A Two-Level Variant of Additive Schwarz Preconditioning for Use in Reservoir Simulation

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Abstract

The computation time for reservoir simulation is dominated by the linear solver. The sets of linear equations which arise in reservoir simulation have two distinctive features: the problems are usually highly anisotropic, with a dominant vertical flow direction, and the commonly used fully implicit method requires a simultaneous solution for pressure and saturation or molar concentration variables. These variables behave quite differently, with the pressure feeling long-range effects while the saturations vary locally. In this paper we review preconditioned iterative methods used for solving the linear system equations in reservoir simulation and their parallelisation. We then propose a variant of the classical additive Schwarz preconditioner designed to achieve better results on a large number of processors and discuss some directions for future research.

1 Introduction

In terms of computing time, the primary element of the majority of reservoir simulations is the solution of a large sparse set of non-symmetric linear equations. The most common mode for reservoir simulation is three-phase fully implicit. Over a given time step in the simulation, a set of non-linear conservation equations is solved, the solution variables typically being cell pressures and either saturations or molar densities (see, for example, [7]). It is also possible to treat just the pressures implicitly, replacing some non-linear functions such as fluid densities and capillary pressures by their start of time step values. Such a method, usually referred to as IMPES (implicit pressure explicit saturation), is now mainly used for compositional reservoir simulation, in which multiple components are tracked using an equation of state to characterise the fluid. IMPES methods are given to oscillatory instability, and fully implicit methods are generally preferred by users.

The required system of conservation equations is typically derived from a finite volume discretisation, and consists of mass accumulation, flow, and well injection and production terms. The system is conservative, and is commonly expressed in residual form, \( R(X) = 0 \), where \( X \) is the set of solution variables to be solved for. In solving these equations using a Newton-Raphson method, a set of solution changes \( x \) is obtained by solving the set of linear equations given by

\[
x = -J^{-1}R(X)
\]  

(1.1)

where

\[
J = \nabla R(X)
\]  

(1.2)

\( J \) is the Jacobian. It is common to treat the set of solution variables associated with a given reservoir simulation cell (for example the pressure, oil saturation and gas saturation) as a single strongly coupled

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sub-vector. So for a three-phase black oil problem the elements of \( X \) and \( R \) would be 3-component sub-vectors and the elements of \( J \) would be 9-component sub-matrices. Given the large size of the ensuing linear system (hundreds of thousands of cells are common in industry, millions becoming so) direct methods are not feasible, and so iterative methods are used.

In this paper we begin in Section 2 by reviewing the iterative methods typically used in reservoir simulation packages, before discussing their adaptation and performance in a parallel computing environment in Section 3. In Section 4 we then present some recent work aimed at improving the parallel performance of multi-phase linear solution by extending the overlap zones to cover the full problem in a coarsened way, similar to a coarse-grid correction but ensuring that local saturation variables are not smeared. Results are presented in Section 5, before discussing our findings and suggesting future avenues of research in Section 6.

2 Review of iterative methods for solving linear system in reservoir simulation

The linear sub-problem can also be expressed in residual form as \( r = b - Ax = 0 \), with \( b = R \), the current non-linear residual, and \( A = -J \). In the early days of reservoir simulation stationary iterative methods such as SOR were common [20], but soon preconditioned conjugate gradients became standard, typically accelerated using ORTHOMIN [18], GMRES [14], or BiCGStab [17]. Preconditioning is usually performed by selecting an invertible approximation to \( A \), \( B \sim A \), such that the inversion of \( B \) is reasonably practical. The most common choice of \( B \) is an incomplete LU factorisation with some degree of fill-in, often zero [13].

In the context of fully implicit reservoir simulation it is typical for ILU methods to be applied to the block structure of the matrix, with the dense sub-matrices inverted directly. Furthermore, the issue of material balance is important in reservoir simulation. In light of this, it is possible to choose \( B \) such that the column sum of the error matrix \( E = B - A \) is zero; this improves convergence and corresponds to selecting a solution in which \( \sum r = 0 \). This has a useful physical interpretation in that it corresponds to zero mass conservation error. As a reservoir simulation can involve many thousand steps, it is useful if the mass accumulation error superconverges: in some reservoir simulation formulations the mass balance error can be zero after one non-linear iteration if using a linear solver which zeros the linear residual sum.

The Jacobian matrices arising from reservoir simulation problems are diagonally dominant, but marginally so, with strong bands representing flow between neighbouring cells – an example is shown in Figure 1. Furthermore, an oil reservoir may be tens of kilometres in areal extent, but a few hundred metres in vertical extent. Flow in the vertical direction is over a shorter distance than in the areal, and occurs over a larger area. The result is that off-diagonal matrix elements representing vertical flow are particularly strong. In light of this, a popular variant of ILU within the context of reservoir simulation is nested factorisation, a series of nested LU factorizations, which is particularly suited to the strong asymmetry of the problem [3]. Nested factorisation produces a preconditioning matrix with no error terms in the vertical direction, as shown in Appendix A, and by eliminating errors in the dominant flow direction results in a very effective and robust preconditioning. Furthermore, by requiring no fill-in, the algorithm is memory efficient. However, it is less suitable for reservoirs with horizontal wells, which destroy the banded sparsity pattern, and those with large heterogeneity, especially in the horizontal direction.

An alternative to preconditioned iterative methods are algebraic multigrid (AMG) methods. These construct a solution based on the application of corrections obtained on a series of successively coarser grids. The corrections are frequently regarded as smoothings, and constructed using Gauss-Seidel or ILU techniques. Such methods are generally effective on the long-range terms which arise in the solution of elliptic equation systems. In reservoir simulation terms this corresponds to the pressure variable part of the solution. However, multigrid methods are less suited to the treatment of saturation or composition variables; these exhibit sharp variations in fluid displacement fronts, and the use of a coarse grid method introduces solution smearing. The result is that, for fully implicit simulation, multigrid methods are usually applied in combination with a second saturation solver: first an approximate pressure-only-equation is set up and solved (using, for example, the constrained pressure residual formulation [19]); then a solver such as ILU(0) is used to obtain the full pressure and saturation solution to the full system [16, 10]. It is then common to use this two-stage solution as a preconditioner within an iterative method.
3 Parallelisation

With the advent of parallel computing architectures in the last twenty or so years reservoir simulation solvers have been adapted to work in parallel. Unfortunately, the use of an invertible LU approximation to the matrix, such as nested factorisation, tends to involve recursive back-substitution techniques which are difficult to run in parallel. One common method for improving the performance of LU factorisation methods when running in parallel is the use of multi-colour domains. Examples are simple block red-black ordering such as parallel nested factorisation [12] and more complex multi-colour methods such as the JALS solver [2]. These preserve the virtue of nested factorisation that error terms in one direction are eliminated, but the preconditioning becomes less effective in the other directions as the number of processors is increased, increasing the iteration count. In addition, the presence of features such as horizontal wells can yield matrix elements which do not fit naturally into the multicolour ordering. Multigrid solvers are more effective as parallel solvers, the number of linear iterations remaining more constant as the number of processors is increased. However, a significant amount of inter-process communication is required to form and solve for the corrections on the coarser grids using all the processors; and an effective parallel method to find the full pressure and saturation solution after the multigrid pressure correction has been applied is still required. Overall, the effect is that solver speed-up still eventually degrades with increasing number of processors.

Whilst the use of up to around 60 processors has been common for some years, computers with hundreds of thousands of processors are now becoming available, so there has been a drive towards finding a new generation of solvers that can scale to work on large clusters of processors. A class of methods that are attractive in this context use sparse approximate inverse (SAI) solvers, which have been widely investigated in the academic literature [5, 8]. These are radically different in that they work in terms of creating approximations to $A^{-1}$ directly rather than an invertible approximation to $A$. In a SAI method the construction of the approximate inverse is thus a completely parallel task; and the construction of a new search direction is done using a matrix multiplication operation. However, in order to render the method practical the approximate inverse must be constrained to be sparse, which means that when constructing a new linear solver search direction a given solution variable is only aware of a small subset of elements of the residual.
Generally SAI methods are similar in performance to ILU methods and have not been heavily used in practical reservoir simulation.

Current methods for solving reservoir simulation linear equations on highly parallel systems include the LSPS solver [9], which uses a power expansion of the inverse of the matrix $A$ to obtain a better approximation to the inverse matrix $A^{-1}$:

$$B^{-1} = \left( I + \sum_{i=1}^{n} (-T^{-1}E)^i \right) T^{-1}$$

(3.1)

where

$$A = T + E$$

(3.2)

and the use of additive Schwarz methods in which each processor uses its own block of the entire matrix, plus some elements of the matrix from other processors by overlapping the computational domains:

$$B_{AS}^{-1} = \sum_{i=1}^{n} R_i^T A_i^{-1} R_i$$

(3.3)

where

$$A_i = R_i A R_i^T$$

(3.4)

and $R_i$ is the rectangular restriction matrix to subdomain $i$.

The draw-back with additive Schwarz methods is that they do not remove small eigenvalues of the coefficient matrix, corresponding to low frequency modes arising from the long range nature of pressure effects in reservoir simulation. Two-level additive Schwarz methods (see, for example, [15]) attempt to alleviate this problem by adding a coarse-grid correction, which acts like the high level coarse grid corrections in a multigrid method:

$$B_{AS2-level}^{-1} = \sum_{i=1}^{n} R_i^T A_i^{-1} R_i + R_C^T A_C^{-1} R_C$$

(3.5)

where

$$A_C = R_C A R_C^T$$

(3.6)

and $R_C$ is a suitable global coarse-grid operator. Alternatively, one can apply the coarse grid correction successively, leading to an overall “two-stage” preconditioner

$$B_{AS2-stage}^{-1} = B_{AS}^{-1} + B_C^{-1} (I - A B_{AS}^{-1})$$

(3.7)

where

$$B_C^{-1} = R_C^T A_C^{-1} R_C$$

(3.8)
4 Boundary conditioning

In the context of multi-phase flow, such a coarse-grid correction suffers from the same problem as multigrid: the saturations are smoothed along with the pressure. In order to circumvent this problem, we propose a modified additive Schwarz preconditioner in which the operator $R_i$, rather than discarding parts of the domain outside of the $i$th subdomain, coarsens them. In matrix terms the operator may be written as

$$R_i = \begin{pmatrix} R_{C,1} & & & & 0 \\ & R_{C,2} & & & \\ & & \ddots & & \\ & & & I_i & \\ 0 & & & & R_{C,n-1} \\ & & & & R_{C,n} \end{pmatrix}$$

(4.1)

where $R_{C,i}$ are local coarse-grid operators. In this way each processor block sees the whole problem to some extent, but avoids applying a coarse grid correction to the saturation variables on that processor. An example of this process for a simple one-dimensional decomposition of a two-dimensional domain is shown in Figure 2.

![Figure 2](image-url)

**Figure 2**: Sketch showing a six-way one-dimensional decomposition of a two-dimensional uniform Cartesian grid (top) and how each processor sees only a coarsened version of the entire problem in which cells outside its own subdomain are lumped together (for clarity, only processors 1, 4, and 5 are shown)
The method proposed differs from traditional methods such as parallel nested factorisation in not using a single invertible approximating matrix $B$; instead each processor constructs and inverts its own approximation to the full matrix. In this way the method is similar to a block sparse approximate inverse; however the reduction in the dimension of each processor matrix is done using coarsening rather than sparsification, so that the reduced system is a coarse rather than a sparse approximate inverse. A similar approach has been taken by [4] in the context of finite element methods; however our approach differs in that the coarsening is performed by simple matrix element summation – the motivation is that solving a system formed in this way corresponds to finding a solution in which residual sums over the coarsened regions are forced to zero, so that material is conserved in a coarse grid sense (see Appendix B).

Once each processor has inverted its own approximation to the full matrix the full linear search direction is obtained by projecting out the on-processor elements for each domain, as in the restricted additive Schwarz method [6]. The solution obtained for the off-processor coarsened variables is discarded; it exists only to set up the boundary conditions for the on-processor variables.

The method can thus be represented as:

$$B^{-1} = \sum_{i=1}^{n} P_i B_i^{-1} \quad (4.2)$$

where

$$B_i^{-1} = R_i^T A_i^{-1} R_i \quad (4.3)$$

$P_i$ is a projection operator into the range of variables corresponding to a processor $i$. The full approximate inverse matrix is thus constructed by taking the rows corresponding to each processor from each of the different preconditionings used on each processor. In practice, the are never explicitly formed: instead the required rows from each are combined to form the full preconditioner. This row-wise combination means that if the original matrix $A$ were symmetric, the preconditioning matrix would not be. A similar effect occurs in SAI preconditioning, in which the approximate inverse is constructed on an independent column by column basis.

In matrix terms, at each iteration of the outer iterative scheme each processor $i$ solves

$$\begin{pmatrix} A_{i,i} & A_{i,C} \\ A_{C,i} & A_{C,C} \end{pmatrix} \begin{pmatrix} \Delta x_i \\ \Delta x_C \end{pmatrix} = - \begin{pmatrix} \Delta r_i \\ \Delta r_C \end{pmatrix} \quad (4.4)$$

where the subscripts $C$ indicates coarsened terms coming from other processors; the global search direction is then taken to be

$$\Delta x = \sum_i \Delta x_i \quad (4.5)$$

Like multigrid, inter-processor communication is required to form the coarsened matrices, but this occurs only at the start of each non-linear iteration. At each linear iteration only the updated coarsened residuals must be communicated. Furthermore, we note that although ideally refinement might steadily increase away from a given processor block, to obtain reasonable computation efficiency matrix elements must be lumped before communication. If all processors required a different coarsening then this algorithm would not scale, and so it is necessary to allow only a fixed number of coarsenings. In particular we use a ‘far-field’ coarse approximation, shared by all processors, and in addition a more refined ‘near-field’ approximation is constructed and shared between neighbouring processors; a sketch of the operations performed is given in Figure 3. This two-level approach is motivated by the multi-phase physics of the problem, with the near-field designed to capture local saturation variables while the far-field characterises the global pressure variations. The idea is to include long range pressure effects in an estimation of the values of the near-field cells. These then provide reasonable boundary values for the calculation on a particular processor.
Figure 3: Sketch showing how each processor coarsens its own grid in three different ways, exchanges data with other processors, and assembles its coarsened version of the full problem.

It is not a requirement that the far-field blocks correspond to processor domains. Generally, the smaller the blocks the better the boundary values that are supplied to each processor; but the price paid is that the total number of variables solved for increases.

5 Results

In order to test the theoretical performance of the method, tests were performed using a Python implementation of the algorithm, with the subdomain problems $A_i \Delta x_i = -\Delta r_i$ solved exactly by Gaussian elimination. The tests were performed on a number of matrices arising from reservoir simulation applications, whose properties are listed in Table 1. The first benchmark test case is the publicly available ORSREG1 matrix from the Harwell-Boeing matrix collection [1], taking the unit vector as the right-hand side. The others are variants of the benchmark test case of Aziz Odeh [11] using water injection instead of gas injection, with four different well configurations, as shown in Figure 4. The original grid ($10 \times 10 \times 3$) has been refined by a factor of two or three in each direction to give larger matrices, although the implementation restricted us to matrices of size less than 105. Both IMPES and fully implicit versions of the problem were considered.

We compare preconditioning using just a near-field (which is effectively an additive Schwarz method), just a far field, (which is a coarse grid correction, but applied within a single stage preconditioning) and a combination of the near and far field methods. For simplicity, the domain decomposition is done only in the $x$-direction.
| Matrix Name | Type    | Size | Number of Non-Zeros | Condition Number |
|------------|---------|------|---------------------|------------------|
| ORSEG1     | IMPES   | 2205 | 14133               | 6745             |
| SPE1a      | IMPES   | 8100 | 53874               | 349422           |
| SPE1b      | IMPES   | 8100 | 54430               | 52436            |
| SPE1c      | IMPES   | 8100 | 54432               | 379882           |
| SPE1d      | IMPES   | 8100 | 54690               | 43969            |
| SPE1a_F    | FULLI   | 9600 | 102878              | 226904602        |
| SPE1b_F    | FULLI   | 9600 | 108964              | 38324890         |
| SPE1c_F    | FULLI   | 9600 | 107790              | 44489039         |
| SPE1d_F    | FULLI   | 9600 | 129399              | 5941993          |

Table 1: Properties of test matrices used

Figure 4: Variants of SPE1 benchmark from which matrices SPE1a,b,c,d are taken. The colour represents the water saturation ranging from zero (blue) to one (red). In all cases the domain decomposition was performed in the x-direction.

In Figure 5 the linear iteration count for solving the ORSEG1 matrix is shown. $K$ is the number of processors used, $C$ is the size of the coarsening (e.g. $C = 2$ means using coarsening blocks of $2 \times 2 \times 2$) and “total blocks” refers to the average size of each $A_i$ and is a measure of how much work goes into building the pre-conditioner. As can be seen, the combination of near and far field consistently yields the minimum number of iterations. However, this does involve solving for more additional variables than the other two methods, which offsets the gain in iteration count to some extent. Nevertheless, the solver compares favourably to the classical two-level Schwarz method and alternative two-stage method, as shown in Figure 6.
Figure 5: Iteration count (histogram values) against number of processors $K$ and size of coarsening $C$ for the ORSREG1 benchmark. The average size of the subdomain problems ("total blocks") is also shown.

Figure 6: Iteration count against number of processors and size of coarsening for the ORSREG1 benchmark, comparing the far-field method to the two-level and two-stage additive Schwartz preconditioners.

For simplicity we have shown results without overlap, so as to compare including coarsened information in our far-field method compared to the classical methods – however similar results are obtained when an overlap (or near-field) is added. The same behaviour was seen for all of the matrices tested, with the near+far method consistently giving the best iteration count – examples are shown in Figures 7 and 8.
Figure 7: Iteration count (histogram values) against number of processors $K$ and size of coarsening $C$ for the fully implicit SPE1a_F benchmark refined to $20 \times 20 \times 6$ cells. The average size of the subdomain problems (“total blocks”) is also shown.

Figure 8: Iteration count (histogram values) against number of processors $K$ and size of coarsening $C$ for the IMPES SPE1d benchmark refined to $30 \times 30 \times 9$ cells. The average size of the subdomain problems (“total blocks”) is also shown.
Finally, tests on a two-dimensional decomposition (in both $x$ and $y$ direction) showed this to be superior to those based on a one-dimensional split, see Figure 9. The only case in which the one-dimensional split worked as well as the two-dimensional split was case b, where the primary direction in which the pressures and saturation vary is orthogonal to the direction in which the problem is divided into processors.

![Figure 9: Iteration count against number of processors $K$ and size of coarsening $C$ for the IMPES SPE1d benchmark refined to $30 \times 30 \times 9$ cells. Results are using the far-field solver with domain decomposition in one and two dimensions.](image)

6 Discussion

The method proposed is an extension of additive Schwarz which takes account not only of the neighbouring processor’s cells, but also of cells further away in a coarsened sense. As the coarse grid problem is effectively solved in a slightly different form on all the processors, this background far field needs to be fairly coarse, both to minimise the number of off-processor cells and the communication time required to pass this information to all the processors. The advantage is that the whole problem is seen, in some sense, by all the processors. The improvement in preconditioning is offset by the number of ‘off-processor’ variables which must be treated by each processor along with the ‘on-processor’ ones that are actually used. Clearly, if the problem is large, there is a case for a second deeper level of coarsening of the far-field in distant regions far from a given processor.

The results presented in this paper were all on small problems with less than 105 variables, with the subdomain problems $A_i \Delta x_i = -\Delta r_i$ solved exactly by Gaussian elimination. This gives us the optimal iteration count for the proposed method, focusing solely on the effect of boundary conditioning. For large-scale reservoir simulations involving tens of millions of cell an exact solution is not feasible, even if hundreds of processors are used. Nevertheless, the method may be generalised to approximately solve the system by inverting a preconditioner $B_i \sim A_i$ instead. In particular, ILU(n), nested factorisation, or even multigrid are all options. Finally, it is also possible to combine boundary conditioning with a global multigrid pressure solver step – however the use of the far-field means that the solver already includes some elements of a multigrid solver.
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Appendix

A Error matrix for nested factorisation

For a hepta-banded matrix of the form

\[ A = D + L_1 + U_1 + L_2 + U_2 + L_3 + U_3 \]  \hspace{1cm} (A.1)

where \( L_i \), \( U_i \) represent lower and upper bands respectively, as typically found from three-dimensional finite volume problems, the nested factorisation preconditioner \( B \) is defined by

\[ B = (P + L_3)(I + P^{-1}U_3) \]  \hspace{1cm} (A.2)

\[ P = (T + L_2)(I + T^{-1}U_2) \]  \hspace{1cm} (A.3)

\[ T = (G + L_1)(I + G^{-1}U_1) \]  \hspace{1cm} (A.4)

where \( G \) is a diagonal matrix. The error matrix is therefore given by

\[ E = B - A = G - D + L_1G^{-1}U_1 + L_2T^{-1}U_2 + L_3P^{-1}U_3 \]  \hspace{1cm} (A.5)

and so we see that by choosing \( G \) such that

\[ G = D - L_1G^{-1}U_1 \]  \hspace{1cm} (A.6)

we eliminate errors coming from the (strongest) inner bands. In practice, one may also preserve residual sum by choosing \( G \) such that

\[ G = D - L_1G^{-1}U_1 - \text{colsum} (L_2T^{-1}U_2) - \text{colsum} (L_3P^{-1}U_3) \]  \hspace{1cm} (A.7)

which nonetheless preserves the virtue of eliminating errors from the inner bands.

B Motivation for use of lumping

Suppose we are iteratively solving the \( n \times n \) linear system \( r = b - ax = 0 \). Define the \( n \times N \) lumping matrix \( E \) consisting of zeros and unit elements, so that, for any \( i \), only one element \( E_{II} \) is non-zero. A typical \( E \) matrix is shown below

\[ E = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 1 & 1 \end{pmatrix} \]  \hspace{1cm} (B.1)

Premultiplying a \( n \)-dimensional vector by \( E \) transforms it to the \( N \)-dimensional space (where it this case \( N = 3 \))

\[ X = Ex, \hspace{1cm} X_I = \sum_{i \in I} E_{II}x_i \]  \hspace{1cm} (B.2)

A coarse-grid lumping matrix, or Watts correction [20], can then be defined as

\[ A = EaE^T, \hspace{1cm} A_{IJ} = \sum_{i \in I \, j \in J} E_{II}a_{ij}E_{JJ}^T \]  \hspace{1cm} (B.3)

so that \( A_{IJ} \) is the sum of the matrix elements projected out by row vectors \( E_I \) and \( E_J \). Starting with some residual \( r \), one can construct the lumped residual \( R = Er \) and then the lumped search direction is given by
\[
\Delta X = A^{-1} R \quad \text{(B.4)}
\]

Projecting \( \Delta X \) back to the \( n \)-space gives us the search direction \( \Delta x = E^T \Delta X \). Then the change in residual is \( \Delta r = -a \Delta x \) and so the new residual is given by

\[
r' = r - a \Delta x = r - aE^T \Delta X \quad \text{(B.5)}
\]

Lumping the residual into the \( N \)-space we find that

\[
R' = Er'
\]

\[
= Er - EaE^T \Delta X
\]

\[
= Er - EaE^T A^{-1} Er
\]

\[
= Er - AA^{-1} Er
\]

\[
= 0
\]

i.e. the residuals that are lumped together by the matrix \( E \) sum to zero.