THE ALGEBRAIC MULTIGRID METHOD (AMG) FOR THE ACCELERATION OF COUPLED SURFACE AND SUBSURFACE FLOW AND TRANSPORT SIMULATIONS

Dr. Peter Thum[1], Dr. Varut Guvanasen[2]
[1] *Fraunhofer Institute for Algorithms and Scientific Computing (SCAI), peter.thum@scai.fraunhofer.de, St. Augustin, Germany*
[2] *HydroGeoLogic, Inc., dguvanasen@hgl.com, Reston, Virginia, USA*

ABSTRACT

This paper introduces the algebraic multigrid technique (AMG) for solving coupled surface and subsurface flow, and transport simulations. AMG approaches commonly used do not work efficiently in the case of coupled flow simulations. Hence, we introduce a specially designed AMG algorithm for this case. The new AMG approach has been developed within the linear solver framework SAMG which is a very mature program that is used for the efficient solution of linear systems of equations in many commercial simulation codes. For the applications in this paper we demonstrate that the new AMG approach is up to 1.8 times faster than PCG on state of the art multi-core machines.

INTRODUCTION

The computationally most expensive task during a coupled simulation is the solution of the linear systems within the Newton or Picard iteration processes. The iterative solution of these linear systems can take up to 80 percent of the overall runtime. Hence, an efficient linear solver can save an enormous amount of run time.

Today, many groundwater simulation codes use algebraic multigrid methods to solve the arising linear systems. These methods are of optimal computational complexity, that is, their numerical work grows only linearly with the number of unknowns. This optimality is achieved by use of a hierarchical approach to solve the linear systems.

However, in the case of coupled simulations the application of classical algebraic multigrid does not always lead to sufficient results. Hence, we have developed a new AMG approach based on aggregative and classical strategies which is especially suited for coupled flow and transport simulations. This hybrid AMG method has been parallelized with state of the art techniques. Hence, it can make efficient use of today’s multi-core computers and CPU clusters.

We compare the hybrid AMG variant to an incomplete LU preconditioned ORTHOMIN solver (PCG) frequently used in the context of coupled flow and transport simulations on two large-scale flow problems.

BRIEF INTRODUCTION TO AMG

AMG accelerates the convergence of the iterative solution of large sparse linear systems by creating a hierarchical process. The motivation for such methods arises from the inability of classical one-level iterative solvers (like Gauss-Seidel or Jacobi) to efficiently reduce the approximation error from iteration to iteration. Hence, classical one-level iterative solvers typically experience a slow convergence, as they cannot handle all error frequencies effectively. To be more specific, the high frequency error components are reduced much faster than the low frequency components. AMG constructs a sequence of lower dimensional systems only based on the matrix itself. Thus, no information about the grid or physical geometry is required beyond what is already contained in the coefficient matrix. On the coarser levels, the low error frequencies of the fine level become higher frequency and, hence, each error frequency can be reduced efficiently at an appropriate level. If combined with some reasonable smoothing process, the lower dimensional systems can be used to correct the higher dimensional ones.

Algebraic multigrid methods proceed in two phases for solving a linear system of equations: a setup phase in which the hierarchical components are set up, and a cycling phase in which the linear system is iteratively solved. Due to its hierarchy, AMG provides optimal complexity, which means that the time for solving a linear system depends on its size only linearly. AMG can be implemented as a plug-in solver, provided that the underlying matrix satisfies certain properties (like sparsity and ellipticity).

One computational advantage of this process is that only the coarsest system requires a direct solution and the operations on all the other levels are simply matrix-vector multiplications. The only drawbacks of AMG are the before-mentioned overhead in terms of the setup phase and its increased memory requirement.

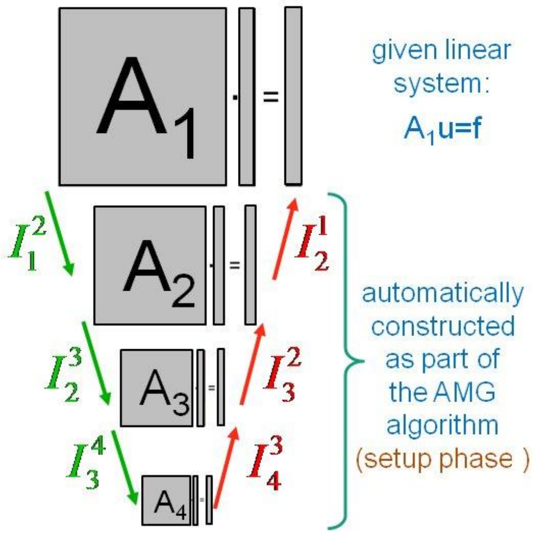

Figure 1. Algebraic multigrid hierarchy

For flow simulations classical AMG has been shown to be fast and robust. However, when looking at coupled surface – subsurface - transport simulations the linear systems have different properties caused by the couplings between the flows. Namely the systems are not fully elliptic anymore and are usually indefinite. Hence, classical AMG strategies do usually not work efficiently. We have developed a new AMG strategy which can deal with the arising difficulties. During the first coarsening step the new strategy applies a coarsening which is based on aggregative techniques instead of the classical approach. After this step, the coarser linear system has much lower coupling strength between the flow regions which leads to better elliptic properties of the coarser system. Hence, we can apply classical techniques during the further coarsening process. The result is an efficient AMG method for coupled surface-subsurface - transport flow.

MODEL PROBLEM DESCRIPTION

The AMG solver was incorporated into the MODHMS code (HydroGeoLogic, 2011) which is a MODFLOW-based code developed for flow and transport simulations in integrated surface water and variably saturated groundwater systems. The solver was tested based on four relatively large-scale flow and transport problems, described below. In all test cases, the system matrices are not symmetric as the Newton-Raphson iterative scheme was used. In all cases, convergence was based on a residual reduction of four orders of magnitude.

Test Case 1: This test case is a steady-state variably saturated groundwater flow problem using approximately 3.5 million nodes. The grid consists of 337 rows, 256 columns and 40 layers, with non-uniform hydraulic properties. The domain is stressed by recharge, and pumping through fracture wells (HydroGeoLogic, 2011).

Test Case 2: This test case is a transient problem with flow in variably saturated groundwater, overland flow, and channel flow with hydraulic structures, Pumping wells in the groundwater domain are allowed provide hydraulic communication between various formations. In terms of unknowns, this problem is smaller than Test Case 1. However, the system matrix is much less structured. It consists of approximately 167 thousand unknowns (approximately 100 thousand cells in the groundwater domain with 5 layers, 196 rows, and 102 columns: 20 thousand cells representing the overland domain; the remaining cells representing channels and the fracture well cells (HydroGeoLogic, 2011)).

Test Case 3: This test case is a steady-state flow problem with one-species transport in variably saturated groundwater. The hydraulic properties for the unsaturated zone are based on the non-linear van

Genuchten relationship (van Genuchten, 1980). The grid consists of approximately 50 thousand cells (1 row, 350 columns and 145 layers), with non-uniform hydraulic properties. A chemical constituent source is present above the phreatic surface.

Test Case 4: This test case is similar to Test Case 2, with integrated surface water/groundwater, but with one-species transport. The system consists of approximately 47 thousand unknowns (approximately 40 thousand cells in the groundwater domain with 4 layers, 97 rows, and 97 columns: 9 thousand cells representing the overland domain; the remaining cells representing channels).

NUMERICAL RESULTS

All the four test problems were solved using the AMG solver and an ILU pre-conditioned Orthomin solver. The test runs were conducted using a computer with an Intel Core2 Duo 3.07 GHz and 4 GB RAM.

For large linear steady-state models, AMG is usually faster than common PCG. The reason for this is the relatively weak diagonal dominance of the linear systems, which effects PCG’s convergence negatively. AMG’s convergence, on the contrary, is nearly independent of the diagonal dominance. Hence, the performance gain can be enormous. Due to AMG’s optimality, the performance gain increases with increasing model size (Thum et al, 2012).

Considering non-linear problems, the performance gain depends not only on the size of the linear system but also on the linearization method used and on the strength of the nonlinearity. Highly nonlinear models usually require the linear systems to be solved much more accurately than in the case of weakly nonlinear models. As a rule of thumb, the more accurately the linear system has to be solved, the higher the performance gain of AMG compared to PCG will be. The reason for this is that one AMG iteration costs as much as 3 to 5 PCG iterations. Hence, if PCG only needs two iterations to reach the required accuracy, say, AMG is not able to beat it.

In the case of non-linear steady-state models and transient models, more than one linear system has to be solved. Our AMG strategy is able to analyze the solver behavior for previous linear systems and (automatically) exploits this information to minimize overall runtime. This is possible due to the fact that subsequent linear systems in non-linear and/or transient simulations typically change only slightly regarding their algebraic properties. This way it is possible to reuse parts or all of previous expensive setup phases whenever feasible which significantly reduces overall run times.

Table 1 shows the Results of the PCG and AMG method. Comparing the transient models 2 and 4, we see that the relative gain in performance for the large is bigger than for the small one. This is due to the fact that AMG’s takes nearly the same number of iterations to solve one linear system for both models. In the case of PCG, however, the number of iterations usually increases with model size.
This is also the reason why AMG does not outperform PCG in test case 3. This case is too small and the required residual reduction for the linear systems is rather low. Hence, the hierarchical approach does not pay off due to its setup costs.

Test Case	No of Nodes	PCG	AMG
1	3,500,000	35	19
2	167,000	2.2	1.6
3	50,000	0.11	0.28
4	47,000	1.63	1.4

Table 1. CPU time (seconds) per solution cycle

SUMMARY

The performance of the AMG solver compared to the PCG solver has been demonstrated four relatively large-scale flow problems in transient as well as steady-state. AMG is extraordinarily efficient for large grids and highly variable conductivity fields as well as steady-state problems. The results show that AMG is up to 1.8 times faster than PCG for large models. Furthermore, we have seen that the parallelization of AMG further improves its performance. The performance gain will increase further with rising cores. More comparison results will be reported in the future.

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