A general software framework for parallel (algebraic) multigrid methods

Serge Gratton[1], Pavel Jiránek[1], Xavier Vasseur[1], and Pascal Hénon[2]

CERFACS, Toulouse, France[1]

Total SA, Centre Scientifique et Technique Jean-Féger, Pau, France[2]

Implicitly Constituted Materials: Modeling, Analysis, and Computing

November 24–27, 2013

Chateau Liblice, Czech Republic

Outline

Outline

Introduction

Ubiquitous need in scientific computing: efficient methods for solving large and sparse linear systems, in particular, iterative methods need efficient preconditioners.

Algebraic multigrid (AMG):

- attempts to retain the performance of the geometric multigrid
- by algebraic means, that is, using the least information possible from the associated PDE problem (ideally only with the information obtained from the system matrix).

AMG is hence particularly attractive when

- the PDE problem is not explicitly available to the iterative solver,
- discretization grids are too complicated for geometric multigrid.

Outline

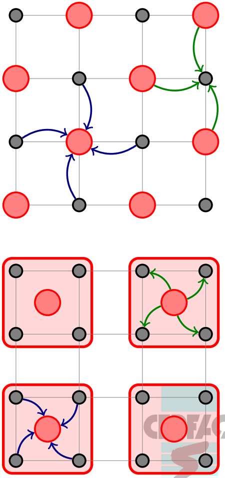
Coarsening in AMG

A vast amount of AMG methods exists nowadays differing mainly in terms of the coarse-grid selection and the construction of interpolation operators.

AMG methods can be usually classified as “classical” AMG mimicing the geometric multigrid coarsening and aggregation-based AMG.

Many modifications and improvements were proposed since 1980’s, e.g.: smoothed aggregation, compatible relaxation coarsening, energy minimizing P-smoothing, AMGe, adaptive AMG, etc.

Software: HYPRE[1] (BOOMERAMG, MLI), TRILINOS[2] (ML, MUELU), SAMG[3],...



[1] http://computation.llnl.gov/casc/hypre

[2] http://trilinos.sandia.gov

[3] http://www.scai.fraunhofer.de

Outline

Design goals

We attempt to create a versatile AMG package which tries to avoid disadvantages of existing AMG codes and allows to implement essentially any kind of (algebraic) multigrid.

- Using an existing algebraic "core" package (TRILINOS).
- Framework for "any" kind of (algebraic) problem (scalar PDEs and systems thereof, coupled problems).
- No particular focus on a fixed coarsening method (classical, aggregation).
- Multiple setup configurations within one hierarchy.
- Possibility to reuse any part of the multigrid hierarchy (particularly useful for partially updating preconditioners for sequences of problems).
- Fine granularity of the AMG setup: reusable and replacable elementary components.
- Behavior controlled by a single XML file for both basic and advanced users.

Example: Smoothed aggregation

The generic setup manager can be controlled by the following “pseudo-code”:

```
...

<Setup>
    <if><not><cond>lastLevel</cond></not></if>
    <block>
        <cmd>Graph           = CouplingGraph(level.A, level.id)                 </cmd>
        <cmd>Aggs            = Aggregator(Graph)                                </cmd>
        <cmd>Nullspace       = SimpleNullspace(level.A)                         </cmd>
        <cmd>Ptent           = TentativeProlongator(Aggs, Nullspace, level.A) </cmd>
        <cmd>level.P         = JacobiPSmoother(Ptent, level.A, Graph)           </cmd>
        <cmd>level.R         = Transposer(level.P)                              </cmd>
        <cmd>level.next.A    = RAPProduct(level.R, level.A, level.P)            </cmd>
        <cmd>level.smoother = Ifpack2Solver(level.A)                            </cmd>
    </block>
    <else/>
    <block>
        <cmd>level.solver    = Amesos2Solver(level.A)                           </cmd>
    </block>
</Setup>

...
```

Outline

Overview

Combining classical AMG and aggregation for anisotropic problems:

- Classical AMG: good convergence of the V-cycle, high complexity.
- Plain aggregation: low complexity and good two-grid convergence, poor V-cycle convergence.
- How about combining plain aggregation and classical AMG?

Scalability tests on Beaufix @ METEO France and Rostand @ Total (Pau) with SPE10 benchmark: pressure systems and CPR-AMG.

Common parameters:

- RS: BoomerAMG with the (more or less) default setting,
- PA: basic Vaněk's aggregation and the "symmetric" strength criterion,
- forward and backward Gauss-Seidel resp. as the pre- and post-smoother,
- LU factorization on the coarsest grid of the size ≤ 128,
- CG/GMRES as the outer solver with a stopping criterion based on the relative decrease of the residual norm and single V-cycle for CPR.

Weak scalability

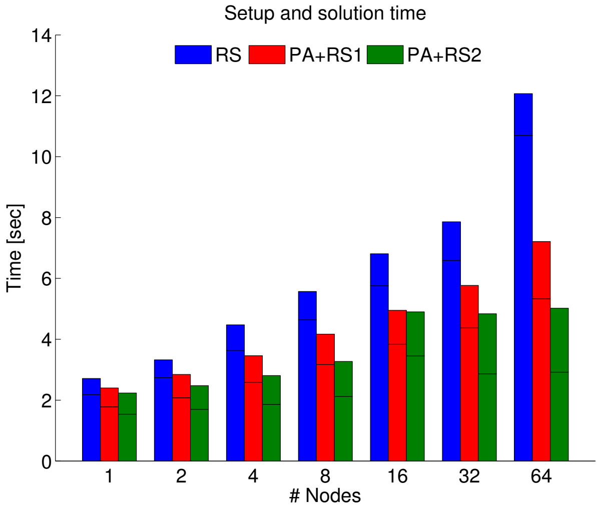
Problem: finite difference discretization of an anisotropic Poisson equation with a grid-aligned strong anisotropy in one direction (about 100^3 grid points per node).

Three schemes:

- RS = stand-alone BoomerAMG preconditioner,
- PA1+RS and PA2+RS = 1 and 2 level(s) of plain aggregation + RS.

	RS		PA1+RS		PA2+RS	
#Nodes	Setup	Total	Setup	Total	Setup	Total
1	2.18E+00	2.72E+00	1.78E+00	2.40E+00	1.54E+00	2.24E+00
2	2.74E+00	3.32E+00	2.08E+00	2.84E+00	1.70E+00	2.48E+00
4	3.64E+00	4.48E+00	2.59E+00	3.46E+00	1.86E+00	2.81E+00
8	4.64E+00	5.57E+00	3.17E+00	4.17E+00	2.12E+00	3.27E+00
16	5.76E+00	6.81E+00	3.84E+00	4.95E+00	3.45E+00	4.89E+00
32	6.59E+00	7.86E+00	4.37E+00	5.77E+00	2.86E+00	4.84E+00
64	1.07E+01	1.20E+01	5.33E+00	7.21E+00	2.92E+00	5.02E+00
C_{op}	4.92 – 6.07		2.83 – 3.54		1.79 – 1.87	
N_{it}	4 – 6		8 – 13		13 – 20	

Weak scalability



AMG in reservoir simulations

Mathematical models involved in reservoir simulations (single/multi-phase flows, compositional flows, etc.) lead to a sequence of coupled pressure-saturation systems

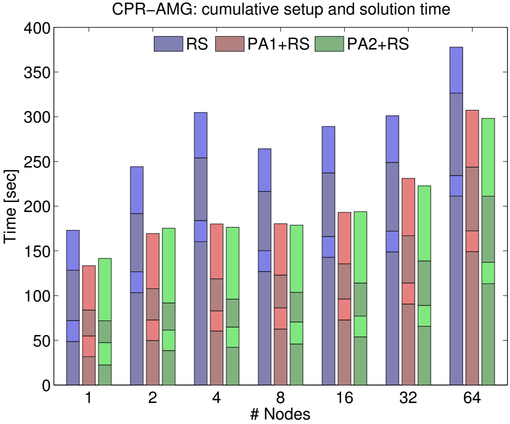
$$\begin{bmatrix} \mathbf{A}_{\mathrm{PP}} & \mathbf{A}_{\mathrm{PS}} \\ \mathbf{A}_{\mathrm{SP}} & \mathbf{A}_{\mathrm{SS}} \end{bmatrix} \begin{bmatrix} \mathbf{u}_{\mathrm{P}} \\ \mathbf{u}_{\mathrm{S}} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{\mathrm{P}} \\ \mathbf{f}_{\mathrm{S}} \end{bmatrix}, \quad \mathbf{G} \begin{bmatrix} \mathbf{A}_{\mathrm{PP}} & \mathbf{A}_{\mathrm{PS}} \\ \mathbf{A}_{\mathrm{SP}} & \mathbf{A}_{\mathrm{SS}} \end{bmatrix} \approx \begin{bmatrix} \tilde{\mathbf{A}}_{\mathrm{PP}} & \mathbf{0} \\ \tilde{\mathbf{A}}_{\mathrm{SP}} & \tilde{\mathbf{A}}_{\mathrm{SS}} \end{bmatrix}$$

Constrained pressure reduction (CPR): decoupling the pressure-saturation dependency by assuming weak global dependency of the pressure on the saturations.

Two-stage preconditioning:

1. Solve the pressure subsystem (AMG),
2. Apply a global preconditioning (ILU) on the updated correction.

SPE10: CPR-AMG @ Rostand, Pau



RS: $N_{\rm it} = 148 - 176$, PA1+RS: $N_{\rm it} = 170 - 213$, PA2+RS: $N_{\rm it} = 228 - 243$.

Outline

Outlook

- Using TRILINOS/TPETRA instead of TRILINOS/EPETRA:
  - MPI/X implementation, where X $\in$ {OpenMP, TBB, PThreads},
  - LARGE-scale problems,
  - ”any” scalar type: single precision, complex.
- Parallel coarsening and interpolation schemes for both aggregation and classical AMG methods.
- Framework for structured problems: saddle point problems, systems of PDEs, coupled problems.

Outlook

- Using TRILINOS/TPETRA instead of TRILINOS/EPETRA:
  - MPI/X implementation, where X $\in$ {OpenMP, TBB, PThreads},
  - LARGE-scale problems,
  - ”any” scalar type: single precision, complex.
- Parallel coarsening and interpolation schemes for both aggregation and classical AMG methods.
- Framework for structured problems: saddle point problems, systems of PDEs, coupled problems.

Thank you for your attention!