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Deflation AMG Solvers for Highly Ill-Conditioned Reservoir Simulation Problems

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Abstract

In recent years, deflation methods have received increasingly particular attention as a means to improving the convergence of linear iterative solvers. This is due to the fact that deflation operators provide a way to remove the negative effect that extreme (usually small) eigenvalues have on the convergence of Krylov iterative methods for solving general symmetric and non-symmetric systems.

In this work, we use deflation methods to extend the capabilities of algebraic multigrid (AMG) for handling highly non-symmetric and indefinite problems, such as those arising in fully implicit formulations of multiphase flow in porous media. The idea is to ensure that components of the solution that remain unresolved by AMG (due to the coupling of roughness and indefiniteness introduced by different block coefficients) are removed from the problem. This translates to a constraint to the AMG iteration matrix spectrum within the unit circle to achieve convergence. This approach interweaves AMG (V, W or V-W) cycles with deflation steps that are computable either from the underlying Krylov basis produced by the GMRES accelerator (Krylov-based deflation) or from the reservoir decomposition given by high property contrasts (domain-based deflation). This work represents an efficient extension to the Generalized Global Basis (GGB) method that was recently proposed for the solution of the elastic wave equation with geometric multigrid and an out-of-core computation of eigenvalues.

Hence, the present approach offers the possibility of applying AMG to more general large-scale reservoir settings without further modifications to the AMG implementation or algebraic manipulation of the linear system (as suggested by two-stage preconditioning methods). Promising results are supported by

a suite of numerical experiments with extreme permeability contrasts.

Introduction

Computational modeling of flow and transport in porous media generally requires the numerical solution of large, sparse systems of equations. In most reservoir simulation scenarios, the complexity and size of problems that can be solved is highly constrained by the efficiency of the solver. This trend has been always present in the oil industry despite significant and sustained advances in high-performance computing technology.

In response to the increasing need to achieve higher resolution and complexity levels (and, therefore, larger and potentially higher ill-posed problems) in many scientific and engineering applications, solver technology has made important advances in seeking to exploit algebraic and physical relations that may be hidden in matrix coefficients. As a result, new algorithms based on Krylov recycling methods (e.g., deflation, augmented, Krylov-secant methods, etc; see Fig. 1)¹⁻⁶, algebraic multigrid/multilevel methods⁷⁻¹¹ and multiscale solvers¹²⁻¹³ have lately been driving the interest of many industrial and academic communities.

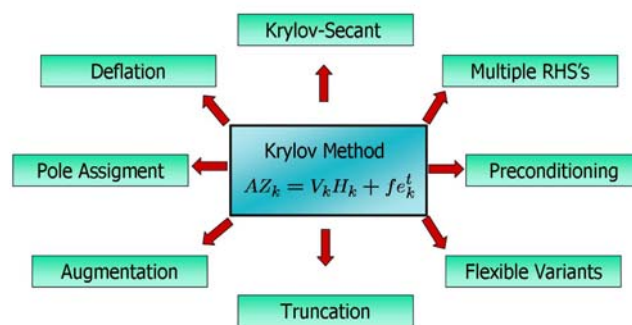


Fig. 1: A family of Krylov recycling methods.

Among the family of Krylov recycling methods, deflation has emerged as an alternative to extend the capability of current preconditioner methods. The key point is that deflation methods provide means to remove the negative effect that extreme (usually small) eigenvalues have on the convergence of Krylov iterative methods³. Nevertheless, we should point out that deflation methods are not strictly confined to the

setting of Krylov subspace iterative methods. They can also be defined in terms of the spatial discretization domain in which the flow and transport equations are defined². Moreover, important connections can be established with domain decomposition methods. Recent results have shown that deflation has greater potentials to further reduce the matrix condition number than coarse grid correction¹⁴ and balancing domain decomposition methods¹⁵.

On the other hand, Algebraic Multigrid (AMG) methods⁷⁻⁹ have been conceived to remedy several of the limitations that geometric multigrid methods show for the definition of smoothing, prolongation (restriction) operators over very complex geometries. The main advantage of AMG methods is that they operate directly on the matrix and, therefore, require no information about the physical grid or the underlying differential equation. This feature has attracted many researchers to extend the convergence theory and develop portable AMG software that may be used effectively in a wide range of scientific and engineering applications⁸.

Despite important advances of AMG from theoretical and computational perspectives, there are still many unresolved issues. The convergence of (traditional) AMG tends to deteriorate when the matrix operator departs from fulfilling the M-matrix condition. This condition may be violated whenever the matrix loses diagonal dominance or becomes highly indefinite or nonsymmetric. In such cases, components of the solution associated with small eigenvalues remain untouched and thus delay convergence towards the solution.

In reservoir simulation, there are many sources where the M-matrix property may be affected (particularly in pressure block systems): (a) highly heterogeneous media (i.e., high permeability and porosity contrasts); (b) complex geometries (e.g., fractures, pinch outs); (c) anisotropic and full tensor permeabilities; (d) drastic changes in well operations; and (e) appearance and disappearance of phases/components, to name a few. In fully implicit formulations, these situations may have more severe implications as the systems are coupled and coefficients inherit a major degree of nonlinearity with respect to the primary variables. We should point out that these difficulties are not exclusive to AMG; they are also shared by all multigrid methods.

The previous discussion suggests that in the event that AMG smoothers and coarse grid corrections are insufficient to remove slow modes from the solution it may be convenient to isolate or extract these modes from the original problem by some alternative method. In other words, AMG may benefit from transforming the original stiff problem into a less-stiff one without incurring major computational costs. Clearly, deflation aims at that objective.

There have been some previous attempts to improve multigrid algorithms based on spectral information using Rayleigh quotients¹⁶. A more powerful idea was recently exploited by Waismann et al.¹⁷⁻¹⁸ for extending geometric multigrid to deal with highly indefinite problems. The basic idea is to construct an intermediate coarse grid problem (between V, W or V-W

cycles) spanned by slowly converging eigenmodes of the multilevel iteration. These slow eigenmodes correspond to the largest eigenvalues of the iteration matrix that generally lie nearby or outside the unit disc. They coined the method as the Generalized Global Basis (GGB); it relies on an out-of-core computation of eigenvalues/eigenvectors from the multilevel iteration matrix using the ARPACK library software for large-scale eigenvalue computations¹⁹. Their approach was used as a preconditioner for either GMRES or QMR accelerators²⁰. Figure 2 illustrates the functionality of this method.

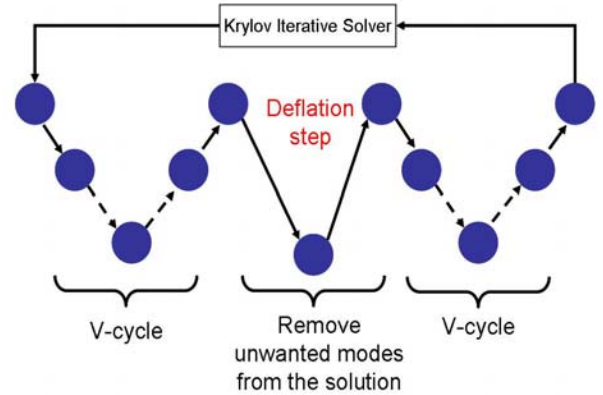


Fig. 2: The GBB approach¹⁷.

In this work, we introduce the GBB ideas with some important modifications: (1) eigenvalue computations are performed in an in-core fashion from the Arnoldi factorization generated by GMRES (or from the Lanczos factorization in the case of symmetric positive definite systems); (2) the coarse-grid construction for slow eigenmodes is replaced by a deflation operator that is applied after all multilevel cycles are carried out; (3) eigenvalues are computed based on the smallest eigenvalues of the preconditioned system which in turn, are equivalent to computing the largest eigenvalues from the multilevel iteration matrix; and (4) AMG is used instead of a geometric multigrid method.

We claim that the present approach is more efficient than the GBB method since it exploits the underlying Krylov information produced within one cycle of GMRES. Additionally, the construction and application of the deflation operator represent a marginal overhead in the overall cost in the preconditioning procedure. Promising results are supported by a suite of numerical experiments ranging from synthetic to large-scale and realistic reservoir data sets.

Krylov Basis Preliminaries

To introduce notation, let us assume that we are required to solve the generic linear system

$$Ax = b, \quad (1)$$

where $A \in \mathbb{R}^{N \times N}$ and $x, b \in \mathbb{R}^{N \times 1}$. Here, the matrix A is generally nonsymmetric, indefinite matrix as it may arise from a fully implicit formulation. Nevertheless, we remark that the approach described below can be efficiently carried out for

symmetric and positive definite systems as well (e.g., pressure block systems arising from IMPES formulations).

Suppose that we employ GMRES(s) for solving (1)²⁰. This means that each cycle of GMRES consists of s iterations before restarting the procedure with an improved solution. At the end of each cycle, if residuals have not met a predefined tolerance, GMRES produces the following Arnoldi decomposition:

$$AV_s = V_s H_s + h v_{s+1} e_s^t, \quad (2)$$

where $H_s \in \mathbb{R}^{s \times s}$ is an upper Hessenberg matrix, $V_s \in \mathbb{R}^{N \times s}$ is an orthonormal matrix holding in its columns a basis for the Krylov subspace $K_s(A, r_0) = \text{span}\{r_0, Ar_0, \dots, A^{s-1}r_0\}$ for a given initial residual r_0 . Here, h is a scalar representing $\|v_{s+1}\|$ and v_{s+1} is a vector orthonormal to V_s .

Provided the Arnoldi decomposition (2), the following reduced minimal residual problem can be solved to approximate the solution to (1) for a given initial guess x_0

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \{b - A(x - x_0)\} &= \min_{x \in \mathbb{R}^n} \{r_0 - Ax\} \\ \Rightarrow \min_{y \in \mathbb{R}^s} \left\{ \beta e_1 - \begin{pmatrix} H_s \\ h e_s^t \end{pmatrix} y \right\}. \end{aligned} \quad (3)$$

Thus, $x_s = x_0 + V y^*$, with y^* representing the solution of (3) and $\beta = \|r_0\|$. If convergence is not yet achieved then $x_0 \leftarrow x_s$ and the process is restarted (i.e., a new GMRES cycle is performed).

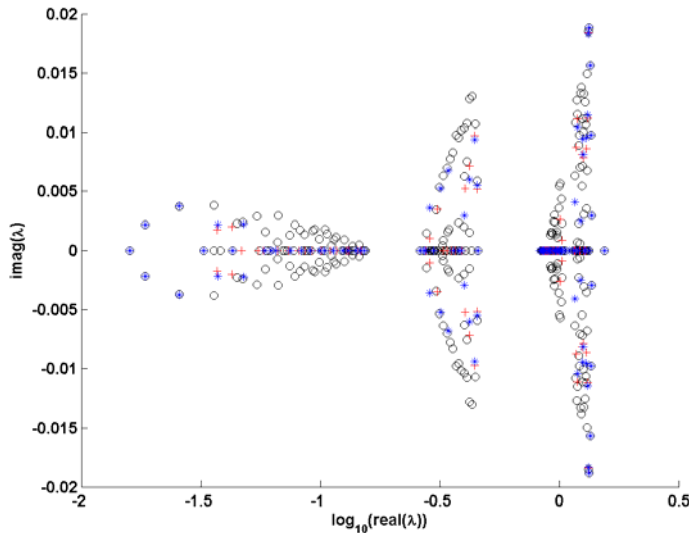


Fig. 3: Ritz values (red crosses), harmonic Ritz values (blue asterisks) and exact eigenvalues (black circles).

The eigenvalues of H_s are known as the Ritz values of A and they tend to approximate well the extreme eigenvalues of A . Additionally, harmonic Ritz values are defined as the Ritz

values of A^{-1} with respect to the space $AK_s(A, r_0)$. The key point about harmonic Ritz values is that they turn out to be even more accurate approximations to the extreme eigenvalues of A than the Ritz values^{1,3,21}. An example illustrating this fact can be seen in Figure 3 for a pressure block system obtained from a fully implicit formulation with a heterogeneous permeability field (values ranging from 10^{-2} to 10^4 md) consisting of 30×30 gridblocks. We compute 50 Ritz and harmonic Ritz values from the pressure block. We can observe how the harmonic Ritz values represent a better approximation to the smallest eigenvalues when compared to the Ritz values. A discussion of the computation of harmonic Ritz values and eigenvectors is provided below.

Deflation Preconditioner

There exists different ways to define deflation, or more generally, spectral or adaptive preconditioners^{2,6,22-24}. Here, we choose to make a presentation based on Frank and Vuik work². Let us define the left and right deflation operators P_1 and P_2 as follows:

$$P_1 = I - Z A_Z^{-1} Z^t A; \quad P_2 = I - A Z A_Z^{-1} Z^t, \quad (4)$$

where $A_Z = (Z^t A Z)^{-1}$. These operators are oblique projectors onto the orthogonal space spanned by Z . Clearly, if A is symmetric and invertible, $P_1 = P_2^t$. Thus, to solve the generic system (1) we can proceed to split the solution into two parts: $x = P_1 x + (I - P_1)x$.

The second component is quite straightforward to compute since $(I - P_1)x = Z A_Z^{-1} Z^t A x = Z A_Z^{-1} Z^t b$. The first component leads to the solution of the following singular but consistent linear system:

$$A P_1 P_1 x = P_2 A P_1 x = P_2 A \hat{x}^{(i)} = P_2 b. \quad (5)$$

It can be shown that if the spectrum of A is $\Lambda(A) = \{\lambda_1, \lambda_2, \dots, \lambda_l, \dots, \lambda_n\}$ and Z holds the eigenvectors associated to the smallest eigenvalues, then $\Lambda(P_2 A) = \{0, 0, \dots, 0, \lambda_l, \dots, \lambda_n\}$.

The previous result implies that the effective condition number of the linear system depicted in (4) is smaller than A . We remark that this is one way of doing deflation. Other authors have used this eigenvalue information to shift those small eigenvalues near to 1^{6,22-23}. In this case, we do not need to solve the singular system (5), and a term of the form $Z A_Z Z^t$ (i.e., coarse grid corrector) is added to the projectors defined in (4). This leads to an invertible system with eigenvalues clustered around 1.

To further illustrate ideas, Figure 4 shows the effect that the deflation operators depicted in (4) has over the original spectrum of A . Here, the operators P_1 and P_2 were constructed based on the harmonic Ritz values shown in

Figure 3. We can clearly observe how several extreme eigenvalues have been removed from the original pressure block.

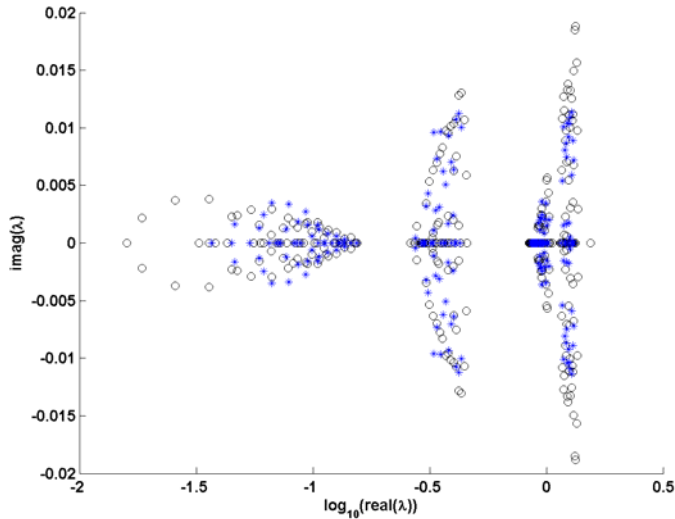


Fig. 4: Eigenvalues of P_2AP_1 (blue asterisks) and eigenvalues of A (black circles).

Computing Eigenvalues

As mentioned above, the Arnoldi decomposition (2) is amenable for approximating some of the eigenvectors and eigenvalues of A . In particular, we are interested in computing an approximation to the eigenvectors associated with the small eigenvalues of A . This is key to constructing a deflation preconditioner capable of eliminating those eigenvalues that are preventing the iterative solver from displaying a faster convergence rate. The overall idea is to generate a transformed operator with a lower condition number. Based on (2), we can compute the harmonic Ritz values, that is, solve the harmonic eigenvalue problem,

$$(AV_s)^t (A - \mu I) V_s u = 0 \Rightarrow (H_s + h^2 H_s^{-t} e_s e_s^t) u = \mu u. \quad (6)$$

The eigenvalue estimation for A is then given by $z = V_s u$. Provided that we are already using a preconditioned GMRES method, the harmonic Ritz values tend to be good approximations of extreme eigenvalues. In order to compute Ritz eigenpairs, we just omit the rank-one term in (6).

Note that the procedure for computing harmonic Ritz and harmonic Ritz eigenpairs is relatively inexpensive since, generally, $s \ll N$. In the event of finding an invariant subspace, i.e., $h = 0$, the harmonic Ritz values coincide with the Ritz values²¹ (i.e., direct eigenvalues of H_s). Moreover, GMRES stagnates whenever h is large or H_s has a very small singular value. From now on, we denote Z as the orthogonal rectangular matrix resulting from the orthogonalization of the set of l eigenvectors z , that is, $Z = [z_1, z_2, \dots, z_l]$.

It is important to remark that the selection of desired eigenvectors (i.e., those strictly associated with the extreme eigenvalues) can be further refined by using implicit shift strategies²⁵ and augmenting the Krylov basis³. In this paper, we do not pursue further these directions for the sake of implementation simplicity.

Algebraic Multigrid (AMG)

The development of algebraic multigrid was driven by the attempt to automate and generalize geometric multigrid so that it can be directly applied to certain (sparse) matrix equations without explicitly referring to geometry and without requiring any pre-defined hierarchy.

In recent years, there has been a remarkable increase of interest in AMG in both science and applications. This is due partially to the increasing geometrical complexity of applications which, technically, limited the immediate use of alternative fast solvers such as those based on geometric multigrid. Another reason is the steadily increasing demand for scalable and robust “plug-in” solvers. In reservoir simulation, this demand was driven by ever-increasing problem sizes, complex structures, heterogeneities, multiphase flows, and wells that have highlighted the limits of classical one-level solvers.

A basic requirement for any multigrid approach, whether geometric or algebraic, is an efficient interplay between smoothing and coarse-grid correction. Although AMG directly mimics geometric multigrid (on a hierarchy of linear systems of equations rather than a hierarchy of grids), there is a very important conceptual difference between geometric and algebraic multigrid, as illustrated in Figure 5.

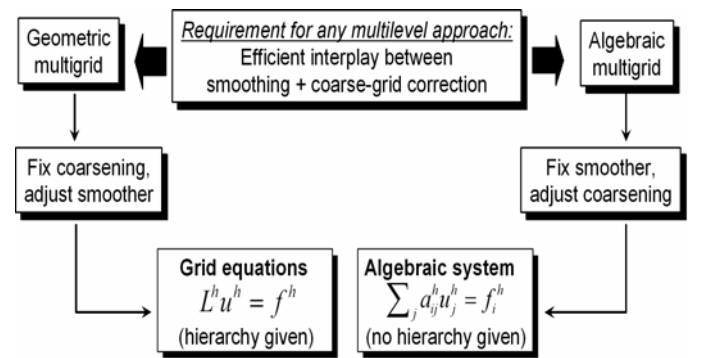


Fig. 5: Algebraic versus geometric multigrid.

In classical multigrid, predefined grid hierarchies are employed and interpolation is defined geometrically, typically linearly. Consequently, an efficient interplay between smoothing and coarse-grid correction requires the careful selection of appropriate smoothing processes such that the error after smoothing is necessarily geometrically smooth, relative to the coarse grid. In other words, the error after smoothing should vary in a geometrically smooth way between fine and neighboring coarse grid points so that linear

interpolation makes sense. While the construction of corresponding "robust smoothers" is not difficult in 2D model situations, for 3D applications on complex meshes their realization tends to become rather cumbersome, if not impossible.

The only way to loosen the requirements on the smoother and still maintain an efficient interplay with the coarse-grid correction is to use more sophisticated coarsening techniques. AMG may be regarded as the most radical attempt to maintain simple smoothers while still achieving robust convergence. Basically, as compared to geometric multigrid, AMG takes the opposite point of view. That is, AMG fixes the smoother to some simple scheme, such as plain Gauss-Seidel relaxation, and attempts to ensure an efficient interplay with the coarse-grid correction by locally adapting coarser levels and (operator-based) interpolations to the smoothing properties of the relaxation method.

Note that it is not important whether relaxation really smoothes the error in a geometric sense. What is important, though, is that the error after relaxation can be characterized algebraically to a degree that makes it possible to perform the coarsening process automatically. For many classes of applications this is possible, the most classical case being represented by weakly diagonally dominant M-matrices. In such cases, AMG is highly flexible in adjusting itself to the problem at hand and is very robust and efficient despite using very simple smoothers.

Generally, the guiding principle in automatic coarsening is to ensure that the range of interpolation approximately contains smooth error, that is, error which is essentially unaffected by relaxation. This is the crucial condition for obtaining robust coarse-grid correction processes as well as fast and (nearly) h -independent convergence. However, in practice, AMG's coarsening process must necessarily be constructed on the basis of compromises between numerical work and convergence. Generally, the more effort put into this construction, the faster the convergence can be. But, unfortunately, the required numerical workload may increase even faster. Typically, the benefit of an improved interpolation in terms of convergence speed is offset by the expense in terms of additional computational work. That is, from a practical point of view, a major problem in designing efficient AMG algorithms is the tradeoff between convergence and numerical workload. Keeping the balance between these aspects is the ultimate goal of any practical algorithm.

Often, sufficiently accurate AMG interpolation cannot easily be computed based only on algebraic information directly contained in the matrix. Typically such cases are indefinite problems or problems with near-zero eigenvalues. In the latter cases, for instance, the major difficulty is caused by the fact that the smaller the eigenvalues of a given problem the more accurately the corresponding eigenvectors must be interpolated. Unfortunately, unless these eigenvectors are close to being constants, the accuracy of interpolation for these eigenvectors cannot really be controlled without additional information. As a consequence, the insufficient

quality of AMG interpolation for just a few modes - namely, the lowest-energy eigenmodes - may severely limit its overall performance.

Rather than investing a lot of additional computational work to improve AMG's coarsening process, in this paper, we investigate the combination of AMG with deflation methods to tackle particular modes that are difficult for AMG to handle efficiently. All investigations are based on the solver package SAMG, developed by Fraunhofer SCAI²⁶.

The Deflation AMG Approach

Based on the aforementioned discussion, we can state that the addition of deflation preconditioning does not impose a major implementation work to AMG solvers that already have a Krylov iterative solver as an accelerator. Obviously, this Krylov iterative solver must allow factorizing the original matrix into a tridiagonal or Hessenberg form to make it amenable for eigenvalue computations. This is provided by Lanczos and Arnoldi decompositions for positive definite and general nonsymmetric/indefinite systems, respectively. After the first GMRES cycle, we should be able to reconstruct the deflation operators based on the harmonic Ritz or Ritz vectors.

The following algorithm summarizes the implementation of a deflation AMG preconditioner for GMRES:

Deflation_AMG_GMRES($A, b, x_0, M_{AMG}, P_1, P_2, \varepsilon, s, l$)

1. *Convergence* = *false*;
2. *While not(Convergence) do*
 - 2.1. $r_0 = P_2(b - AM_{AMG}^{-1}x_0)$;
 - 2.2. *Apply Arnoldi decomposition and obtain (2)*
 - 2.3. *Solve (3) and obtain $x_s = x_0 + Vy^*$,*
 - 2.4. *If $\|b - Ax_s\| < \varepsilon \|r_0\|$ then*
 - 2.4.1. *Convergence* = *true*;
 - 2.4.2. $x^* = P_1 M_{AMG}^{-1} x_s + x^*$;
 - Else*
 - 2.4.3. $x_0 = x_s$;
 - 2.4.4. *Compute l harmonic Ritz vectors (or Ritz vectors) according to (6) and form the corresponding eigenvector approximation Z ;*
 - 2.4.5. *Construct the deflation operators P_1 and P_2 according to (4) for the preconditioned system AM_{AMG}^{-1} ;*
 - 2.4.6. *Compute $x^* = (I - P_1)x = ZA_Z^{-1}Z'b$.*
- End If*
- End While*

Several comments are in order:

1. Initially, at the first GMRES cycle, the deflation operators may be defined as $P_1 = P_2 = I$; however, strategies to provide physically insightful eigenvectors have been explored by Vuik and collaborators²⁷. The idea is to

algebraically define eigenvectors according to regions or subdomains sharing the same permeability coefficients (as in a domain decomposition approach). The set of resulting eigenvectors is the basis for domain-based deflation operators.

2. The AMG preconditioner has been used as a right preconditioner, whereas the deflation operators are acting from the left side of the equation.
3. The computation of harmonic Ritz vectors or Ritz vectors may imply the use of complex arithmetic for nonsymmetric systems. However, due to the relatively small size of the associated Hessenberg matrix H_s , this computation can be efficiently carried out via Lapack library calls²⁸.
4. Since most deflation or spectral preconditioners share the same principle for computing harmonic Ritz vectors or Ritz vectors, the implementation of other varying and adaptive preconditioners can be easily realized using the above algorithmic presentation.
5. As iterations progresses, the Ritz vectors and harmonic Ritz vectors tend to be mutually closer as the variable h progressively becomes smaller. In this case, the GMRES algorithm will be approaching a “happy breakdown”, that is, an invariant subspace for A will be generated and the computed eigenpairs will be very accurate.
6. The proposed algorithm does not imply modifications to AMG or GMRES if desired. The point is that all the required spectral information can be generated after calling each cycle of GMRES. Hence, each subsequent deflation operator construction may be performed alternatively, outside GMRES.
7. In contrast to the GBB approach¹⁷, there is no need to make out-of-core eigenvalues computations from scratch and directly from the original matrix operator. The underlying Krylov information is basically reused to generate the required eigenvector approximations. In this sense, the proposed approach has an in-core blend in the computation that is not intrusive upon AMG cycling or coarsening steps.
8. Special care must be taken for efficiently carrying out the action of the deflation operators. For instance, it is recommended to factorize the constrained matrix A_z to save computations during the application of P_2 in step 2.2 and P_1 in step 2.4.6. Also, algebraic operations must be performed giving precedence to vector-matrix products over matrix products.

Numerical Experiments

In this preliminary set of experiments we consider the following two cases:

1. IMPES pressure systems arising from a set of different 30x30 reservoir meshes with permeability distributions varying according to variance and correlation length; and
2. A fully implicit pressure system arising from a 12x44x17 upscaled reservoir version of the SPE 10th Comparative Project²⁹.

Numerical cases are performed on the parallel reservoir simulation framework IPARS³⁰. For all cases we define a water injection well at the lower left corner and a production well at the opposite corner of the reservoir. All wells are bottomhole pressure specified. The first set of IMPES cases was based on an oil-water system. The fully-implicit case was defined for a black-oil system. Pressure block systems were obtained after 100 timesteps and at the first Newton iteration for fully implicit formulations. No special treatment was performed on time stepping to enforce the generation of ill-posed linear systems. Instead, we restrict our observations on high heterogeneity effects.

We basically distinguish two types of solver approaches: (1) AMG with GMRES acceleration (AMG); and (2) deflation AMG with GMRES acceleration (DAMG). We consider the following default settings for SAMG²⁶ in all cases that were analyzed:

- pre- and post-smoothing steps at each level consisting of one Gauss-Seidel iteration;
- V-cycle coarsening/refinement pattern consisting of a maximum of 25 levels; and
- sparse Gaussian elimination at the very coarsest level.

GMRES was run with a tolerance of 10^{-12} and a fixed restart of $s = 5$ due to the relative small size of the problems. For each DAMG computation the size of the deflation space was set as $l = s$. We computed only one set of deflation operators per problem, thus freezing the deflation operators for subsequent GMRES cycles. This allows us to lower the computational burden and evaluate the effectiveness of the first spectral approximation in retrieving those “hard” modes from AMG iterations.

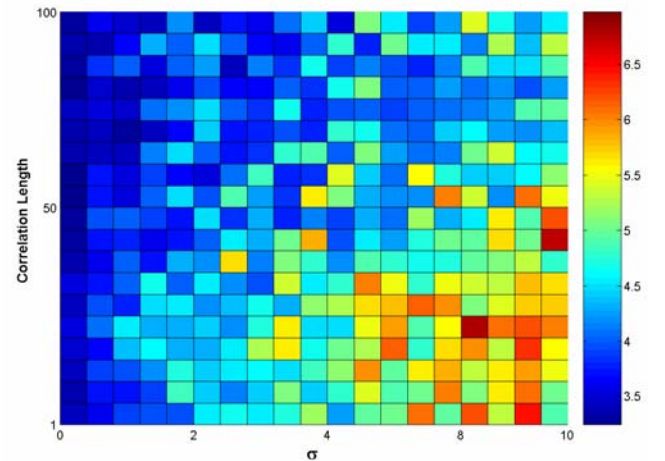


Fig. 6: Matrix condition number as a function of variance and correlation length for a 30x30 mesh (colors are in log10 scale).

For the first set of experiments, we generate the permeability distribution according to the following exponential covariance function:

$$\text{Cov}(X, Y) = \sigma e^{|X-Y|/L}.$$

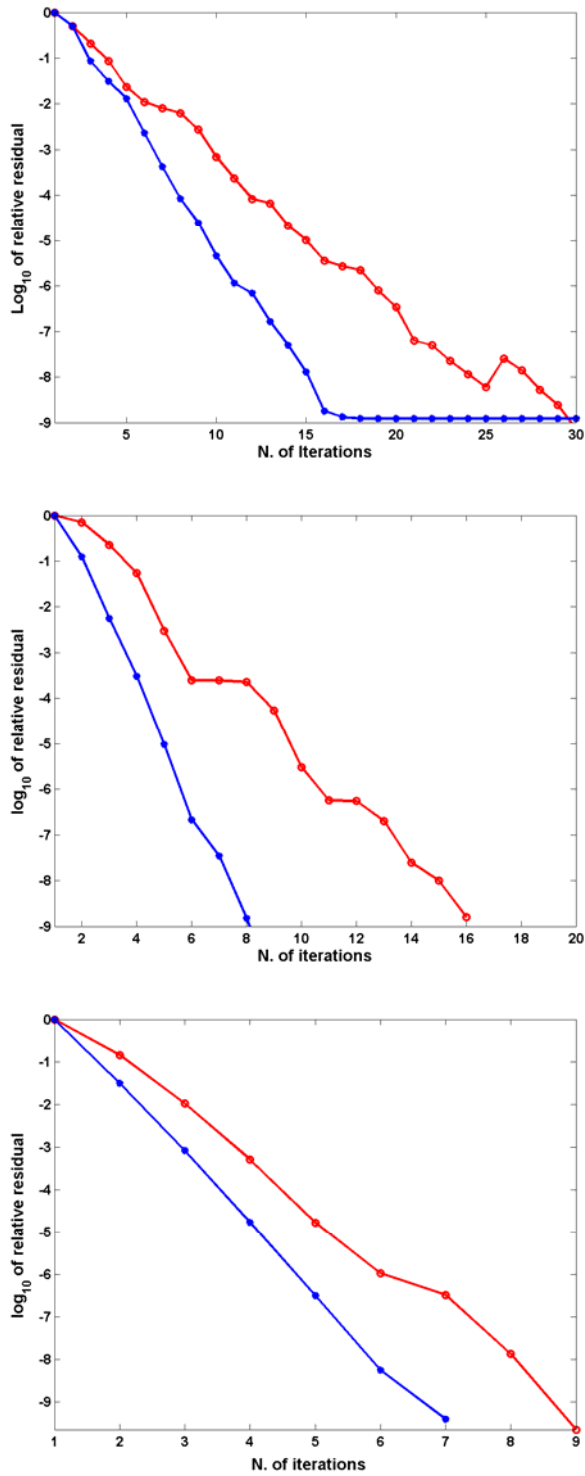


Fig. 7: Convergence results of DAMG (blue asterisks) and AMG (red circles) solvers for $\sigma = 30, 20$ and 10 (from top to bottom) and a fixed correlation length of 10% .

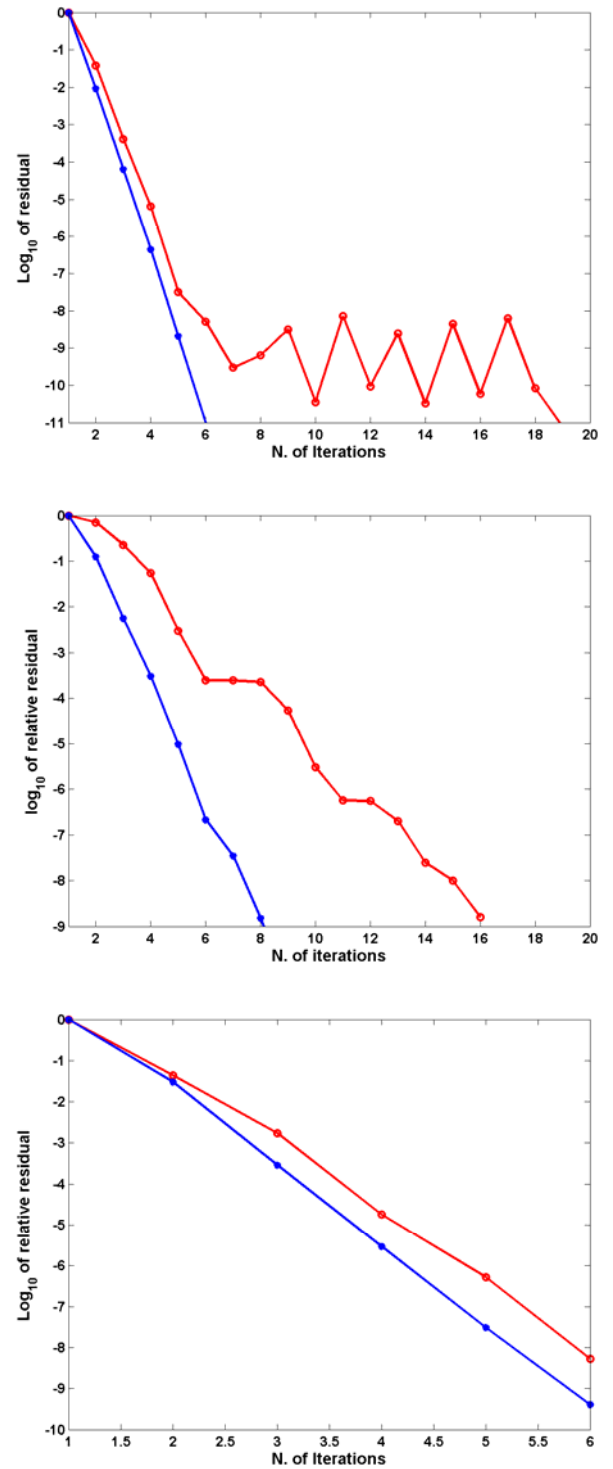


Fig. 8: Convergence results of deflation DAMG (blue asterisks) and AMG (red circles) solvers for $L = 5, 10$ and 30% (from top to bottom) and fixed $\sigma = 20$.

Here, σ represents the variance and L represents the correlation length. Figure 6 illustrates how the condition number of an IMPES pressure system behaves with respect to these two parameters. The general trend is that the condition number increases steeply as both the variance increases and the correlation length decreases; that is, when the permeability field lacks any particular structure and varies significantly between adjacent cells. For the cases considered here the permeability may vary by up to 10 orders of magnitude.

Figure 7 compares the behavior of DAMG and AMG for different permeability variations and a fixed correlation length. It can be observed that the higher the variation the greater the effectiveness of DAMG compared to AMG. Nevertheless, it should be noted that for $\sigma = 30$ the deflation process was unable to maintain the rate of convergence at very low residuals. This is an indication that there may be some bad nodes that were not captured by the deflation operators and refreshing the basis may be a reasonably thing to do.

Figure 8 performs a similar comparison in terms of the permeability correlation length. As expected, the greater the correlation length the greater the number of adjacent cells with similar values and, therefore, the better conditioned the associated linear system. DAMG seems to be less prone to stagnation and oscillations as the spatial correlation decreases. It is worth to add, that AMG does, in overall, a good job decreasing the relative residuals. GMRES may be having difficulties to deal with slight variations on how AMG satisfies its own tolerances for remaining hard modes (see top graph of Figure 8). DAMG seems to be approaching the solution fast enough to avoid this oscillatory behavior.

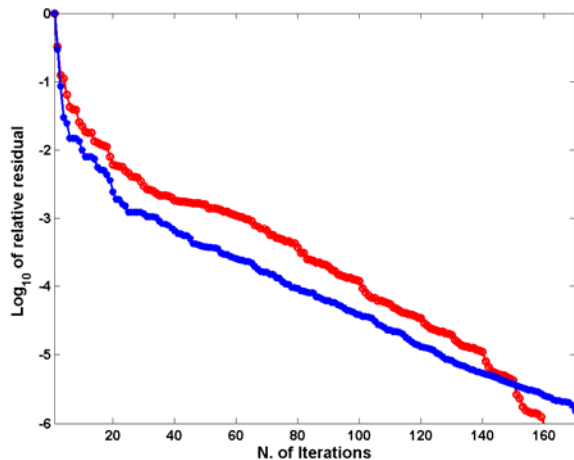


Fig. 9: Convergence results of DAMG (blue asterisks) and AMG (red circles) solvers for the upscaled version 12x44x17 of the SPE 10th Comparative Project.

The fully implicit case results are depicted in Figure 9. Due to the larger size and lost of symmetry, the problem imposes major difficulties to both AMG and DAMG. Yet, there is slight advantage for DAMG over AMG for the first 150 GMRES iterations. However, the deflation vectors may be reaching an exhausted point that does not allow for discovering other bad modes from the problem. Note how AMG recovers after 140 iterations and end up surpassing the

DAMG. This may reveal that the deflation vectors should have been refreshed some cycles before in order to quickly reach low residual values.

Conclusions and Further Remarks

This work establishes how deflation preconditioning strategies may be used to complement the preconditioning strength of AMG methods. The basic principle is to rely on Krylov iterative methods that maintain an orthogonal basis for the underlying Krylov subspace. We show that this information can be useful to construct deflation operators for subsequent restart cycles. Nevertheless, the proposed deflation strategy may also accommodate domain-based approaches. The proposed DAMG algorithm has the potential to remove components of the solution associated with these undesired eigenvalues and thereby provide more robustness to AMG.

We can draw the following conclusions:

1. Deflation AMG preconditioners are an attractive alternative to extend convergence capabilities of plain AMG preconditioning strategies.
2. The additional effort of implementing DAMG solvers is relatively low if the Krylov basis is available in some factorized form.
3. The proposed strategies may be primarily convenient in situations where matrix symmetry and positive definiteness are lost. These situations typically arise in fully implicit formulations for coupled pressure and saturation/concentration operators involving abrupt flow changes due to high permeability/porosity heterogeneities.

Despite the encouraging results, further testing is certainly required to formalize more solid conclusions. Many lessons were obtained during the implementation that needs to be further evaluated and related to a wider range of physical situations. The challenge here is to identify what physical and algebraic scenarios may lead to a small number of negative eigenvalues and, preferably, have them arranged in a clustered fashion that could be amenable for deflation processes. There has been evidence that pressure systems resulting in fully implicit systems can generate very small and even negative eigenvalues as a consequence of negative well production contributions to main diagonal terms. This topic is ongoing research of the authors in conjunction with two-stage preconditioning strategies³¹.

Indefinite and highly nonsymmetric operators are prone to appear when disparate physical processes are coupled to increase the predictive capabilities of current reservoir models. The proposed deflation and AMG methodology should be evaluated in multiphysics settings such as compositional flow, thermal, fracture models, geomechanics, surface networks and sophisticated well models. As indicated in the text, there are many ways to compute spectral preconditioners that may be beneficial to evaluate with AMG approaches in the near future.

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References

1. Parks, M.L., E. de Sturler, G. Mackey, D. D. Johnson, and S. Maiti, "Recycling Krylov Subspaces for Sequences of Linear Systems", SIAM J. Sci. Comput. 5: pp. 1651-1674, 2006.
2. Frank, J. and Vuik, C. "On the Construction of Deflation-based Preconditioners". SIAM J. Sci. Comput. **23**:2:442-462, 2001.
3. Morgan, R. "GMRES with Deflated Restarting". SIAM J. Sci. Comput. **24**:1:20-37, 2002.
4. Klie, H. and M.F. Wheeler, "Krylov-Secant Methods for Accelerating the Solution of Fully-Implicit Formulations", SPE Reservoir Simulation Symposium, SPE 92863, The Woodlands, Texas, Jan. 31 - 2 Feb., 2005.
5. Simoncini V. and D. B. Szyld, "Recent Computational Developments in Krylov Subspace Methods for Linear Systems", Research Report 05-9-25, Department of Mathematics, Temple University, September 2005 (revised May 2006). To appear in Numerical Linear Algebra with Applications.
6. L. Giraud and Gratton S. "On the Sensitivity of Some Spectral Preconditioners". SIAM J. Matrix Anal. Appl., Vol. 27, pp. 1089-1105, 2006
7. Stüben, K.: "An Introduction to Algebraic Multigrid" Appendix in the book "Multigrid" by Trottenberg, U., Oosterlee C.W. and Schuller, A. Academic Press, pp. 413-532, 2001.
8. Stüben, K. "Review of Algebraic Multigrid", J. of Comp. and Appl. Math., 128, pp. 281-309, 2001.
9. Stüben K., Delaney P. and Chmakov, S. "Algebraic Multigrid (AMG) for Ground Water Flow and Oil Reservoir Simulation", Proceedings of the Conference "MODFLOW and More 2003: Understanding through Modeling", International Ground Water Modeling Center (IGWMC), Colorado School of Mines, Golden, Colorado, Sept 17-19, 2003.
10. Axelsson, O. "A Survey of Algebraic Multilevel Iteration (AMLI) Methods". BIT Num. Math. Vol. 43, pp. 863-879, 2003.
11. Brezina M., Falgout, R., Maclahan, S., Manteuffel, T., McCormick S. and Ruge, J. "Adaptive Smoothed Aggregation (α SA)". SIAM J. Sci. Comput. Vol. 25, N. 6, pp. 1896-1920, 2004.
12. Aarnes, J. and T.Y. Hou, "Multiscale Domain Decomposition Methods for Elliptic Problems with High Aspect Ratios", Acta Math. Appl., 2002, 18(1): 63-76.
13. Graham, I.G. and P.O. Lechner. "Domain Decomposition for Heterogeneous Media", Domain Decomposition Methods in Science and Engineering, XVI, Lecture Notes in Computational Science and Engineering, Vol. 55 O. Widlund and D. Keyes (Eds), 2006.
14. Nabben R. and C. Vuik. "A Comparison of Deflation and Coarse Grid Correction Applied to Porous Media Flow". SIAM J. Numer. Anal. Vol. 42, N. 4, pp. 1631-1647, 2004.
15. Nabben R. and C. Vuik. "A Comparison of Deflation and the Balancing Preconditioner". SIAM J. Sci. Comput. Vol. 27, N. 5, pp. 1742-1759, 2006.
16. Ruge J.W. and Stüben, K. "Algebraic Multigrid (AMG)", Multigrid Methods, S.F. McCormick ed., pp. 73-130, vol. 3 of Frontiers of Applied Mathematics, SIAM, Philadelphia, PA, 1987.
17. Waismann, H., J. Fish, R.S. Tuminaro and J. Shadid. "The Generalized Global Basis (GBB) Method". Int. J. Numer. Meth. Engng. Vol. 61, pp. 1243-1269, 2004.
18. Waismann, H., J. Fish, R.S. Tuminaro and J. Shadid. "Acceleration of the Generalized Global Basis (GBB) Method for Nonlinear Problems". J. Comp. Physics. Vol. 210, pp. 274-291, 2005.
19. Lehoucq, R., D. Sorensen and C. Yang. "ARPACK User's Guide: Solution of Large-Scale Eigenvalue Problems with Implicit Restarted Arnoldi Methods", SIAM Philadelphia, 1997.
20. Saad, Y. Iterative Methods for Sparse Linear Systems. SIAM, 2003. 2nd. edition.
21. Goossens S. and Roose, D. "Harmonic Ritz Values and the Convergence of FOM and GMRES". Numer. Lin. Alg., pp. 281-293, 1999.
22. Burrage, K and J. Erhel. "On the Performance of Various Adaptive Preconditioned GMRES Strategies", Numerical Linear Algebra with Applications, 5, pp. 101-121, 1998.
23. Carpentieri, B., I.S. Duff and L. Giraud. "A Class of Spectral Two-Level Preconditioners", SIAM J. Sci. Comput., 25, pp. 749-765, 2003.
24. Baglama J., D. Calvetti, G.H. Golub and L. Reichel. "Adaptively Preconditioned GMRES Algorithms", SIAM J. Sci. Comput., 20, pp. 243-269, 1998.
25. Sorensen, D.C. "Implicit Application of Polynomial Filters in a k-Step Arnoldi Method", SIAM J. Matrix Anal. Appl., 13, pp. 357-385, 1992.
26. Stüben, K. and Clees, T. "SAMG User's Manual", <http://www.scai.fhg.de/samg>.
27. Vuik, C. A. Segal and J.A. Meijerink. "A Comparison of Various Deflation Vectors Applied to Elliptic Problems with Discontinuous Coefficients", Appl. Numer. Math., 41, pp. 219-233, 2002.
28. Anderson, E. et al. "LAPACK User's Guide", SIAM, Philadelphia, 1992.
29. Christie M.A. and Blunt, M.J.: "Tenth SPE Comparative Solution Project: A Comparison of Upscaling Techniques", SPE Reservoir Simulation Symposium, SPE 72469, Houston, Feb 11-14, 2001.
30. Wheeler, J.: "IPARS User's Manual", Tech Report CSM, ICES, The University of Texas at Austin, Austin, TX, 2000.
31. Clees T. and L. Ganzer: "An Efficient Algebraic Multi-Grid Solver Strategy for Adaptive Implicit Methods in Oil Reservoir Simulation" paper SPE 105789 presented at the 2007 SPE Reservoir Simulation Symposium, Houston, TX, Feb. 26-28.