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Decoupling preconditioners in the implicit parallel accurate reservoir simulator (IPARS)

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SUMMARY

This paper presents an overview of two-stage decoupling preconditioning techniques employed in the implicit parallel accurate reservoir simulator (IPARS) computational framework for modelling multi-component multi-phase flow in porous media. The underlying discretization method is implicit Euler in time and mixed finite elements or cell-centred finite differences in space. IPARS permits rigorous, physically representative coupling of different physical and numerical flow models in different parts of the domain and accounts for structural discontinuities; the framework currently includes eight physical models. For simplicity of exposition, we have restricted our discussion to a two-phase oil–water model and a three-phase black oil model. Our decoupling approach involves extracting a pressure equation from the fully coupled linearized system thus allowing for a more accurate preconditioning of a discrete elliptic problem of lower dimension. Copyright © 2001 John Wiley & Sons, Ltd.

KEY WORDS: multi-phase flow; generalized minimum residual method; decoupling preconditioner

1. INTRODUCTION

The implicit parallel accurate reservoir simulator (IPARS) computational portal or framework is research software developed mainly for the purposes of investigating different physical models and different numerical algorithms for modelling multi-phase flows in porous media. The IPARS framework supports three-dimensional transient subsurface flow of multiple phases containing multiple components plus immobile phases (rock and absorbed components) and an arbitrary number of wells each with one or more completion intervals. The vertical well models in IPARS are based on Peaceman's correction [1]. This simulator provides all the memory management, message passing, table lookup, solvers input/output so that a developer

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only needs to code the relevant physics. A detailed description of IPARS can be found in References [2, 3]. In this paper, we will focus on the solution of the coupled multi-component non-linear time-dependent flow equations which are solved using a fully implicit time-stepping scheme and mixed finite element or cell-centred finite difference methods in space.

An inexact Newton method is used to approximate the Jacobian. The resulting system is sparse, non-symmetric and ill-conditioned and is solved by applying a preconditioned generalized minimum residual (GMRES) procedure. The preconditioner is referred to as two-stage. In the first stage, a decoupling preconditioner is introduced which decouples a given pressure from saturations. This decoupling allows for a second stage, a preconditioning of the diagonal pressure block of the Jacobian *independently* of the saturation blocks. Furthermore, construction of a global preconditioner implies certain coupling between saturations and pressure which is a complementary issue to decoupling. In this paper, we address different techniques for coupling/decoupling, leaving the second stage for presentation elsewhere.

The contents of this paper are as follows. In Section 2, we consider the general formulation of a multi-component multi-phase isothermal model with wells and the linearization of this model. The equations comprise accumulation, transport, and well terms. Each of the terms is linearized using Newton's method and the resulting linear system is written in the form of increments. We restrict our attention to a particular set of primary variables, namely a chosen pressure and one or more saturations and make two assumptions regarding this choice. We remark that our selection of primary variables is standard in the petroleum industry [4–6]. Our third assumption is based on Impes time splitting [7]. Here Impes refers to solving a pressure equation implicitly and a saturation equation explicitly. In Section 3, several decoupling techniques are formulated. Construction of the global preconditioner for the coupled system is based on one of two methods, a block Gauss–Seidel method [8, 9], and a combinative technique [10, 9]. Numerical experiments comparing these approaches are discussed for a collection of SPE benchmark problems [11]. Several of these technique such as the constrained pressure have been applied successfully in commercial software. Conclusions are provided in the last section.

2. GENERAL MODEL FORMULATION AND ITS LINEARIZATION

2.1. General model equations

In this section, we follow the formulation presented in Reference [7] for the general model equations. A multi-phase flow model consists of $n + m$ equations associated with each grid block (grid cell). The first n equations are those for conservation of n species M_i:

$$\Delta_t M_i = Q_i \Delta t, \quad i = 1, \ldots, n \tag{1}$$

Here, Q_i represents inter-block flow and well terms:

$$Q_i = \sum_{\kappa} T_{i\kappa}(p_\kappa - p) - q_i \tag{2}$$

$\sum_\kappa$ denotes the summation over all neighbour grid blocks κ, p and p_κ stand for a grid block and a neighbour block pressure, q_i denotes the production rate of species i, and $T_{i\kappa}$ is a transmissibility for flow of species i between a grid block and its neighbour κ. Although the

capillary pressure and gravity terms are taken into account in IPARS, for the sake of brevity we neglect them in the course of the presentation.

In the case of fully implicit schemes, both $\Delta_t M_i = M_i^{k+1} - M_i^k$ and $Q_i = Q_i^{k+1}$ are unknown. They are computed by the Newton method. Let M_i^{l+1}, Q_i^{l+1} be the new iterates approximating M_i^{k+1}, Q_i^{k+1}, respectively. Then, Equation (1) may be rewritten as

$$M_i^{l+1} - M_i^l + M_i^l - M_i^k - Q_i^l \Delta t = (Q_i^{l+1} - Q_i^l)\Delta t \tag{3}$$

Since $M_i^{k+1} - M_i^k = Q_i^{k+1}\Delta t$, the residual of Newton iteration is

$$r_i = M_i^l - M_i^k - Q_i^l \Delta t$$

and (3) may be written in the form of increments:

$$\delta M_i + r_i = \delta Q_i \Delta t, \quad i = 1, \ldots, n \tag{4}$$

Given a set of n species, there always exists a set of $n+m$ variables $\{Y_j\}$, $j = 1, \ldots, n+m$, such that each M_i is a unique function of $\{Y_j\}$. The first n variables from $\{Y_j\}$ are called primary, and the remained variables are referred to as secondary. Although a wide set of primary variables is available [12], we restrict our attention to a very particular set of primary variables.

Assumption 1
We assume that Y_1 is the grid block pressure and $\{Y_j\}$, $j = 2, \ldots, n+m$, are the grid block saturations (or concentrations).

We remark that no special phase pressure has been chosen. However, the optimal choice of the component turns out to be very important in computational practice. In order to close the system (4), we need additional m constraint equations. They may express phase equilibrium, saturation constraint, and other model constraints. A general form of the additional differential equations is

$$\delta L_i + r_i = 0, \quad i = n+1, \ldots, n+m \tag{5}$$

These additional constraint equations (7) may be chosen to possess local properties. Thus, we may assume that the constraint equations (7) state relationships between our variables in each grid block independently of other grid blocks. On the other hand, the equations of conservation (1)–(2) contain three terms: accumulation $\Delta_t M_i$, transport $\sum_\kappa T_{i\kappa}(p_\kappa - p)$, and well terms q_i. By definition, the transport term provides interaction between grid blocks through the pressure differences. Accumulation term $\Delta_t M_i$, responsible for a change in amount of a given species, is likely to have a dominant local interaction within a grid block. The well term may yield an inter-block coupling but be dominated mainly by the pressure variable.

Taking into account the above considerations, we conclude that *the interaction between variables other than pressure is chiefly local*. In algebraic terms, it allows us to make

Assumption 2
Consider the block representation of matrix A associated with grid cell blocks. The off-diagonal block entries responsible for interaction between different variables, are small compared to the respective entries of the diagonal block.

2.2. Newton linearization

Linearization of (4) yields linear equations

$$\sum_{j=1}^{n+m} g_{ij}^{M}\delta Y_j + r_i = \sum_{j=1}^{n+m} g_{ij}^{Q}\delta Y_j, \quad i=1,\ldots,n \tag{6}$$

where g_{ij}^{M}, g_{ij}^{Q} are the entries of the accumulation and transport–well Jacobian's terms.

Linearization of (5) results in

$$\sum_{j=1}^{n+m} g_{ij}^{L}\delta Y_j + r_i = 0, \quad i=n+1,\ldots,n+m \tag{7}$$

The system (6), (7) may be presented in an algebraic form

$$\begin{pmatrix} B & C \\ D & E \end{pmatrix}\begin{pmatrix} \delta Y_I \\ \delta Y_{II} \end{pmatrix} = \begin{pmatrix} \delta Z_I \\ \delta Z_{II} \end{pmatrix} \tag{8}$$

The dependence of the secondary variables is eliminated by the reduction to the Schur complement counterpart of the system (8)

$$\begin{gathered} A := B - CE^{-1}D, \quad Z := Z_I - CE^{-1}Z_{II}, \quad Y := \delta Y_I \\ AY = Z \end{gathered} \tag{9}$$

System (9) is obtained by the reduction of linearized equations to the primary variables. These equations are the linearization of the residual formulation for the system of conservation equations. Since Y stands for the vector of primary variables, (9) may not be reduced to a smaller system. It is to be solved by an iterative technique. Although (9) is a Schur complement reduction of the Jacobian system (8), for the sake of brevity we shall refer to it as the Jacobian system.

According to Assumption 1, our formulation is presented in terms of pressure and saturations. At least for the black oil isothermal models, the studies [13–15] show that: the pressure equation is essentially parabolic or elliptic and the saturation equations are hyperbolic or transport-dominated parabolic. These features are expected to be inherited by compositional models as well [16]. A well-known consequence is that the pressure equation must be treated implicitly and the saturation equations *may* be treated explicitly (Impes models).

Applicability of the Impes models is a starting point of our considerations. We note that implicit pressure and explicit saturation advancing in time approximates the original parabolic equations. It implies that in the cases we consider, the solutions due to Impes and fully implicit time stepping are close to each other. Therefore, the respective time step non-linear operators are close in a sense, and their linearizations (Jacobian) are expected to possess a similar nature as well. Thus, given a meaningful guess to the pressure variable, an explicit update of the saturations hopefully yields a meaningful guess to the saturation variables. It means that an explicit saturation calculation based on a physically reasonable pressure computation, results in a meaningful approximation for the inversion of the fully implicit Jacobian.

Assumption 3
Consider a reduced system with the fully implicit Jacobian (9). Let the matrix A and the vectors Y, Z be split into pressure and saturation blocks:

$$A = \begin{pmatrix} A_{\mathrm{p}} & A_{\mathrm{ps}} \\ A_{\mathrm{sp}} & A_{\mathrm{s}} \end{pmatrix}, \quad Y = \begin{pmatrix} Y_{\mathrm{p}} \\ Y_{\mathrm{s}} \end{pmatrix}, \quad Z = \begin{pmatrix} Z_{\mathrm{p}} \\ Z_{\mathrm{s}} \end{pmatrix}$$

and let a meaningful approximation $\tilde{Y}_{\mathrm{p}}$ to Y_{p} and an easy-to-invert approximation $\tilde{A}_{\mathrm{s}}$ to A_{s} be known. Then $(\tilde{Y}_{\mathrm{p}}, \tilde{A}_{\mathrm{s}}^{-1}(Z_{\mathrm{s}} - A_{\mathrm{sp}}\tilde{Y}_{\mathrm{p}}))^{\mathrm{T}}$ is a meaningful approximation to $(Y_{\mathrm{p}}, Y_{\mathrm{s}})^{\mathrm{T}}$.

The choice $\tilde{A}_{\mathrm{s}} = A_{\mathrm{s}}$ implies solution of a saturation system. Lesser stiffness of A_{s} allows us to approximate A_{s} by a simple approximation (ILU(0) or cell block Jacobi). As we shall see, the latter choice results in moderate convergence dependence on the number of grid blocks.

We note, however, that Assumption 3 is not applicable to the solution of (9) directly, since a meaningful guess $\tilde{Y}_{\mathrm{p}}$ is to be found. Computation of such a guess is the main target of decoupling techniques.

3. DECOUPLING PRECONDITIONERS

In the case of multi-phase flow, the system matrix A is sparse, non-symmetric, ill conditioned, and its blocks have different nature. The basic linear solver within IPARS is chosen to be the right preconditioned GMRES method [17]. The GMRES method is known to be the most robust method for solving non-symmetric non-singular systems, and it has a modification (flexible GMRES) capable of converging with a non-linear preconditioner. The essential drawback of the GMRES method is its memory requirements. However, fast convergence can be obtained by the use of a good preconditioner. Since the blocks of the system matrix have different characteristics (elliptic and hyperbolic), the sensible approach to the construction of a preconditioner is to precondition different blocks separately, taking the advantage of their nature. Since the blocks are coupled through non-trivial off-diagonal blocks, the issues of decoupling the blocks are to be considered.

3.1. Decoupling techniques

3.1.1. Basic framework. Our goal is an efficient iterative solution of system (9). To this end, we need a physically meaningful preconditioner for the matrix of this system. In this section, we address those preconditioners which minimize the number of systems to be solved at each preconditioned step and do not require high accuracy for such systems. This reduces both computer memory requirements and CPU time for solving a system with the preconditioner. We shall focus on preconditioners based on the pressure equation solution and block Gauss–Seidel update of saturations. Different updates as well as more advanced preconditioners [9, 18] are considered in Section 3.3.

According to Assumption 3, we need a meaningful guess $\tilde{Y}_{\mathrm{p}}$ to Y_{p}. The pressure equation reads as

$$A_{\mathrm{p}}Y_{\mathrm{p}} + A_{\mathrm{ps}}Y_{\mathrm{s}} = Z_{\mathrm{p}}$$

Here the pressure variable is coupled to the saturation variables by matrix A_{ps}. This coupling is chiefly local (Assumption 2) which means that the entries of matrix A_{ps} not belonging to the diagonal cell blocks $\{A\}_{ii}$ of A may be neglected. Therefore, any transformation of system (9) which makes the diagonal cell blocks $\{A_{\mathrm{ps}}\}_{ii}$ of A_{ps} to be zero, essentially decouples pressure from saturation and allows us to find $\tilde{Y}_{\mathrm{p}}$. We consider several such transformations. Hereinafter, we denote by $\{A\}_{ii}$ the diagonal blocks of a matrix A reordered according to grid cell blocks. Within these notations we consider transformations of (9) such that $\{A_{\mathrm{ps}}\}_{ii} = 0$.

3.1.2. Constrained pressure decoupling. The approach [9, 19] also named constrained pressure reduction (CPR) is based on inversion of local matrices $\{A\}_{ii}$. Let $e_1 = (1, 0, \ldots, 0)^{\mathrm{T}} \in \mathbf{R}^n$, I be the identity matrix of order n, and

$$G_{ii}^{\mathrm{W}} = I + e_1 e_1^{\mathrm{T}} (\{A_{\mathrm{p}}\}_{ii} \{A\}_{ii}^{-1} - I) \tag{10}$$

where in our case and according to Assumption 1

$$\{A_{\mathrm{p}}\}_{ii}$$

is a real. It is easy to check that

$$G_{ii}^{\mathrm{W}} \{A\}_{ii} = \begin{Bmatrix} A_{\mathrm{p}}^{\mathrm{W}} & O \\ A_{\mathrm{sp}}^{\mathrm{W}} & A_{\mathrm{s}}^{\mathrm{W}} \end{Bmatrix}_{ii} \tag{11}$$

which implies decoupling pressure from saturations within the diagonal cell block $\{A\}_{ii}$. Introducing the block diagonal matrix

$$G^{\mathrm{W}} = \mathrm{blockdiag}\{G_{ii}^{\mathrm{W}}\} \tag{12}$$

and multiplying (9) by G^{W}, we get the transformed system

$$A^{\mathrm{W}} = G^{\mathrm{W}} A, \quad A^{\mathrm{W}} Y = G^{\mathrm{W}} Z$$

Decomposition of A^{W} into blocks corresponding to primary variables

$$A^{\mathrm{W}} = \begin{pmatrix} A_{\mathrm{p}}^{\mathrm{W}} & A_{\mathrm{ps}}^{\mathrm{W}} \\ A_{\mathrm{sp}}^{\mathrm{W}} & A_{\mathrm{s}}^{\mathrm{W}} \end{pmatrix}$$

Expressions (11)–(12), and Assumption 3 result in the preconditioner

$$\tilde{A}^{\mathrm{W}} = \begin{pmatrix} A_{\mathrm{p}}^{\mathrm{W}} & O \\ A_{\mathrm{sp}}^{\mathrm{W}} & \tilde{A}_{\mathrm{s}}^{\mathrm{W}} \end{pmatrix} \tag{13}$$

to matrix A^{W}. Here, $\tilde{A}_{\mathrm{s}}^{\mathrm{W}}$ denotes a preconditioner to $A_{\mathrm{s}}^{\mathrm{W}}$ (cell block Jacobi). In order to solve a system $\tilde{A}^{\mathrm{W}} x = r$, one has to solve the pressure equation $A_{\mathrm{p}}^{\mathrm{W}} x_{\mathrm{p}} = r_{\mathrm{p}}$, compute the residual $r_{\mathrm{s}} - A_{\mathrm{sp}}^{\mathrm{W}} x_{\mathrm{p}}$ and precondition the residual $(\tilde{A}_{\mathrm{s}}^{\mathrm{W}})^{-1}(r_{\mathrm{s}} - A_{\mathrm{sp}}^{\mathrm{W}} x_{\mathrm{p}})$. We note that inverting $\tilde{A}_{\mathrm{s}}^{\mathrm{W}}$ requires either additional storage for keeping $(\tilde{A}_{\mathrm{s}}^{\mathrm{W}})^{-1}$ or to invert $\tilde{A}_{\mathrm{s}}^{\mathrm{W}}$ whenever we solve a system with A^{W}. In the latter case the inversion may be performed cell-by-cell resulting in a sequence of inversions of order $n - 1$. Furthermore, one property of the decoupling is that $A_{\mathrm{sp}}^{\mathrm{W}} = A_{\mathrm{sp}}$, $A_{\mathrm{s}}^{\mathrm{W}} = A_{\mathrm{s}}$, that is, large part of system (9) remains unchanged.

3.1.3. Householder reflection decoupling. An alternative to CPR decoupling is the Householder reflection [8]. Let G_{ii}^{H} be a product of $n-1$ Householder matrices:

$$G_{ii}^{\mathrm{H}} = P_{1,ii} \cdot P_{2,ii} \ldots P_{n-1,ii} \tag{14}$$

Multiplication of a matrix by $P_{k,ii}$ zero the kth row of the upper triangular part of $\{A\}_{ii}$. Hence,

$$G_{ii}^{\mathrm{H}}\{A\}_{ii} = \begin{Bmatrix} A_{\mathrm{p}}^{\mathrm{H}} & O \\ A_{\mathrm{sp}}^{\mathrm{H}} & A_{\mathrm{s}}^{\mathrm{H}} \end{Bmatrix}_{ii} \tag{15}$$

where $A_{\mathrm{s}}^{\mathrm{H}}$ is lower triangular matrix. This implies not only decoupling pressure from saturations, but a virtual factorization of the saturation block $A_{\mathrm{s}}^{\mathrm{H}}$ within a grid block. Multiplication of (9) by the block diagonal matrix

$$G^{\mathrm{H}} = \mathrm{blockdiag}\{G_{ii}^{\mathrm{H}}\}$$

result in the transformed system

$$A^{\mathrm{H}} = G^{\mathrm{H}}A, \quad A^{\mathrm{H}}Y = G^{\mathrm{H}}Z$$

Block representation of A^{H} and its preconditioner $\tilde{A}^{\mathrm{H}}$ related to primary variables are

$$A^{\mathrm{H}} = \begin{pmatrix} A_{\mathrm{p}}^{\mathrm{H}} & A_{\mathrm{ps}}^{\mathrm{H}} \\ A_{\mathrm{sp}}^{\mathrm{H}} & A_{\mathrm{s}}^{\mathrm{H}} \end{pmatrix}, \quad \tilde{A}^{\mathrm{H}} = \begin{pmatrix} A_{\mathrm{p}}^{\mathrm{H}} & O \\ A_{\mathrm{sp}}^{\mathrm{H}} & \tilde{A}_{\mathrm{s}}^{\mathrm{H}} \end{pmatrix} \tag{16}$$

Here, $\tilde{A}_{\mathrm{s}}^{\mathrm{H}}$ denotes the cell block Jacobi approximation to $A_{\mathrm{s}}^{\mathrm{H}}$. The solution procedure for matrix $\tilde{A}^{\mathrm{H}}$ is similar to that for the matrix $\tilde{A}^{\mathrm{W}}$. The first advantage is that neither additional memory nor additional inversion is needed to evaluate $(\tilde{A}_{\mathrm{s}}^{\mathrm{H}})^{-1}$, since it is lower triangular. Another profit of Householder reflections is that they preserve the L_2 norm of a vector. This property is important in the case of the inexact Newton method, when the forcing term technique is used to relax the tolerance of the linear iterative solver. The L_2-norm conservation implies direct applicability of advanced modifications of the Newton method.

3.1.4. Quasi-Impes decoupling. Quasi-Impes decoupling uses an Impes reduction [7] approach to zero the block $\{A_{\mathrm{ps}}\}_{ii}$. Let $X_i \in \mathbf{R}^n$ satisfy the system

$$\{A\}_{ii}^{\mathrm{T}} X_i = e_1 \tag{17}$$

Due to (17) multiplication of $\{A\}_{ii}$ by X_i^{T} yields

$$X_i^{\mathrm{T}} \begin{Bmatrix} A_{\mathrm{p}} & A_{\mathrm{ps}} \\ A_{\mathrm{sp}} & A_{\mathrm{s}} \end{Bmatrix}_{ii} = \{A_{\mathrm{p}}^{X} \quad O\}_{ii}$$

Therefore, if we define the cell block diagonal matrix

$$G^{X} = \mathrm{blockdiag} \begin{Bmatrix} X_i^{\mathrm{T}} \\ \overset{\circ}{I}_{n-1} \end{Bmatrix}, \quad \overset{\circ}{I}_{n-1} := (O \quad I_{n-1}) \in \mathbf{R}^{(n-1)\times n}$$

and multiply it by both sides of (9), we obtain the transformed system

$$A^X = G^X A, \quad A^X Y = G^X Z$$

Block representations of A^X and its preconditioner $\tilde{A}^X$ are similar to those of A^{W} and $\tilde{A}^{\mathrm{W}}$:

$$A^X = \begin{pmatrix} A^X_{\mathrm{p}} & A^X_{\mathrm{ps}} \\ A^X_{\mathrm{sp}} & A^X_{\mathrm{s}} \end{pmatrix}, \quad \tilde{A}^X = \begin{pmatrix} A^X_{\mathrm{p}} & O \\ A^X_{\mathrm{sp}} & \tilde{A}^X_{\mathrm{s}} \end{pmatrix} \tag{18}$$

where $\tilde{A}^X_{\mathrm{s}}$ is the cell block Jacobi preconditioner to A^X_{s}. The solution procedure for the matrix $\tilde{A}^X$ is just the same as for $\tilde{A}^{\mathrm{W}}$ with same properties.

3.1.5. True Impes decoupling. The main idea of the above approaches is to extract the pressure equation which is not coupled to saturations locally within grid cells. Then the construction of the preconditioner for the modified system matrix is performed in two steps: neglecting the remained pressure–saturation ties in the pressure equation; replacing the saturation block by an easy-to-invert approximation. All the approaches are similar in a sense that they construct the *slightly* coupled pressure equation algebraically, based on system (9). An alternative is to construct a decoupled pressure equation along with the generation of matrix A. Such an equation may be obtained in the framework of the Impes approach [7]. We remind that if only accumulation term is linearized in (6), the reduction procedure (6)–(9) yields a matrix denoted by A^M. Let us find such a linear combination of rows of the cell diagonal blocks $\{A^M\}_{ii}$, that the pressure is decoupled within the cells. Let vector $X_i^M \in \mathbf{R}^n$ satisfy the system

$$\{A^M\}^{\mathrm{T}}_{ii} X_i^M = e_1 \tag{19}$$

Analogous to the quasi-Impes decoupling, multiplication by $(X_i^M)^{\mathrm{T}}$ eliminates dependency of pressure on saturations:

$$(X_i^M)^{\mathrm{T}} \begin{Bmatrix} A^M_{\mathrm{p}} & A^M_{\mathrm{ps}} \\ A^M_{\mathrm{sp}} & A^M_{\mathrm{s}} \end{Bmatrix}_{ii} = \{A^M_{\mathrm{p}} \quad O\}_{ii}$$

The modified system is obtained by the multiplication of system (9) by the cell block diagonal matrix

$$G^M = \mathrm{blockdiag} \begin{Bmatrix} (X_i^M)^{\mathrm{T}} \\ \overset{\circ}{I}_{n-1} \end{Bmatrix}$$

If we assume that the well terms are implicit in pressure only, the pressure equation of the modified system is the Impes pressure equation [7]. The modified matrix and its preconditioner are

$$A^I = \begin{pmatrix} A^I_{\mathrm{p}} & A^I_{\mathrm{ps}} \\ A^I_{\mathrm{sp}} & A^I_{\mathrm{s}} \end{pmatrix}, \qquad \tilde{A}^I = \begin{pmatrix} A^I_{\mathrm{p}} & O \\ A^I_{\mathrm{sp}} & \tilde{A}^I_{\mathrm{s}} \end{pmatrix} \tag{20}$$

The true Impes reduction is different from the quasi-Impes one in the vectors X_i^M and X_i only. Vector X_i^M is defined on the basis of accumulation term, while X_i depends on all three terms of the Jacobian. Therefore, the quasi-Impes decoupling is more efficient from the algebraic point of view, though the true Impes decoupling is more physically meaningful.

Table I. Performance of decoupling preconditioners.

Case	$\tilde{A}^{\mathrm{W}}$	$\tilde{A}^{\mathrm{H}}$	$\tilde{A}^{X}$	$\tilde{A}^{I}$
1	4	4	4	5
2	4	4	4	5
3	5	5	5	27
4	7	7	7	12
5	7	7	7	12
6	14	14	15	>100

Table II. Exact saturation solve versus the block Jacobi approximation.

Case	$\tilde{A}^{\mathrm{H}}$	$\tilde{A}^{\mathrm{H}}_{\mathrm{exact}}$
1	4	4
2	4	4
3	5	5
4	7	6
5	7	6
6	14	14

3.2. Numerical comparison for the decoupling techniques

The decoupling preconditioners have been tested for several matrix equations (9). The comparative characteristic is the number of GMRES(20) iterations needed to reduce the residual L_2-norm by a factor of 10^3 (initial guess is supposed to be trivial). We consider the black oil model (water pressure as a primary variable) [20, 21]. Case 1 is the first Newton iteration of the first time step of the ninth SPE comparison problem ($15 \times 24 \times 25$ grid blocks), with a one day time step. Case 2 is different from Case 1 only in the time step increased to 10 days. Case 3 is the same as Case 2 but for the second Newton iteration. Cases 4–6 are similar to Cases 1–3 but correspond to a finer mesh ($30 \times 48 \times 50$ grid blocks). Table I summarizes the performance of the preconditioners $\tilde{A}^{\mathrm{W}}$, $\tilde{A}^{\mathrm{H}}$, $\tilde{A}^{X}$, $\tilde{A}^{I}$, with the cell block Jacobi approximations of saturation blocks $A_{\mathrm{s}}^{\mathrm{W}}$, $A_{\mathrm{s}}^{\mathrm{H}}$, A_{s}^{X}, A_{s}^{I}, and almost exact solution of the pressure equation.

We may conclude that the true Impes results in larger number of iterations compared to other types of decoupling which perform similarly.

In the above experiments, we used the cell block Jacobi preconditioner $\tilde{A}_{\mathrm{s}}$ in the block Gauss–Seidel update of saturations. However, it is not clear how accurate should be the saturation preconditioner $\tilde{A}_{\mathrm{s}}$, or, in other words, what is the price for the replacement of the saturation block A_{s} by a computationally cheap preconditioner. In Table II, we compare two block Gauss–Seidel preconditioners for the Householder decoupling (16) and the above described data set. The first one takes the cell block Jacobi approximation $\tilde{A}_{\mathrm{s}}^{\mathrm{H}}$ for the saturation block $A_{\mathrm{s}}^{\mathrm{H}}$, and the second, $\tilde{A}^{\mathrm{H}}_{\mathrm{exact}}$, uses $\tilde{A}_{\mathrm{s}}^{\mathrm{H}} = A_{\mathrm{s}}^{\mathrm{H}}$.

It is clear that the usage of cell block Jacobi approximation to the saturation block almost does not affect the convergence rate. Hence, it is decoupling preconditioner that makes the convergence sensitive to the mesh size.

3.3. Combinative techniques

The assumption that pressure 'governs' saturations but is not 'governed' by saturations may be too strong. The preconditioner providing a feedback for the pressure–saturation interaction is likely to converge faster. An example of such a preconditioner is the combinative two-stage preconditioner [10, 9, 19]. Consider, for example, a Jacobian system transformed by the Householder reflection decoupling (16). The action of the two-stage combinative preconditioner $Y = (\tilde{A}_2^{\mathrm{H}})^{-1} Z$ is

1. Solve the pressure equation $A_{\mathrm{p}}^{\mathrm{H}} Y_{\mathrm{p}} = Z_{\mathrm{p}}$.
2. Compute the total residual:

$$\begin{pmatrix} R_{\mathrm{p}} \\ R_{\mathrm{s}} \end{pmatrix} = \begin{pmatrix} Z_{\mathrm{p}} \\ Z_{\mathrm{s}} \end{pmatrix} - \begin{pmatrix} A_{\mathrm{p}}^{\mathrm{H}} \\ A_{\mathrm{sp}}^{\mathrm{H}} \end{pmatrix} Y_{\mathrm{p}}$$

3. Precondition the total residual and update the pressure:

$$\begin{pmatrix} Y_{\mathrm{p}} \\ Y_{\mathrm{s}} \end{pmatrix} := (\hat{A}^{\mathrm{H}})^{-1} \begin{pmatrix} R_{\mathrm{p}} \\ R_{\mathrm{s}} \end{pmatrix} + \begin{pmatrix} Y_{\mathrm{p}} \\ O \end{pmatrix}$$

Here, $\hat{A}^{\mathrm{H}}$ stands for a preconditioner to A^{H} providing a pressure dependence of saturations. The difference between the combinative $\tilde{A}_2^{\mathrm{H}}$ and block Gauss–Seidel preconditioner $\tilde{A}^{\mathrm{H}}$ (16) is in computing and preconditioning the residual, as well as the presence of the feedback update of the pressure. The algebraic form of the combinative preconditioner is

$$\left(\tilde{A}_2^{\mathrm{H}}\right)^{-1} = \begin{pmatrix} (A_{\mathrm{p}}^{\mathrm{H}})^{-1} & 0 \\ 0 & 0 \end{pmatrix} + (\hat{A}^{\mathrm{H}})^{-1} \left(I - \begin{pmatrix} A_{\mathrm{p}}^{\mathrm{H}} \\ A_{\mathrm{sp}}^{\mathrm{H}} \end{pmatrix} (A_{\mathrm{p}}^{\mathrm{H}})^{-1} \right) \tag{21}$$

Two important remarks are pertinent here. First, the block $(A_{\mathrm{p}}^{\mathrm{H}})^{-1}$ may be replaced by any pressure preconditioner. Second, according to numerical evidence, the preconditioner $\hat{A}^{\mathrm{H}}$ to the whole matrix may be chosen to be rather weak, since its goal is to provide a pressure–saturation feedback. Possible candidates are ILU(1) [19], DILU [22], or one LSOR iteration, or even a couple of Richardson iterations with a block Jacobi preconditioner.

We compare the combinative preconditioner (21) with the block Gauss–Seidel preconditioner (16). The preconditioner $\tilde{A}^{\mathrm{H}}$ uses the cell block Jacobi approximation $\tilde{A}_{\mathrm{s}}^{\mathrm{H}}$ of $A_{\mathrm{s}}^{\mathrm{H}}$. The global preconditioner $\hat{A}^{\mathrm{H}}$ in the combinative method $\tilde{A}_2^{\mathrm{H}}$ is just two Richardson iterations with matrix A^{H} and the cell block Jacobi preconditioner and zero initial guess ($\tilde{A}_{2,\mathrm{R}}^{\mathrm{H}}$), or one LSOR iteration with blocks associated to vertical grid lines ($\tilde{A}_{2,\mathrm{L}}^{\mathrm{H}}$). We note that in the case of the black oil (and compositional) model, the cost of $\hat{A}^{\mathrm{H}}$ evaluation approaches the cost of multiplication by the Jacobian matrix A^{H}. Therefore, the cost of one GMRES iteration with the combinative preconditioners $\tilde{A}_{2,\mathrm{R}}^{\mathrm{H}}$, $\tilde{A}_{2,\mathrm{L}}^{\mathrm{H}}$ exceeds that for $\tilde{A}^{\mathrm{H}}$ by an additional matrix-vector multiplication for A^{H}. In the case of two-phase flow (hydrology model) the relative weight of $\hat{A}^{\mathrm{H}}$ becomes larger in the overall cost of the combinative preconditioner.

In our comparison, we consider four cases related to the hydrology (Cases 1,2) and to the black oil (Cases 3,4) models. The physical properties of the reservoir are similar in all the cases: vertical permeability has a 4-fold jump in a thin horizontal layer (Plate 1), and in two

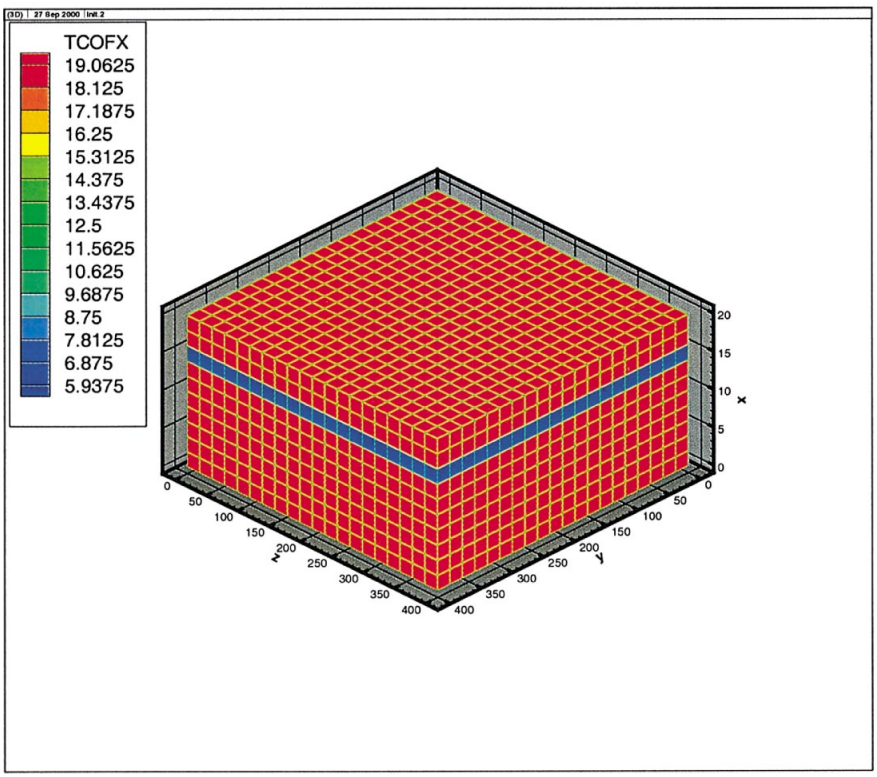

Plate 1. Layered media.

Table III. Block Gauss–Seidel and the combinative preconditioners.*

Case	No. of GMRES iteration			No. of GMRES per Newton step			CPU time		
	$\tilde{A}^{\mathrm{H}}$	$\tilde{A}^{\mathrm{H}}_{2,\mathrm{R}}$	$\tilde{A}^{\mathrm{H}}_{2,\mathrm{L}}$	$\tilde{A}^{\mathrm{H}}$	$\tilde{A}^{\mathrm{H}}_{2,\mathrm{R}}$	$\tilde{A}^{\mathrm{H}}_{2,\mathrm{L}}$	$\tilde{A}^{\mathrm{H}}$	$\tilde{A}^{\mathrm{H}}_{2,\mathrm{R}}$	$\tilde{A}^{\mathrm{H}}_{2,\mathrm{L}}$
1	158	130	120	7.9	6.5	6	8.5	9.5	9.6
2	361	257	241	17.2	11.7	10.5	177	166	168
3	141	114	108	5.6	4.6	4.3	11.3	12.9	15.4
4	653	363	345	15.5	9.5	8.6	431	355	397

*Pressure block is preconditioned by LSOR(6).

Table IV. Block Gauss–Seidel and the combinative preconditioners.*

Case	No. of GMRES iteration			No. of GMRES per Newton step			CPU time		
	$\tilde{A}^{\mathrm{H}}$	$\tilde{A}^{\mathrm{H}}_{2,\mathrm{R}}$	$\tilde{A}^{\mathrm{H}}_{2,\mathrm{L}}$	$\tilde{A}^{\mathrm{H}}$	$\tilde{A}^{\mathrm{H}}_{2,\mathrm{R}}$	$\tilde{A}^{\mathrm{H}}_{2,\mathrm{L}}$	$\tilde{A}^{\mathrm{H}}$	$\tilde{A}^{\mathrm{H}}_{2,\mathrm{R}}$	$\tilde{A}^{\mathrm{H}}_{2,\mathrm{L}}$
1	58	49	52	2.9	2.5	2.6	4.8	5.6	6.2
2	115	82	72	5.5	3.7	3.4	72	76	73
2′	184	113	73	9.2	5.6	3.6	79	73	59
3	147	112	108	5.9	4.5	4.3	11.5	13.5	16
4	604	372	343	15.5	9.5	8.3	417	384	423
4′	971	551	292	19.4	11	5.8	651	484	344

*Pressure block is preconditioned by AMG.

opposite corners there are injection and production wells. The mesh in Cases 1 and 3 has $10 \times 20 \times 20$ cells, while in Cases 2 and 4 the mesh has $20 \times 40 \times 40$ cells. The simulation is done for 18 days within 10 time steps. The relative tolerance for the Newton iterations is 10^{-4} and for the linear solver 10^{-2}. The pressure equation is solved by 6 LSOR iterations. In Table III, we show the total number of linear iterations accumulated in the whole simulation and the average number of GMRES(20) iterations per Newton step, as well as CPU time of all linear solves measured on a PC-II(400 MH).

As it stems from the data in Table III, the combinative preconditioner results in a faster convergence although one GMRES iteration is more costly than that for the block Gauss–Seidel. The advantage of the combinative preconditioner becomes more evident for large number of unknowns. The drawback of the considered two Richardson iterations is that the iterative parameter is not known *a priori*. The value of the parameter affects the convergence. The chosen value (1.0) accelerates the method considerably for the above cases. But in other cases, the convergence may be even worse compared to the block Gauss–Seidel preconditioner. LSOR preconditioning is robust and may be considered to be parameter-independent. Our experience shows that the combinative technique is more efficient than the block Gauss–Seidel method, if the pressure block is not preconditioned very well or if the media is heterogeneous. Table IV illustrates this by the results of the same experiments with algebraic multi-grid preconditioner [23] for the pressure block, which is the best preconditioner at hand. Cases 2′ and 4′ differ from cases 2 and 4 only in 10-fold heterogeneous permeability.

4. CONCLUSIONS

We considered several issues related to the iterative solution of the systems of non-linear partial differential equations. The systems appear in the fully implicit simulation of multi-phase flow in porous media. Three-phase black oil model (with species oil, water and gas) and two-phase hydrology model (with species oil and water) have been examined. We made the comparative study of several coupling and decoupling methods in order to derive some practical conclusions.

The preconditioned GMRES method is a robust algorithm for solving sparse linear systems appearing in the porous media flow simulations. The set of decoupling techniques has been examined. The goal of the techniques is to decouple a pressure equation from saturation ones. This approach seems to be very promising in compositional models. Four approaches to decoupling have been tested for the black oil model. Three of them have exhibited the same convergence properties. The Householder reflection decoupling is more preferable since it minimizes memory requirements. Two techniques for construction of the global preconditioner have been considered: the combinative and block Gauss–Seidel. The combinative technique accelerates the convergence of GMRES method and may reduce the overall CPU time in spite of more expensive iterations. The advantage of the combinative technique may be seen in the case of weak pressure preconditioner or large number of grid blocks.

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REFERENCES

1. Peaceman DW. Interpretation of well–block pressures in numerical reservoir simulation. *Society of Petroleum Engineering Journal*, *Transactions of the AIME* 1978; **253**:183–194.
2. Lu Q, Peszynska M, Wheeler MF. A parallel multi-block black-oil model in multi-model implementation. *2001 SPE Reservoir Simulation Symposium*, SPE 66359, Houston, TX, 2001.
3. Wheeler MF, Wheeler JA, Peszynska M. A distributed computing portal for coupling multi-physics and multiple domains in porous media. *Computational Methods in Water Resources*, vol. XII, Calgary, Alta., Canada, 25–29 June 2000.
4. Miffin RT, Watts JW. A fully coupled, fully implicit reservoir simulator for thermal and other complex reservoir processes. SPE 21252.
5. Watts JW. A compositional formulation of the pressure and saturation equations. *SPE Reservoir Engineering* 1986; **1**:243–252.
6. Young LD, Stephenson RE. A generalized compositional approach for reservoir simulation. *Society of Petroleum Engineering Journal* 1983; **23**:727–742.
7. Coats KH. A note on Impes and some Impes-based simulation models. Presented at the *SPE 1999 Reservoir Simulation Symposium*, SPE 49774, Houston, TX, February 14–17, 1999.
8. Edwards HC. A parallel multilevel-preconditioned GMRES solver for multi-phase flow models in the implicit parallel accurate reservoir simulator (IPARS). *TICAM Report* 98-04, The University of Texas, Austin, 1998.
9. Dawson CN, Klie H, Wheeler MF, Woodward C. A parallel implicit, cell-centered method for two-phase Krylov-secant methods for solving large scale systems of coupled non-linear parabolic equations. *Ph.D. Thesis*, Rice University, Houston, 1996.
10. Behie G, Vinsome P. Block iterative methods for fully implicit reservoir simulation. *Society of Petroleum Engineers Journal SPE9303* 1980; 658–558.
11. Killough JE. *Ninth SPE Comparative Solution Project*: *A Reexamination of Black-Oil Simulation*. *Society of Petroleum Engineering Journal* 1995 SPE 29110.
12. *Proceedings of the 15th Symposium on Reservoir Simulation*, Society of Petroleum Engineers Inc., Richardson, TX, 1999.

13. Aziz K, Settari A. *Petroleum Reservoir Simulation*. Applied Science Publishers Ltd.: London, 1979.
14. Bell JB, Trangenstein JA, Shubin GR. Conservation laws of mixed type describing three-phase flow in porous media. *SIAM Journal on Applied Mathematics* 1986; **46**:1000–1017.
15. Peaceman D. *Fundamentals of Numerical Reservoir Simulation*. Elsevier Scientific Publishing Company: Amsterdam, 1977.
16. Watts JW. A compositional formulation of the pressure and saturation equations. *SPE Reservoir Engineering* 1986; **1**:243–252.
17. Saad Y. *Iterative Methods for Sparse Linear Systems*. PWS Publishing Co.: Boston, 1996.
18. Watts JW. A total-velocity sequential preconditioner for solving implicit reservoir simulation matrix equations. Presented at the *SPE 1999 Reservoir Simulation Symposium*, SPE 51909, Houston, TX, February 14–17, 1999.
19. Wallis JR, Kendall RP, Little TE. Constrained residual acceleration of conjugate residual methods. Presented at the *SPE 1985 Reservoir Simulation Symposium*, SPE 13536, Dallas, TX, February 10–13, 1985.
20. Lu Q. A parallel multi-block/multi-physics approach for multi-phase flow in porous media. *Ph.D. Thesis*, TICAM, The University of Texas, Austin, 2000.
21. Trangenstein JA, Bell JB. Mathematical structure of the black-oil model for petroleum reservoir simulation. *SIAM Journal on Applied Mathematics* 1989; **49**:749–783.
22. Dean R. *Private Communication*.
23. Stuben K. Algebraic multigrid (AMG): experiences and comparisons. *Applied Mathematics and Computation* 1983; **13**:419–452.
24. Bank R, Wagner C. Multilevel ILU decomposition. *Numerische Mathematik* 1999; **82**(4):543–576.

