedules for training run 2

Figure 3.28: Producer BHP schedules for training run 3
3.2. SIMULATION RESULTS USING TPWL PROCEDURE

rate, Figure 3.31 depicts the water rate and Figure 3.32 provides the injection rates for wells I1 and I2. TPWL results are generally quite accurate, though slight errors are evident at some points in the simulation.

![Figure 3.29: Test K: BHP schedules for all production wells](image)

![Figure 3.30: Results for test K: Oil rate for each production well](image)

Errors in the TPWL solutions for tests I through M are presented in Table 3.3. Recall that producer BHPs for tests I, J and K are within the range of the training runs, while those for tests L and M are outside of this range. The errors in Table 3.3 are overall higher, but generally of comparable magnitude, relative to those presented in Table 3.1 for tests A–E. Errors clearly trend higher as we proceed from test I to test M, as expected, though the increase is not strictly monotonic. Water production errors are fairly high for tests K, L and M. The results in Table 3.3 reiterate that the TPWL model provides accurate results.
Figure 3.31: Results for test K: Water rate for each production well

Figure 3.32: Results for test K: Injection rate for each injection well
3.3. ADDITIONAL ISSUES

within an appropriate range, but that solution accuracy can degrade outside of the range of the training runs.

Table 3.3: Errors in TPWL solutions for tests I–M

<table>
<thead>
<tr>
<th></th>
<th>Test I</th>
<th>Test J</th>
<th>Test K</th>
<th>Test L</th>
<th>Test M</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oil prod</td>
<td>0.0109</td>
<td>0.0132</td>
<td>0.0170</td>
<td>0.0461</td>
<td>0.0432</td>
</tr>
<tr>
<td>Water prod</td>
<td>0.0215</td>
<td>0.0215</td>
<td>0.0520</td>
<td>0.0809</td>
<td>0.1596</td>
</tr>
<tr>
<td>Water inj</td>
<td>0.0088</td>
<td>0.0095</td>
<td>0.0085</td>
<td>0.0204</td>
<td>0.0244</td>
</tr>
<tr>
<td>MBE oil</td>
<td>0.0021</td>
<td>0.0022</td>
<td>0.0030</td>
<td>0.0061</td>
<td>0.0067</td>
</tr>
<tr>
<td>MBE water</td>
<td>0.0022</td>
<td>0.0039</td>
<td>0.0029</td>
<td>0.0067</td>
<td>0.0250</td>
</tr>
</tbody>
</table>

The runtime speedups offered by TPWL relative to the high-fidelity simulations are even larger in this case than in the previous example. Specifically, the GPRS simulations for this model required about 30 minutes of CPU time, while each TPWL run required only 0.9 seconds if material balance errors were not computed. These timings correspond to a runtime speedup factor of about 2,000. If material balance errors are computed at every time step, the TPWL runs require about an order of magnitude more computation, so the speedup relative to GPRS is reduced to about a factor of 200.

3.3 Additional Issues

The results presented in the previous section demonstrate the potential of the TPWL method for subsurface flow modeling. Reasonable accuracy was achieved for two realistic example cases for test simulations in which the production well controls (BHPs) were quite different from those used in the training simulations. There remain, however, several issues that must be addressed before the TPWL procedure can be used for a wide range of practical subsurface flow problems.

Because the method is based on linearization around previously simulated (saved) states, degradation in accuracy is to be expected when higher order terms in the expansion (Eq. 3.2) become significant. It will therefore be useful to develop efficient estimators for these terms as well as heuristics that indicate when the TPWL solution is likely to degrade. For the latter, empirical error estimates that relate error in oil and water production rates and injection rate to, for example, mass balance error and some measure of the distance between the saved state $\mathbf{x}^{i+1}$ and the computed state $\mathbf{x}^{n+1}$, could be of value.
In the next chapter we apply TPWL for production optimization problems. Within this context, error estimators could be used to determine when model retraining is required. Retraining could then be accomplished by performing one or more new high-fidelity simulations using control schedules consistent with those at the current stage of the optimization. This would provide additional saved states which should be closer to those encountered during subsequent stages of the optimization.

As discussed in Chapter 2, the underlying POD representation requires more basis functions as the relative permeability functions become highly nonlinear and in the case of strong density differences. The use of higher numbers of basis functions leads to reduced efficiency, as all computations involving the basis matrix $\Phi$ become more costly. Another concern when using a large number of basis functions is that, due to computational precision issues, the condition number of $\Phi$ may begin to deviate from unity. As a result, as the number of basis functions becomes large, the use of additional basis functions does not always lead to better simulation accuracy, as the information incorporated in the additional columns of $\Phi$ is counterbalanced by a loss of precision. Degradation in accuracy has also been observed when the injection well BHPs were varied along with the production well BHPs. Thus it will be important to develop improved procedures for constructing $\Phi$. This will benefit both the standalone approach, i.e., the POD-based ROM described in Chapter 2, as well as the TPWL procedure. Along these lines, the goal-oriented optimization procedure for constructing the basis matrix presented in [15] may be useful to consider.

In total, the results presented in this chapter demonstrate the applicability of the TPWL procedure for modeling oil-water flow. A number of issues must still be addressed, however, before the method can be used for general practical cases. In the next chapter, we apply the TPWL approach to optimization problems.
Chapter 4

Production Optimization Using the TPWL Procedure

A target application for the TPWL procedure is as a fast function evaluator in optimization procedures. Within the context of oil reservoir management, one is often interested in maximizing oil production or the net present value of the project. In this chapter the reduced-order TPWL representation developed in the previous chapter is evaluated for production optimization problems involving waterflood. Three different heterogeneous 3D reservoir models will be used. We maximize the net present value for a waterflooding process by optimizing the BHPs of the production wells. In the first example, both gradient-based and generalized pattern search optimization algorithms are considered. For the other two cases only the gradient-based algorithm is applied. We demonstrate that the TPWL representation provides results for the objective function that are in close agreement with those generated using the high-fidelity model. Finally, a multiobjective optimization is performed for one of the models using the TPWL representation. For this problem only limited high-fidelity simulations are performed due to the very high computational demand required, though close correspondence between these results and those from TPWL is demonstrated.
4.1 Optimization Problem 1

4.1.1 Description of the Simulation Model

The reservoir model, shown in Figure 4.1, is a portion of a synthetic geological model developed by Castro in [23]. This is a smaller version (fewer gridblocks) of the model considered in Chapter 2. The model used here contains 20,400 grid blocks \((n_x=30, n_y=40, n_z=17)\) and has four production wells and two water injection wells.

Figure 4.1: Synthetic reservoir model with four production wells and two injection wells

Figure 4.2 shows the permeability in the \(x\)-direction for selected layers (layer numbers indicated under each figure). The production wells are completed in layers 1 through 5 and the injection wells in layers 15 through 17.

Figure 4.2: Permeability in the \(x\)-direction for selected layers
For this reservoir model capillary pressure is neglected and the fluid densities are set to be equal. The other fluid and rock-fluid properties are different from those used in Chapter 2. Here, the initial saturations of oil and water are 0.8 and 0.2, respectively, and the residual oil saturation is 0.2. The oil viscosity at standard conditions is 3.0 cp and the water viscosity is 0.5 cp. The relative permeabilities for the oil and water phases are shown in Figure 4.3.

![Relative permeability curves for oil and water](image)

**Figure 4.3:** Relative permeability curves for oil and water

### 4.1.2 Training and Testing Results Using TPWL

To generate the states and Jacobian matrices needed by the TPWL procedure, a number of high-fidelity training simulations are required, as explained in section 3.2.1. The quality of the TPWL representation in the subsequent optimization computations depends on the well conditions applied in the training simulations, so it is important that these conditions be selected carefully. Ideally, the well conditions used in the training simulations should correspond as closely as possible to those encountered during the optimization. At this initial stage, however, the optimal conditions are not known. A possible approach, which we plan to consider in future work, is to ‘re-train’ the TPWL during the course of the optimization. Such a procedure would assure that the TPWL is always trained for states along the optimization trajectory.

Our approach here, however, is more straightforward. In our optimizations, the injection wells are prescribed to have constant bottom hole pressures (BHPs) of 6,000 psia, so this
injection BHP is maintained in all training runs. For the production wells, rather than re-train the TPWL model during the optimization runs, we apply schedules for the producer BHPs in the training runs that we expect to capture the required range of behavior. For the first training simulation, the BHPs of the production wells are held constant at 1,000 psia. For the second training simulation, the producer BHPs are changed every 200 days such that the total flow rate of each producer well is approximately constant at 2,000 stb/d. For the third training run, we vary the BHPs of the producer wells randomly and independently between 2,000 and 4,000 psia. For the fourth training simulation, the producer BHPs are again varied randomly, but this time between 1,000 and 3,000 psia. The four training schedules are shown in Figures 4.4 – 4.7. Because these schedules differ significantly from each other, it is reasonable to expect that the resulting TPWL model can describe flow over a wide variation of producer BHP schedules. We note that these training simulations correspond closely to those used in section 3.2.1 where our goal was to explore the accuracy and robustness of the general TPWL model.

All training simulations were run for 5,000 days with a maximum timestep of 30 days. A total of 752 snapshots for the oil pressure and water saturation states and Jacobian matrices were recorded from these four training runs. Applying the proper orthogonal decomposition approach described in Chapter 2, a reduced basis $\Phi$ containing a total of 400 columns, with 200 columns corresponding to the oil pressure states and 200 to the water saturation states, was constructed. Following the trajectory piecewise linear formulation presented in Chapter 3, we use this basis to project all states and Jacobian matrices into the reduced space.

Prior to using the reduced-space TPWL model (Eq. 3.24) for production optimization computations, it is important to assess the accuracy of the TPWL representation. Because we did not consider this model in Chapter 3, we now evaluate its ability to reproduce results from training and testing simulations. Figures 4.8 and 4.9 present comparisons for oil rate and water rate for the four production wells for training simulation 4, where the solid lines represent the solution using the high-fidelity simulation model (labeled ‘GPRS’) and the circles the reduced-order TPWL representation. There is clearly very close agreement between the high-fidelity results and the TPWL results for all wells. Similar levels of agreement between the high-fidelity and TPWL results are achieved for the other three training simulations.

We next evaluate the accuracy of the TPWL representation for test simulations, which
4.1. OPTIMIZATION PROBLEM 1

Figure 4.4: Producer BHP schedules for training run 1

Figure 4.5: Producer BHP schedules for training run 2

Figure 4.6: Producer BHP schedules for training run 3
CHAPTER 4. OPTIMIZATION USING TPWL

Figure 4.7: Producer BHP schedules for training run 4

Figure 4.8: Oil rate for high-fidelity GPRS and TPWL (training run 4)

Figure 4.9: Water rate for high-fidelity GPRS and TPWL (training run 4)
differ from the training runs. Figures 4.10 – 4.15 show the BHPs for the production wells and the oil production rates for three different testing simulations. Tests 1 and 2 show very close agreement between the high-fidelity GPRS results and the TPWL results. In test 3, producers P1, P2 and P4 are in agreement, though the TPWL results for P3 (red circles) do show some discrepancy with the GPRS results after 1,500 days, though the error is not excessive. These results are representative of the oil and water production rates and water injection rates for the several testing runs considered. Having established a reasonable level of accuracy for the TPWL model, we are now ready to proceed with the optimization computations.

Figure 4.10: Producer BHPs using GPRS and TPWL for test simulation 1

Figure 4.11: Producer oil flow rates using GPRS and TPWL for test simulation 1
CHAPTER 4. OPTIMIZATION USING TPWL

Figure 4.12: Producer BHPs using GPRS and TPWL for test simulation 2

Figure 4.13: Producer oil flow rates using GPRS and TPWL for test simulation 2

Figure 4.14: Producer BHPs using GPRS and TPWL for test simulation 3
4.1. OPTIMIZATION PROBLEM 1

We will now optimize the production well BHPs using the TPWL representation. The objective function is the net present value (NPV) of the reservoir over a period of 3,000 days. Two different cases, corresponding to different oil prices and water costs, will be considered. The discount rate is 10%. Each well setting will persist for 500 days, which means that we have six control variables for each production well (24 total control variables). We will apply two different optimization algorithms. The first algorithm (fmincon in Matlab [47]) is a gradient-based procedure. The gradients in this case are computed numerically using a finite difference approach as applied by Yeten et al. [72, 73]. The second algorithm (patternsearch in Matlab) is a generalized pattern search (GPS). This is a direct search algorithm that applies an adaptive stencil as it moves through the search space. Our specific concern here is not necessarily to establish the better algorithm for this particular problem, but rather to assess the performance of TPWL with two different types of optimization procedures.

For each case we will run the optimization using TPWL and using the high-fidelity model (GPRS). We will in addition apply the optimal producer BHPs determined using the TPWL model to the high-fidelity model in order to obtain a more direct comparison. For both cases the injection wells are kept at constant pressure (6,000 psia), the producer BHPs are constrained to stay between 1,000 psia and 4,000 psia, and the maximum change in BHP from one control step to the next is 500 psia.
4.1.4 Results for Optimization Case 1

For this case the oil price is specified to be $80/stb and the water injection and water production costs are $15/stb. The initial guess for the BHPs of all four production wells is 2,500 psia. Table 4.1 presents the NPV (in $10^6) for the gradient-based method and the generalized pattern search. Initial and final NPV are shown for optimizations using GPRS and TPWL. The final NPV using GPRS with the well settings determined by TPWL, designated ‘GPRS(TPWL)’ in the table, is also presented.

It is evident that the NPVs using GPRS are about 1-2% higher than those computed using TPWL. However, using the final controls from the TPWL optimization in the high-fidelity (GPRS) simulator gives NPVs that differ by only about 0.15% (using the gradient-based method), or are essentially identical (using generalized pattern search), compared to those achieved using GPRS for the optimizations. We see that the gradient-based method gives better results than the generalized pattern search and provides an increase of 11.8% in NPV over the initial guess. The optimized BHPs and the resulting cumulative fluid injection and production are shown in Figures 4.16 and 4.17. These results were generated using the gradient-based method. From Figure 4.16, it is evident that the BHP sequence differs slightly between the GPRS (solid lines) and TPWL (circles) optimizations, but the cumulative production and injection are nonetheless very close as can be observed in Figure 4.17. In this figure the solid lines represent the high-fidelity model (GPRS), the open circles the TPWL model, and the dots the solution using GPRS with the well settings determined by TPWL.

Consistent with the observations in Chapter 3, the CPU requirements for the TPWL and GPRS optimizations differ considerably. Specifically, for the gradient-based optimizations, four iterations were performed and each iteration required 25 simulation runs (for a total of 100 simulations). Each GPRS simulation consumed 6 minutes of CPU time (10 hours for 100 simulations), while each TPWL simulation required only 0.8 seconds (80 seconds for 100 simulations). Thus the runtime speedup using TPWL is about 450. Recall that the overhead associated with TPWL is the equivalent of about eight GPRS simulations.
4.1. Optimization Problem 1

Table 4.1: NPV ($10^6$) for problem 1, case 1 (oil $80/\text{stb}$, produced and injected water $15/\text{stb}$)

<table>
<thead>
<tr>
<th>Simulator</th>
<th>Gradient-based method</th>
<th>Generalized pattern search</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>NPV(initial)</td>
<td>NPV(final)</td>
</tr>
<tr>
<td>GPRS</td>
<td>733.6</td>
<td>820.3</td>
</tr>
<tr>
<td>TPWL</td>
<td>725.2</td>
<td>805.8</td>
</tr>
<tr>
<td>GPRS(TPWL)</td>
<td></td>
<td>819.1</td>
</tr>
</tbody>
</table>

Figure 4.16: Producer BHPs for case 1 (problem 1)

Figure 4.17: Cumulative production and injection for case 1 (problem 1)
4.1.5 Results for Optimization Case 2

For this case the oil price is $60/stb, the water injection cost is $3/stb and the water production cost is $30/stb. The initial guess for the producer BHPs is 2,000 psia. Results for NPV are presented in Table 4.2. These results are consistent with those for case 1, with the NPVs using GPRS approximately 1-2% higher than the NPVs computed using TPWL. Again, however, if we use the final controls from the TPWL optimization in GPRS, we obtain NPVs that are very close to those achieved using GPRS for the optimizations (with differences of 0.1% using the gradient-based method and 0.8% using generalized pattern search). As was observed for case 1, the gradient-based method provides a higher NPV, here achieving an increase of 7.8% over the initial guess.

The optimized BHPs (using the gradient-based method) and the resulting cumulative fluid injection and production are shown in Figures 4.18 and 4.19. As was observed in case 1, the BHP schedule differs slightly between the GPRS and TPWL optimizations, but the cumulative production and injection are in close agreement. Less water is produced here than in case 1 because of the higher cost of produced water ($7.728 \times 10^6$ stb in case 2 compared to $9.271 \times 10^6$ stb in case 1). We note finally that the timings for this case are essentially the same as those for case 1.

Table 4.2: NPV ($10^6$) for problem 1, case 2 (oil $60/stb$, produced water $30/stb$ and injected water $3/stb$)

<table>
<thead>
<tr>
<th>Simulator</th>
<th>Gradient-based method</th>
<th>Generalized pattern search</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>NPV(initial)</td>
<td>NPV(final)</td>
</tr>
<tr>
<td>GPRS</td>
<td>636.4</td>
<td>685.8</td>
</tr>
<tr>
<td>TPWL</td>
<td>628.9</td>
<td>676.3</td>
</tr>
<tr>
<td>GPRS(TPWL)</td>
<td>684.9</td>
<td></td>
</tr>
</tbody>
</table>
4.1. OPTIMIZATION PROBLEM 1

Figure 4.18: Producer BHPs for case 2 (problem 1)

Figure 4.19: Cumulative production and injection for case 2 (problem 1)
4.2 Optimization Problem 2

We next consider the determination of optimal production well BHPs for the reservoir model described in section 3.2.1 (SPE 10 model containing 24,000 cells). The objective function is the net present value (NPV) of the reservoir over a period of 3,000 days and two different cases, corresponding to different oil prices and water costs, will again be considered. The discount rate (10\%) and the total number of control variables (24) are the same as were used in problem 1. For this and subsequent optimizations, we apply only the gradient-based optimization algorithm (fmincon in Matlab).

As in problem 1, 100 simulations (four iterations of the optimization algorithm) were performed using TPWL and the high-fidelity model (GPRS). The optimal producer BHPs determined using the TPWL model are also applied to the high-fidelity model. For this reservoir model the injection wells are kept at a constant pressure of 10,000 psia and the producer BHPs are constrained to stay between 1,000 psia and 4,000 psia with the maximum change in BHP from one control step to the next being 500 psia. For the TPWL optimizations, we use the TPWL model developed in section 3.2.1 (see section 3.2.1 for a description of the training runs).

4.2.1 Results for Optimization Case 1

For this case the oil price is specified to be $80/stb and the water injection and water production costs are $10/stb. The initial guess for the BHPs of all four production wells is 2,500 psia. Table 4.3 presents the NPVs (in $10^6$) computed using the gradient-based method. Initial and final NPV are shown for optimizations using GPRS and TPWL, as well as the final NPV using GPRS with the well settings determined by TPWL, designated ‘GPRS(TPWL).’

From the table we see that the NPV using GPRS is about 0.66\% higher than that computed using TPWL. However, using the final controls from the TPWL optimization in the high-fidelity simulator gives an NPV that is within 0.1\% of that achieved using GPRS for the optimizations. The optimized BHPs are shown in Figure 4.20, where it is apparent that the BHP sequences show small differences. The cumulative production and injection are nonetheless very close, as shown in Figure 4.21. The runtime speedup using TPWL was a factor of 500, the same as was reported in section 3.2.1.
Table 4.3: NPV ($10^6$) for problem 2, case 1 (oil $80$/stb, produced and injected water $10$/stb)

<table>
<thead>
<tr>
<th>Simulator</th>
<th>NPV(initial)</th>
<th>NPV(final)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GPRS</td>
<td>655.5</td>
<td>682.1</td>
</tr>
<tr>
<td>TPWL</td>
<td>648.9</td>
<td>677.6</td>
</tr>
<tr>
<td>GPRS(TPWL)</td>
<td></td>
<td>681.6</td>
</tr>
</tbody>
</table>

Figure 4.20: Producer BHPs for case 1 (problem 2)

Figure 4.21: Cumulative production and injection for case 1 (problem 2)
4.2.2 Results for Optimization Case 2

For this case we decreased the oil price to $60/stb, the water injection cost to $5/stb, and increased the water production cost to $15/stb. The initial guess for the producer BHPs is 1,000 psia and the results for NPV are presented in Table 4.4. These results are different from those for case 1, with the NPV using GPRS approximately 0.06% lower than the NPV computed using TPWL. Using the final controls from the TPWL optimization in the high-fidelity simulator gives an NPV that is about 0.41% higher than that achieved using GPRS for the optimizations.

The optimized BHPs and the resulting cumulative fluid injection and production are shown in Figures 4.22 and 4.23. There are some significant differences in the BHP schedules between the GPRS and TPWL optimizations for production wells P1, P2 and P3. However, the cumulative production and injection are in close agreement. Less water is produced here than in case 1 because of the higher cost of produced water. We note finally that the timings for this case are essentially the same as those for case 1.

Table 4.4: NPV ($10^6$) for problem 2, case 2 (oil $60/stb$, produced water $15/stb$ and injected water $5/stb$)

<table>
<thead>
<tr>
<th>Simulator</th>
<th>Gradient-based method</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>NPV(initial)</td>
</tr>
<tr>
<td>GPRS</td>
<td>472.7</td>
</tr>
<tr>
<td>TPWL</td>
<td>467.0</td>
</tr>
<tr>
<td>GPRS(TPWL)</td>
<td></td>
</tr>
</tbody>
</table>
Figure 4.22: Producer BHPs for case 2 (problem 2)

Figure 4.23: Cumulative production and injection for case 2 (problem 2)
4.3 Optimization Problem 3

The optimization procedure is now applied to the 79,200-cell reservoir model described in section 3.2.2 (60 × 220 × 6 SPE 10 model). The optimization parameters, the producer BHP range and the maximum change in BHP are the same as were used for optimization problem 2, though the injection wells in this case are kept at a constant pressure of 8,000 psia. Four iterations of the gradient-based algorithm are again applied.

4.3.1 Results for Optimization Case 1

For this case the oil price is specified to be $80/stb, the water injection and water production costs are $15/stb, and the initial guess for the BHPs of all four production wells is 2,500 psia. Table 4.5 presents the NPV (in $10^6). The final NPV using GPRS is about 1.25% higher than that computed using TPWL. However, using the final controls from the TPWL optimization in GPRS gives an NPV that is 0.7% higher than that using GPRS. From Figure 4.24, it is clear that the BHP sequence between the GPRS and TPWL optimizations is very close for production wells P2, P3 and P4, but differs significantly for well P1. Figure 4.25 shows once more that the cumulative production and injection are very close. A factor of 2,000 runtime speedup was achieved using TPWL, which is the same as reported in section 3.2.2.

Table 4.5: NPV ($10^6) for problem 3, case 1 (oil $80/stb, produced and injected water $15/stb)

<table>
<thead>
<tr>
<th>Simulator</th>
<th>NPV(initial)</th>
<th>NPV(final)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GPRS</td>
<td>643.7</td>
<td>696.4</td>
</tr>
<tr>
<td>TPWL</td>
<td>638.9</td>
<td>687.8</td>
</tr>
<tr>
<td>GPRS(TPWL)</td>
<td></td>
<td>701.2</td>
</tr>
</tbody>
</table>
4.3. OPTIMIZATION PROBLEM 3

Figure 4.24: Producer BHPs for case 1 (problem 3)

Figure 4.25: Cumulative production and injection for case 1 (problem 3)
4.3.2 Results for Optimization Case 2

For this case the oil price and water injection cost are decreased to $60/stb and $2/stb, respectively, and the water production cost is increased to $20/stb. The initial guess for the producer BHPs is 2,000 psia. Results for NPV are presented in Table 4.6. The final NPV using GPRS is about 1.14% higher than that computed using TPWL. Using the final controls from the TPWL optimization in GPRS gives an NPV that is essentially the same as that achieved using GPRS for the optimizations.

The optimized BHPs and the resulting cumulative fluid injection and production are shown in Figures 4.26 and 4.27. As was observed in case 1, the BHP schedule between the GPRS and TPWL optimizations differs the most for well P1. Consistent with case 1, the cumulative production and injection from the two simulations are in close agreement.

Table 4.6: NPV ($10^6$) for problem 3, case 2 (oil $60/stb$, produced water $20/stb$ and injected water $2/stb$)

<table>
<thead>
<tr>
<th>Simulator</th>
<th>Gradient-based method</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>NPV(initial)</td>
</tr>
<tr>
<td>GPRS</td>
<td>587.2</td>
</tr>
<tr>
<td>TPWL</td>
<td>583.9</td>
</tr>
<tr>
<td>GPRS(TPWL)</td>
<td></td>
</tr>
</tbody>
</table>
4.3. OPTIMIZATION PROBLEM 3

Figure 4.26: Producer BHPs for case 2 (problem 3)

Figure 4.27: Cumulative production and injection for case 2 (problem 3)
4.4 Multiobjective Optimization

Finally, we apply TPWL for a more challenging multiobjective optimization in which we consider conflicting goals. Specifically, we seek to maximize cumulative oil production while minimizing cumulative water injection. Thus the goal of the optimization is to determine the Pareto front on a plot of cumulative oil produced versus cumulative water injected. Any point on this curve represents the ‘most’ oil (as determined from the optimization) that can be produced for the corresponding amount of water injected. The curve can also be viewed as providing the least amount of water that must be injected to produce a given amount of oil. The solution of this optimization problem is computationally demanding if the high-fidelity model is used, as the optimization procedure must be run for many points along the Pareto front.

We consider the model used in optimization problem 2. The model contains 24,000 grid blocks and is described in section 3.2.1. The multiobjective optimization seeks to maximize the net present value (NPV) of the reservoir over a period of 3,000 days. The discount rate is 10% and the cost of both the produced and injected water is fixed at $10/stb. The oil price is varied from $10/stb to $150/stb in increments of $2/stb, and the optimization is performed for each oil price.

As in problem 2, the injection wells are specified to operate at 10,000 psia and the minimum and maximum producer BHPs are prescribed as 1,000 psia and 4,000 psia respectively. The producer BHPs are updated more frequently in this case (every 250 days) than in problem 2. As the simulation is run for 3,000 days, there are a total of 48 control variables (12 for each production well). We further specify that the maximum change in BHP from one control step to the next is 250 psia. The gradient-based algorithm is applied and a total of four iterations of the optimization are performed, meaning that each point on the curve requires 196 simulations. The initial guess for the producer BHPs is 2,500 psia.

The optimization results are presented in Figure 4.28, where we plot cumulative oil produced versus cumulative water injected. The ×’s represent TPWL solutions (71 points were generated), while the blue dots represent high-fidelity results computed using the optimal well settings as determined from the TPWL optimizations. For a few points (shown as red triangles) we performed the full optimization using the high-fidelity model. The general correspondence between these three sets of points is quite close, indicating the applicability of the TPWL procedure for this application.
4.4. **MULTIOBJECTIVE OPTIMIZATION**

The speedup achieved by TPWL for this case is very significant. A total of 13,916 simulations are required for the multiobjective optimization. The TPWL computations required 0.85 seconds per run, while the high-fidelity simulations consumed 430 seconds per run. Thus the full optimization entailed 3.3 hours using TPWL. We did not perform the full optimization using the high-fidelity model – had we done this, it would have required about 69.3 days. These timings highlight the potential benefits of the TPWL procedure for challenging multiobjective optimization problems.

In this chapter, we applied the TPWL model for several production optimization problems. We saw consistently that, although there were some differences (e.g., 1%) between the TPWL and high-fidelity results for optimized NPV, when the controls from the TPWL optimization were used in high-fidelity simulations, the resulting NPVs were nearly identical. Our overall conclusion is that the TPWL representation appears to be very well suited for use in computational optimization procedures, at least for the class of problems considered here.

![Figure 4.28: Optimized cumulative oil production versus cumulative water injected](image)
Chapter 5

Summary and Future Work

This dissertation addressed the application of reduced-order modeling procedures for reservoir simulation. In this chapter this work is summarized and recommendations for future research are presented. We reiterate that, although our interest here is the application of ROM for oil reservoir simulation, our findings are useful for other areas such as aquifer management and the geological storage of carbon dioxide.

5.1 Summary and Conclusions

We summarize this work as follows:

POD-Based Reduced-Order Modeling

- A reduced-order modeling (ROM) procedure based on the proper orthogonal decomposition (POD) technique was extended, incorporated into a general purpose simulator, and applied for subsurface flow applications. The POD procedure provides a mechanism to extract a reduced-order basis of small dimension that contains the key features of the states encountered during the simulation of a full (high-fidelity) reservoir model. This requires the recording of snapshots of the solution states (oil pressure and water saturation) at many time steps during a ‘training’ simulation followed by a singular value decomposition of the resulting covariance or data matrix. Use of this basis in subsequent simulations provides runtime speedups, assuming the dimensions of the basis matrix are sufficiently small.
CHAPTER 5. SUMMARY AND FUTURE WORK

• Two procedures were introduced to decrease the size of the basis matrix. A snapshot clustering method enables the use of fewer vectors in the reduced-order basis. Further reduction of the computational burden was achieved through application of the missing point estimation (MPE) technique. Using a condition number criterion, MPE allows the most important grid blocks to be selected, leading to a reduction in the number of rows in the basis matrix.

• Proper orthogonal decomposition, clustering, and missing point estimation are all off-line (pre-processing) computations and were implemented in a stand-alone Matlab application. The reduced-order modeling framework was implemented in Stanford’s general purpose research simulator (GPRS). Using this implementation ROMs with different complexities can be applied, specifically, ROM with POD only, ROM using clustered snapshots and POD, and ROM using clustered snapshots, POD and MPE, for oil-water flow simulations.

• All of these ROM procedures were tested using a realistic 3D reservoir model with 60,000 grid blocks. This corresponds to 120,000 unknowns (oil pressure and water saturation in each block) at each time step. The ROMs were able to capture the dynamics of these models using only about 40 unknowns (the exact number varied depending on the specific ROM procedure). Results for production and injection rates, which are typically the key inputs to an optimization procedure, were shown to be in fairly close agreement with reference (high-fidelity) simulation results for different production schedules. For all cases the same sets of basis vectors were used, meaning that only one full-order simulation was required to generate the information needed to construct the ROMs. This indicates that these models retain a reasonable level of robustness, which is important if they are to be used in optimization applications.

• Computational speedups for the ROM using clustered snapshots, POD and MPE, evaluated relative to full-order GPRS simulations using a specialized linear solver and preconditioner combination (GMRES solver and CPR preconditioner), were between 6 and 10 depending on the case. Comparison to a full-order GPRS simulation using a much simpler preconditioner (ILU(0)) showed a speedup of about 700. This highlights the fact that the ROM procedures considered here are very well suited for situations where the linear solver occupies the great majority of the computational time. Otherwise, the maximum speedup attainable is more limited.
• The POD-based ROM procedure was shown to be less effective in cases with strong
density differences between phases, highly nonlinear relative permeability curves, or
significant variation in injection BHPs. For such cases, improved treatments are re-
quired.

TPWL Formulation

• We also developed a trajectory piecewise linearization (TPWL) procedure for the
modeling of two-phase flow in subsurface formations. This ROM technique entails
representation of new states in terms of linear expansions around states previously
simulated and saved during training runs. The method is tractable and efficient
because all computations are performed in a low-dimensional space generated using
the POD basis matrix.

• TPWL was applied to heterogeneous reservoir models derived from the SPE 10 and
Stanford VI reservoir models. Reasonable levels of accuracy in TPWL computations
were observed for oil and water production rates and water injection rate for test cases
in which the production well bottom hole pressures were within the general range of
the training simulations. When the production well BHP schedule in the test runs
differed significantly from that of any of the training runs, the accuracy of the TPWL
model degraded.

• The preprocessing overhead required for the construction of the TPWL model corre-
sponds to about the time required to simulate 6-8 high-fidelity models. The TPWL
model provided runtime speedups of about 500-2000 for the cases considered if mass
balance error was not computed. Speedups were less dramatic but still very substanc-
tial if mass balance error was assessed frequently, though in practice this error need
be computed only occasionally.

Use of TPWL Model for Optimization

• The TPWL procedure was applied for waterflood optimization using three hetero-
geneous 3D models containing 20,400, 24,000 and 79,200 grid blocks. Each model
contained two injection wells and four production wells. Two different optimization
cases, corresponding to different oil prices and water costs, were considered for each
reservoir model. The BHPs for the four production wells at six different times were
determined in the optimizations using a gradient-based algorithm with gradients computed numerically and a generalized pattern search algorithm (the latter algorithm was applied only for the reservoir model with 20,400 grid blocks).

- Results for net present value using the controls determined from TPWL optimizations in GPRS simulations were shown to be very close to those achieved by performing the optimizations with the high-fidelity model. Optimization using TPWL provided runtime speedups of a factor of 450 – 2,000, depending on the reservoir model used.

- A significant advantage of the TPWL approach is that, once the preprocessing computations are completed and the TPWL model is constructed, additional optimizations or multiobjective optimization can be run at very little cost. Thus, the sensitivity of the optimized BHPs to oil price, water costs, constraints, etc., can be assessed inexpensively. The optimizations can also be run using a number of different initial guesses. Runs of this type will be very expensive if the high-fidelity model is used. We demonstrated the use of the TPWL procedure for a multiobjective optimization problem to determine the Pareto front. Limited high-fidelity simulations suggest that the TPWL results are of sufficient accuracy for this problem.

5.2 Recommendations for Future Work

- Our current procedure for specifying the controls (BHP settings) used in the training runs is heuristic, so it will be useful to explore more rigorous approaches. An interesting starting point might be the work of Kunisch and Volkwein [43], who address the problem of un-modeled dynamics, as occurs when the optimum solution is considerably different from the training simulation. Another approach that employs a greedy algorithm for the selection of snapshots in high-dimensional space was proposed by Bui-Thanh et al. [15].

- The accuracy and runtime speedup provided by the POD-based ROM are closely related with the amount of energy retained by the basis functions selected, as explained in section 2.3. The development of a methodology to evaluate the compromise between accuracy and speedup could give a reduced-order basis with the optimum number of basis functions.
• The models considered here (oil-water systems, capillary pressure neglected) are still relatively simple, in terms of multiphase flow physics, compared to many of the models that arise in practice. The presence of strong gravitational effects as well as high degrees of nonlinearity in the relative permeability functions was shown to limit the effectiveness of the POD-based ROM procedures implemented in this work. Variable injector BHPs also led to reduced accuracy. These issues require further investigation. Alternatives to the POD approach used here should be considered.

• Other strategies for using TPWL in optimizations should be studied. For example, additional high-fidelity training runs could be performed occasionally during the course of the optimization to ensure that the TPWL model retains accuracy. Along these lines, it will additionally be useful to develop approaches for estimating error in the TPWL predictions.

• The TPWL method and the underlying POD procedure should be extended for use in three-phase flow problems. They should also be tested for larger models containing $O(10^5)$ grid blocks and many wells.

• All of the ROM procedures developed in this work considered wells to be controlled by bottom hole pressure (BHP). Extending the method for wells under flow rate control will broaden the applicability of the methods.

• It will be useful to consider the use of POD-based ROMs and/or TPWL models for the combined production optimization – history matching problem (i.e., closed-loop reservoir modeling). This will require the development of procedures for updating the reduced basis matrix.
Nomenclature

Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>BHP</td>
<td>bottom hole pressure</td>
</tr>
<tr>
<td>CPR</td>
<td>constrained pressure residual</td>
</tr>
<tr>
<td>CVT</td>
<td>centroidal Voronoi tesselation</td>
</tr>
<tr>
<td>GPRS</td>
<td>general purpose research simulator</td>
</tr>
<tr>
<td>LTI</td>
<td>linear time invariant</td>
</tr>
<tr>
<td>LTV</td>
<td>linear time variant</td>
</tr>
<tr>
<td>MBE</td>
<td>material balance error</td>
</tr>
<tr>
<td>MPE</td>
<td>missing point estimation</td>
</tr>
<tr>
<td>NPV</td>
<td>net present value</td>
</tr>
<tr>
<td>POD</td>
<td>proper orthogonal decomposition</td>
</tr>
<tr>
<td>ROM</td>
<td>reduced-order modeling or reduced-order model</td>
</tr>
<tr>
<td>SQRD</td>
<td>sequential QR decomposition</td>
</tr>
<tr>
<td>SVD</td>
<td>singular value decomposition</td>
</tr>
<tr>
<td>TPWL</td>
<td>trajectory piecewise linearization</td>
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Variables

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a, b$</td>
<td>Corey exponents</td>
</tr>
<tr>
<td>$A$</td>
<td>area of grid block face</td>
</tr>
<tr>
<td>$A$</td>
<td>accumulation term</td>
</tr>
<tr>
<td>$B$</td>
<td>formation volume factor</td>
</tr>
<tr>
<td>$D$</td>
<td>depth</td>
</tr>
<tr>
<td>$C$</td>
<td>covariance matrix</td>
</tr>
</tbody>
</table>
NOMENCLATURE

\( D \)  accumulation matrix for incompressible systems
\( E \)  energy
\( f_w \)  Buckley-Leverett fractional flow function
\( F \)  flow term or flux
\( g \)  gravitational acceleration
\( g \)  residual vector
\( J \)  Jacobian matrix
\( k \)  permeability tensor
\( K \)  condition number
\( k_r \)  relative permeability
\( \ell \)  number of columns retained in the reduced basis
\( N_c \)  number of grid blocks
\( p \)  pressure
\( q \)  source term
\( Q \)  well flow rate
\( Q \)  source/sink term
\( S \)  saturation
\( S \)  number of snapshots recorded
\( t \)  time
\( T \)  transmissibility matrix
\( u \)  Darcy velocity or well controls
\( V \)  grid block volume
\( W \)  well index
\( x \)  vector of primary unknowns
\( X \)  data matrix
\( z \)  reduced vector of primary unknowns

Greek

\( \delta \)  solution update
\( \lambda \)  mobility or eigenvalues
\( \mu \)  viscosity
\( \rho \)  density
\( \phi \)  porosity
**NOMENCLATURE**

- \( \Phi \) orthonormal reduced basis matrix
- \( \Phi_w \) \( \Phi \) with only well block entries
- \( \Phi^* \) \( \Phi \) after applying MPE
- \( \Psi \) eigenvectors

**Subscripts**
- \( i \) grid block index
- \( j \) phase
- \( \ell \) number of basis functions retained
- \( o \) oil phase
- \( p \) pressure
- \( r \) reduced representation
- \( s \) saturation
- \( t \) total
- \( w \) water phase

**Superscripts**
- \( i \) saved state in the training simulations for TPWL
- \( m \) well number
- \( n \) time level
- \( v \) iteration level
- \( w \) well
- \( 0 \) reference
Bibliography


