Advanced Multigrid Solvers for Fluid Dynamics

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Summary of Research

1. Overview

The main objective of this project has been to support the development of multigrid techniques in computational fluid dynamics that can achieve "textbook multigrid efficiency" (TME), which is several orders of magnitude faster than current industrial CFD solvers.

Toward that goal we have assembled a detailed table which lists every foreseen kind of computational difficulty for achieving it, together with the possible ways for resolving the difficulty, their current state of development, and references.

We have developed several codes to test and demonstrate, in the framework of simple model problems, several approaches for overcoming the most important of the listed difficulties that had not been resolved before. In particular, TME has been demonstrated for incompressible flows on one hand, and for near-sonic flows on the other hand. General approaches were advanced for the relaxation of stagnation points and boundary conditions under various situations. Also, new algebraic multigrid techniques were formed for treating unstructured grid formulations. More details on all these are given below.

2. Table of Barriers

During this period we have completed (in collaboration with D. Sidilkover, C. Swanson, J.L. Thomas and S. Taasan) a detailed table called "Barriers to Achieving Textbook Multigrid Efficiency in CFD" [C1],[C3]. It lists every foreseen kind of computational difficulty for achieving that goal, together with the possible ways for resolving the difficulty, their current state of development, and references.

Included in the table are staggered and nonstaggered, conservative and non-conservative discretization of viscous and inviscid, incompressible and compressible flows at various Mach numbers, as well as a simple (algebraic) turbulence model and comments on chemically reacting flows. The listed difficulties include: non-alignment of streamlines or sonic characteristics with grid directions; recirculating flows; stagnation points; discretization and relaxation on and near shocks and boundaries; far-field artificial boundary conditions; small-scale singularities (meaning important features, such as the complete airplane, which are not visible on some of the coarse grids); large grid aspect ratios; boundary layer resolution;

and grid adaptation.

3. Solution methods on structured grids

As shown before (see [A1], [A2] and [A3]), to obtain TME for any discretized partial differential system of equations (PDE), it is necessary and usually (with proper boundary treatment) also sufficient to attain that efficiency for each factor of the PDE principal determinant. Each such factor is a scalar differential operator of first or second order, so its efficient solution is a vastly simplified task. The way for separating the factors is by a *distributed* (and possibly also *weighted*) relaxation scheme in which to each factor there corresponds a *"ghost"* discrete function. The latter can be directly relaxed for its corresponding factor, dictating a resulting pattern of changes to be distributed to the *actual* discrete functions (see details in Sec. 3.7 of [A1] and also in [A5]). To obtain the top efficiency, the relaxation of each ghost function should incorporate an essential part of an efficient multigrid solver for its corresponding operator: sometimes this essential part is just the relaxation part of that solver, sometimes this may even be the entire solver (applied at some proper subdomain).

3.1 Incompressible systems

For the *incompressible* Euler and Navier-Stokes equations, the relevant factors are the Laplace and the convection (or convection-diffusion) operators. The former's multigrid solver is classical; the latter's can be based on downstream relaxation [A3], with additional special procedures for recirculation flows [A4], [A6]. Indeed, it has been shown that incorporating such procedures into the relaxation schemes for the appropriate ghost functions yields very efficient solvers for incompressible flows even at high Reynolds numbers and at second-order accuracy [A3].

In the first year of the NASA contract we have extended the results of [A3] to 2D flows with *more general (grid cutting) boundaries*. Near such boundaries the interior DGS relaxation scheme is inefficient. Instead, we have used a very robust *box relaxation* (cf. [A1]). As anticipated, the "interior efficiency" of the multigrid cycles could be attained, *provided* a couple of *extra* passes of this box scheme along the boundaries is added to the usual (interior) relaxation sweep. The amount of added computer work is negligible. The textbook efficiency of the FMG algorithm has been demonstrated for problems with a smooth bump in one of the side walls. See more details in Appendix A of [D1].

3.2 The full-potential factor

The main factor of flow systems for which no general adequate multigrid solver had previously been developed is the *"full potential"* operator

$$(u\partial_x + v\partial_y + w\partial_z)^2 - a^2\Delta \, , \tag{1}$$

where (u, v, w) is the flow velocity vector and a is the speed of sound. This

operator appears as a factor in the principal determinant of the 3-D compressible Euler equations.

In the deep *subsonic* case ($u^2 + v^2 + w^2 \leq .5a^2$, say) the operator (1) is uniformly elliptic, hence a usual multigrid V-cycle, employing red/black Gauss-Seidel relaxation at all levels, yields top-efficiency solvers. In the deep *supersonic* case ($u^2 + v^2 + w^2 \geq 1.5a^2$) the full potential operator is uniformly hyperbolic (with the stream direction serving as the time-like direction), and an efficient solver can be obtained using downstream relaxation (marching in the time-like direction).

The most difficult situation for solving the full potential operator is the *near sonic* regime ($u^2 + v^2 + w^2 \approx a^2$), especially in the (usual) case of non-alignment with the grid (e.g., when the grid is cartesian and no velocity component is consistently much smaller than the others). No previous multigrid approach had attained good efficiency in this case.

Since (1) is just a factor of the Euler system principal determinant, its solution is only a (DGS) relaxation step in a multigrid Euler solver. It is therefore enough to confine this step to one subdomain at a time (whose size, however, is not $O(h)$ but $O(1)$). Without loss of generality we could therefore limit the algorithm to the case that throughout this subdomain the velocity is, e.g., *vertically-inclined.* In this case, the multigrid solver we have developed for (1) uses *horizontal* semi coarsening (coarsening only in the x and y directions), possibly together with *vertical* line relaxation. (This z-line relaxation is actually not needed on the finest levels, but may be required after several levels of semi-coarsening.) With this semi coarsening, the inherent cross-characteristic numerical dissipation at the coarse level is *smaller* than at the fine one (opposite to their relation upon *full* coarsening); we can therefore stably add artificial dissipation terms at the coarse level so that its total cross-characteristic dissipation matches the local fine-level average.

The resulting algorithm can fully exploit massively parallel processing. It can be extended to other non-elliptic operators, including the convection operator. (The approach mentioned in Sec. 3.1 for relaxing the convection operator, based on downstream relaxation, is not fully efficient on massively parallel machines.)

Extensive numerical tests have been performed with this algorithm: first in 2D, then in 3D, starting with constant-coefficients, then variable. Simple boundary conditions were chosen in a box: Dirichlet conditions on two opposite faces and periodic on the others. In 2D we have also carried out comprehensive half-space FMG mode analyses. All the results show that at any Mach number the algorithm always attains the "textbook" efficiency. The methods and results are summarized in several publications [C5], [C6], [C7], [C10], [C11].

4. New methods for unstructured grids

The methods described above are suitable for *structured* grids or *semi-structured* grids (i.e., uniform grids with overset patches of finer uniform grids creating

local refinements — which is the ideal setting for obtaining the highest efficiency of multigrid solvers). However, discretization schemes very common today in industrial CFD codes (e.g., in terms of finite elements or finite volumes) are highly unstructured. We have therefore decided to add to our program a special study on fast multigrid solvers for unstructured discretizations.

Algebraic multigrid (AMG) algorithms are solvers of linear systems of equations which are based on multigrid principles but do not explicitly use the geometry of grids; see [C8], [C9], [C2], [C12], [C13]. The emphasis in AMG is on automatic procedures for *coarsening* the set of equations, relying exclusively on its algebraic relations. AMG is widely employed for solving discretized partial differential equations (PDEs) on unstructured grids (or even on structured grids when the coarse grid can no longer be structured, or when the PDE has highly disordered coefficients). The scope of AMG solvers had been rather limited, though. Its coarsening procedures had been inadequate for general non-scalar, or high-order, or non-elliptic and anisotropic PDE systems, and also for non-variational discretizations. The purpose of our recent work [C4] has been to delineate general algebraic coarsening techniques that can be employed in all those cases and, in particular, be applicable to CFD.

Two types of devices have been developed in [C4]. The first is a general criterion for gauging, and a method to control, the quality of the *set* of coarse-level variables, prior to deriving the coarse-level equations. The second includes general approaches for deriving the coarse-level *equations* once the coarse variables are given.

Two such approaches have been advanced. The first one is based on the premise that although in principle each coarse variable depends on *all* others, this dependence decays exponentially with distance. Hence a highly accurate coarse equation can be constructed locally. This is done by solving a certain local optimization problem. We call this approach *direct coarsening*.

The second approach is based on the traditional *Galerkin coarsening*, where the interpolation and restriction operators can again be very accurately derived by solving local optimization problems.

In both these approaches one can control the level of coarsening accuracy, and the corresponding amount of computational work per coarse equation, by choosing the size of certain stencils: The error in approximating sufficiently "smooth" components (i.e., those slow to converge in relaxation) decreases *exponentially* with the size of those stencils, while the work per coarse equation increases proportionally to some *power* of that size.

Numerical results for the advection equation are presented in [C4].

5. Studies with NASA scientists

Collaborating with NASA/Langley researchers Drs. James L. Thomas, Thomas W. Roberts, and R. Charles Swanson, and with Boris Diskin at ICASE, we have

studied several particular issues of multigrid flow solvers, especially those related to boundary treatment and flow stagnation points. Resulting publications include [D2], [D3]. Some emerging general conclusions are summarized below.

- When multigrid cycles slow down, a general useful practice is to print out, just before the fine-to-coarse transition, a table of the *normalized* residuals (i.e., the residuals for the discrete equations, each being normalized so that the sum of its coefficients in absolute value is 1). If the normalized residuals near boundaries are much larger than elsewhere, one can mend the cycles by one of two options: either to have more accurate residual transfers near the boundary, or to add extra local relaxation steps wherever needed to reduce the residuals to their overall average magnitude. The latter option is generally easier to implement, since the accurate fine-to-coarse-transfer weights sensitively depend on distances of various fine and coarse gridpoints to the boundary, and on the type of the boundary conditions.

- The usual Distributed Gauss-Seidel (DGS) relaxation of the interior PDE system should in principle be extend only over those equations whose DGS relaxation does not touch the boundary conditions.

- Near the boundary and on it, a *simultaneous* relaxation of interior equations and the boundary equations coupled to them should be performed. Two general approaches (for constructing such simultaneous relaxation steps when there is no natural set of discrete unknowns corresponding to each relaxed set of discrete equations) are the following.
  (A) A simultaneous Kacmarz scheme. (One can often just use *simple* Kacmarz for each of the boundary and near-boundary equations; but simultaneous schemes are more robust.)
  (B) A more specific distributive scheme; e.g., to each of the interior equations in the relaxed set assign the same distribution as in the interior DGS scheme, just avoiding distribution to variables participating in the discrete boundary conditions.

- In the case that (due to aligned anisotropy of the equation or of the grid) the interior DGS needs be done simultaneously in *lines* (similarly: planes), one should solve simultaneously with each such line of interior equations the boundary equations which are coupled to them.

- In the case of a stretched grid, which requires such line relaxation schemes, the interior DGS allows to relax each line of discrete equations resulting from the same PDE (e.g., the line of continuity equations) *separately* from all other equations — with proper coupling at the boundary as specified above.

- On a *boundary with radius of curvature comparable to the meshsize*, the velocity error after relaxation is not smooth in the usual sense; instead, the *tangential* velocity error is smooth. Hence, the course-to-fine interpolation should be done in terms of the tangential velocity. In particular this is true near the leading and trailing edges of airfoils.

- *Near a stagnation point* the relaxation scheme should be modified; one can no longer regard the advection coefficients as non-principal (i.e., neglect their imminent change when calculating a relaxation step). Thus, a full linearization of the advection terms should enter into the design of the relaxation steps near the stagnation point. Also, one cannot generally relax each momentum equation on the corresponding velocity alone. A general possible approach is to solve simultaneously all the nonlinear system in a box around the stagnation.

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