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System-AMG for Fully Coupled Reservoir Simulation with Geomechanics

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Abstract

The consideration of geomechanical effects is becoming more and more important in reservoir simulations. Ensuring stable simulation processes often enough requires handling the entire process with all types of physical unknowns fully implicitly. However, the resulting fully coupled linear systems pose challenges for linear solvers. The number of approaches that can efficiently handle a fully coupled system is extremely limited.

System-AMG has demonstrated its efficiency for isothermal and thermal reservoir simulations. At the same time, AMG is known to be a robust and highly efficient linear solver for mere linear elasticity problems. This paper will discuss the combination of the advantages that AMG approaches have for both types of physics. This results in a robust and efficient solution scheme for the fully coupled linear system. The Automatic Differentiation General Purpose Research Simulator (AD-GPRS) is used to produce the Jacobians that are guaranteed to be exact.

In a single-phase case, the overall Jacobian matrix takes the form of a constrained linear elasticity system where the flow unknowns serve as a Lagrangian multiplier. In other words, a saddle point system needs to be solved, where the flow and the mechanics problem might come at very different scales. A natural relaxation method for this kind of systems is given by Uzawa smoothing schemes which provide a way to overcome the difficulties that other smoothers may encounter.

This approach appears intuitive for single-phase problems, where Gauss-Seidel can be applied in an inexact Uzawa scheme. However, in the multiphase case, incomplete factorization smoothers are required for the flow and transport part. We will discuss the incorporation in an inexact Uzawa scheme, where different realizations are possible, with different advantages and disadvantages. Finally, we propose an adaptive mechanism along with the outer Krylov solver to detect the best-suited realization for a given linear system. In the multiphase case, also the matrix preprocessing, for instance, by Dynamic Row Summing, needs to be considered. However, the process now also needs to reflect the requirements of the Uzawa scheme to be applicable.

We demonstrate the performance for widely used test cases as well as for real-world problems of practical interest.

Introduction

In fully coupled reservoir simulations with geomechanics, for reasons of stability, accuracy, and performance, the resulting linear systems often enough need to be handled in a fully coupled manner (Garipov 2018, Hu et.al. 2013, Yang et.al. 2014). Because the models are further increasing in size, direct solver approaches are hardly applicable due to their memory and time consumption. Therefore, finding robust and efficient iterative linear solvers for the coupled sparse linear systems is of high interest. We will describe how a System-AMG approach can fulfill these requirements.

For detailed information on the physical background of the considered simulations, we, for instance, refer to Aziz and Settari (1979) and Coussy (2004). Regarding the linear solver part, we note that both sub-problems of the coupled system, the flow-transport and the geomechanics, are governed by elliptic PDEs, or elliptic parts of PDEs. Thus, the application of Algebraic Multigrid (AMG) methods appears to be a natural option to be considered. AMG methods (cf. Ruge and Stüben 1986, Stüben 2011 and Cleary et.al. 1998) are known to be robust and efficient linear solvers for elliptic problems. They especially do not rely on geometric or physical information. Thus, they can be directly applied also in problems based on unstructured grids and with high heterogeneities. These properties can in principle also be transferred (Clees 2005) to problems where multiple physical unknowns are involved.

For the mechanics, which is most of the time based on linear elasticity, the application of AMG is well studied (cf. Baker et.al. 2010, Brezina et.al. 2006, Griebel et.al. 2006 and Stüben 2000). Due to the typical material parameters of rock, the application of unknown-wise AMG can be expected to be rather straight- forward for this sub-problem. It is, in particular, known to be much more robust for these kinds of problems than single level methods. Incomplete factorizations, for instance, need a high amount of fill-in to appropriately converge.

Also for the flow-transport reservoir simulations, AMG is known to provide an efficient solver method. There is the constrained pressure residual method (CPR, cf. Wallis 1983 and Wallis et.al. 1985) that uses the original AMG for solving an extracted pressure sub-system. This serves as a convergence accelerator for an incomplete factorization method for the full system. However, the way how the pressure sub-system is extracted may affect the applicability of AMG.

System-AMG provides an alternative approach (cf. Gries 2016 and 2018, and the references therein). While it has similarities with CPR in the Black-Oil case, it has the advantage of handling the entire linear system in the context of AMG. Thus, it can be extended to more sophisticated situations where also thermal effects (Gries and Plum 2015) or, like in this paper, geomechanical processes are considered. Therefore, our AMG-based solution approach for the fully coupled systems of reservoir simulation with geomechanics will follow the System-AMG methodology.

However, while the AMG-based approaches for each of the two considered sub-problems can simply be taken over from earlier work, there still is a major challenge: a System-AMG approach for the full coupled systems here. One way is to approximately decouple flow-transport and mechanics and iterate between both sub-systems (Klevtsov et.al. 2016, White et.al. 2018). However, with AMG involved, like in CPR, such approximate decouplings and the inherent algebraic operations carry the risk of loosing the applicability of AMG. Therefore, we intend to handle the entire system by a single AMG approach. The main challenge is that, depending on the time step size, the two sub-systems may drastically differ regarding their scale. This can pose serious troubles for the AMG-smoothing scheme, since round-off effects may simply dominate with the given machine accuracy.

The inexact Uzawa smoothing scheme (Schöberl and Zulehner 2003 and Metsch 2013) for AMG provides a way to handle the two sub-systems independently in the smoother. The construction of the AMG hierarchy is not affected by any decoupling. This exploits the fact that the overall system features matrix properties as they are known from saddle-point problems. We will discuss how this Uzawa smoothing can be applied

in the case of coupled multiphase reservoir simulation with geomechanics. This will also include some adaptive mechanism for adjusting the method such that it fits best for a particular linear system.

In the end, the scaling differences can be properly handled by this smoothing scheme. Our results with representative linear systems and full simulations demonstrate the robust applicability of the System-AMG approach for a broad range of practically relevant simulations. Compared to other applicable linear solvers, this holds in terms of computational performance but also in terms of memory requirement and robustness. These results have been studied with Fraunhofer's SAMG software for problems from Stanford's ADGPRS simulator (ADGPRS, Voskov et.al. 2017 and Rin et.al. 2017).

This paper is structured as follows. In the following section we will briefly describe the physical model behind the simulations that we consider. In the third section we then give an overview of AMG and recapitulate its application for both the flow-transport and geomechanical sub-systems. This is followed by an introduction to Uzawa-based AMG smoothing and its application here in the fourth section. In the following fifth and sixth section we will describe some mechanisms to further improve the robustness of the System-AMG approach. And, finally, in the seventh section we will show results of the System-AMG approach with single linear systems and full simulation runs.

Linear Systems in Coupled Reservoir Simulations with Geomechanics

In coupled problems of reservoir simulation with geomechanics, we are concerned with a simultaneous solution of two different physical problems. We will only give a brief overview here and refer to the literature, e.g., Aziz and Settari (1979), for detailed information.

For the sake of simplicity, we limit our description to the immiscible isothermal formulation for flow and transport. However, in terms of the linear systems, the effects of flow-transport being coupled to geomechanics is comparable in the general compositional non-isothermal case. We will demonstrate the applicability of our System-AMG approach with representative simulation examples later on.

The mass balance equation has to be fulfilled for all phases in any place of the reservoir at any time. For each phase α (e.g., oil, gas or water), this equation reads as:

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

Here, t is time, φ the porosity and $\vec{g}$ is gravity. ρ_α is the density of phase α and λ_α its mobility. The absolute permeability of the rock is given as K and the source term q_α accounts for external influences like wells. S_α and p_α are the phase's saturation and pressure – that are to be solved for in each time step. Finally, the mass balances are supplemented by saturation constraints and capillary pressure relations.

In addition to the mass balance equations, the consideration of geomechanics results in the need of the momentum to be balanced:

$$\nabla \cdot \vec{\vec{\sigma}} + \rho_b \vec{g} = 0, \tag{2}$$

where σ is the stress, ρ_b is the combined bulk density for fluid and solid in a volume. By Biot's effective stress relation, we obtain a connection between the effective stress σ′ and the total fluid pressure p_{tot}:

$$\vec{\vec{\sigma'}} = \vec{\vec{\sigma}} + \alpha_{Biot} p_{tot} \vec{\vec{1}}, \tag{3}$$

where α_{Biot} is Biot's coefficient for the characterization of the fluid-structure interaction. We refer to the poroelasticity literature for additional details (Coussy 2004 and Wan 2002). For our further discussion, we just note that (3) yields the one coupling between the flow and the geomechanics part of the simulation. The back-coupling, the influence of the mechanics on the flow, is resulting from a strain dependency of the porosity:

$$\varphi = \frac{1}{M_{Biot}} p_{tot} + \alpha_{Biot} \epsilon_v. \tag{4}$$

Equation (1) then turns into:

$$\frac{\partial}{\partial t}\left[\rho_\alpha S_\alpha \left(\frac{1}{M_{Biot}} p_{tot} + \alpha_{Biot}\epsilon_v\right)\right] - \nabla \cdot \left[\rho_\alpha \lambda_\alpha \vec{\vec{K}}(\nabla p_\alpha - \rho_\alpha \vec{g})\right] + q_\alpha = 0, \tag{5}$$

where M_{Biot} is Biot's modulus and ϵ_v is the volumetric strain, the trace of the strain tensor $\vec{\vec{\epsilon}}$.

To close the gap between (3) and (5), we need a relation between the effective stress and the volumetric strain. For isotropic linear elastic materials, this is described by:

$$\vec{\vec{\sigma'}} = \tilde{\lambda}\epsilon_v \vec{\vec{1}} + 2\tilde{\mu}\vec{\vec{\epsilon}}, \tag{6}$$

where $\tilde{\lambda}$ and $\tilde{\mu}$ are the first and second Lamé constant, respectively. $\vec{\vec{\epsilon}} = \frac{1}{2}(\nabla\vec{u} + \nabla^T\vec{u})$ is the strain and $\vec{u}$ is the mechanical displacement.

Due to pressure and saturation dependencies in densities, mobilities and source terms, the mass conservation equations (1) and (5) are highly non-linear. The necessary linearization is typically realized with Newton's method.

The outcome of discretization and linearization is a coupled linear system for flux and mechanics of the following form:

$$J_{coupled}\begin{pmatrix} x_F \\ x_M \end{pmatrix} =: \begin{pmatrix} J_{FF} & J_{FM} \\ J_{MF} & J_{MM} \end{pmatrix}\begin{pmatrix} x_F \\ x_M \end{pmatrix} = \begin{pmatrix} f_F \\ f_M \end{pmatrix}. \tag{7}$$

We should note that the flow and the geomechanics may well be discretized in different grids. The mechanical grid may especially cover a bigger domain than the reservoir itself, to properly account for mechanical effects also in the surrounding rock.

The flow-related sub-system J_{FF} essentially has the same properties as a linear system from a mere reservoir simulation with no coupling to geomechanics. If we assume a point- or cell-wise ordering of the Jacobian matrix with n_p reservoir-cells, which matches the situation in typical reservoir simulators, then the resulting linear system reads as

$$\begin{aligned} J_{FF}x_F =: & \begin{pmatrix} [A]_{11} & \cdots & [A]_{1n_p} \\ \vdots & \ddots & \vdots \\ [A]_{n_p1} & \cdots & [A]_{n_pn_p} \end{pmatrix}\begin{pmatrix} [x_F]_1 \\ \vdots \\ [x_F]_{n_p} \end{pmatrix} = f_F \\ \text{with } [x_F]_i = \begin{pmatrix} p_i \\ S_i \end{pmatrix} & \text{ and } [A]_{ii} = \begin{pmatrix} [A_{pp}]_{ii} & [A_{ps}]_{ii} \\ [A_{sp}]_{ii} & [A_{ss}]_{ii} \end{pmatrix}. \end{aligned} \tag{8}$$

The only difference to the case where no geomechanics are considered affects the pressure-related sub-systems A_{pp} and A_{sp}, i.e., the first matrix column per cell in the ordering of (8). The strain-dependent porosity involves a pressure dependency as well. Hence, these pressure-related sub-systems, compared to the non-mechanical case, involve an additional term P_M. The matrix P_M is diagonal, since the discretized form of (5) per cell only considers the porosity of that cell. Moreover, since $M_{Biot}>0$, we have $P_M>0$.

The coupling sub-system J_{FM} is resulting from the volumetric strain in (5), which results in the divergence of the displacement. Additionally, a multiplication with α_{Biot} is involved, i.e., "$J_{FM} = \alpha_{Biot}\nabla\cdot$".

The back-coupling, J_{MF} results from the pressure dependence in the effective stress relation (3). Hence, essentially we have "$J_{MF} = -\alpha_{Biot}\nabla$". The negative sign results from the one in (6).

Finally, the mechanical sub-system J_{MM} results from Equation (6). The solution vector x_M consists of the displacements per grid direction (u_x, u_y, u_z). The respective sub-problems are known to be of elliptic type.

System-AMG for the Flow-Transport Part and for the Geomechanics Part

As indicated above with (7), the linear systems that we need to solve consist of two different coupled sub-parts. For each of the sub-systems J_{FF} and J_{MM}, the efficient application of AMG-based solution approaches is well-established. Here we will briefly review them and provide references for further details. Our solution approach for the coupled system described in the next section will then combine the respective AMG strategies.

For both the flow-transport and the geomechanical sub-problem, linear solution approaches based on the Algebraic Multigrid (AMG) idea are exploited in order to provide an efficient and robust solver. AMG methods have originally been developed as an efficient solver for problems that are described by sparse, positive definite, symmetric M-matrices. Properties that typically arise when discretizing scalar, elliptic partial differential equations. A cheap smoothing method is applied at each level of an automatically constructed hierarchy, which provides a scalable solver strategy. In contrast to geometric multigrid, AMG is based only on matrix information. It can especially adapt the exploited hierarchy to the particular problem. This makes AMG particularly suited for unstructured and heterogeneous problems. We refer to the literature for further information on AMG (Ruge and Stüben 1986, Stüben 2001 and Cleary et.al. 1998).

Since we are concerned with different physical unknowns in flow-transport and mechanical problems, we should note that AMG can also be applied to such coupled linear systems. We refer to Clees (2005) for a detailed discussion on how scalar AMG is extended to these situations.

System-AMG Approach for Flow-Transport Reservoir Simulation

System-AMG is a well-suited, efficient solver approach for linear systems (8) from flow-transport reservoir simulations, as described in the earlier work by Gries (2016). It essentially works 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 (Wallis 1983 and Wallis et.al. 1985). However, synergies can be exploited by System-AMG and just a single interface is used for the entire linear solution process. Moreover, as described by Gries and Plum (2015) and in the following section, the System-AMG approach is extendable also to applications where multiple components or thermal and mechanical effects are considered. And finally, the full set of AMG components is available and all physical information can be used by AMG.

Especially the latter aspect is important for the matrix pre-processing that is applied before actually solving the linear system. This pre-processing aims at ensuring the applicability of AMG in a robust manner. While the pressure sub-problem in (8) in principle has an elliptic background, especially influences from wells can have drastic impacts on the matrix properties and the applicability of AMG.

The earlier described Dynamic RowSum pre-processing (Gries et.al. 2014) aims at exactly this issue. It left-scales the point-wise Jacobian (8) with a block-diagonal matrix:

$$C_{DRS} = \begin{pmatrix} [C_{DRS}]_1 & \square & \square \\ \square & \ddots & \square \\ \square & \square & [C_{DRS}]_{n_p} \end{pmatrix} \text{ with the blocks as } [C_{DRS}]_i = \begin{pmatrix} \delta_1^i & \delta_2^i & \cdots & \delta_{n_u}^i \\ \square & 1 & \square & \square \\ \square & \square & \ddots & \square \\ \square & \square & \square & 1 \end{pmatrix}. \quad (9)$$

The weights δ_j^i consider the properties of the respective pressure-related parts of the linear system. 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.

System-AMG Approach for Linear Elasticity

Algebraic multigrid methods are a well-established efficient solver option for linear elasticity problems. We refer, for instance, to Baker et.al. (2010), Brezina et.al. (2006), Griebel et.al. (2006) and Stüben (2000) for further details. To give a brief overview, we exemplarily consider a simple two-dimensional homogeneous problem. The three-dimensional case is analogously.

In terms of the underlying PDE operators, the linear system to be solved reads as:

$$\begin{pmatrix} " -2\frac{1-\nu}{1-2\nu}\partial_{xx} - \partial_{yy} " & " -\frac{1}{1-2\nu}\partial_{xy} " \\ " -\frac{1}{1-2\nu}\partial_{xy} " & " -\partial_{xx} - 2\frac{1-\nu}{1-2\nu}\partial_{yy} " \end{pmatrix} \begin{pmatrix} u_x \\ u_y \end{pmatrix} = f_M, \quad (10)$$

where the quotation marks indicate that we are dealing with the discretizations of the respective PDE operators. ν is Poisson's ratio that describes the mechanical compressibility.

We especially note that the two sub-matrices on the diagonal do have an elliptic background. Thus, the unknown-wise System-AMG approach from Clees (2005) should in principle be applicable. However, we should be aware of two conditions that can result in quite ill-conditioned matrices with resulting difficulties for multigrid:

- The closer Poisson's ratio is to 0.5, which corresponds to a mechanically incompressible material, the more dominant the off-diagonal blocks become compared to the diagonal. According to the analysis by Clees (2005), this results in convergence issues for an unknown-wise AMG approach. More sophisticated System-AMG approaches are required then.
- The higher the amount of von-Neumann boundary conditions (i.e., free boundaries) is, the closer the eigenvalues of the matrix are to zero. This is because with only free boundaries, shifts or rotations of the entire domain result in displacements but do not lead to stress or strain. Special coarsening approaches are needed then. These can reflect this fact and transfer near kernel eigenmodes through the AMG hierarchy. An example is adaptive smoothed aggregation (Brezina et.al. 2006).

In classical simulations of reservoirs coupled with geomechanics, however, we are not concerned with these two potential problems: typical Poisson's ratios for rock are between 0.1 and 0.4, bounded away from 0.5. And the sub-surface region that is considered for the geomechanical problem is typically surrounded by rock. This implies Dirichlet boundary conditions.

Hence, unknown-wise System-AMG can be expected to be applicable for the geomechanics sub-problem.

System-AMG for the Coupled Problem, based on Uzawa Smoothing

We do have AMG-based approaches for the sub-systems J_{FF} and J_{MM} of (7) available and, in fact, could apply them in an unknown-wise manner to solve the full system. However, unfortunately, both sub-systems

can feature heavy differences in scale. This in turn can lead to a dominance of round-off effects even with double precision arithmetic.

Moreover, this effect is also influenced by the time step size, which is included in the flow-transport sub-problem J_{FF}. Thus, with a time step that outweighs the scale differences between flow and mechanics, the unknown-wise application of AMG might work properly. However, another time step size, even with the same simulation, can lead to a drastic scale difference and, thus, serious convergence issues.

A way to overcome these round-off effects is by applying smoothers that consider each of the two sub-parts individually. We should note that this really only affects the smoother. The construction of the AMG hierarchy is performed in an unknown-wise manner, so that the scaling differences between different types of unknowns do not matter. Therefore, all decoupling attempts that we will describe in the following are limited to the smoothing method of AMG. This especially implies that the linear system itself is never affected by any kind of (approximate) decoupling, but they will only be implicitly incorporated in the smoothing scheme. Hence, this does not have impacts on the applicability of AMG itself.

For the smoother, we formally re-arrange the coupled system (6) such that it is multiplied with −1:

$$\begin{pmatrix} -J_{FF} & -J_{FM} \\ -J_{MF} & -J_{MM} \end{pmatrix} \begin{pmatrix} x_F \\ x_M \end{pmatrix} = \begin{pmatrix} -J_{FF} & -J_{FM} \\ J_{FM}^T & -J_{MM} \end{pmatrix} \begin{pmatrix} x_F \\ x_M \end{pmatrix} = \begin{pmatrix} -f_F \\ -f_M \end{pmatrix}, \tag{11}$$

where $-J_{MM}$ is a positive semi-definite operator, $-J_{MF} = J_{FM}^T$ is a gradient operator, and $-J_{FM}$ is a negative divergence operator. This linear system belongs to the class of *saddle point systems* with both positive and negative eigenvalues. Classical (algebraic) multigrid methods cannot be applied straight-forwardly to this kind of matrices, as they are designed for (symmetric) positive definite, diagonally dominant operators.

The starting point for our Saddle Point AMG method is a suitable smoother. A commonly used choice is an inexact Uzawa relaxation.

The Uzawa scheme also recently was the method of choice in a geometric multigrid approach for a coupled problem of single-phase flow and poroelasticity (Luo et.al. 2017a and 2017b). With geometric multigrid, the (potentially) different grids for flow and mechanics require different grid transfer operators. Then also the smoothing operator needs to distinguish the two different sub-systems. This was realized by the decoupled Uzawa scheme, where the coupled system matrix is splitted as

$$\begin{pmatrix} -J_{FF} & -J_{FM} \\ J_{FM}^T & -J_{MM} \end{pmatrix} = \begin{pmatrix} \frac{1}{\omega} Id & -J_{FM} \\ 0 & -\widetilde{J_{MM}} \end{pmatrix} - \begin{pmatrix} J_{FF} + \frac{1}{\omega} Id & 0 \\ -J_{FM}^T & J_{MM} - \widetilde{J_{MM}} \end{pmatrix}, \tag{12}$$

with $\widetilde{J_{MM}}$ some easily invertible approximation of J_{MM}, for instance, by some relaxation method. ω is some under-relaxation parameter. The left matrix is now considered for smoothing, while the right one is incorporated to the right-hand-side. This leads to a two-step Uzawa scheme: the displacements are updated first, based on a relaxation method, and the flow-transport is updated afterwards.

On the one hand, this scheme allows to treat the smoothing separately for the flow and the mechanics part. This is crucial in the geometric multigrid context. But, due to the round-off effects, it is also beneficial for algebraic multigrid, although AMG does not exploit the grid information. However, on the other hand, it does only apply a Richardson step in the flow update of the second step of the resulting Uzawa scheme.

To gain a higher robustness, we choose to use an Uzawa scheme with a Schur complement approximation, as it is, for instance, described by Schöberl and Zulehner (2003). This higher robustness is especially required in the multiphase case, where we need to include an incomplete factorization step in the flux-update, as we will discuss further below. The Schur-Uzawa scheme consists of three steps, a relaxation on the mechanics' part as first and third step and a flow update as a second step:

$$\begin{aligned} x_M^* &= x_M - \widetilde{J_{MM}}^{-1}(J_{MM}x_M - J_{FM}^T x_F - f_M) \\ x_F^{new} &= x_F + \tilde{S}^{-1}(J_{FF}x_F + f_F + J_{FM}x_M^*) \\ x_M^{new} &= x_M - \widetilde{J_{MM}}^{-1}(J_{MM}x_M - J_{FM}^T x_F^{new} - f_M), \end{aligned} \tag{13}$$

where $\widetilde{J_{MM}}$ and $\tilde{S}$ denote easily invertible preconditioners for J_{MM} and the Schur complement matrix $S = J_{FF} - J_{FM}\widetilde{J_{MM}}^{-1}J_{FM}^T$, respectively. A quick analysis (Schöberl and Zulehner 2003 and Metsch 2013) shows that a single Uzawa sweep essentially consists of a block relaxation using the matrix

$$\begin{pmatrix} J_{FF} - J_{FM}\widetilde{J_{MM}}^{-1}J_{FM}^T & 0 \\ 0 & -J_{MM} \end{pmatrix}, \tag{14}$$

followed by two coupling steps. This suggests to use the matrices J_{MM} and $J_{FF} - J_{FM}\widetilde{J_{MM}}^{-1}J_{FM}^T$ to compute the next level of the AMG hierarchy. An extensive description of this approach can be found at Metsch (2013).

However, the computation of the approximate Schur complement $-J_{FM}\widetilde{J_{MM}}^{-1}J_{FM}^T$ is expensive and not always needed. A cheaper alternative is to only use the matrix J_{FF}, but this only works well if the characteristics of J_{FF} well represent those of $J_{FF} - J_{FM}\widetilde{J_{MM}}^{-1}J_{FM}^T$. To this end, we compare the diagonal of the latter matrix with the diagonal of J_{FF}. For all rows whose diagonal entry of J_{FF} is "not large enough", we do not take the respective variable into the next level, i.e., we do not perform AMG coarsening there.

Summarizing this discussion, a coarse AMG level for the saddle point system (11) can be constructed based on the coarse levels for J_{MM} and J_{FF}. In the previous section, we have already described how AMG levels for the geomechanics matrix J_{MM} and the flow matrix J_{FF} can be built. We compose them to a coarse level for (11). During the AMG cycling phase, we then use the Uzawa smoothing (13) to handle flow and mechanics.

This requires an approximation $\tilde{S}$ of the Schur complement $S = J_{FF} - J_{FM}\widetilde{J_{MM}}^{-1}J_{FM}^T$, which makes the flow update more robust than the plain Richardson iteration from (12). We have simply chosen a diagonal approximation of the Schur complement: $\tilde{S} = J_{FF} - diag(J_{FM}\widetilde{J_{MM}}^{-1}J_{FM}^T)$. This can be calculated rather easily, especially due to the equality of $J_{MF} = -J_{FM}^T$. Moreover, for relaxation schemes like Gauss-Seidel that are used for approximating $\tilde{S}^{-1}$, this only requires an additional scaling per update in the x_F vector:

$$(x_F^{i+1})_k = \frac{1}{\tilde{S}_{kk}}\left((f_f)_k - \sum_{j=1}^{k-1}(J_{FF})_{kj}\left(x_F^{i+1}\right)_j - \sum_{j=k+1}^{n}(J_{FF})_{kj}\left(x_F^{i}\right)_j\right) \tag{15}$$

At the same time, due to the rather well-conditioned J_{MM} that is based on standard linear elasticity PDEs, this diagonal approximation turned out to be already quite robust.

Regarding the order of the Uzawa steps (13), we should note that we also could have started with a flow-transport update, followed by a mechanical update and another flow-transport update. However, then our Schur complement approximation would involve the approximation of the inverse of J_{FF}. In contrast to the linear-elasticity-based J_{MM}, the flow-transport-related sub-system, at least in the multi-phase case, is non-symmetric. Moreover, depending on the wells, it can be much more ill-conditioned and, depending on the number of components, much bigger than the mechanical sub-problem. Hence, the approximation of the inverse of J_{MM} simply appeared to be less error-prone, but we will get back to this aspect later on.

With the exemplary *CubeCoup* test case (Janna et.al. 2012), we can demonstrate the necessity of Uzawa smoothing in the System-AMG approach (see Figure 1). It is a single-phase problem in three dimensions with about 540 thousand verticies (finite-element discretization with collocated displacement and pressure degrees of freedom). Two linear systems are considered that only differ in the underlying time-step size: 1 second and 10^6 seconds, respectively. This allows to also observe the time-step dependency of the Uzawa-necessity, as we have discussed at the beginning of this section. For the bigger time-step size, the scale difference between the flow-transport and the mechanical sub-problem is in the order of 10^{10}. The standard smoother with double precision arithmetics can here still cope with this difference. The same holds for strong single-level methods like FGMRes/ILUT,200.

However, for the smaller time-step size, the scale difference increases to 10^{13}. Along with the additionally included material heterogeneities, this is too much for the standard smoother to work properly here. In contrast, the Uzawa scheme does not significanty suffer from this condition. With this smoother, System-AMG converges properly for both time step sizes.

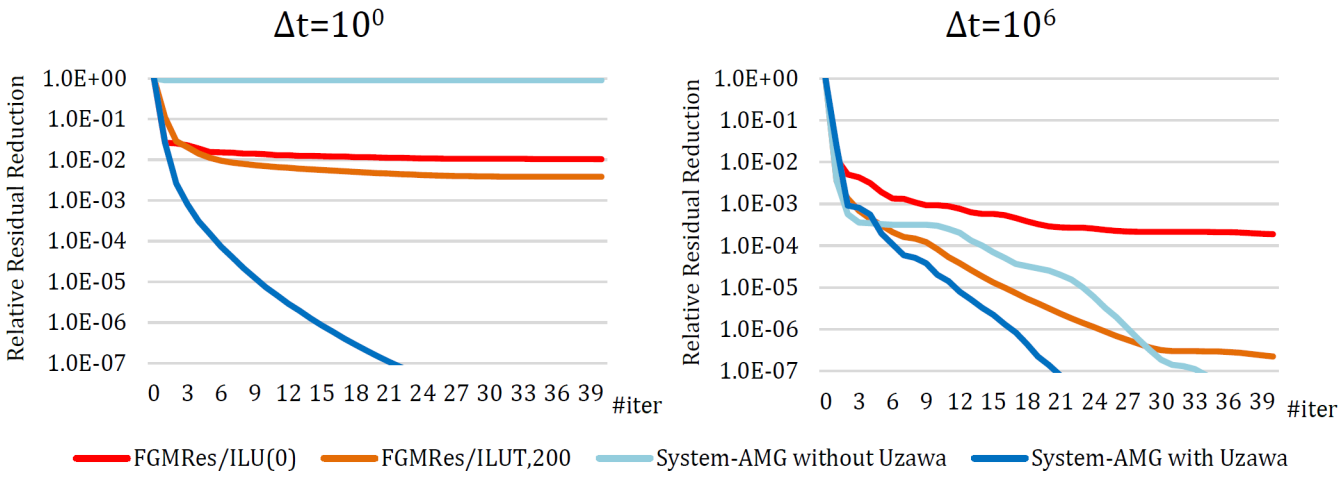

Figure 1—Convergence history for System-AMG and one-level methods for the CubCoup problem at different time-step sizes.

Adjusting the DRS Pre-Processing for Use with Uzawa Smoothing

As soon as multiple phases are involved, the DRS pre-processing needs to be adjusted in order for the Uzawa smoothing to be reliably applied. In its original form (9), the DRS would not only have an effect in the flow part J_{FF}, but also on the coupling J_{FM} to the mechanics. As a consequence, the flow-mechanics coupling would no longer be the transpose of the mechanics-flow one. However, this transposition property, along with the symmetry of J_{MM} is exploited in the computation of the Schur complement approximation $\tilde{S}$. An explicitly calculated transposition would need to be considered otherwise, the computation of which is cost-intensive and hardly parallelizable with sparse matrices.

Analogue implications would hold for any kind of matrix pre-processing that was applied to the flow part of the problem. However, waiving a matrix pre-processing imposes the risk of AMG no longer being robustly applicable for the flow sub-problem of the coupled system. We refer to the discussion and examples from Gries et.al. (2014).

The DRS pre-processing can be adjusted in order to maintain the transpose property of the cross-couplings, which is a pre-requisite for applying the Uzawa-scheme reliably. The J_{FM} coupling results from the displacement-derivative of the discretization of the term $\frac{\partial}{\partial t}\rho_\alpha S_\alpha \alpha_{Biot} \nabla \cdot \vec{u}$ from the geomechanics-aware mass balance (5). This derivative is the same for each coordinate direction (u_x, u_y, u_z). For each reservoir cell it only differs by a phase-dependent factor.

The DRS does have an effect only on the pressure-related matrix rows of J_{FM} anyway. Hence, we can adjust the DRS weights in (9) such that per cell we maintain the relation of the pressure-related row in J_{FM} to the other rows that are affiliated with the same cell.

The matrix stencil of J_{FM} is the same for each row that is affiliated with the same reservoir cell: they are all influenced by the same mechanical displacement. Thus, the above DRS-adjustment maintains $J_{FM} = -J_{MF}^T$.

For the mechanical part (i.e., sub-system J_{MM}) a pre-processing is neither necessary nor applied. That is, the left-scaling operator that is used for pre-processing the full system (7) is the DRS operator in the flow-related part and the identity in the mechanics-related one.

Incorporating ILU Smoothing for the Flow-Transport Part

The fine-level post-smoother requires special attention in the System-AMG case. The diffusion based pressure and, if applicable, temperature unknowns have just been transferred back from the AMG-hierarchy. The fine-level post-smoothing now does not only need to post-smooth these unknowns, but also update the saturation and concentration unknowns that have been remaining at the finest level. As discussed by Gries (2018), this requires an ILU smoothing scheme: due to the particular matrix structure of J_{FF}, the ILU factorization in fact includes an approximate Schur-complement regarding those unknowns that are involved in the flow part.

In order to sufficiently solve for all involved unknowns, the flow-related update in the Uzawa scheme needs to involve an ILU iteration in the multiphase case. In particular, the Richardson iteration from (12) often enough is no longer sufficient. We should mention that sometimes block-ILU is preferred due to its higher robustness. But the situation regarding the Uzawa scheme is just the same with ILU and block-ILU.

Using an ILU instead of a Gauss-Seidel iteration as approximation of $\tilde{S}^{-1}$ in the second stage of the Uzawa scheme (13) seems rather straight-forward: the residual vector is computed, considering the already updated mechanical-part of the solution vector, x_M. Then the incomplete factors are used to get a correction of the flow-related part of the solution vector, x_F.

However, the incomplete factorization needs to consider the Schur complement approximation $\tilde{S} = J_{FF} - diag(J_{FM}\widetilde{J_{MM}}^{-1}J_{FM}^T)$. And computing this ILU factorization for $\tilde{S}$ in practice often resulted in a break-down of the factorization process, since the diagonal of J_{FF} is weakened further.

Therefore, we incorporated the Schur approximation in a different way: in the single-phase case with Gauss-Seidel smoothing (15), the Schur approximation resulted in an additional scaling by $\frac{1}{\tilde{s}_{kk}}$ per element k in the Gauss-Seidel scheme. With ILU we simply use the same scaling when updating the k-th element with the correction that was based on the ILU factorization of J_{FF}. Since the Gauss-Seidel scheme can be seen as an ILU with just a smaller sparsity pattern (namely, the upper triangle), we can expect this scaling also for a full ILU to serve as a rough Schur approximation. Moreover, in our System-AMG approach, we went for the Uzawa smoother only because of the round-off effects caused by the scaling differences between mechanics and flow. This scaling difference now is outweighed by the element-wise scaling, even though we involve some error in approximating the correct Schur complement. Since we intend to use our System-AMG as a preconditioner, we can safely accept such an approximation error.

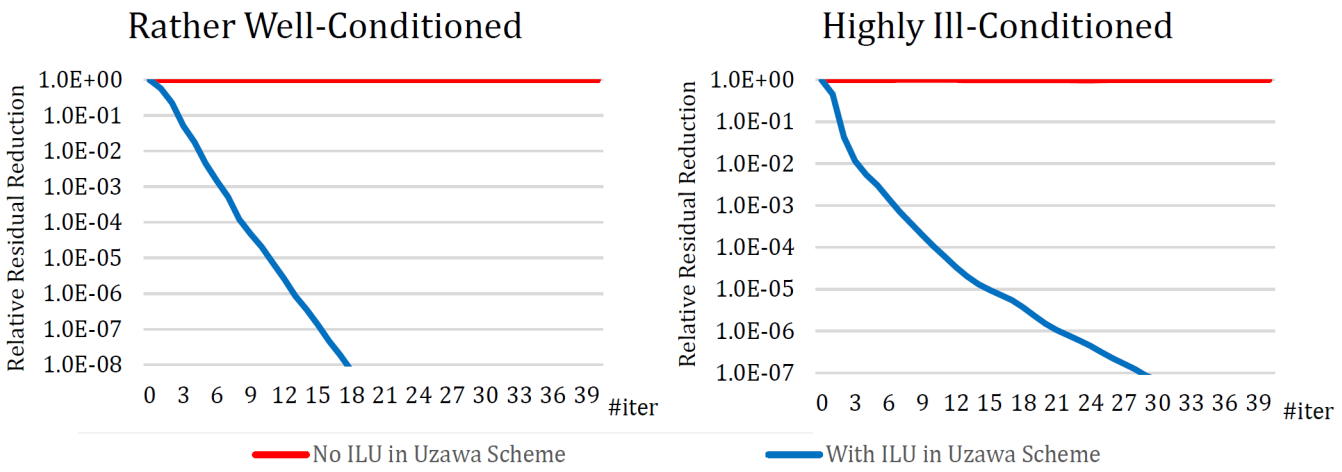

Figure 2—Convergence history for System-AMG with and without ILU in the Uzawa scheme (in the non-ILU case, only Gauss-Seidel is used). Results for the rather well-conditioned first linear system from the isothermal, compositional cold-water-injection simulation (5 components, 3 phases; a full description is provided in the Results-Section below). And for a rather ill-conditioned problem from the fractured cold-water-injection simulation (details are also provided in the Results-Section). In the ill-conditioned case, an adaptive setup modification and an adaptive smoothing control is used both with and without ILU in the Uzawa scheme (cf. Figure 3).

The results in Figure 2 show that our incorporation of ILU in the Uzawa scheme is not only working. It is also crucial to obtain a reliable convergence already in rather well-conditioned problems.

We should emphasize that the incorporation of ILU in the Uzawa scheme only holds for the flow-transport part at the finest level, where saturation/concentration unknowns need to be updated. Regarding the mechanical part of the system, i.e., the first and the third step of the Uzawa scheme (13), we still use Gauss-Seidel smoothing, also at the finest level. And on all other levels of our AMG hierarchy we can properly use Gauss-Seidel in all steps of the Uzawa-scheme (13).

Uzawa Stabilization for Highly Ill-Conditioned Problems

The above-described System-AMG with Uzawa smoothing can already properly handle the difficulties that result from the scaling differences between flow and mechanics in by far most of the cases that we have considered. However, in some rare cases the scaling differences, at least for portions of the domain, are that severe that even the Schur complement approximation in the Uzawa scheme (13) suffers. The resulting element-wise scaling by $diag^{-1}(J_{FM}\widetilde{J_{MM}}^{-1}J_{FM}^{T})$ then may result in floating point exceptions.

It might appear questionable then whether the model is well-posed for a computation on a double precision machine. However, since only a small number of cells might be affected in a limited number of time steps, one may accept this in practical applications. The linear solver should not cause a break-down then. We simply use an averaged $\tilde{s}$ (averaged over all rows) in those cells where the Schur complement is attempted to be approximated by a "near-zero".

We should note that the way we approximated the Schur complement of the Uzawa scheme with the ILU smoothing does not cause an additional error here. The ILU factorization process itself may otherwise just have resulted in a floating point exception and we needed a comparable stabilization technique there.

Adaptive Smoother Control Mechanism

In our fine-level Uzawa scheme, we have involved some error in the way we approximated the Schur complement by a diagonal matrix and with an element-wise scaling. However, whether or not the Uzawa is really necessary to outweigh scaling differences depends on the time step size. Thus, if the Uzawa scheme in fact was not necessary for a particular linear system, we would not want to accept the approximation

error. Moreover, the choice to have an update of the mechanical parts in the first and third step of the Uzawa scheme (13) was arbitrary to some extent, although we had good reasons to prefer this order over the reverse one.

In summary, with our System-AMG setup (including the ILU factorization), we can in fact realize three different fine-level post-smoothers:

- Uzawa scheme as described above
- Uzawa scheme in reversed order That is, the flow part would be updated in the first step and the Schur approximation was applied with updating the mechanics in the second step. While this requires a different diagonal matrix for the Schur approximation, the compute-intensive ILU factorization of J_{FF} for the first step was the same as in the original Uzawa scheme above.
- No Uzawa scheme

This corresponds to simply using the identity as Schur approximation in our Uzawa scheme (13).

All the three options are influenced in a different way by the scaling differences of the two sub- problems of the full system, as well as by the approximation errors in the Uzawa scheme. Consequently, although the initial Uzawa scheme empirically appears to give the most robust setting, in practice we find examples for each of the three options to give the best solver option. Unfortunately, the concrete strength of the round-off effect and approximation error can hardly be estimated reliably beforehand in practice.

Thus, we simply moved towards an adaptive approach. The three different options simply transfer to small differences in the applied Uzawa scheme, while those ingredients that require a cost-intensive setup (AMG, ILU) remain unchanged. Therefore, we can easily effort computing three different results as an outcome of the fine-level post-smoother. While this comes at some additional computational efforts, the impact is rather negligible in terms of the overall computational performance of the full System-AMG approach.

Moreover, really only the post-smoother at the finest level is of concern here: at all other levels no ILU is combined with an element-wise Schur approximation. And, moreover, the result of the fine-level post-smoother is not further corrected by any other smoothing or coarse-grid correction scheme. Consequently, the portion of the algorithm where three different options are handled simultaneously is rather limited.

However, having all three options available enables the Krylov-method, which uses our System-AMG as a preconditioner, to choose the one option that gives the best result. And this decision does not only have to be made once, but it is made per iteration. In fact, in practical cases, the optimal choice does differ for different iterations.

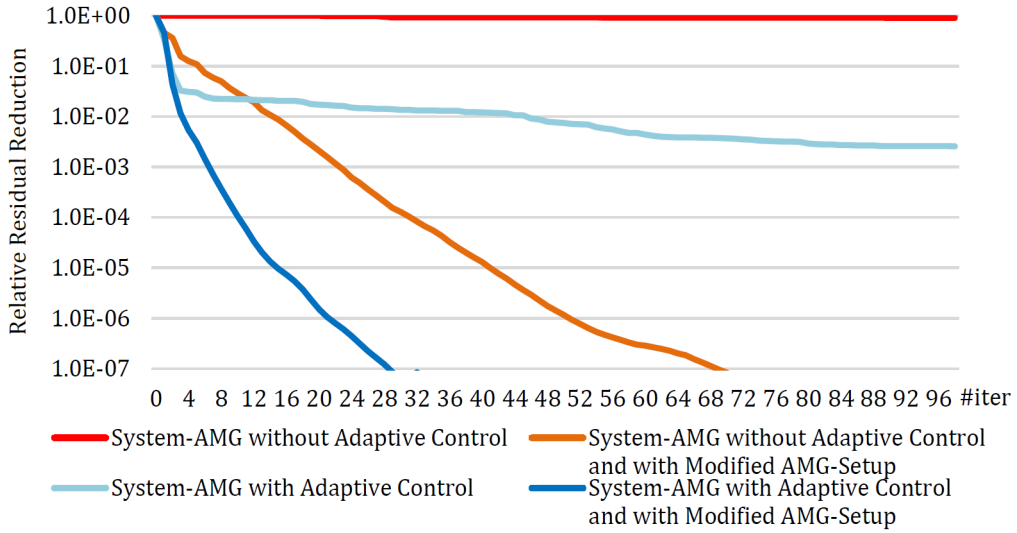

Figure 3—Convergence history for System-AMG with and without adaptive smoother control. In addition, an adaptively activated setup modification is included that aims at higher robustness in highly ill-conditioned cases. The problem is a rather ill-conditioned system from the fractured cold-water-injection simulation from the Results-Section.

While System-AMG with the Uzawa scheme often enough works properly also without this mechanism, the adaptive control has turned out to be beneficial especially in ill-conditioned problems. In Figure 3 the convergence histories of System-AMG are compared with different System-AMG approaches for an ill-conditioned problem of the second time step of the fractured cold-water-injection simulation from the Results-Section. With standard AMG coarsening, the adaptive smoother control is crucial to achieve some convergence. Due to the detected ill-conditioning of the problem, our implementation of System-AMG activates a modification in the AMG setup that aims at a higher robustness. With this modification, convergence is also achieved without the adaptive smoother control. However, the mechanism still is very beneficial for the convergence. In this particular problem, the adaptive mechanism decides to use the initially described Uzawa scheme (first variant) in about 22 % of the iterations. The reversed-order scheme (second variant) is chosen in roughly 33 % of the iterations. And not to use a Schur approximation (third variant) gave the best solution in 44 % of the iterations in this particular case.

Results

In this section, we will demonstrate the applicability of our System-AMG approach for a set of representative reservoir simulations with geomechanics. We will consider different problem sizes as well as different physical complexities, including simulations considering thermal effects and fractures.

We use Stanford's ADGPRS reservoir simulator along with the System-AMG implementation in Fraunhofer's SAMG solver library, both in the 2018 version. Our benchmarks have been run on an Intel E2650 architecture. However, we are mainly interested in the numerical performance, i.e., the convergence properties, of the described approach. This also includes the comparison to other solver approaches.

Extended SPE 10

The extended SPE 10 dataset (Garipov et.al. 2018) has original relative permeability curves, porosity and permeability distributions, fluid properties, and well controls, plus additional geomechanical parameters. The simulation domain of 365.8 m × 670.6 m × 51.8 m is discretized using a regular Cartesian grid of 60 × 220 × 85 cells. The top 35 layers have a permeability (porosity and Young's modulus) with a Gaussian distribution, and the bottom 50 layers have channelized high-contrast properties. Using a simple volume-averaging upscaling, we considered a set of coarsened models from 24 960 to 399 360 cells. We refer to

Garipov et.al. (2018) for a detailed description of the physical models, also regarding the model variations that we will consider further below.

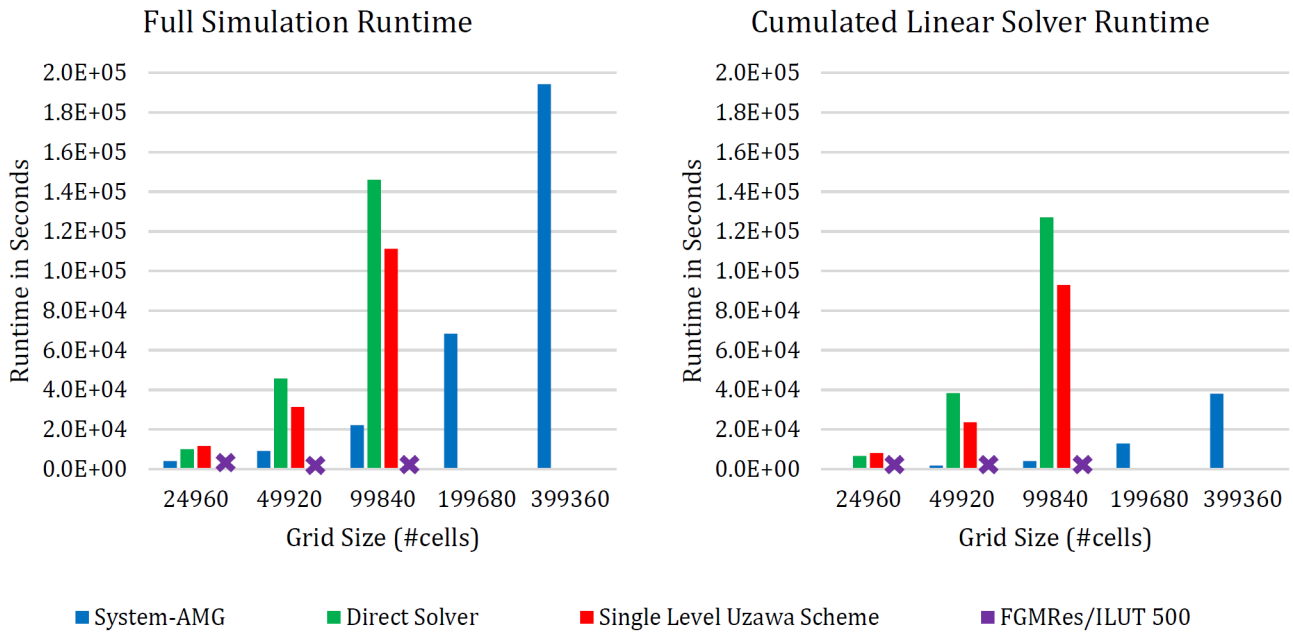

Figure 4—Total simulation runtime and cumulated linear solver runtime for different problem sizes of the extended SPE10 problem. Up to 99 840 cells, also a direct solver (Pardiso) and the single-level Uzawa-scheme are included in the comparison. For the bigger problems, only System-AMG has been considered. The non-Uzawa variant with ILUT has not converged for any considered problem size.

In Figure 4 we compare the runtime in a full simulation of 1000 days for different grid sizes and a two-phase flow with linear elasticity. In addition, the direct solver and the single-level Uzawa-scheme are included up to a size of 99 840 cells. In comparison to these methods, our System-AMG approach allows to exploit the major strength of multigrid methods also for reservoir simulations with geomechanics. It scales roughly linearly with the problem size. For the single-level and direct solver approach, the increase in runtime is much higher with a growing problem size.

The quality of the linear solution seems to be comparable with all considered methods, as the number of time steps and the number of Newton iterations is roughly the same for all cases of the same problem size. Finally, we observe the necessity of the Uzawa scheme in the iterative approaches. Without, even a strong ILUT does not properly converge for this simulation.

In addition to the problem size, we are interested in the effects of different physical complexities. We exemplarily consider the problem size of 199 680 cells and vary the physical complexity in two regards:

- We consider a stronger and weaker geomechanics coupling. This is realized by applying a multiplier of 0.1 and 10, respectively, to Young's modulus.
- In addition to a two-phase flow with linear elasticity, we also consider a single-phase flow with linear elasticity and a two-phase flow with nonlinear plastic deformation.

The runtimes are presented in Figure 5. Our System-AMG approach is working for all types of simulations that we have tested here. The drastically better performance in the single-phase case is due to no ILU factorization being needed in System-AMG here on the one hand. And due to the better convergence of linear and nonlinear solver with the better conditioned problems on the other hand. Both iteration counts are about 15 times lower in the single-phase case.

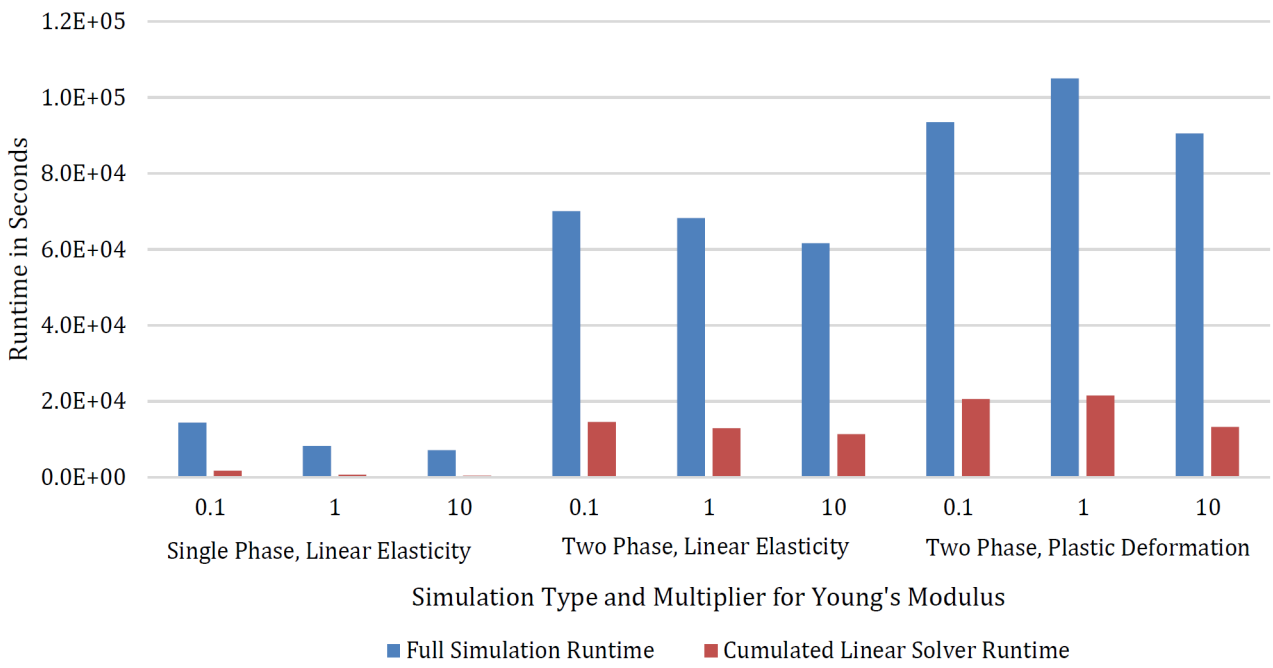

Figure 5—Runtimes for the full simulation and the linear solver for different variations of the 199 680-cell problem.

Cold Water Injection

Here, we consider a problem that includes coupled compositional flow-transport and mechanics. We consider two cases: with and without thermal effects included. The model is based on a modified version of the SPE 9 dataset (Killough 1995). We extend the description from three-phase black-oil to a 5- components system (H_2S, C_1, C_5, C_{13}, H_2O). A K-values flash is used for the phase equilibrium calculations. There are 25 producers and 1 injector, all operating with a BHP control. The simulation covers 1000 days. More details can be found at Rin et.al. (2017).

	Non-Thermal	Thermal
Full Simulation Runtime	1149 sec.	1517 sec.
Cumulated Linear Solver Runtime	365.5 sec.	499.6 sec.
Number of Time Steps	16	16
Number of Newton Iterations	60	61
Number of Linear Iterations	993	962
Av. Number of Linear Iter. per Newton	16.55	15.77

Figure 6—Runtimes and iteration counts for the cold-water-injection simulation in the non-thermal and thermal configuration.

From the results in Figure 6 we see that the described System-AMG approach can also cope with compositional and thermal cases. In the thermal simulation, the temperature is handled in an unknown- wise manner within the flow-transport sub-problem. See Gries (2016) for further details. The increased runtime for linear solution and full runtime is due to the additionally involved thermal effects. Both the increase for the solver runtime and the full simulation are in the same range of about 33 %.

Discrete Fracture Modeling On Unstructured Grids

9-Fractures. A 2.5 dimensional domain of 200 × 200 × 100 meters is considered. The domain contains nine fractures of different size and orientation: one central fracture of 120 m and eight other fractures of 60 meters. The central group contains vertical fractures, while others have the orientation of 80°. The model is discretized using an unstructured mesh generator producing a tetrahedral grid. One injector in the center

of the domain operates with a constant flow rate of 50 m^3/day. Four producers in the corners of the domain operate with constant bottom hole pressure of 100 bar. For mechanical boundary conditions, we fix bottom, left, and front boundaries, while a constant uniform loading is applied to the others. The model is designed in the way that fractures quickly turn in the sliding mode after the start of fluid injection. We refer to Shovkun et.al. (2018) for a detailed description of the case. From the results in Figure 7 we see that our System-AMG approach can properly handle the presense of fractures. However, the resulting material heterogeneities lead to less well-conditioned linear systems. Thus, we observe a higher number of linear iterations per Newton step than in the non-fractured cases.

	9-Fractures	Fractured Cold Water Injection
Full Simulation Runtime	1660 sec.	24762 sec.
Cumulated Linear Solver Runtime	474.7 sec.	10161 sec.
Number of Time Steps	10	69
Number of Newton Iterations	50	295
Number of Linear Iterations	3311	25489
Av. Number of Linear Iter. per Newton	66.22	86.40

Figure 7—Runtimes and iteration counts for the 9-Fractures case and simulation of cold water injection in a fractured reservoir.

Cold Water Injection in Fractured Reservoir. This case is a synthetic model, designed to study thermo-hydro-mechanical effects that occur during injection of cold water into a fractured carbonate reservoir (Garipov and Hui). The well in the middle of the domain for 30 days injects cold water with a temperature of 50°C, while the initial reservoir temperature is 100°C. The domain of 2000 m × 2000 m is discretized into about 25 000 cells. The reservoir is highly fractured with a distorted grid of fractures. Several physical phenomena occurring during injection have a dramatic impact on the properties of the fractures: their conductivity changes with stress change, shear, surface cooling, opening due to matrix contraction. All this results in highly nonlinear behavior and ill-conditioned systems to solve.

In fact, the time step sizes are therefore more restrictive than in the 9-Fractures case above. However, from the results in Figure 7 we see that the number of nonlinear iterations per time step is roughly constant. Also the number of linear iterations per Newton step does only slightly increase. We should mention that with a direct solver the numbers of time and Newton steps are almost the same (68 and 293, respectively). However, the direct linear solver takes 15218 seconds for the entire simulation, an increase by 50 %. The full simulation runtime then increases accordingly to 29411 seconds.

Conclusions and Outlook

We have described how the System-AMG framework can be extended to reservoir simulations that couple the flow-transport process with geomechanics. By using Uzawa smoothing, the full, coupled system can be handled properly. We have described how the classical Uzawa scheme can be adjusted to the needs also in multiphase simulations and how adaptive controls can further improve the robustness. We have demonstrated the robust applicability for a set of representative reservoir simulations with geomechanics. Also thermal effects and fractures have been considered in these results.

Future research will target at further improving the convergence properties, especially by further adjusting the Uzawa smoothing scheme to the needs in reservoir simulation. Moreover, we intend to further investigate the handling of fractures. Our System-AMG approach has worked properly for the test cases under considerations, and has recently also successfully been applied in further simulations with fractures by Ren et.al. (2018). However, due to the worse condition of the respective linear systems, some increase in the

number of iterations per Newton step is observed, compared to the non-fractured cases. Further research will target on reducing this increase.

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