

### On the Convergence of System-AMG in Reservoir Simulation

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#### **Abstract**

System-AMG provides a flexible framework for linear systems in simulation applications that involve various different types of physical unknowns. Reservoir simulation applications, with their driving elliptic pressure unknown, are principally well-suited to exploit System-AMG as a robust and efficient solver method.

However, in order to be efficient and robust, the coarse grid correction process of AMG on the one hand needs to be possible, i.e., the matrix needs to fulfill certain requirements. It has been demonstrated earlier how to ensure this by the dynamic rowsumming (DRS) method.

On the other hand, the coarse grid correction must be physically meaningful in order to speed up the overall convergence. It has been common practice in CPR-type applications to use an approximate pressure-saturation decoupling to fulfill this requirement. This, however, can have drastic impacts on AMG's applicability and, thus, is not performed by the DRS-method.

In this work, we are going to see that the pressure-saturation decoupling indeed is not necessary for ensuring an efficient interplay between the coarse grid correction process and the fine-level problem. We will find that a comparable influence of the pressure on the different involved PDEs is much more crucial.

As an extreme case w.r.t. the outlined requirement, we will discuss linear systems from compositional simulations under the volume balance formulation. In these systems, the pressure typically is associated with a volume-balance, rather than a diffusion process. The corresponding coarse grid correction does, hence, not provide any benefit regarding the overall convergence: the other PDEs involve pressure-based diffusive parts that have a drastically different structure than the volume-balance has. We will see how System-AMG can still be used in such cases.

#### Introduction

Solution approaches based on algebraic multigrid (AMG) have demonstrated to be efficient methods for solving linear systems in reservoir simulations. Especially the continuous growth in size and complexity of such simulations creates a need for efficient solver methods. However, in order for AMG to be robust and efficient, certain conditions have to be met that we will discuss in this work. In reservoir simulations [1], as soon as multiple phases are considered, we are concerned with a system of partial differential equations (PDEs) that is discretized and linearized. Consequently, the linear solver has to deal with different types of physical unknowns and the couplings in-between.

In Black-Oil and in compositional simulations only two types of physical unknowns are involved, namely pressure and saturations/concentrations. The constrained pressure residual method (CPR, [15][16]) is an established way of how classical AMG can be exploited in such simulations by solving an extracted pressure problem. A common practice (e.g., [2][10]) is to approximately decouple this system from the saturations. The idea behind this procedure is to make the coarse grid correction by AMG independent of the saturation unknowns. Of course, given that AMG was properly applicable to this decoupled sub-system, a good convergence can be expected. However, the properties of the pressure sub-system are heavily influenced by the decoupling procedure and the system might not be suited at all for AMG anymore.

System-AMG [5][12] provides an alternative methodology by considering the full linear problem in an AMG context. It has been described earlier [8] that for Black-Oil problems this results in a method comparable to the principal CPR approach – just without the decoupling. However, the System-AMG methodology can be extended to systems in more advanced simulations, where, for instance, thermal or mechanical effects are considered. AMG hierarchies can then be exploited for the respective unknowns as well. Moreover, applying it to the full system allows AMG to exploit the original physical information and to benefit from synergies. Finally, when applying AMG not only to an extracted sub-system, there arises the question of the necessity of decoupling a sub-system for applying classical AMG.

The Dynamic RowSumming (DRS) pre-processing [7] has been introduced as an alternative to decoupling different unknowns. Its primary objective is maintaining those matrix properties that allow for the construction of an AMG hierarchy. This does not only mean that potential problems from approximate decouplings are avoided. The pre-processing also copes with challenging matrix properties that result from the modelling, for instance, of well-bores. Such properties might cause serious difficulties for AMG.

The DRS approach does, however, not focus on cross-couplings between unknowns. It does especially not decouple them. In this work, we are going to see that a decoupling of pressure and saturation is not necessary for an efficient interplay of the AMG coarse grid correction and the fine-level problem, i.e., for a good overall convergence. We will find that the comparability of the pressure's influence on the different involved PDEs is more crucial – and we discuss how DRS has a positive influence in this regard.

As an extreme case regarding this requirement, we will discuss a System-AMG approach for simulations under a molar formulation (e.g., [6][17]), where the pressure is associated with a volume balance equation. The resulting pressure sub-system is a diagonal matrix, which drastically differs from the diffusion-based influence of the pressure on the other involved equations. However, with an adjusted pre-processing, System-AMG can nevertheless be used as an efficient linear solver method.

This paper is organized as follows: In the following two sections we briefly recapitulate the properties of typical systems from reservoir simulations and the System-AMG solution approach with DRS matrix pre-processing. In the third section, we will then discuss the convergence properties of System-AMG for a model problem. This discussion is transferred to the general Black-Oil case in the fourth section. Finally, in the fifth section, we will describe the application of System-AMG for linear problems from simulations under the volume-balance, or molar formulation.

# **Linear Systems in Reservoir Simulation**

The objective of a reservoir simulation essentially is to fulfill mass balance equations in all places of the reservoir at any time. We will only give a brief overview here and refer to the reservoir simulation literature, e.g. [1], for detailed information.

In simulations under the natural variable formulation, for each phase  $\alpha$  (e.g., oil, gas or water), this equation reads as:

$$0 = \frac{\partial}{\partial t} (\varphi \rho_{\alpha} S_{\alpha}) - \nabla \left[ \rho_{\alpha} \lambda_{\alpha} \vec{\vec{K}} (\nabla p_{\alpha} - g \nabla D) \right] + q_{\alpha}. \tag{1}$$

Here, t is time,  $\varphi$  the porosity and g and D are gravity and depth.  $\rho_{\alpha}$  is the density of phase  $\alpha$  and  $\lambda_{\alpha}$  its mobility. The absolute permeability of the rock is given as K and the source term  $q_{\alpha}$  accounts for external influences like wells. Finally,  $S_{\alpha}$  and  $p_{\alpha}$  are the phase's saturation and pressure – that are to be solved for in each time step.

With well-bores being present, additional balance equations need to be considered that describe the flow inside the well. Analogously, the consideration of thermal or mechanical effects results in additional PDEs for energy and momentum, respectively. We will not discuss this in detail here and limit our following discussion to mere Black-Oil simulations.

We should mention that it is possible to use a different, so-called volume-balanced, or molar formulation for the description of the reservoir flux. We will get back to this formulation at the end of this paper. For the moment, we note that this formulation results in principally comparable balance equations that need to be fulfilled.

The mass conservation equations (1), but also all other types of mentioned balance equations, are highly non-linear due to pressure and saturation dependencies in densities, mobilities and source terms. Newton's method is usually used for the required linearization. In this process, additional, non-PDE relations like capillary pressures and saturation constraints are used to avoid an under-constrained system.

If we assume a pointor cell-wise ordering of the Jacobian matrix with  $n_p$  cells, which matches the situation in typical reservoir simulators, then the resulting linear system reads as

$$J_{point\_wise}u =: \begin{pmatrix} [A]_{11} & \cdots & [A]_{1n_p} \\ \vdots & \ddots & \vdots \\ [A]_{n_p1} & \cdots & [A]_{n_pn_p} \end{pmatrix} \begin{pmatrix} [u]_1 \\ \vdots \\ [u]_{n_p} \end{pmatrix} = f \text{ with } [u]_i = \begin{pmatrix} p_i \\ S_i \\ \vdots \end{pmatrix}. \tag{2}$$

Linear systems of this kind need to be solved within a reservoir simulation during each Newton iteration in each time step. Consequently, the linear solver typically is a significantly dominating component in terms of runtime. At the same time, the linear solver's robustness is crucial for the overall simulation.

# System-AMG and Dynamic RowSumming in Reservoir Simulation

Algebraic Multigrid methods have originally been developed to efficiently solve linear systems of equations that are described by sparse, positive definite, symmetric M-matrices - properties that typically arise when discretizing scalar, elliptic partial differential equations. The application of a rather cheap smoothing method at each level of an automatically constructed hierarchy provides a scalable solver strategy. In the case of algebraic multigrid, in contrast to geometric variants, this strategy relies on matrix information, only. It can adapt itself to the particular problem, which makes AMG suited also for unstructured and heterogeneous problems. Detailed information on AMG methods and the different components can be found in the literature [4][12][14].

The AMG idea can also be extended to coupled linear systems, i.e., systems that involve different types of physical unknowns and typically result from systems of PDEs. A detailed discussion of such extensions is given in [5].

#### **System-AMG Approach in Reservoir Simulation**

System-AMG is a well-suited, efficient solver approach for linear systems (2) from reservoir simulations, as described in the earlier work [8]. The fact that the elliptic pressure component dominates the system makes the exploitation of a hierarchy crucial for obtaining an efficient linear solver approach. At the same time, the different natures of the different physical unknowns need to be considered.

For Black-Oil systems (2), a System-AMG approach is found as:

• Construct an AMG hierarchy based on the pressure unknown, which is driving the fluid flow.

- To properly handle cross-couplings between unknowns, use ILU-smoothing where pressure and saturation are present.
- Due to its non-elliptic background, do not apply the hierarchy to the saturation unknowns. Because
  of their diagonal dominance, the respective matrix parts will typically not cause problems for the
  solution process.

In fact, for the Black-Oil case, this System-AMG approach is quite comparable to the well-known CPR approach [15][16]. However, as described in [8], the System-AMG approach has the advantage of being extendable also to applications where thermal and mechanical effects are considered. Moreover, also in the Black-Oil case the algorithmic versatility is advantageous: The full set of AMG components is available and all physical information can be used by AMG. This is of particular importance regarding matrix preprocessings that we will discuss next. Finally, System-AMG, by combining the full set of AMG components for the full system, can exploit synergies for providing more efficiency and it uses just a single user interface.

### Matrix pre-processing: Dynamic RowSumming

Constructing the AMG hierarchy based on the pressure sub-problem requires this sub-problem to be well-suited from AMG's perspective. Due to the, principally, elliptic background, this appears to be given at first glance. Real-life simulations, however, may result in challenging linear problems for all types of hierarchical solvers. Especially influences from wells, but also from considering compressibility, can have drastic impacts on the applicability of AMG.

The earlier described Dynamic RowSum pre-processing [7] aims at exactly this issue. It left-scales the point-wise Jacobian (2) with a block-diagonal matrix:

$$C_{DRS} = \begin{pmatrix} [C_{DRS}]_1 & & \\ & \ddots & \\ & & [C_{DRS}]_{n_p} \end{pmatrix} \text{ with the blocks as } [C_{DRS}]_i = \begin{pmatrix} \delta_1^i & \delta_2^i & \cdots & \delta_{n_u}^i \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix}.$$
(3)

Cell-wise, the different weights  $\delta_j^i$  are computed according to the properties of the corresponding pressure related parts of the Jacobian. This results in a compromise between the total pressure equation, which would be used in IMPES-simulation approaches, and shielding AMG from problematic structures. According to practical experience, this ensures the efficient applicability in reservoir simulations.

However, in contrast to the classical realization of CPR approaches, DRS does not at all focus on decoupling pressure and saturations. Such (approximate) decouplings turned out to often enough impose additional problems for the applicability of AMG by the way the pressure sub-problem is altered. As a consequence of the following discussion on the convergence of System-AMG, we will see that DRS, apart from ensuring the applicability of AMG, is nevertheless beneficial for the convergence speed.

# **Convergence Considerations in a Model Case**

So far, we have described and motivated a solution approach for the linear system (2). However, we have not yet discussed what, apart from the mere applicability, is crucial for the convergence speed of the System-AMG approach. Our discussion essentially follows the one from [9], where also further details can be found. The results analogously hold for CPR-like solution approaches as well.

For practical reasons, we do not attempt to discuss the convergence properties for a completely general linear system from a Black-Oil simulation. Instead, we limit our discussion to some special, yet representative, model case. Afterwards, we will motivate that these results can be expected to also hold in more general cases.

More precisely, we discuss the situation of only two phases involved, some production wells being present and we neglect compressibility. These assumptions essentially lead to a pressure sub-problem that is prototypically suited for AMG and we can, hence, exploit the established AMG theory.

In the next step, we will introduce a further assumption (5) regarding the relation of the properties of both involved phases.

In the linearization, we choose the pressure unknown to be the first one – followed by the saturation. We moreover assume an unknown-wise ordering of the linear system. From the cell-wise ordering (2) that typical reservoir simulators produce, this implies a reordering, which, however, does not have an impact on the further argumentation. It would essentially work cell-wise as well – just being more complicated in terms of notation.

This model results in a linear system that is described by the following Jacobian:

$$J_{model} = \begin{pmatrix} A & -B \\ \hat{A} & \hat{B} \end{pmatrix}, \text{ and, hence, } \begin{pmatrix} A & -B \\ \hat{A} & \hat{B} \end{pmatrix} \begin{pmatrix} p \\ S \end{pmatrix} = \begin{pmatrix} f_p \\ f_S \end{pmatrix}, \tag{4}$$

where the pressure-related A and  $\hat{A}$  are sparse, symmetric positive definite M-matrices. Both matrices result from the pressure-derivatives of the discretized mass balance equation (1) of the first and second phase, respectively. The saturation-related B and  $\hat{B}$  are sparse, strongly diagonally dominant M-matrices. Regarding the mentioned relation between the two phases, we assume

$$\hat{A} = VA$$
 and  $\hat{B} = WB$  with diagonal matrices  $V, W > 0$ . (5)

Due to the comparable background of  $\hat{A}$  and A, as well as  $\hat{B}$  and B, some rather close relation between the two respective matrices can be expected in any case. Limiting our discussion to V and W being diagonal essentially results in neglecting non-linear dependencies between both phases. The dominating linear dependency, however, is reflected (how, for instance, the water density relates to the oil density). Also cell-wise changes in this dependency are reflected, as V and W might have different entries per row, i.e., cell. Both matrices being positive is a consequence of the four sub-matrices in (4) being M-matrices – and, hence, is no further limitation.

Let us now describe the iteration matrix that our System-AMG approach results in for the system (4) with (5). Convergence properties of the solution approach can then be concluded from this iteration operator.

The AMG hierarchy can be constructed based on A, which, due to our assumptions, is perfectly suited for AMG. Let us denote  $M_{AMG}$  the multigrid iteration operator that we could use to solve the system  $A_P = f_p$  and let  $Q_{AMG}$  the respective approximation of A (i.e.,  $M_{AMG} := I - Q_{AMG}^{-1}A$ ). Then, as we do not apply the hierarchy to the saturation, the iteration operator that represents the exploitation of the hierarchy is

$$H = \begin{pmatrix} M_{AMG} & Q_{AMG}^{-1}B\\ 0 & I \end{pmatrix}. \tag{6}$$

We now need to discuss the ILU smoothing, which we apply as post-smoother. We denote the corresponding operator as S. The full System-AMG operator is then given as M=SH. Let the ILU(0) factorization  $J_{model}=LU-R$  be given with some rest matrix R. Then we have  $S=I-U^{-1}L^{-1}A$ .

Just as with the hierarchical part, we will simplify the structure of S to a 2x2 block-matrix. To do so, we make use of two facts:

- The rest matrix is zero within the given non-zero pattern ([13], Proposition 10.2).
- An ILU(0) factorization of an arbitrary  $n \times n$  matrix, if it exists with regular factors, is unique. This can be seen by tracking how the  $2n^2$  entries of the two factors are recursively set by the ILU factorization algorithm and which entries a priori are zero or one.

Consequently, if we find L and U as 2x2 blocks that give a valid ILU(0)-factorization of  $J_{model}$ , then we have found the ILU(0) factorization.

Let us denote the ILU(0) factorization of A as  $L_A$  and  $U_A$ . Due to A being a symmetric M-matrix, the existence is guaranteed [11]. Moreover, let  $L_{VWB}$  and  $U_{VWB}$  the ILU(0) factorization of (V+W)B, which is a diagonally dominant M-matrix and, though it is unsymmetric, the factorization should exist.

Then, with some matrix T, we can propose the factors L and U to read as:

$$L = \begin{pmatrix} L_A & 0 \\ VL_A & L_{VWB} \end{pmatrix} \text{ and } U = \begin{pmatrix} U_A & T \\ 0 & U_{VWB} \end{pmatrix}. \tag{7}$$

This yields:

$$LU = \begin{pmatrix} L_A U_A & L_A T \\ V L_A U_A & V L_A T + L_{VWB} U_{VWB} \end{pmatrix}. \tag{8}$$

The fact that the rest matrix is zero in the non-zero pattern yields that  $L_AT$  equals -B within this pattern. Hence, LU equals  $J_{model}$  in the non-zero pattern and (7) is the desired ILU(0) factorization.

We could compute the iteration operator S now. However, we will proceed in a different way that will directly allow us to find that S is block-triangular. This structure of S will then make convergence considerations feasible.

More precisely, for the moment we will consider the linear system where the saturation is decoupled from the pressure:

$$\bar{J}_{model} := CJ = \begin{pmatrix} A & -B \\ 0 & (V+W)B \end{pmatrix}, \text{ with } C := \begin{pmatrix} I & 0 \\ -V & I \end{pmatrix}. \tag{9}$$

The ILU(0) factorization of this system obviously reads as:

$$\bar{L} = \begin{pmatrix} L_A & 0 \\ 0 & L_{VWB} \end{pmatrix} \text{ and } \bar{U} = \begin{pmatrix} U_A & T \\ 0 & U_{VWB} \end{pmatrix}.$$
(10)

The two lower factors of both factorizations (7) and (10) are connected via the matrix C from (9). This is a consequence of the fact that an ILU factorization performs row-wise eliminations. As the two pressure related blocks A and  $\hat{A}$  of (4) are connected via the diagonal V, the same needs to hold for the incomplete ones.

That is, the ILU(0) factorization of  $J_{model}$  incorporates the decoupling from (9). Hence, the ILU operators for both systems, S and  $\bar{S}$ , should be equal. We can also formally find this:

$$\bar{S} = I - \bar{U}^{-1}L^{-1}\bar{J}_{model} = I - U^{-1}L^{-1}C^{-1}CJ_{model} = S. \tag{11}$$

When computing  $\bar{S}$ , we directly find the block-triangular structure of the operator without further algebra. That is, with  $S_A$  and  $S_{VWB}$  the ILU iteration operators for the systems described by A and (V+W)B, respectively, we have:

$$S = \bar{S} = \begin{pmatrix} S_A & X \\ 0 & S_{VWB} \end{pmatrix}, \tag{12}$$

where X is some matrix that depends on the coupling between pressure and saturation. However, it turns out that X does not influence the spectral radius of the final iteration operator – at least as long (5) holds. This System-AMG operator, M, is computed as:

$$M = SH = \begin{pmatrix} S_A M_{AMG} & S_A Q_{AMG}^{-1} B + X \\ 0 & S_{VWB} \end{pmatrix}.$$
 (13)

We can now discuss the convergence properties of System-AMG. We will find that the spectral radius of M, which is directly linked to the asymptotic convergence rate of System-AMG, is bounded away from one. The block-triangularity drastically simplifies this discussion, as it allows to state:

$$\rho(M) = \max(\rho(S_A M_{AMG}), \rho(S_{VWB})). \tag{14}$$

Hence, we can discuss the two spectral radii separately.

To start with  $S_{VWB}$  (i.e., ILU for the system described by (V+W)B), we again note that (V+W)B is diagonally dominant in each row. According to practical experience, ILU converges for such systems – the better the stronger the diagonal dominance is. Since (V+W)B is an M-matrix, the link between diagonal dominance and the spectral radius can also be shown formally. We refer, for instance, to [9] for details and do not further discuss this here.

The situation is a bit more involved with the other, pressure-related, spectral radius. It results from the combination of AMG and ILU for the system described by A. Both operations are necessary for an efficient solver:

- Without AMG, the overall convergence would be bounded by ILU's convergence for the system described by A. Due to A being a weakly diagonally dominant M-matrix, this convergence will be the closer to one the higher the dimension of A is.
- Without ILU (i.e., with ILU only for the saturation part of the overall system), we would not have the elimination of the two pressure related parts of the system matrix. Hence, the operator *M* would not be upper triangular and the coupling between pressure and saturation would have a major impact.

Because A is a symmetric, positive definite M-matrix, we know that both ILU and AMG do converge and, hence, the spectral radii of  $S_A$  and  $M_{AMG}$  are below one ([11] and [14], respectively). However, because both operators do not commute, we cannot simply multiply both spectral radii. Instead, we can show that both operations do converge in the same matrix norm, namely the energy norm.

Regarding AMG, i.e.,  $M_{AMG}$ , the properties of A allow to conclude this from the general AMG-theory, e.g. in [14]. Regarding ILU, showing the convergence in the A energy norm requires some work. We refer to [9] for details and take the result as given here.

For some arbitrary e this implies

$$||S_A M_{AMG} e||_{en} < ||M_{AMG} e||_{en} < (1 - \tau_A)||e||_{en}$$
 and, hence,  $\rho(S_A M_{AMG}) < (1 - \tau_A)$ . (15)

Here,  $\tau_A$  is in (0;1] and depends on the quality of the AMG interpolation for A. For matrices that are well-suited for AMG, such as A, we can expect it to be bounded away from zero.

From the above results we can conclude that the convergence of System-AMG for the model problem (4) depends on

- The convergence of AMG for the pressure sub-problem.
- The convergence of ILU for the saturation sub-problem.

With the given matrix properties both can be expected to be bounded away from one.

# **Convergence Considerations in the Black-Oil Case**

In the general Black-Oil case (2) there is one additional aspect that influences the convergence of System-AMG: the comparability of the pressure-related blocks.

In the above model case we have assumed that  $\hat{A} = VA$  with a diagonal, non-negative V. However, in the general case we will have  $\hat{A} = VA + E$ . The quality of the approximation of the Schur complement (9)

by the ILU factorization is directly linked to E. The "bigger" E, the worse the approximation quality – and the "less triangular" will M be. The effect of a strong E will especially be that the coarse grid correction for the pressure by AMG is not meaningful for the overall problem and the ILU sweep will have to correct this accordingly. We will see an extreme case for this phenomenon in the next section where we discuss volume-balance formulations.

In practical applications under the natural variable formulation we can, however, expect E to be rather small. All pressure-related parts of the Jacobian, i.e., A and  $\hat{A}$  from (4), do result from pressure derivatives of mass balance equations of different phases (or components). These mass balance equations are all of the same type – just the material parameters and their dependence on the unknowns, pressure and saturation, might differ. Any such difference that can be expressed by the linear relation V from (5) is properly captured by our above model problem. We have only neglected non-linear dependencies – which do not dominate in practical applications. Figure 1 exemplarily compares the Frobenius norm of E in a SPE10 case [3] with those of the pressure-related blocks, which are orders greater. Figure 2 shows the good quality of the approximation of the Schur complement (9) by ILU for a representative J from a Dead-Oil simulation: The lower left matrix block of  $U^{-1}L^{-1}J$  is orders smaller than all other blocks.

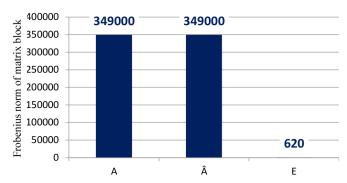


Figure 1—Frobenius norms of the matrix blocks  $A, \hat{A}$  and E for a linear system from an SPE10 simulation.

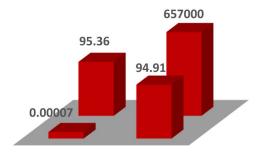


Figure 2—Frobenius norms of the four matrix blocks of  $U^{-1}L^{-1}J$  with LU the ILU(0) factorization of a representative J

We have described three criteria that determine the convergence speed of our solution approach and we will now discuss how the matrix pre-processing by Dynamic RowSumming does reflect these three criteria:

- Applicability of AMG for the pressure part
  - As this is the primary objective of DRS, we can expect the pressure sub-block to be as well-suited for the construction of an AMG hierarchy as it is possible with a given matrix. With practical simulations no problems with this regard have been observed.
- Applicability of ILU for the saturation part
   This is not actively reflected by DRS. However, the DRS pre-processing does not modify the saturation-related sub-blocks of the matrix and, due to the typical diagonal dominance of these blocks, we do not expect any difficulties for ILU.

• Comparability of pressure-related blocks

As long as no impacts for the applicability of AMG are expected, DRS produces an averaged pressure sub-problem, comparable to a total pressure problem. That is, the pressure sub-block can be expected to "fit" for all phases and, hence, the *E* from above should be small.

### System-AMG and Volume-Balance Formulation

We will now consider linear systems from volume-balance (or molar) formulation simulations, as they provide an extreme case regarding the comparability of pressure-related blocks. Such formulations are sometimes preferred especially in compositional simulations, as the flash calculations can be separated from the linearization process. These formulations are, for instance, described in [6] and [17]. We will follow the latter one.

The mass balance equation per component c, in contrast to the natural-variable formulation (1), is stated in terms of number of moles  $N_c$ :

$$0 = \frac{\partial}{\partial t} (M_c^{mol} N_c) - X_{c,oil} \nabla T_{c,oil}^{mol} [(\nabla p_{oil} - g \nabla D)] - X_{c,gas} \nabla T_{c,gas}^{mol} [(\nabla p_{gas} - g \nabla D)] + q_c^{mol}, \tag{16}$$

where  $M_c^{mol}$  is the molar mass of component c.  $X_{c,oil}$  and  $X_{c,gas}$  are the oil and gas concentrations of c and  $T_{c,oil}^{mol}$  and  $T_{c,gas}^{mol}$  are the oily and gaseous molar transmissibilities, respectively. For the water phase, an analogue equation is formulated.

Because no saturations are used, the summation of saturations cannot be used as volume balance anymore. Instead, the following relation is used

$$0 = \sum_{k=1}^{n_{comp}} \frac{N_k M_k^{mol}}{\rho_k} - \varphi, \tag{17}$$

which typically is associated with the pressure in the linearization process. With each number of moles,  $N_c$ , associated with the respective mass balance, linear systems of the following structure arise:

$$J_{VBF} \begin{pmatrix} p \\ N \end{pmatrix} = \begin{pmatrix} f_p \\ f_N \end{pmatrix}, \text{ with } J_{VBF} = \begin{pmatrix} A_{VB,p} & A_{VB,N} \\ A_{MB,p} & A_{MB,N} \end{pmatrix}, \tag{18}$$

where  $A_{MB,p}$  and  $A_{MB,N}$  have properties comparable to the pressureand saturation-related blocks from (2), respectively. The blocks  $A_{VB,p}$  and  $A_{VB,N}$ , however, are non-zero only in the diagonal blocks, which especially means that the pressure sub-system  $A_{VB,p}$  is a diagonal matrix. An AMG hierarchy based on this subsystem would obviously not accelerate the convergence. In this sense, (18) is an extreme case regarding the similarity requirement from above: the pressure related  $A_{VB,p}$  and  $A_{MB,p}$  drastically differ.

A necessary condition for a reasonable AMG approach is to construct the hierarchy with a diffusion-based sub-block of the matrix. The easiest way to achieve this is to simply exchange the rows based on volumeand mass-balance by a simple left scaling of the linear system (18).

This, however, does not resolve the different properties of the pressure-related blocks. As a consequence, while a pressure-based AMG hierarchy would now be based on diffusion, this AMG hierarchy would not at all consider the explicitly stated volume balance condition (17). That is, the coarse grid correction for the pressure would now be possible, but the result might be meaningless in terms of the overall system. Consequently, the ILU sweep will have to correct this - just as in the case with a giant E from above.

What an AMG approach needed was a diffusion-based pressure system that is independent of the volume balance, so that the different sub-blocks' properties do not matter anymore. This can be realized by simply decoupling the pressure from the volume balance. Let us separate the last column of the matrix blocks from molar derivatives and denote them with the superscript *B*, while the other columns are labeled with

A (i.e.,  $A_{VB,N} := \begin{pmatrix} A_{VB,N}^A & A_{VB,N}^B \end{pmatrix}$ ). Then we can formulate the combination of the association of pressure with diffusion and this decoupling from the volume balance as:

$$C_{1}J_{VBF}: = \begin{pmatrix} -A_{MB,N}(A_{VB,N}^{B})^{-1} & I \\ I & 0 \end{pmatrix} \begin{pmatrix} A_{VB,p} & A_{VB,N}^{A} & A_{VB,N}^{B} \\ A_{MB,p} & A_{MB,N}^{A} & A_{MB,N}^{B} \end{pmatrix}$$

$$= \begin{pmatrix} A_{MB,p} - A_{MB,N}^{B}(A_{VB,N}^{B})^{-1} A_{VB,p} & A_{MB,N}^{A} - A_{MB,N}^{B}(A_{VB,N}^{A})^{-1} A_{VB,N}^{A} & 0 \\ A_{VB,p} & A_{VB,N}^{A} & A_{VB,N}^{A} \end{pmatrix}$$
(19)

Because the volume-balance related blocks are zero in the off-diagonal, this yields a pressure subproblem that is independent of the volume balance. Hence, all unknowns that are effected by the coarse grid correction with AMG are now comparably influenced by the pressure.

However, we need to check whether the pressure sub-block is well-suited as a basis for AMG. Regarding  $A_{MB,p}$  this is true, as this has comparable properties to the pressure-based blocks from the natural variable formulation. In this special case, also the decoupling does not impose problems for AMG:  $A_{MB,N}^B$  has comparable properties to saturation-related blocks from the natural variable formulation, i.e., it is a diagonally dominant Z-matrix.  $A_{VB,N}^B$  and  $A_{VB,p}$  are both diagonal matrices with the first being positive and the second non-positive. Hence, we are adding a diagonally dominant Z-matrix to the – ideally – M-matrix  $A_{MB,N}^B$ , which should not cause problems for AMG.

The disadvantage of (19) is the possible additional fill-in in the non-zero structure in the "A"-columns of the first block-row. This, however, can be avoided by separating the scaling from (19) in the row-exchange from the left and the decoupling from the right:

$$C_{2}J_{VBF}C_{3} := \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \begin{pmatrix} A_{VB,p} & A_{VB,N}^{A} & A_{VB,N}^{B} \\ A_{MB,p} & A_{MB,N}^{A} & A_{MB,N}^{B} \end{pmatrix} \begin{pmatrix} I & 0 \\ -(A_{VB,N}^{B})^{-1} A_{VB,p} & I \end{pmatrix}$$

$$= \begin{pmatrix} A_{MB,p} - A_{MB,N}^{B} (A_{VB,N}^{B})^{-1} A_{VB,p} & A_{MB,N}^{A} & A_{MB,N}^{B} \\ 0 & A_{VB,N}^{A} & A_{VB,N}^{B} \end{pmatrix}$$
(20)

Both pre-processings do not yield exactly the same overall problem. However, they do give the same pressure sub-problem. We should note that the left-scaling in both cases can be combined with the Dynamic RowSum pre-processing in order to deal with problematic matrix properties. By using this modified pre-processing, System-AMG works properly, as demonstrated for representative test problems in Figure 3 and Figure 4 with about 95 and 950 thousand grid cells, respectively.

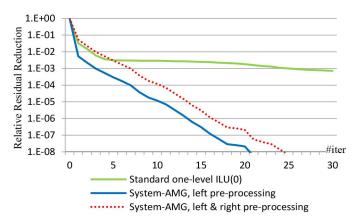


Figure 3—Convergence-comparison of System-AMG with both pre-processing schemes and ILU(0) for a problem with roughly 95,000 cells. Both methods are used as preconditioner for FGMRes.

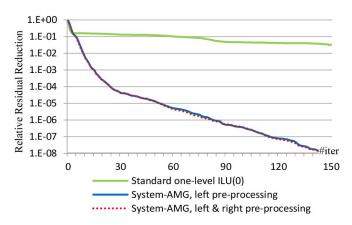


Figure 4—Convergence-comparison of System-AMG with both pre-processing schemes and ILU(0) for a problem with roughly 950,000 cells. Both methods are used as preconditioner for FGMRes.

### **Conclusions and Outlook**

It has been demonstrated that an efficient application of AMG in reservoir simulations does not require to decouple different physical unknowns. Instead, the comparability of the involved PDEs, especially regarding the influence of those unknowns that the AMG hierarchy is intended to be based on, is crucial for an efficient interplay of fine level smoothing and coarse grid correction. We have seen that the DRS preprocessing approach reflects this requirement – as well as this is possible along with its primary objective of ensuring the applicability of AMG. Consequently, regarding the overall convergence, it is not a problem that DRS does not decouple any unknowns.

In linear systems from simulations under the volume balance, we have seen how drastic differences regarding the pressure influences on different sub-problems impose challenges for the application of AMG. With an appropriate pre-processing, it was possible to completely decouple the volume-balance condition from the system – in a way that does not result in problems for the applicability of AMG. This decoupling resulted in all sub-problems that are effected by the coarse grid correction with AMG are comparably influenced by the pressure.

Further research on the convergence properties of AMG could consider additional physical unknowns such as thermal and mechanical ones. Especially in the latter case, the potential need of special smoothing schemes should be subject of further research.

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