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# Combining Aggregation and Classical Algebraic Multigrid in the CPR-AMG Linear Solver

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## Abstract

Algebraic multigrid (AMG) represents a class of efficient preconditioners for large and sparse linear systems arising in particular from discretized elliptic partial differential equations. In the context of reservoir simulation, a standard preconditioner for the linear solver is the so-called CPR-AMG in which AMG is applied to an approximated pressure subsystem. In this method, AMG is the bottleneck for scalability because it involves a lot of communications across processors in particular for the setup phase, which constructs the coarse levels according to the coefficients of the Jacobian matrix. The goal of this work is to decrease the overall cost of the CPR-AMG in parallel by combining two different coarsening strategies: the first levels are computed using an aggregation scheme whereas the coarsest levels are treated using a classical point-wise Ruge-Stüben (RS) scheme. AMG preconditioners constructed using classical coarsening schemes are able to achieve good convergence rates of the preconditioned iterative method. The complexities of the multigrid hierarchies can be quite high and thus the classical AMG may be expensive in terms of memory requirements and computational times. Aggregation AMG methods, on the other hand, provide better means of complexity control and consequently the setup time required to construct the preconditioner can be considerably lower. The efficiency of the aggregation AMG methods, however, deteriorates with the increasing problem size although the two-level convergence rates can be very good. To take advantage of both the aggregation and classical AMG, we consider combining both approaches within one hierarchy in order to decrease the setup time of the AMG preconditioner while retaining the convergence properties of the two-level aggregation method.

## Introduction

Algebraic multigrid (AMG) is one of the most efficient methods for solving large sparse linear algebraic systems that arise in a wide range of scientific and engineering applications governed by elliptic partial differential equations. Multigrid methods (including AMG) are based on a careful interplay of smoothing and coarse-grid correction. While the smoothing attempts to diminish the oscillatory components of the errors, the coarse-grid correction is designated to eliminate the complementary smooth components of the errors by transferring the fine-grid problem to a coarse-grid and solving a problem with fewer unknowns.

These two fundamental components are combined in a recursive fashion in a multigrid hierarchy of successively coarser levels.

Fully implicit formulations of coupled pressure-saturations problems in multi-phase flow models require solving a system of non-linear algebraic equations at each time-step. This is typically done by a Newton-type iterative method and, consequently, a sequence of linear systems with linearized Jacobian matrices (coupling together the pressure and saturation unknowns) has to be solved at each time-step. A common class of preconditioners applied to accelerate the convergence of iterative solvers in this context is based on the *constrained pressure reduction* (CPR) approach [see, e.g., (Wallis et al., 1985) and (Stüben et al., 2007)], which decouples the pressure-saturation dependency and approximates the solution of the coupled algebraic system in two stages: by first solving the pressure sub-system (approximately, usually by a single V-cycle of an AMG method) and then applying a global preconditioner such as a block incomplete factorization. This two-stage process defines a preconditioner for an outer iteration, e.g., the GMRES method (Saad and Schultz, 1986).

The AMG setup time (the time required to build the AMG preconditioner) can dominate the overall setup time of the combined CPR-AMG preconditioner. The computational costs and memory requirements of the classical AMG methods, which are commonly used in the context of reservoir simulations, can be relatively high compared to the AMG methods based on aggregation of unknowns. In this work, we investigate a possibility to reduce the overhead associated with the AMG setup by combining the two approaches within one multigrid hierarchy. We also investigate an option of further reducing the setup time by partially reusing the previously computed multigrid preconditioner in a sequence of linear algebraic systems.

## Classical and aggregation AMG

We recall briefly in this section the basic principles of AMG with classical and aggregation-based coarsening. AMG can be generally considered as an algebraic counterpart of the traditional geometric multigrid method. In the geometric multigrid, a sequence of levels is typically defined by discretizing the original partial differential equation (PDE) on a sequence of consecutively coarsened grids and occasionally the smoothers require certain adjustments in order to obtain an efficient and scalable solver. On the other hand, the multigrid hierarchy in AMG [see, e.g., Ruge and Stüben (1987) and Stüben (2001)] is built during the setup phase “automatically” entirely by algebraic means. In contrast to the geometric methods, the smoothers in AMG are normally fixed to some simple relaxation scheme such as the Jacobi or Gauss-Seidel iterations. Consequently, the coarse systems and the associated inter-level operators must be constructed such that they capture accurately the error components, which are not efficiently eliminated by the smoother. Such a construction often utilizes a concept of the strength of coupling between the algebraic variables deduced by a certain comparison of the nonzero entries of the system matrix. Using this concept, the AMG methods attempt to mimic the so-called semi-coarsening geometric method suitable in the context of solving problems with anisotropies in the PDE coefficients. Furthermore, several components of the AMG setup such as the construction of the restriction operators and of the coarse-level matrices are usually fixed and dependent only on the prolongation operators and fine-level matrices. Therefore, the AMG methods are typically characterized by the construction of the coarsening (the choice of the coarse-level variables) and of the interpolation operators realizing the transfers from coarse to fine levels.

In terms of coarsening schemes AMG methods can generally be classified as *classical* and *aggregation* AMG methods. The classical AMG (see Figure 1, left), proposed in the early 80’s of the last century (Brandt et al., 1982), in a sense mimics the geometric multigrid coarsening. In these methods, a certain subset of the fine-level variables is identified with the variables on the coarse level and linear interpolation rules, defining the values in the remaining fine-level variables in terms of the coarse ones in some close neighborhoods, are deduced from the entries of the fine-level matrix.

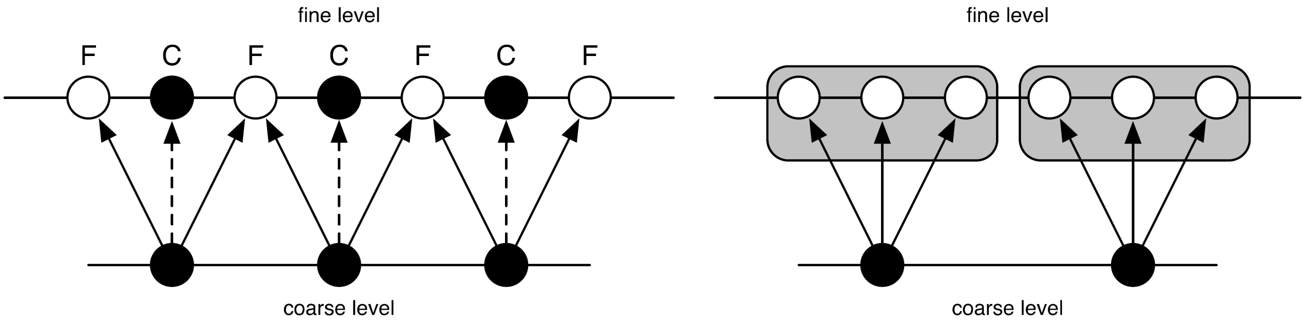

**Figure 1—Coarsening and interpolation in the classical (left) and aggregation (right) AMG.**

The classical AMG coarsening algorithms are typically implemented as a modified coloring procedure applied on a graph associated with strong couplings between the algebraic variables. This coupling is often determined by inspecting the signs and magnitudes of the entries of the system matrix with the help of a suitable strength criterion. The coarse-level variables cannot be chosen arbitrarily but must satisfy some restrictive conditions implied by the chosen interpolation scheme. For illustration, one of the most conservative (classical) distance-one interpolation requires that each fine point is adjacent either to a coarse point or a fine point, which shares with the given fine point a common (strongly connected) coarse point. This often requires a relatively large amount of coarse points to be created during the coarsening procedure in order to ensure that the interpolation weights are well defined. Consequently, the coarsening can be rather slow leading to relatively large number of levels and high operator complexities[1].

In parallel implementations, it is possible to execute any sequential coarsening on the local portions of the system matrix distributed across the processors. This is typically followed by some sort of "special" treatment of the points close to the inter-process boundaries as the interpolation operator needs to be well-defined on the whole domain. Various classical coarsening schemes exist for parallel AMG including more aggressive variants relaxing the strict conditions on the fine-coarse point splitting and allowing for faster coarsening rates, which, however, require constructing transfer operators with wider interpolation ranges. Various related algorithms are implemented in the BoomerAMG (Henson and Yang, 2002) package of the Hypre preconditioning library.

Coarsening by aggregation (see Figure 1, right) is based on a different idea. Instead of classifying certain algebraic variables as coarse ones, they are partitioned to a collection of disjoint contiguous "patches" of variables called aggregates, which represent the variables on the coarse level. Essentially any graph-coarsening algorithm (applied, similarly to the classical AMG, to a certain graph deduced from strong connections in the system matrix) can be directly used or adapted for aggregation. A simple coarsening algorithm is used by (Vaněk et al., 1996). In the first pass, the initial aggregates are constructed from strongly connected patches of unaggregated points. The second pass follows, where the remaining unaggregated points are appended to the adjacent aggregates. We adopt a similar two-pass aggregation procedure in our coarsening algorithm.

In the simplest case of Poisson-like problems, the interpolation operators are given by the adjacency matrix between the fine-level points and their associated aggregates. Hence the nonzero patterns of the aggregation interpolation and coarse-level matrices are usually very sparse. However, this method does not lead to a scalable convergence behavior of the resulting multigrid cycle. Typically, certain post-treatment of the interpolation operator is required such as smoothing (Vaněk et al., 1996) or using "exotic"

[1] The operator complexity is defined by $C_{\mathrm{op}} = \frac{1}{\mathrm{nz}(A_1)}\sum_{\ell=1}^{L}\mathrm{nz}(A_\ell)$, where nz(·) denotes the number of nonzero entries in the matrix and $A\ell$ denotes the matrix on the level $\ell = 1, \ldots, L$ (the finest level has the index 1).

multigrid cycles with over-correction (Blaheta, 1988) or generally a polynomial acceleration (Notay and Vassilevski, 2008).

Parallel aggregation methods are often implemented in a completely decoupled way, where each process aggregates only its local portion of the variables. There is, at least on the finest levels, no strict need for any particular treatment of the inter-process boundaries in contrast to the classical AMG. Since we use the aggregation coarsening only on a fixed number of finest levels, we adopt this approach as well.

## Hybrid aggregation-classical AMG

The classical AMG with a short-distance interpolation often exhibits a very good V-cycle convergence behavior for a wide range of problem sizes. However, the operator complexities, which approximately characterize the memory requirements and the computational costs of the V-cycle (ignoring the costs associated with the transfer operators), can be high. The (plain) aggregation methods, on the other hand, are relatively fast and cheap. However, they are not much recognized in the multilevel setting as the convergence rates may deteriorate with the increasing number of levels.

An option to reduce the complexity of the (classical) AMG method consists of first applying the aggressive coarsening with the long-range multi-pass interpolation (Stüben, 2001) on a prescribed number of fine levels followed by a more accurate and less aggressive coarsening with an accurate short-distance interpolation. Even though the iteration numbers of the preconditioned iterations often increase, this is compensated by substantially reduced costs associated with the setup and solution phases of the preconditioner. Motivated by this idea, we consider instead of using the aggressive coarsening the combination of the classical AMG with a fixed number of aggregation method on fine levels. Although the aggregation AMG does not lead to scalable V-cycles, limiting the number of levels reasonably compensates this drawback. In our implementation, we use a similar strength criterion and aggregation procedure as in Vaněk et al. (1996). The strength criterion is modified so that the positive off-diagonal elements are classified as weak couplings and the weights are compared symmetrically to their maxima in both corresponding rows and columns. In this way, it cannot happen that a connection is classified as weak in one direction and strong in the other. The aggregation procedure considers a larger set of strongly connected patches, which allows for more aggressive coarsening. In order to improve the performance of the aggregation method, we use a single step of over-correction to accelerate the convergence of the multigrid cycle. For more details, we refer the reader to (Gratton et al., 2014).

For illustration, we consider a two-dimensional Poisson equation in a unit square with a constant right-hand side and homogeneous Dirichlet boundary conditions discretized by the 5-point finite difference stencil on a uniform Cartesian grid. We consider eight different schemes: the two- and three-level aggregation method with the “exact” coarse-level solver (AGG-2L, AGG-3L) and the coarse-level solver given by the classical AMG (AGG-2L-CAMG, AGG-3L-CAMG), the (full) aggregation method with a V- and W-cycle (AGG-V, AGG-W) and the same methods with the over-correction step (AGG-V+, AGG-W+). In Table 1, we report the numbers of iterations of the flexible GMRES method required to reduce the norm of the residual by six orders of magnitude for various sizes of the discretization grids. The experiments were run on a single node of a BULL cluster described in the next section. We can observe that the performance of both the exact and inexact two- and three-level methods scales well with the problem size with a mild deterioration in terms of the iteration numbers of the inexact method (combined aggregation-classical AMG). On the other hand, the convergence of the V- and W-cycle with the aggregation AMG preconditioner scales very poorly with the problem size. This can be somewhat compensated by using the over-correction approach in particular in the combination with the W-cycle. However, the W-cycle is much more computationally expensive in contrast to the V-cycle (especially in parallel) and we do not consider it in this work.

**Table 1—Iteration counts associated with different AMG schemes in dependence on the grid size for the two-dimensional Poisson problem.**

| | Grid size $N$ (number of unknowns = $N \times N$) | | | | | | |
|---|---|---|---|---|---|---|---|
| **Method** | **64** | **128** | **256** | **512** | **1024** | **2048** | **4096** |
| AGG-2L | 11 | 13 | 14 | 14 | 15 | 15 | 16 |
| AGG-2L-CAMG | 12 | 15 | 16 | 18 | 20 | 22 | 24 |
| AGG-3L | 12 | 15 | 18 | 21 | 22 | 22 | 22 |
| AGG-3L-CAMG | 12 | 15 | 19 | 22 | 24 | 27 | 30 |
| AGG-V | 25 | 37 | 57 | 83 | 145 | 474 | >1000 |
| AGG-V+ | 12 | 15 | 20 | 25 | 31 | 40 | 53 |
| AGG-W | 21 | 27 | 36 | 46 | 64 | 84 | 123 |
| AGG-W+ | 11 | 13 | 14 | 15 | 15 | 16 | 17 |

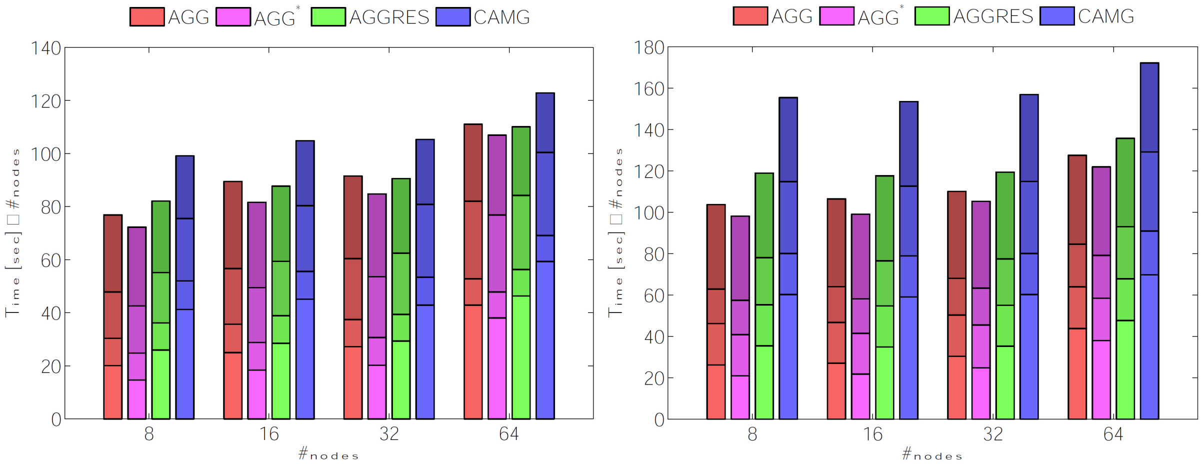

**Figure 2—Setup and solution times of AMG and CPR for the SPE10 (left) and QUARTER5SPOT (right) problems.**

## Strong scalability experiments

We compare the performance of the proposed hybrid AMG preconditioner on two types of problems. We test the strong scalability on two benchmark problems arising in reservoir simulations. The experiments were run on the Beaufix BULL cluster with 1080 computational nodes (each consisting of two sockets equipped with the 12-core Intel® Xeon processor) located at Météo-France in Toulouse. We implemented the aggregation method in our multigrid framework based on the Epetra package of the Trilinos library (Heroux et al., 2005).

In our experiments, we compare four different AMG schemes. The classical AMG (denoted by CAMG) is realized using the BoomerAMG implementation. For coarsening, we use the PMIS algorithm combined with the classical distance-one interpolation and the distance-two interpolation for fine points, which do not share a common coarse point. This choice leads to reasonable coarsening rates in contrast to the algorithms derived from the original RS coarsening algorithm. We consider also a variant with one level of the aggressive coarsening (denoted by AGGRES) followed by the CAMG method on the subsequent levels. Similar setup is considered for the combined aggregation-classical method (denoted by AGG), where the first level is coarsened by a relatively aggressive aggregation method and with the CAMG scheme on the remainder of the hierarchy. In order to further improve the setup times when solving a sequence of linear systems, we compute the AGG preconditioner for the first system in the sequence (corresponding to the Jacobian matrix in the first Newton iteration) and for subsequent systems we reuse the transfer operators of the aggregation part and update only the second-level matrix together with the classical AMG solver. We denote this variant by AGG*. For all methods, the local symmetric Gauss-Seidel method is used as the smoother.

We test the methods on two model problems: the highly heterogeneous and anisotropic SPE10 (Christie and Blunt, 2001) with 1094421 pressure unknowns and the anisotropic homogeneous QUARTER5SPOT problem with 2700000 pressure unknowns. We consider a sequence of 8 (for SPE10) and 5 (for QUARTER5SPOT) Jacobian matrices corresponding to a single time-step of the implicit Euler method. The flexible GMRES method is used as the outer solver. The iteration is stopped when the residual norm decreases by three orders of magnitude.

In Figure 2, we report the timing results for both problems and all considered AMG preconditioners run on up to 64 nodes (denoted by "#nodes"). Each bar in the plots is divided to four parts. From bottom to top, they represent: the setup time of the AMG preconditioner, the remaining setup time of CPR, the solution time spent in applying the multigrid cycle to approximate solutions of the pressure sub-systems, and the remaining time of the CPR solution phase including the overhead from the flexible GMRES method. For convenience of the presentation, the times are scaled by the number of nodes.

In all our tests, the setup times of AGG and AGG* are considerably reduced in comparison with the setup times of the classical AMG. In terms of total time, the aggregation leads to improvements of about 10–27% for SPE10 and 26–36% for QUARTER5SPOT. The operator complexities associated with the aggregation and classical methods are about 1.6 and 2.6 for SPE10 and 1.8 and 3.4 for QUARTER5SPOT, respectively. The complexities obtained by the AGGRES scheme are similar to the ones of the aggregation (but slightly higher). The differences between the AGG and CAMG schemes are less apparent for the SPE10 problem due to the slightly increased number of iterations (by approximately 10%). It is worth mentioning that reusing of the aggregation part of the hierarchy in AGG* does not substantially improve the setup times (on the other hand, without a visible harm to the convergence behavior). This is mainly due to the fact that the classical AMG still takes a considerable portion of the overall setup time of AGG* because it is updated at every Newton iteration. In addition, the current implementation of the matrix-matrix products to recompute the coarse-level matrices does not take full advantage of reusing the structures of products from the previous steps.

## Conclusions

The classical AMG preconditioners are often of high quality in terms of the convergence rates of the preconditioned iterative methods. However, they can be quite expensive in terms of memory requirements and computational costs. On the other hand, aggregation methods are relatively fast and cheap but efficient only with a limited number of levels unless they are combined with a suitable post-processing of the interpolation operators such as in the smoothed aggregation, which leads generally to denser matrices and higher complexities. We proposed a combined aggregation-classical AMG preconditioner, that is, we first generate a fixed number of aggregation levels followed by the coarsening by the classical AMG. By this strategy, we essentially retained the convergence properties of the exact aggregation methods and improved the costs of the setup and solution phases. The combination has a similar effect as the use of the aggressive classical coarsening with the multi-pass interpolation.

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