PROPER ORTHOGONAL DECOMPOSITION FOR PRESSURE PRECONDITIONING FOR THE GMRES ALGORITHM.

A Thesis

by

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ABSTRACT

The linear solver in a typical reservoir simulator consumes around 60 to 70 % of the total simulation time. To speed up the solution of the linear systems we will use a two stage preconditioner, where the first stage is the ILU preconditioner and the second stage is obtained with a technique of Reduction of Order Modelling (ROM) called Proper Orthogonal Decomposition (POD). The benefits of using this method is that it is relatively easy to implement because it doesn't require big modifications in existing code. There is already research in this area with positive results, but the method has been tested with the Richardson Algorithm. This is not a very realistic scenario given that there are better solvers widely available. The objective of this thesis is to test the method with the Generalized Minimal Residual Method (GMRES). The results validate the findings that two stage preconditioner improves the performance of the Richardson algorithm, however it doesn't improve the performance of the GMRES algorithm. The drawback is that although the two stage preconditioner increases convergence it is too costly to compute. And the time saved by the decrease in the number of iterations is offset by the increase in time in preconditioner computation.

DEDICATION

I dedicate this thesis to my brothers Luis and Fernando.

ACKNOWLEDGEMENTS

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NOMENCLATURE

POD	Proper Orthogonal Decomposition
SVD	Singular Value Decomposition
ROM	Reduced Order Modeling
ILU	Incomplete LU Factorization
LU	Lower Diagonal, Upper Diagonal
GMRES	Generalized Minimum Residual Method
CPR	Constrained Pressure Residual
AMG	Algebraic Multigrid
M_{ILU}	Incomplete LU Preconditioner
M_{POD}	POD Preconditioner
$M_{POD+ILU}$	Two Stage POD + ILU Preconditioner
M^{-1}	Inverse of the Preconditioner
Φ	Orthogonal Basis
Ψ	Projection Operator
P	Pressure
S	Saturation
P_o	Oil Pressure
S_w	Water Saturation
U	Left Basis Vectors
S	Diagonal Matrix With Singular Values
V	Right Basis Vectors

σ	Singular Value
ρ	Density
c	Compressibility
ϕ	Porosity
μ	Viscosity
k	Permeability
g	Gravity
z	Depth
q	Flow
t	Time
$\|\| \cdot \|\|$	Matrix and Vector Norm

TABLE OF CONTENTS

Page

LIST OF FIGURES

LIST OF TABLES

1. INTRODUCTION

1.1 Introduction

In the early stages of reservoir simulation development, the reservoir models were small and two dimensional, with 10^2 to 10^3 cells. Current modern reservoir simulators run giant three dimensional reservoir models with a number of cells in the order of 10^6 and upwards [3, 4]. Depending on the type of discretization of the partial differential equations and on the number of fluid phases being simulated, this leads to very large systems of linear equations that have to be solved for each timestep. The capability that we have today of performing this type of simulations is possible thanks to the steady increase in the computing power of computers and the availability of high performance computing.

Despite all of this computing power, it becomes time consuming to run simulations in the context of history matching and optimization , where thousands of simulations must be run to obtain the solution to a problem [4]. Therefore, it is important to find ways to speed up the solution of the simulations. We should point out that this is not a new problem, and many techniques have been developed to achieve this.

The bottleneck of the typical reservoir simulator is the linear solver, which consumes around 60 to 70% of the total simulation time [5] . An improvement in the linear solver improves the simulator greatly, so in this thesis we will focus on enhancing the preconditioner for the linear system solvers. Some of the methods to decrease the simulation time are preconditioning techniques and reduced order modeling (ROM) techniques. Preconditioning consists of multiplying the linear system by a preconditioner matrix that makes the system easier to solve and increases the order of convergence of the iterative solvers [6]. There are many types of precondi-

tioners, but the most widely used in the context of reservoir simulation is the ILU preconditioner (M_{ILU}) [5]. On the other hand, ROM reduces a high order system to a low order system that accurately represents the main characteristics of the high order model but that is faster to solve due to its lower number of equations [7, 5, 8, 9]. This leads to cases were it is possible to decrease the number of equations that describe the reservoir from hundreds of thousands to a few dozen equations, that is a three to four fold reduction [4].

One of the disadvantages of ROM techniques is that they require to make modifications to the linear solver module of the simulator [10], and depending on the simulator this may or may not be straightforward to implement.

In this thesis we will study the pressure preconditioner proposed by Rui in [10]. It is derived from the ROM technique called Proper Orthogonal Decomposition (POD), and it has the advantage that its implementation in the simulator does not require to make intrusive modifications to existing code. This preconditioner also has the potential of performing better than typical preconditioners, such as M_{ILU}. The goal is to enhance the capabilities of M_{ILU} by means of POD.

1.2 Literature Review

Reservoir simulation began in the mid 1950's and since its inception it has become an important quantitative and qualitative tool for predicting the flow of the different fluid phases in the subsurface [3]. Reservoir simulation has evolved from handling two dimensional reservoir models with simple geometry to solving highly complex heterogenoeus models with complex geometry and millions of cells .

The main advances in reservoir simulation have been closely tied to advances in linear solvers and preconditioning techniques. This is because about 60 % and up to 90 % of the total simulation time is spent solving the linear system of equations

resulting from the discretization of the partial differential equations that describe the porous media fluid flow [5, 11]. Solving these linear systems is challenging because of their size and because they are highly sparse.

The linear solvers can be classified as either direct solvers or iterative solvers. The direct solvers, such as Gaussian elimination and LU factorization, are only suitable for small matrices because they consume much more resources than iterative solvers and also because they scale poorly with the number of cells [12]. For that reason iterative solvers are preferred.

There are many iterative linear solvers but the most widely used in reservoir simulation are the Generalized Minimal Residual Method (GMRES) and ORTHOMIN [13, 14]. However , the most advanced solvers belong to the Algebraic Multigrid (AMG) Methods [15, 16, 17, 18]. According to the authors in [19], AMG methods are an "ideal solver for large-scale scientific simulation", because they can solve linear systems with N unknowns with $\mathcal{O}(N)$ work. Also, with the use of parallel computing, ever larger problems can be solved on proportionally larger parallel computers in constant time. Figure 1.1 shows how the computational requirements of the algorithms scale with the number of cells in the model. The "x" axis of the plot correspond to the size of the linear system being solved, and the "y" axis to the the number of operations required to solve the system. As the size of the system increases the number operations, and the time, required to solve the system increase with respect to the relation expressed in the $\mathcal{O}$ notation. Linear solvers such as Gaussian elimination, are $\mathcal{O}(N^3)$, which means that the time required to solve the linear system increase in cubic form as the size of the model increase. GMRES and ORTHOMIN are $\mathcal{O}(N^2)$. And, as stated above, AMG methods are $\mathcal{O}(N)$, which makes them the best option.

As mentioned earlier, the performance of the iterative solvers can be improved

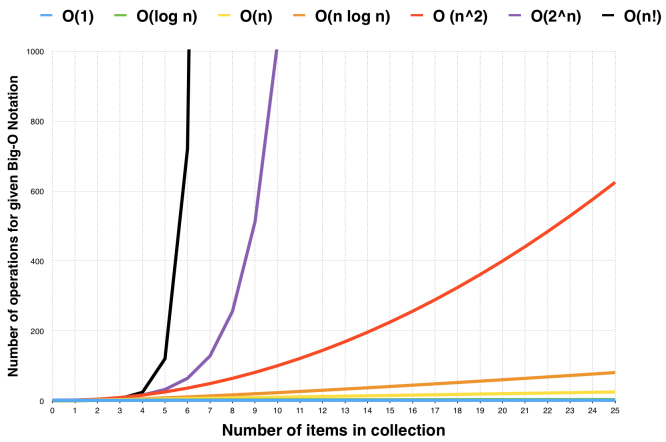


Figure 1.1: Big O complexity and its effect in the number of computations. From [1].

with the use of preconditioners. The use of preconditioners is not something new and they have been studied for decades [20, 21, 22, 23]. The main effect of the preconditioner is that it decreases the condition number of the of the problem and increases the rate of convergence of the solver, thus reducing the number of iterations required to solve the linear system. The most used preconditioners in reservoir simulation are the incomplete LU preconditioner, Nested Factorization and Constrained Pressure Residual Preconditioning (CPR) [24].

The ILU preconditioner is the most basic of the three, and its available is practically all simulator platforms. This preconditioner is obtained with the Cholesky factorization of the linear system in one upper and one lower diagonal matrix. The nested factorization differs from the previous preconditioner in that the preconditioning matrix is not formed from striclty upper and lower factors. It constructs block lower and upper factors using a procedure which adds one dimension at a time to the preconditioning matrix [25].

Finally, the state of the art in preconditioners is the CPR preconditioner [4]. The

CPR preconditioner is more efficient that the ILU preconditioner. The CPR preconditioner is a two-stage preconditioner, which solves a submatrix from the pressure equation using multigrid methods and then uses the ILU methods to solve the whole system [26].

Preconditioners can also be obtained by exploiting the nature of the problem being solved, this type of preconditioners are called called physics based preconditioners. In [10] a POD based pressure preconditioner for a reservoir simulator is derived. From this, a two stage preconditioner $M^{-1}_{ILU+POD}$ was created. This preconditioner was tested in a water flooding simulation with the Richardson algorithm as the linear iterative solver. The findings were that the $M^{-1}_{ILU+POD}$ preconditioner increases the order of error reduction in the iterative solver. Nevertheless, the Richardson algorithm is not the state of the art in iterative linear solvers, as explained above the most sophisticated solver is AMG, but because this solver is not available in all commercial and research simulators, the most widely available and second best option would be the GMRES + ILU combination [4]. That is the reason that the focus of this thesis is in that solver and preconditioner combination and how to improve upon them.

Regarding ROM and POD, the application of model reduction techniques, and in specific, the Proper Orthogonal Decomposition technique is very wide. It has been used to create reduced order models of the pressure and saturation matrix in reservoir simulators [4]. It has been used to replace the first stage preconditioner of a reservoir simulator [27], it has also been used in history matching, in inverse problems, and in probabilistic inverse modeling to speed up Monte Carlo simulations.

We will implement proper orthogonal decomposition to reservoir simulation with the snapshot based algorithm. There are many recommendations for the successful implementation of this algorithm found in the literature. To this end, it was

determined that the number of basis vectors required to capture the behavior of the system is at most two times the number of wells in the reservoir [27]. For the case where the pressure and saturation equations are uncoupled, snapshots of both variables are collected and then the POD procedure is applied to each set of snapshots independently to precondition each linear system [4]. It was also found that clustering of the snapshots with the k-means method is beneficial. The clustering is relatively inexpensive and allows for a more representative basis space and decrease the number of basis vectors required in the reduced basis matrix [4]. Another practical recommendation was to compute the quality of the basis, it is inexpensive to compute and it indicates if the current reduced basis is a good basis for the current problem being solved [10].

1.3 Scope of this Thesis

The scope of this thesis is to implement a physics based preconditioner derived with the aid of POD in the Matlab Reservoir Simulation Toolbox (MRST), and to test whether the GMRES solver performs better with it than with the most commonly used preconditioner M_{ILU}.

We began with a literature review in Section 1.2 to explore the state of the art in linear solvers and preconditioners in reservoir simulators. Then, in Section 3, we will introduce Proper Orthogonal Decomposition and we will use this technique to derive a preconditioner. To this end, we will also suggest a framework, or step by step procedure, to implement this method in the already existing reservoir simulator MRST without tedious modifications of the original code. In Section 4, this framework is first tested in a simple square reservoir model with increasing geometric complexity to study the conditions in which this preconditioner performs better. Then, we will test the framework in a realistic reservoir model. We will also compare the two

preconditioners with two linear solvers, the Richardson algorithm and the GMRES method. Finally, Section 5 contains the conclusions and recommendations for future work in this topic.

2. LINEAR SOLVERS AND RESERVOIR SIMULATION

In this section we will introduce linear solvers and preconditioners. And we will focus on the iterative solvers such as Richardson iteration and GMRES. We will also give an overview of the reservoir simulator and then we will explain where the linear solver and preconditioner come into play. We will also show how to obtain the discretized version of the partial differential equation (PDE) that describes the flow of oil and water in the subsurface.

2.1 Linear Solvers

For the following explanations we will consider the linear system of equations in Equation (2.1). Where $A \in \mathbb{R}^{n \times n}$ is a non-sigular square matrix. And $x \in \mathbb{R}^n$, $b \in \mathbb{R}^n$, are vectors. We wish to solve for the vector of unknowns x.

$$Ax = b \tag{2.1}$$

A linear solver is an algorithm that solves for the vector of unknowns, x. There are many linear solvers, but they can be classified as either direct or iterative. As mentioned in Section 1.2 the direct solvers are not suitable for solving the large system of equations in a reservoir simulator.

2.1.1 Iterative Solvers

The two iterative solvers that are going to be considered in this thesis are the Richardson iteration and the Generalized Minimal Residual Method (GMRES). The algorithms are shown in pseudocode in Algorithm 2.1 and Algorithm 2.2. For an in depth explanation of the solution of linear systems in reservoir simulation please

refer to [11].

Algorithm 2.1 Richardson algorithm

1: $A, b \leftarrow given$
2: $k \leftarrow 0$, initialize iteration counter
3: $tol \leftarrow$ set error tolerance
4: $x^0 \leftarrow$ initial guess
5: $r_0 \leftarrow ||b - Ax^0||$
6: **while** *(error* $<$ *tol)* **do**:
7: $\quad x^{k+1} \leftarrow x^k + (b - Ax^k)$
8: $\quad k \leftarrow k + 1$
9: $\quad$ error $\leftarrow \frac{||b-Ax||}{||r_0||}$

A concept that is going to become useful in Section 4 is that of the order of error reduction. The residual error is defined as Equation (2.2), where the exponent k of vector x denotes the iteration number. If we make a plot of the log of residual error in the y axis and the iteration number in the x axis, as in Figure 2.1, we can see how rapidly the residual error is decreased. The slope of that plot is called the order of error reduction. The higher this number is the better, because it means that less iterations, and therefore less computation time, is required to reach the solution of the linear system.

$$\text{residual error} = \frac{||b - Ax^k||}{||b - Ax^0||} \tag{2.2}$$

The data in Figure 2.1 comes from solving a random linear system of equations with the Richardson solvers, and plotting the residual error after each iteration. As it is expected, the order of error reduction is higher when the system is preconditioned.

Algorithm 2.2 GMRES from [11]

1: $x \leftarrow$ initial guess
2: $r^0 \leftarrow b - Ax^0$
3: $\beta = ||r^0||_2$
4: $v^1 = \frac{r^0}{\beta}$
5: For the$(k+1) \times kmatrix H^k = h_{ij}, set H^k = 0$
6: **for** j = 1,2,...,k **do**
7: $w^j = Av^j$
8: $h_{ij} \leftarrow (v^i)^T w^j$for $i = 1, 2, ..., j$
9: $w^j \leftarrow w^j - \sum_{i=1}^{j} h_{ij} v^i$
10: $h_{j+1,j} \leftarrow ||w^j||_2$
11: **if** $h_{j+1,j} = 0$ **then**
12: $k = j$
13: **else**
14: $v^{j+1} = \frac{w^j}{h_{j+1,j}}$
15: $q^k \leftarrow min(||\beta e_1 - H^k q^k||_2)$
16: $x^k = x^0 + V^k q^k$

2.2 Preconditioners

In this section we will give a small introduction to preconditioners and in specific to the M_{ILU} preconditioner. For the linear system (2.1), the condition number is defined as (2.3), where $||\cdot||$ is a matrix norm. The condition number gives an estimation of the loss of accuracy when solving the linear system (2.1). If the condition number is (2.4), then we can estimate a loss of accuracy of k digits. If the condition number is infinite the linear system is singular and can't be solved. When the condition number is "too large" then the system is ill conditioned [28].

$$cond(A) = ||A|| \cdot ||A^{-1}|| \tag{2.3}$$

$$cond(A) = 10^k \tag{2.4}$$

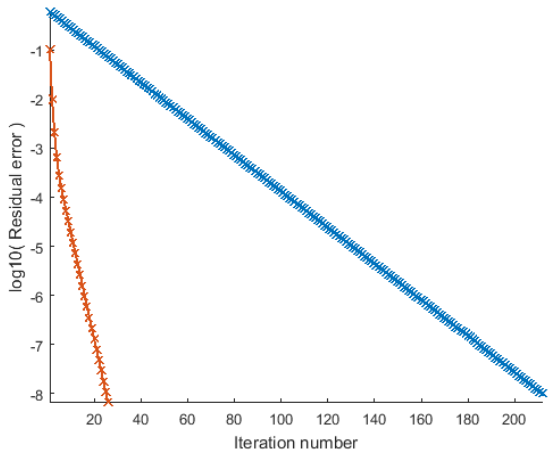


Figure 2.1: Example of residual error vs iteration number. The blue line corresponds to when the system is preconditioned and the red line to when the system is not preconditioned.

In some cases, the condition number can be improved and the system can be made better conditioned, with a preconditioner $M \in \mathbb{R}^{n \times n}$. A preconditioner is a non-singular matrix that decreases the condition number of the original system and that increases the order of convergence of the original system. One desirable property of the preconditioner is that it should approximate the inverse of matrix A, while at the same time being less computationally expensive to compute. Equation (2.5), is an example of a preconditioner multiplying the original system from the left, also called left preconditioning. The objective is to lower the condition number of the system as shown in Equation (2.6).

$$M^{-1}Ax = M^{-1}b \tag{2.5}$$

$$cond(A) > cond(M^{-1}A) \tag{2.6}$$

2.2.1 ILU Preconditioner

There are different options for a preconditioner, but we should emphasize thath there is not a correct "option" for all systems. Designing and picking a good preconditioner is problem dependent and may require several experiments. For reservoir simulation the incomplete LU factorization, M_{ILU}, (2.10) has been the most commonly used preconditioner for two-phase flow [4]. In the complete LU decomposition, see Equation (2.7), the original matrix is decomposed into a lower (L) and an upper (U) triangular matrix. For sparse matrices, as is the case for reservoir simulation, L and U are usually less sparse than A, so computing the exact decomposition can become very expensive. Thus instead we compute an approximation, or incomplete LU factorization, as shown in (2.9). If in the incomplete LU factorization, the matrices L and U are selected so that they conserve the sparsity pattern of the original matrix, the ILU is called ILU(0). The visual representation of this decomposition is in Figure 2.2. One important parameter in ILU algorithms, as the one available in MATLAB, is `droptol` [29]. This is a specified threshold below which nonzero entries are replaced by zeros. By increasing this value, the number of nonzero entries increases. There exists a trade off, by increasing the `droptol`, the preconditioner is computed faster, but the quality of the preconditioner decreases, and so does the converge rate of the solver.

Figure 2.3 shows the effect of the value of `droptol` of M_{ILU} in the rate of convergence of the GMRES algorithm. For this plot, M_{ILU} was computed with varying values of `droptol` and then it was used to precondition the solver. The plot shows that as `droptol` increases the order of error reduction also increases.

$$A = LU \tag{2.7}$$

$$A^{-1} = (LU)^{-1} = U^{-1}L^{-1} \tag{2.8}$$

$$A \approx \tilde{L}\tilde{U} \tag{2.9}$$

$$A^{-1} \approx M_{ILU}^{-1} = \left(\tilde{L}\tilde{U}\right)^{-1} = \tilde{U}^{-1}\tilde{L}^{-1} \tag{2.10}$$

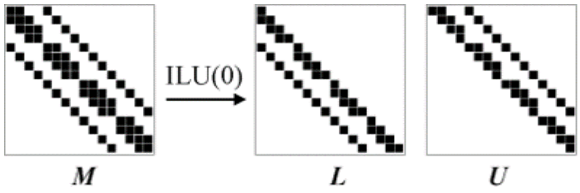


Figure 2.2: Observe the structure of L and U, in the ILU(0) decomposition. From [2].

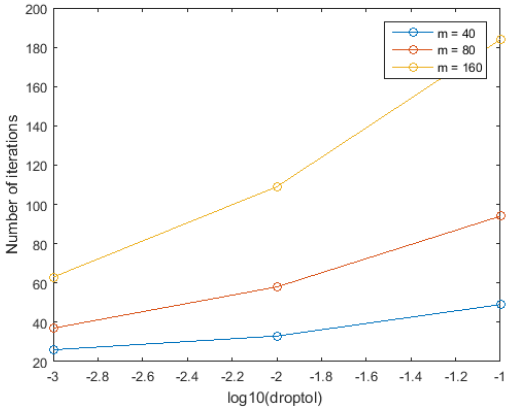


Figure 2.3: Effect of `droptol` in number of iterations required to solve the system of equations.

2.3 Reservoir Simulator Overview

A reservoir simulator is a type of porous media flow simulator that is used to simulate the flow of oil, gas and water in the reservoir rock [3].

The partial differential equation that describe the fluid flow in three dimensions is Equation (2.11). Where l stands for the fluid phase, o for oil and w for water.

$$\nabla \cdot \left(\left[k \frac{h_l}{B_l} \left(P_l + \gamma_l z \right) \right] \right) = \frac{d}{dt} \left(\frac{\phi S_l}{B_l} \right) - Q_l \tag{2.11}$$

$$\left(T + \frac{1}{\delta t} B \right) P_o^{n+1} = \frac{-1}{\delta t} B P_o^n + Q \tag{2.12}$$

$$R(P_o^{n+1}) = \frac{-1}{\delta t} B P_o^n + Q - \left(T + \frac{1}{\delta t} B \right) P_o^{n+1} \tag{2.13}$$

The discretized form of the partial differential equations can be written in matrix form as (2.12). Where T is the transmissibility matrix, B is the accumulation matrix, P_o is the oil pressure vector, and Q is the flow vector. And where the subscript n denotes the current timestep and $n+1$ denotes the next timestep. In this case the equations were written with the Fully Implicit formulation. The residual form of the equation is (2.13).

The structure of the matrices in Equation (2.12) depends on the grid ordering, the number of dimensions of the problem, and on the type of discretization applied to Equation (2.11). For a 3D problem, with a Cartesian grid, natural grid ordering and with the finite difference method the matrices result as follow. Matrix T is a square heptadiagonal block matrix, with a size of $(n * f) \times (n * f)$, where n is the number of cells and f is the number of fluid phases. Matrix B, is a block diagonal

matrix with the same dimensions as T. Vector Q, has a length of $(n * f)$.

Figure 2.4 shows the basic workflow of a reservoir simulator. The diagram shows a linear solver that solves for the oil pressure vector for a determined timestep. For this thesis we use the Fully Implicit formulation of the equations. In Figure 2.4 it is shown how nested inside each timestep iteration there is a Newton Raphson iteration. For each Newton Raphson iteration the iterative linear solver solves (2.14).

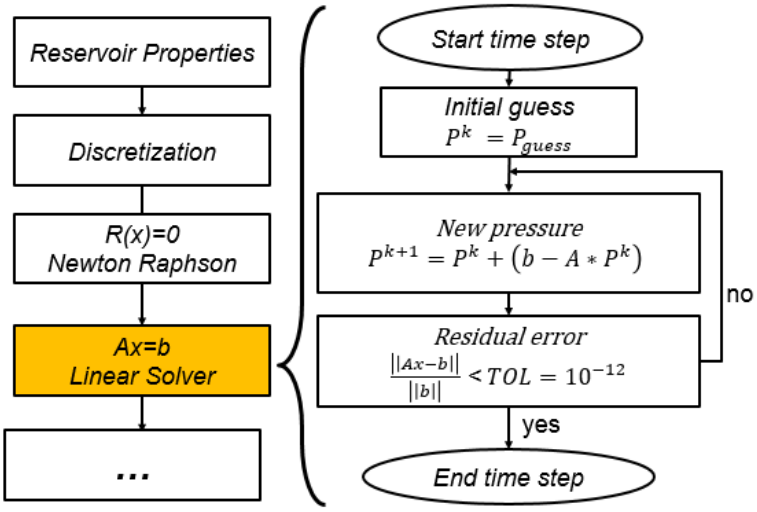


Figure 2.4: Reservoir simulation workflow.

For the Fully Implicit Method we solve (2.14) for the oil pressure, and (2.15) for the water saturation for each time step. J_{P_o} and J_{S_w} are the Jacobian of the oil pressure and of the water saturation respectively. The inverse of the Jacobian is constructed explicitly, because constructing the Jacobian and then performing the inverse function would be too expensive. For small systems this equation can be solved with a direct solver but for bigger systems an iterative solver is employed. For the iterative solvers the solution from the previous timestep is usually used as the

first guess of the solution of the next timestep.

$$P_o^{n+1} = P_o^{n+1} - J_{P_o}^{-1} \cdot R(P_o^{n+1}) \tag{2.14}$$

$$S_w^{n+1} = S_w^{n+1} - J_{S_w}^{-1} \cdot R(S_w^{n+1}) \tag{2.15}$$

3. POD BASED PRECONDITIONING

In this section we will explain the Proper Orthogonal Decomposition method and then use it to derive the preconditioner M_{POD}. We will use this preconditioner to create the two stage preconditioner $M_{POD+ILU}$. In the last part of the section we will show and explain the framework that is going to be used to implement this preconditioner in a reservoir simulator.

3.1 Introduction to Model Reduction by Proper Orthogonal Decomposition

The aim of Reduced Order Modeling (ROM) is to transform a high dimensional model to a lower dimensional one without losing accuracy to a certain degree [7]. By reducing the number of dimensions, in other words, the number of equations that represent the system, the model can be solved faster. There are many techniques in ROM, one of them is Proper Orthogonal Decomposition (POD) [30]. POD is used to extract basis functions from experimental data or detailed simulations of high dimensional systems for subsequent use in Galerkin projections that yield low dimensional models. A very straightforward introduction to proper orthogonal decomposition and its application in data analysis can be found in [7]. The author of the tutorial defines POD as a "powerful and elegant method of data analysis aimed at obtaining low dimensional approximate descriptions of high dimensional systems (HDS)". For other introductory material also refer to [31] and [32].

We will explain POD in the infinite dimensional case, then in the finite dimensional case, and finally we will point the correspondence between the two. For the infinite dimensional case, we begin with the objective of approximating (3.1) over some domain of interest as a finite sum. $z(x,t)$ is a function with a spatial coordinate x and a temporal coordinate t. The approximation becomes exact as M approaches

infinity. There are many options for the space function $\Phi_k(x)$, for each choice of $\Phi_k(x)$, the sequence of time functions $a_k(t)$ is different. For the choice of POD the sequence of functions $\Phi_k(x)$ is orthonormal to each other. To choose the functions, apart of orthonormality, the other criteria for selection is that "the approximation for each M is as good as possible in least square sense" [7], as to minimize Equation (3.2) That is that the first n basis functions give the best possible n-term approximation. These ordered orthonormal functions are the proper orthogonal nodes for the function $z(x,t)$. The expression in (3.1) is called the POD of $z(x,t)$.

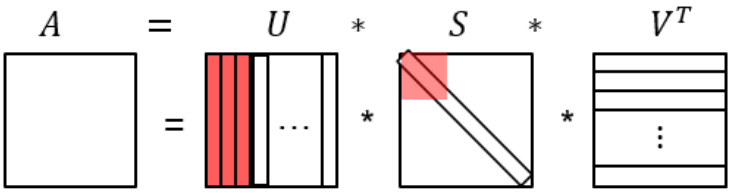
$$z(x,t) \approx \sum_{k=1}^{M} a_k(t)\Phi_k(x) \tag{3.1}$$

$$\sum_{i=1}^{M} \int_0^T ||z(x,t) - a_k(t)\Phi_k(x)||^2 dt \tag{3.2}$$

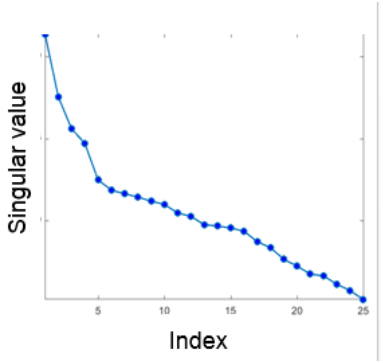
For the finite dimensional case, we will consider the data matrix $A \in \mathbb{R}^{N\times m}$. Composed of n data points over m samplings. We can perform Singular Value Decomposition (SVD) to matrix A, as in Equation (3.3), to obtain the matrices $U \in \mathbb{R}^{n\times n}$, $S \in \mathbb{R}^{n\times m}$, and $V \in \mathbb{R}^{m\times m}$. This is depicted in a visual way in Figure 3.1a.

$$A = USV^T \tag{3.3}$$

U and V are orthogonal matrices, and S is a diagonal matrix with the singular values of A. The singular values , σ_i, are ordered in descending order, and each one corresponds to one orthogonal vector in matrix U. The concept of energy should be



(a) Graphical depiction of SVD.



(b) Energy plot. The vertical axis is the $log(\sigma_i)$.

Figure 3.1: Singular value decomposition.

introduced now. Energy is defined as σ_i^2. The cumulative energy is defined as (3.4). Where $k \leq m$. The energy can be though as the information contribution of each orthogonal vector. A typical plot of energy vs. vector number is Figure 3.1b. It can be seen that most of the energy is represented by a few orthogonal vectors.

$$\text{Cumulative Energy} = \frac{\sum_{i=1}^{k} \sigma_i^2}{\sum_{i=1}^{m} \sigma_i^2} \tag{3.4}$$

The correspondence between the infinite case and the finite case is illustrated as follows. Equation (3.3) can be written as (3.5). Where q_k and v_k are the k columns of Q and V correspondingly. Equation (3.5) is the discrete form of (3.1). The function $z(x,t)$ is represented by matrix A, the function $a_k(t)$ is represented by q_k and $\Phi(x)$

by v_k^T.

$$A = (US)V^T = QV^T = \sum_{k=1}^{m} q_k v_k^T \tag{3.5}$$

To obtain a lower dimensional approximation of A we need only to select the first k basis vectors corresponding to the first k singular values. Equation (3.6), where $\tilde{U} \in \mathbb{R}^{n\times k}$, $S \in \mathbb{R}^{k\times k}$, and $V \in \mathbb{R}^{k\times n}$, is the optimum k order approximation of A, in the least squares sense. The value of k is selected as to conserve a desirable amount of energy of the original system, usually k is selected so that (3.4) is 0.99 or more.

$$A \approx \tilde{U}\tilde{S}\tilde{V}^T \tag{3.6}$$

3.2 POD Preconditioner Derivation

In [10] the derivation of the preconditioner starting from the linear system of equations is explained. The derivation starts with ROM-POD, then proceeds to explain how to create the preconditioner and how to measure the quality of the basis. The projection preferred is the Galerkin Projection. It is preferred because stability is guaranteed for SPD matrices and the Jacobian matrices for the pressure equation are usually SPD matrices.

The derivation of the preconditioner proceeds as follows.

$$Ax = b \tag{3.7}$$

Where A is $n \times n$. To reduce the order of (3.7)

$$\tilde{x} = \Phi z \tag{3.8}$$

Where Φ is the POD basis, with l columns , and $l << n$

$$A\Phi z = b \tag{3.9}$$

(3.9) is an overdetermined system, we need to project the full set of equations into a lower dimensoinal space. With the projeciton operator Ψ

$$\Psi^T A\Phi z = \Psi^T b \tag{3.10}$$

$$z = (\Psi^T A\Phi)^{-1}\Psi^T b \tag{3.11}$$

Substituting previous equation in (3.8)

$$\tilde{x} = \Phi(\Psi^T A\Phi)^{-1}\Psi^T b \tag{3.12}$$

And from (3.7)

$$\tilde{x} = \Phi(\Psi^T A\Phi)^{-1}\Psi^T b \approx A^{-1}b \tag{3.13}$$

If the projection scheme is the Galerkin projection, then

$$\Psi = \Phi \tag{3.14}$$

$$\tilde{x} = \Phi(\Phi^T A\Phi)^{-1}\Phi^T b \approx A^{-1}b \tag{3.15}$$

Rui shows in [10] that of the three possible choices for the projection operator; identity matrix, least-squares projector (LSP) or Petrov-Galerkin, and Galerkin; the Galerkin projector is better than the other two. We choose this projector.

Therefore, the preconditioner becomes,

$$M_{POD}^{-1} = \Phi(\Phi^T A \Phi)^{-1} \Phi^T \tag{3.16}$$

To create the two-stage preconditioner with M_{POD} and M_{ILU}, we follow the procedure in [33]. To advance from iteration i to iteration i+1 in a two-stage preconditioner can be expressed as Equation (3.17) and (3.18).

$$x_{i+\frac{1}{2}} = x_i + d_1 = x_i + M_1^{-1}(b - Ax_i) \tag{3.17}$$

$$x_{i+1} = x_{i+\frac{1}{2}} + d_2 = x_{i+\frac{1}{2}} + M_2^{-1}(b - Ax_{i+\frac{1}{2}}) \tag{3.18}$$

By combining the two equations we obtain the following

$$x_{i+1} = x_i + M_3^{-1}(b - Ax_i) \tag{3.19}$$

Where

$$M_3^{-1} = M_1^{-1} + M_2^{-1}(I - AM_1^{-1}) \tag{3.20}$$

So, for our case, the two stage preconditioner becomes

$$M_{POD+ILU}^{-1} = M_{POD}^{-1} + M_{ILU}^{-1}\left(I - AM_{POD}^{-1}\right) \tag{3.21}$$

To measure if the basis used to create the preconditioner is good for the current linear system being solved we can measure the quality of it. The quality of the basis is defined as Equation (3.22) for the Galerkin projection and it should be less than 10^{-1}. If the quality is less than this value, then we can continue using the same basis, if it is higher than this, then we should recompute the basis.

$$\frac{||(I - AM_{POD}^{-1}b)||_2}{||b||_2} \tag{3.22}$$

3.3 Snapshots Method Framework

The framework used in this thesis can be described as in Figure 3.2. Each step will be explained in detail in the sections below.

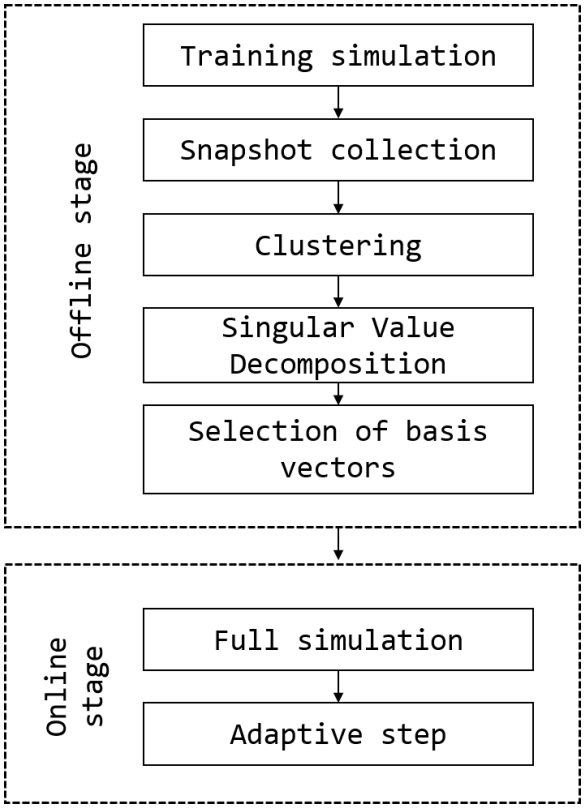


Figure 3.2: Framework.

3.3.1 Offline Stage

1. **Training simulation.**

   The training simulation consists of running the reservoir for a "short" period of time with the objective of capturing the most relevant information about the reservoir as possible. To accomplish this, during the training period the injector and producer wells are run on a schedule that permits to explore the most representative behavior of the reservoir. There is not an specific criteria for the selection of the training schedule, but some examples can be found in [27, 4, 10, 5]. We will use an schedule where the producers maintain a constant bottom hole pressure, while the water injectors are being turn on and shut down one by one in sequence.

2. **Snapshots.**

   The snapshots consist of the solution of the linear system for each timestep of the training simulation. In our case, the snapshots are the vectors of the pressure solution. These vectors are saved in a matrix with shape $n \times k$, where n is the number of cells in the reservoir and k is the number of timesteps in the training simulation.

3. **Clustering**.

   The snapshots are clustered with the `k-means` method. Mathworks defines k-means clustering, or Lloyd's algorithm , as an iterative, data-partitioning algorithm that assigns n observations to exactly one of k clusters defined by centroids, where k is chosen before the algorithm starts [34]". The benefit of clustering is that we obtain average snapshots that are more representative of the behavior of the solution, and this in turn decreases the number of basis vectors required to represent the same amount of energy in the reduced basis

matrix [4].

4. **Singular Value Decomposition.**

   In this step we perform the SVD of the snapshots matrix as depicted in Equation (3.3) and in Figure 3.1a. Here, only the full basis matrix U, and the singular value matrix S, are of interest.

5. **Selection of basis vectors.**

   In this step we construct the reduced basis matrix, U_k , by selecting the basis vectors that contribute the most energy and discarding the rest. Usually, the basis vectors are selected so that at least 99 % of the cumulative energy is conserved. Following the recommendation in [27], at most two times the number of vectors as the number of wells are needed in the reduced basis matrix.

   The previous steps correspond to the *offline* part of the process. Unless an adaptive approach is desired, once the basis vectors have been selected they will remain fixed for the rest of the subsequent simulations.

3.3.2 Online Stage

1. **Full simulation.**

   In this step, the full simulation is run. For each time step of the simulation the preconditioner (3.21) has to be calculated and then the iterative linear solver is ran.

2. **Adaptive step.**

   If an adaptive approach is desired, the quality of the reduced basis is evaluated at each time with Equation (3.22). If the quality is not good, then the basis needs to be updated. There are two approaches that can be used to update the basis. One is to perform a SVD on all the previous solutions and recompute

the full reduced basis. The drawback of this method is that it required to store all the previous pressure solutions. A second option, presented in [35], is to expand the basis matrix by one column with the previous solution. This method has the advantage that it is inexpensive to compute.

4. NUMERICAL EXPERIMENTS

We will perform numerical experiments with the Matlab Reservoir Simulation Toolbox (MRST). in two reservoir models. Model 1 is a simple square reservoir and Model 2 is a realistic reservoir model consisting of the first layer of the SPE10 benchmark model.

The objective of the experiments is to test the framework presented in Section 3.3 and discover whether the GMRES performs better when it is preconditioned with the two stage preconditioner $M_{POD+ILU}$ than when it is preconditioned with the single stage M_{ILU}. To measure the performance improvements we will use two metrics. The first metric will be the order of error reduction, as explained in Section 2.1.1, of the algorithm. The order of error reduction will tell use how rapidly the residual error decreases per each iteration. A positive result will be obtained if the order of error reduction increases, because that means than the number of iterations required to solve the system decrease. The second metric is the computational cost, measured as the total time required to run the simulation, and the memory requirements. The MATLAB profiling tool is going to be used for this purpose. A positive result will be obtained if the total computational cost decrease.

4.1 The Reservoir Models

4.1.1 Model 1: Simple Model

The simple reservoir model is a square reservoir with a size of $L \times L \times H$. Where L is the number of cells in one side of the reservoir and H is the number of layers. L takes the values of 10, 15 and 20. And H takes the values of 1, 2 and 3. That means that the smallest reservoir has 100 cells while the biggest has 1,200 cells. In all the cases, there are five wells in a five spot pattern. Four oil producers surrounding a

water injector in the middle of the reservoir to simulate a water flooding scenario. The reservoir is shown in Figure 4.1 and its parameters in the rock Table 4.1.

The fluid used in all the simulations is composed of two phases, water and oil. The phases are immiscible and incompressible. The properties of the fluid are in Table 4.2. The capillary pressure curve and the relative permeability curves, are in Figure 4.2.

The rock is incompressbile. The porosity field comes from a random gaussian distribution calculated using the function `gaussianField` of MRST. The target values for the porosity are $[0.002, 0.3]$, with a standard deviation of 0.65. The permeability was calculated with the Carman Kozeny relation, as in Equation (4.1) [3].

$$K = \frac{\phi^3 \times (1E^{-5})^2}{(0.81 * 72 * (1 - \phi)^2)} \tag{4.1}$$

Dimensions	$L \times L \times H$
Number of cells	from 100 to 1200
Injectors	1
Producers	5
Fluid	black oil
Rock	incompressible

Table 4.1: Model 1. Simple reservoir model specifications.

4.1.2 Model 2: Realistic Model

The second reservoir model is the first layer of the SPE10 reservoir model. With a total of 13,200 cells. This model has 5 water injector wells and 5 oil producer wells in an irregular pattern. In this model we will also be simulating a water

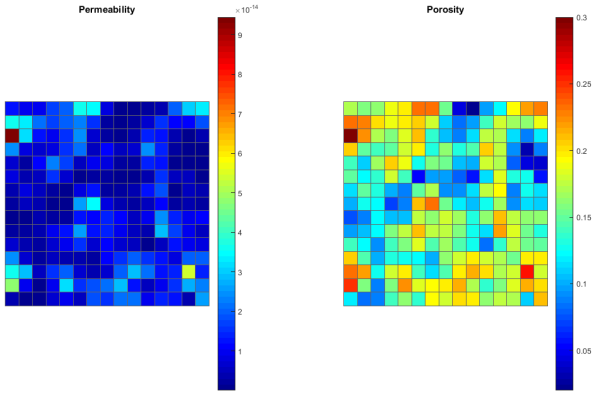
Fluid	Water	Oil
Density ($\frac{kg}{m^3}$)	1,000	700
Viscosity (cp)	1	10
Compressibility (psi^{-1})	0	0

Table 4.2: Fluid properties.

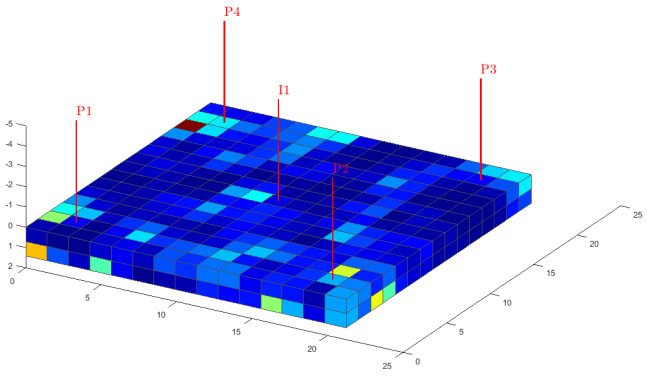
flooding scenario. This model with the well locations is shown in Figure 4.3. The rock properties are heterogeneous and are the original properties included with the benchmark model [36]. The fluid properties are the same as the ones used in Model 1.

Dimensions	1st layer of SPE10
Number of cells	13,200
Injectors	5
Producers	5
Fluid	black oil
Rock	incompressible

Table 4.3: Model 2. Realistic reservoir model specifications.

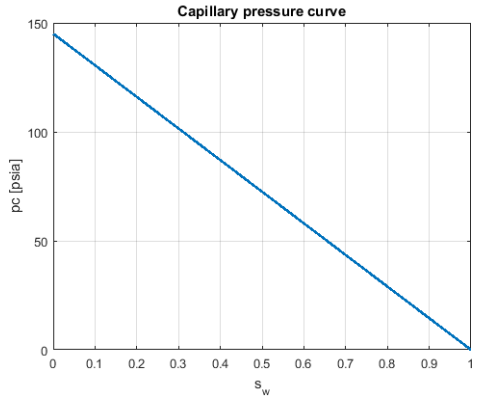


(a) Petrophysical properties. Porosity and permeability fields.

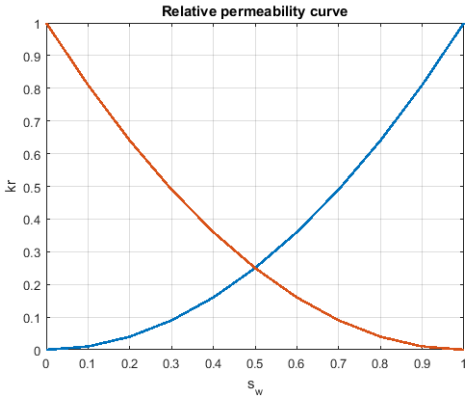


(b) 3D Model View

Figure 4.1: Model 1. Simple square reservoir.

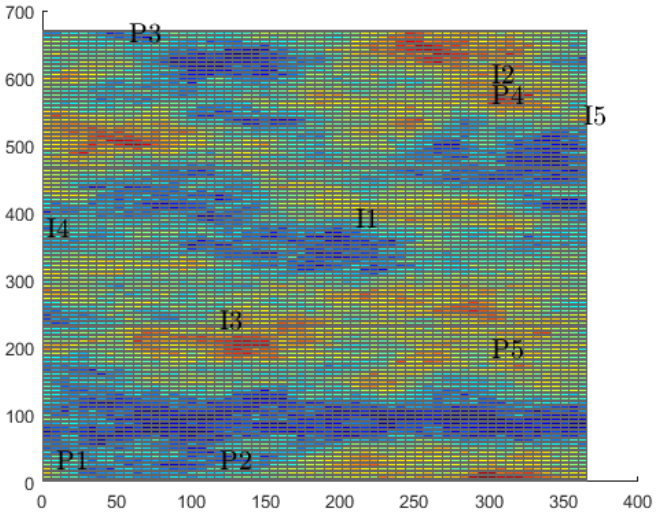


(a) Capillary pressure.



(b) Relative permeability. The red line is k_{r_o} and the blue line is k_{r_w}.

Figure 4.2: Fluid properties.



(a) 3D Model View

Figure 4.3: Model 2. Realistic reservoir model.

4.2 Numerical Experiments. Model 1

For the first numerical experiment we use Model 1 with the objective to compare the performance of the GMRES and Richardson solvers, see Section 2.1.1, preconditioned with M_{ILU} and $M_{ILU+POD}$. For the reduced orthogonal basis we use the criteria of conserving at least 99 % of the energy, that was accomplished by using the first five basis vectors. For the training period we will run the simulation for 25 timesteps corresponding to a total of 86 days, while we turn on and off the oil producers in sequence. During this training period, when a producer is turned on, the bottom hole pressure is maintained at 5,500 psia. The injector well is set at 300 bbl/day.

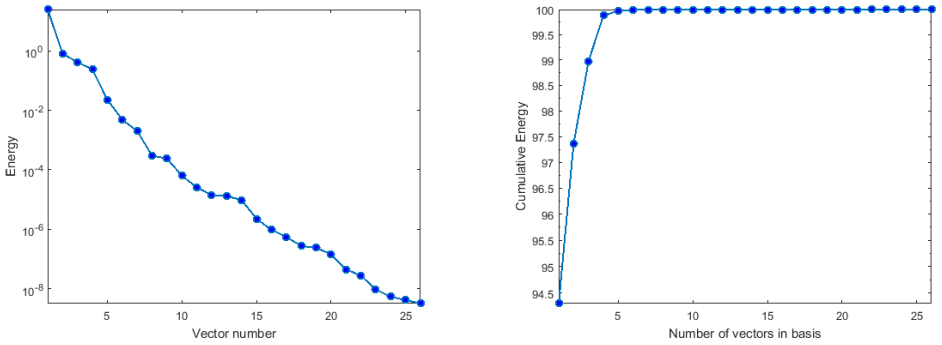
The criteria for stopping the solvers is when the relative error of $1E^{-8}$ has been reached. To obtain the LU decomposition, the MATLAB function `ilu` was used with a droptol of $1E^{-3}$.

4.2.1 Energy vs Basis Number

The snapshots matrix of the pressure solution has the dimensions of $n \times k$. Where n is the number of cells and k is the number of timesteps in the training schedule, in this case 25. SVD was performed to the snapshots matrix to obtain the basis vectors and their singular values. Figure 4.4 shows the energy of the basis vectors. Figure 4.4a shows the plot of the energy contributed by each of the basis vectors. Figure 4.4b shows the cumulative energy vs. number of basis vectors. As can be seen, with just five basis vectors we capture 99.99% of the energy of the system.

4.2.2 Residual Error Analysis

Figure 4.5 shows the residual error vs. the iteration number for the Richardson and GMRES solvers when they are preconditioned with M_{ILU} and $M_{POD+ILU}$.



(a) Log of energy vs basis vector number.

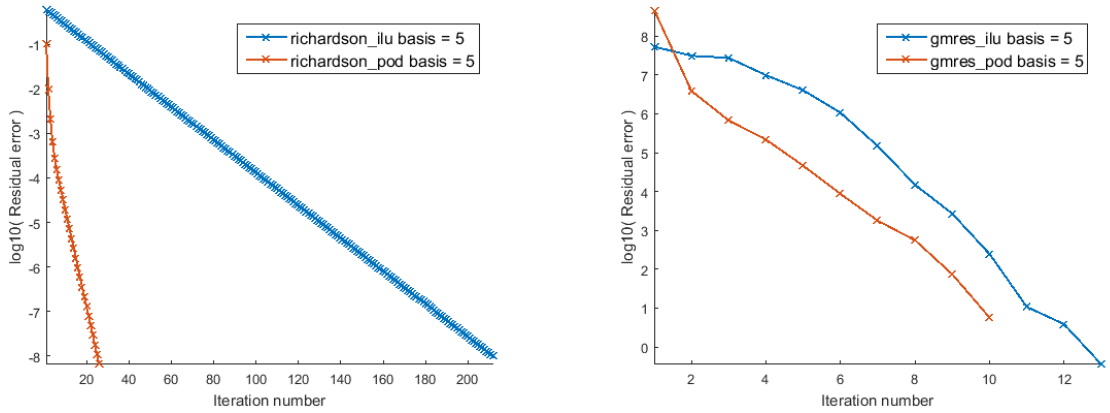
(b) Cumulative energy vs basis vector number.

Figure 4.4: Model 1. Energy of POD basis vectors.

These two plots are for the case of three layers, and for a single timestep, but these results are similar for all timesteps and number of layers. The error reduction for the GMRES algorithm is shown in Figure 4.5b. When the solver is preconditioned with M_{ILU} it takes 13 iterations to converge. On the other hand, when the preconditioner $M_{POD+ILU}$ is used, it converges in only 10 iterations. The order of error reduction is 0.62 and 0.85, correspondingly. In Figure 4.5a the error reduction for the Richardson algorithm is shown. The M_{ILU} converges in 337 iterations while $M_{POD+ILU}$ converges in 23 iterations. The order of error reduction increased from 0.024 to 0.28. Table 4.4 and Table 4.5 show the improvement in the order of error reduction when M_{ILU} is substituted by $M_{POD+ILU}$.

4.2.3 Performance Improvement

Figure 4.6 and Figure 4.7 show the time improvement for the preconditioner calculation time, solver time and total simulation time. For the Richardson solver, for all cases, the $M_{ILU+POD}$ preconditioner performs better, with savings in time of at least 60% and up to 85%. For the GMRES solver there are not savings in time



(a) Richardson (b) GMRES

Figure 4.5: Model 1. Relative residual error vs. iteration number, for the Richardson and GMRES algorithm preconditioned with M_{ILU} and $M_{ILU+POD}$.

	Number of cells		
Number of layers	10	15	20
1	31.45	39.64	229.98
2	197.90	212.36	878.17
3	400.5	423.3	1,099.2

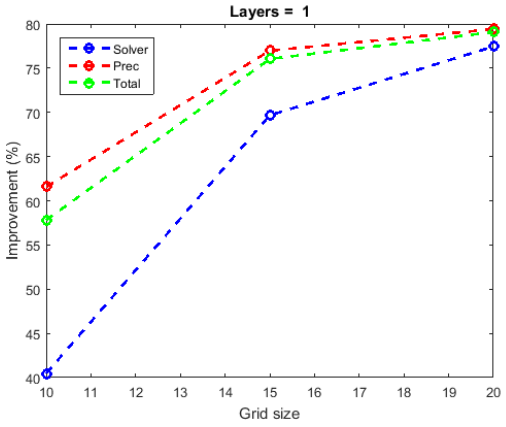
Table 4.4: Model 1. Percentage improvement in the order of error reduction. Richardson algorithm.

	Number of cells		
Number of layers	10	15	20
1	15.87	17.53	-1.38
2	34.50	43.49	21.87
3	23.72	15.03	37.02

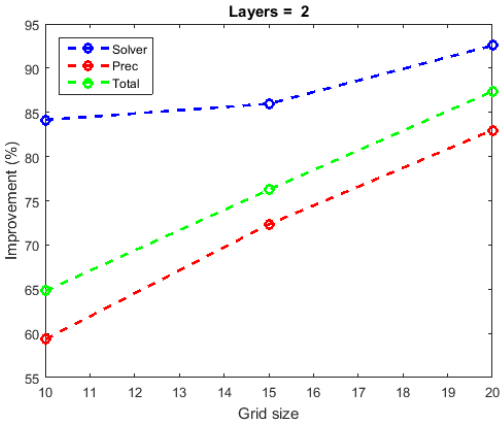
Table 4.5: Model 1. Percentage improvement in the order of error reduction. GMRES algorithm.

with the two stage preconditioner. The total simulation time increases by at least 50% and up to 500 %. The reasons for this will be explained in detail in Section 5. But the main reason is that for the GMRES algorithm, the increase in the order of converge and decrease in the number of iterations is not big enough to offset the increased cost of computing the two stage preconditioner. It can also be seen in the plots that the most consuming part of the solution procedure is to generate the preconditioner.

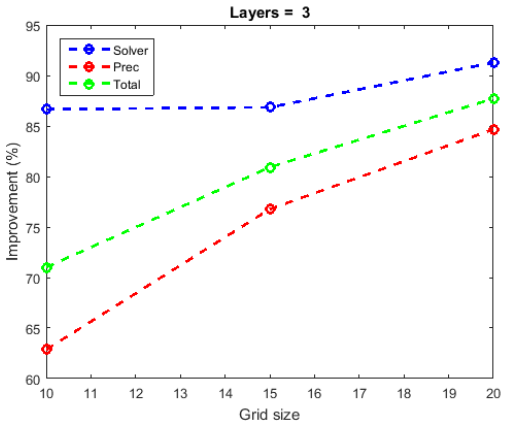
Another numerical experiment was run to understand the reason behind the bad performance of the two stage preconditioner. We simulated the three layer square reservoir for the condition where the well schedule for the full simulation is the same as the schedule for the training simulation. The results are shown in Figure 4.8. Once again, we obtain that the two stage preconditioner increases the total simulation time from -180 % to -600 %. Because the two schedules were the same one, we can narrow the bad performance cause to the implementation of the method. This is confirmed when we do the code profiling in Section 4.3.



(a) One layer. Richardson.

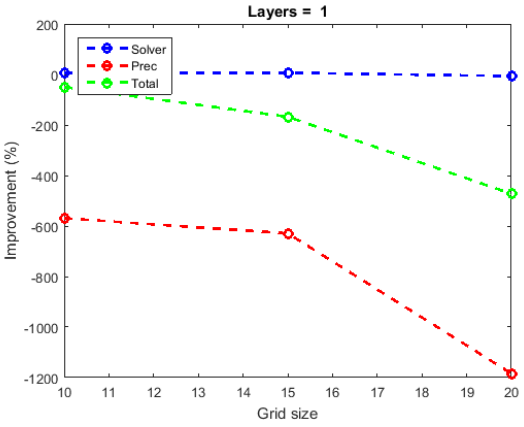


(b) Two layers. Richardson.

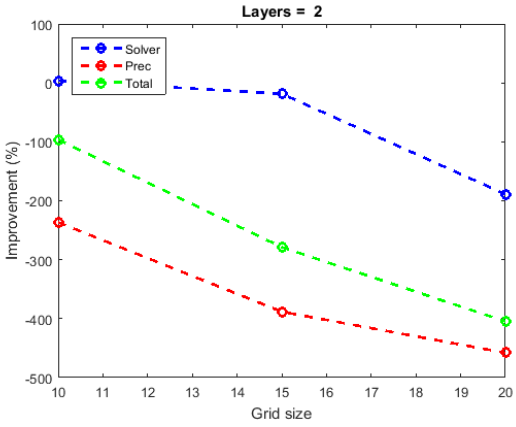


(c) Three layers. Richardson.

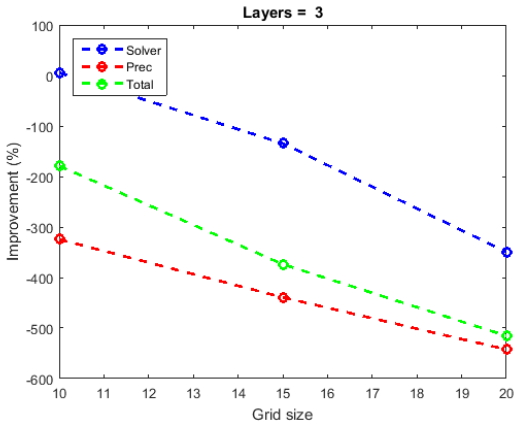
Figure 4.6: Model 1. Simulation time improvement for the Richardson algorithm. Effect of number of layers and number of cells.



(a) One layer. GMRES.



(b) Two layers. GMRES.



(c) Three layers. GMRES.

Figure 4.7: Model 1. Simulation time improvement for the GMRES algorithm. Effect of number of layers and number of cells.

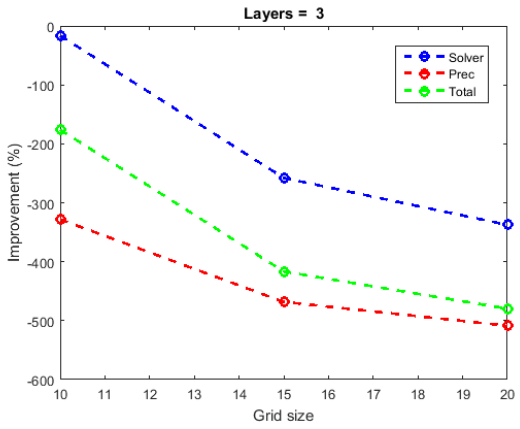


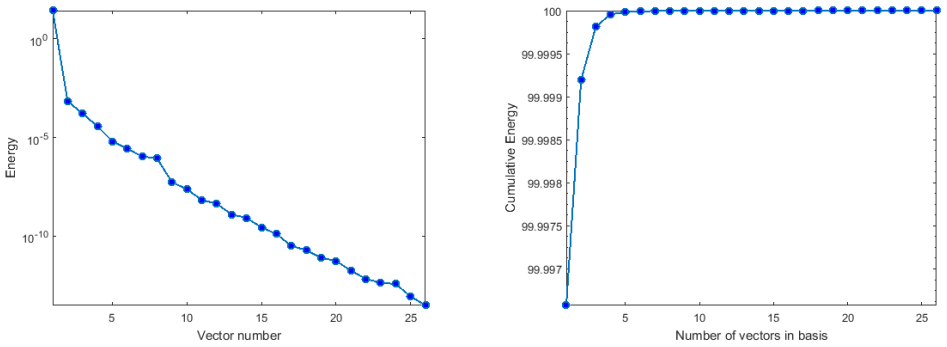
Figure 4.8: Model 1. Simulation time improvement for the GMRES algorithm. Case when the full simulation schedule is the same as the training schedule.

4.3 Numerical Experiments. Model 2

For the second numerical experiment we use Model 2. The training schedule has 26 timesteps and adds to 86.5 days, while the full simulation schedule has a duration of 866 days and consists of 103 timesteps . For this model we will measure the performance of the GMRES algorithm preconditioned with M_{ILU} and $M_{POD+ILU}$.

4.3.1 Energy vs Basis Number

The plots of the energy of the basis vectors for Model 2 are in Figure 4.9. As in the previous model, there are a total of 25 basis vectors, Figure 4.9a. The cumulative energy plot, Figure 4.9b shows that with only 5 basis vectors almost 100% of the energy of the system is represented, nevertheless we decided to use 10 basis vectors in the reduced basis matrix.



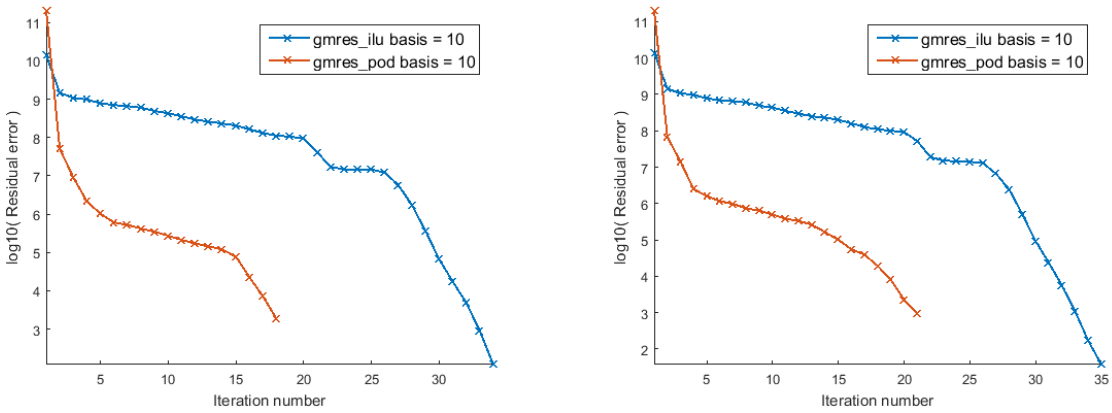
(a) Log of energy vs basis vector number.

(b) Cumulative energy vs basis vector number.

Figure 4.9: Model 2. Energy of POD basis vectors.

4.3.2 Residual Error Analysis

Figure 4.10 shows the order of the error reduction for the GMRES solver with the M_{ILU} and $M_{ILU+POD}$ preconditioners. The order of error reduction is 0.244 for the first case and 0.4114 for the second case, resulting in an improvement of 68.67 %. The number of iterations needed to solve for the pressure inside the Newton Raphson iteration was 35 for M_{ILU} and 20 for $M_{POD+ILU}$.



(a) Day 10. (b) Day 236.

Figure 4.10: Model 2. Residual error vs. iteration number for the GMRES algorithm.

4.3.3 Performance Improvement

The time improvement is shown in Table 4.6. When the GMRES solver is preconditioned with $M_{ILU+POD}$ the solver performs worse than when it is preconditioned with M_{ILU}. In both categories, total time spent solving the system and total time spent computing the preconditioner, the two stage preconditioner performance is worse. The total simulation time increased from $0.122E^3$ seconds to $1.189E^3$ seconds, this represents an increase of 873 %.

	M_{ILU}	$M_{ILU+POD}$
Total solver time	0.117	0.184
Total preconditioner computation time	0.005	1.005
Total	0.122	1.189
Improvement		-873 %

Table 4.6: Model 2. Performance of $M_{ILU+POD}$ over M_{ILU}. The units of time are 10^3 seconds.

Operation	Time %	Memory(MB)
`[L,U] = ilu(A)`	3.1	171
`M_pod = basis * ((basis'* A *basis)\basis')`	18.5	70,977
`M_ilu_pod= U \(L \(eye(m)-A*M_pod)) + M_pod`	77.6	70,977

Table 4.7: $M_{ILU+POD}$ computation time and memory allocation for Model 2.

5. CONCLUSIONS

The results from the numerical experiments with Model 1 and Model 2 clearly show that the the new preconditioner $M_{POD+ILU}$ is an improvement over M_{ILU} only if it used with the Richardson solver. For GMRES, the time performance is lowered with $M_{POD+ILU}$.

First we will talk about the improvement in the order of error reduction of $M_{POD+ILU}$ over M_{ILU}. For the Richardson algorithm, see Table 4.4 , the improvement increases as the size and the number of layers of the reservoir model increase. For one layer and 100 cells the improvement is of 31.45%, and for 3 layers with 1,200 cells the improvement is of 1,099.2 %. This is visualized in the plots of residual error vs. iteration number in Figure 4.5. For GMRES, Table 4.5, there is not a clear pattern for the improvement in error reduction. It increases and decreases as the number of layers and number of cells increase. And for the case of one layer and 400 cells, the new preconditioner in fact has a negative effect. Also, for GMRES the improvements range from 15 to 44 %, while for Richardson algorithm they range from 31 to 1,100 %.

Continuing with the analysis of the time improvements of the preconditioners. Figures 4.6 and 4.7 show the time improvements resulting with the two stage preconditioner. For the Richardson solver the simulation time decreases by at least 60% and up to 85%.

For the GMRES algorithm, on the other hand, there is no time improvements. Even tough the number of iterations per timestep are decreased, preconditioning the solver with $M_{POD+ILU}$ takes much more time and the total time to solve the system increases from 50 % to 500 %.

There are two main reasons why $M_{POD+ILU}$ is more time consuming. The first reason is that it is more time consuming to compute the two stage preconditioner than the one stage ILU preconditioner and the second reason is that it is also more time consuming to apply the preconditioner to the linear system. For the first point, M_{ILU} only requires an ILU decomposition, while $M_{POD+ILU}$, besides an ILU decomposition requires to compute M_{POD} and $M_{ILU+POD}$ for each iteration loop. Analysis of the Model 2 simulation with the Matlab profiling tool are shown in Table 4.7. Computing M_{ILU} consumes 3.1% of the time, while M_{POD}^{-1} consumes another 18.5 %. The remaining 77.6 % of the time is spent computing the two stage preconditioner. These operations are costly because the reduced basis matrix Φ is fully dense. This results in M_{POD} and $M_{POD+ILU}$ being also fully dense. This bring us to the second point. Applying the dense preconditioner is more costly than applying a sparse preconditioner. As shown in 4.6, GMRES plus the two stage precondioner, consumes more total time, even though the number of iterations was decreased in average from 35 to 20 in each timestep.

Also, another drawback with the two stage preconditioner is that it consumes more memory storing the dense matrices. Table 4.7 also shows the memory consumption. MATLAB allocates 414.6 times more memory for M_{POD} and $M_{POD+ILU}$, than for M_{ILU}.

So, we can conclude that when the time spent creating and applying the two stage preconditioner is offset by the decreased number of iterations, using the two stage preconditioner makes sense. This condition is only met for the Richardson algorithm, where the number of iterations is decreased greatly as discussed before.

We also want to mention that the conclusions obtained have only been observed for the solvers and models that we simulated and that more extensive test with other reservoir models and solvers are necessary to make a more general conclusion.

Furthermore, for this thesis we only performed numerical experiments. A theoretical analysis of the algorithm would be better to make a general statement about the method.

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