Barriers to Achieving Textbook Multigrid Efficiency (TME) in CFD

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Barriers to Achieving
Textbook Multigrid Efficiency (TME) in CFD

Achi Brandt†

Abstract

"Textbook multigrid efficiency" (TME) means solving a discrete PDE problem in a computational work which is only a small (less than 10) multiple of the operation count in the discretized system of equations itself. As a guide to attaining this optimal performance for general CFD problems, the table below lists every foreseen kind of computational difficulty for achieving that goal, together with the possible ways for resolving that difficulty, their current state of development, and references.

Included in the table are staggered and nonstaggered, conservative and non-conservative discretizations 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 listing of associated computational barriers involves: non-alignment of streamlines or sonic characteristics with the grids; 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 adaption.

Introduction (by James L. Thomas, NASA LaRC)

Computational fluid dynamics (CFD) is becoming a more important part of the complete aircraft design cycle because of the availability of faster computers with more memory and improved numerical algorithms. As an example, all of the external cruise-surface shapes of the new Boeing 777 wide-body subsonic transport were designed with CFD [R1]. The cruise shape of such a vehicle is designed to minimize viscous and shock wave losses at transonic speeds and can be analyzed with potential flow methods coupled with interacting boundary layers. Off-design performance associated with maximum lift, buffet, and flutter and the determination of stability and control derivatives, involving unsteady separated and vortical

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flows with stronger shock waves, are determined largely by experimental methods. Computational simulations of these flowfields require the use of Reynolds-averaged Navier-Stokes (RANS) methods; these computations for high-Reynolds flows over complex geometries are very expensive, the turnaround time is too long to impact the design cycle, and the turbulence models for separated flows have a high degree of variability. Thus in these areas experiments, rather than computations, are preferred for reasons of cost and uncertainty.

Inroads are being made into these off-design areas with RANS methods. A major lesson learned from industrial use of RANS methods is that both the numerics and the physics must be improved substantially for a new procedure to replace an older procedure. Also, there is a synergistic interplay between the speed of the simulation and the fidelity of the turbulence model, since a larger parameter variation and/or model formulation can be explored on fine enough grids with a faster simulation. For example, the TLNS3D Navier-Stokes code [R2] found its way into use because it was the first three-dimensional Navier-Stokes code to show true multigrid performance, in which the cost scales linearly with the number of unknowns, and it incorporated a better turbulence model than the algebraic models then in use. Solutions with 1 million grid points could be converged in approximately 1 hr of Cray-2 time, which allowed spatial convergence studies to be conducted to ensure that the level of truncation error is sufficiently low, and the prediction of the angle of attack to attain a desired lift coefficient was improved over interacted potential methods [R3]. The faster turnaround of the multigrid procedure enabled the extension and calibration of the original two-dimensional turbulence model to three-dimensions, thus allowing a more accurate prediction of the transonic shock/boundary-layer interaction.

The current RANS solvers with multigrid require on the order of 1500 residual evaluations to converge the lift and drag to one percent of their final values for wing-body geometries near transonic cruise conditions. Complex geometry and complex physics simulations require many more residual evaluations to converge, if indeed convergence can even be attained. It is well-known for elliptic problems that solutions can be attained using full multigrid (FMG) processes in far fewer, on the order of 3-6, residual evaluations; this efficiency is known as textbook multigrid efficiency (TME). Thus, there is a potential gain of two orders of magnitude in operation count reduction if TME could be attained for the RANS equation sets. This possible two order of magnitude improvement in convergence represents an algorithmic floor since it is unlikely that faster convergence for these nonlinear equations could be attained. This algorithmic speed-up, however, coupled with further increases in computational speed can open up avenues and accelerate progress in many areas, including: the application of steady and time-dependent simulations in the high-lift, off-design, and stability and control areas; the usage of RANS solvers in the aerodynamic and multidisciplinary design areas; and the development of improved turbulence models.

The RANS equation sets are a system of coupled nonlinear equations which
are not, even for subsonic Mach numbers, fully elliptic, but contain hyperbolic factors. The theory of multigrid for hyperbolic and mixed-type equations is much less developed than that for purely elliptic equations. Resolution of complex geometries and the thin boundary layers at high Reynolds number cause the grid to be highly irregular and stretched, leading to a slowdown in convergence. Discontinuities, such as shocks and slip surfaces, introduce additional difficulties. These difficulties are illustrated in the sketch in Fig. 1 for a typical multi-element section of a three-dimensional wing with the flaps deployed at takeoff and landing conditions. Overcoming these difficulties poses a formidable challenge, especially because in order to attain optimal and robust convergence rates for the applications of interest in aircraft design, they must all be overcome.

Brandt, in 1984 [G84], summarized the state of the art for attaining multigrid performance for fluid dynamics. Since that time, there has been considerable progress in the field, although optimal results have only been shown for inviscid flows, viscous flows at low Reynolds number, and simple geometries. The methodology and theory that Brandt and others have developed is applicable to the RANS equations and can lead to optimal convergence rates; however, a rational and systematic attack on the barriers which stand in the way needs to be mounted. The purpose of this paper is to delineate clearly the barriers which exist to attaining optimal convergence rates for solutions to the fluid dynamic equations for complex geometries. The following sections identify the barriers, possible solutions, and current status of the problem. The paper is intended as a guide to attaining the optimal convergence goal and is written for the most part in a tabular form so that new solutions and updates to the current status can be made. When completed, the document is intended to list every type of computational difficulty encountered on the road to attaining TME for RANS and the solution paths taken. The insights, lessons learned, and methodologies gained from aerodynamic applications should be applicable to other areas such as acoustics, electromagnetics, hypersonic propulsion, and aerothermodynamics.

Preliminary comments

The table below does not refer to a vast literature on multigrid methods in CFD (see for example [AJ]), in which enormous improvements over previous (single-grid) techniques have been achieved, but without adopting the systematic TME approach. This approach insists on obtaining basically the same ideal efficiency to every problem, by a very systematic study of each type of difficulty, through a carefully chosen sequence of model problems. Several fundamental techniques are typically absent in the multigrid codes that have not adopted the TME strategy. Most important, those codes fail to decompose the solution process into separate treatments of each factor of the PDE principal determinant, and therefore do not identify, let alone treat, the separate obstacles associated with each such factor. Indeed, depending on flow conditions, each of those factors may have different ellipticity measures (some are uniformly elliptic, others are non elliptic at some or all of the relevant scales) and/or different set of characteristic surfaces,
requiring different combinations of relaxation and coarsening procedures.

The table deals only with steady-state flows and their direct multigrid solvers, i.e., not through pseudo-time marching. Time-accurate solvers for genuine time-dependent flow problems are in principle simpler to develop than their steady-state counterparts. Using semi implicit or fully implicit discretizations, large and adaptable time steps can be used, and parallel processing across space and time is feasible [R88]. The resulting system of equations (i.e., the system to be solved at each time step) is much easier than the steady-state system because it has better ellipticity measures (due to the time term), it does not involve the difficulties associated with recirculations, and it comes with a good first approximation (from the previous time step). A simple multigrid "F cycle" at each time step can solve the equations much below the discretization errors of that step [Par]. It is thus believed that fully efficient multigrid methods for the steady-state equations will also yield fully efficient and highly parallelizable methods for time-accurate integrations.

Acknowledgement

Contributions to the table were made by David Sidilkover (ICASE), Jerry C. South (NASA Langley Research Center, retired), R. Charles Swanson (NASA Langley Research Center), and Shlomo Ta’asan (Carnegie Mellon University).
Textbook Multigrid Barriers
(After Brandt, 1997)

Far-Field Boundary Conditions

Grid Aligned with Characteristics

Grid Skewness

High-Aspect-Ratio Grids

Boundary-Layer Separations

Grid Near Boundaries

Inviscid Transonic Flows and Sonic Lines

Separated Cove Flows Possible Unsteadiness

Stagnation Regions

Laminar Separation bubbles

Boundary-Layer Separations
# Attaining Ideal Multigrid Efficiency in CFD: Difficulties and Cures

<table>
<thead>
<tr>
<th>Difficulty</th>
<th>Possible Solutions</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uniformly elliptic scalar equation on uniform grids in general domains</td>
<td>Multigrid cycles, guided by local mode analyses + FMG</td>
<td>TME demonstrated 1971 [B73], [B77] and rigorously proved [RLMA], [RQMA]</td>
</tr>
<tr>
<td>Nonlinearity</td>
<td>FAS + FMG continuation</td>
<td>Demonstrated 1975 [South], [B77], [G, §8.3.2]</td>
</tr>
<tr>
<td>Fluid dynamics – general</td>
<td>See a review in [R88, §2]; at some points it is not fully up to date, but it concisely summarizes the main procedures needed for obtaining TME</td>
<td></td>
</tr>
<tr>
<td>Non-scalar PDE systems</td>
<td>(1) General rules for the inter-grid transfers are given in [G, §4.3], with some more details in [RQMA, §3.3] (2) General approach to the design of relaxation, based on the operator principal matrix $L$ and on the factors of det $L$. Distribution matrix $M$ and weighting (or preconditioning) matrix $P$ are constructed so that PLM is triangular, containing the factors of det $L$ on the main diagonal (separated from each other as much as possible, to avoid the complication described next). This (if necessary – together with the technique described next), leads to decomposing relaxation into simple schemes for the (scalar) factors of det $L$ (3) For systems of PDE which are of mixed type (elliptic-hyperbolic) another possibility is to introduce new unknowns in terms of which elliptic and hyperbolic parts are separated</td>
<td>TME demonstrated in a number of cases (see below). TME proved for uniformly elliptic systems [RLMA], [RQMA]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TME demonstrated for incompressible and compressible cases [T1]–[T5]</td>
</tr>
<tr>
<td>Difficulty</td>
<td>Possible Solutions</td>
<td>Status</td>
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</tbody>
</table>
| Product operator: an equation $LU = f$, where $L = L_2L_1$, with the Fourier symbols $L_j(\theta) = e^{-i\theta \cdot x/h}Le^{i\theta \cdot x/h}$. Assume a relaxation process for $L_j$ is given, with the amplification factor $\mu_j(\theta)$ and the smoothing factor $\bar{\mu}_j$, $(j = 1, 2)$ | Two possible approaches:  
(1) Introduce an explicit new unknown function $V$, replacing the equation with the pair of equations $L_1U - V = 0$ and $L_2V = f$, throughout the MG solution process (including, e.g., transferring residuals of both equations to coarse grids and correcting both $u$ and $v$ by interpolations from the corresponding coarse-grid values). The smoothing factor for this process is $\bar{\mu} = \max(\bar{\mu}_1, \bar{\mu}_2)$ 
(2) Use $V$ only as an auxiliary function in relaxation. That is: starting with $v = L_1u$, where $u$ is the current approximation to $U$, perform $\nu_2$ sweeps on the equation $L_2V = f$, yielding a new value $\tilde{v}$. Then perform $\nu_1$ sweeps on the equation $L_1u = \tilde{v}$. The resulting amplification factor is $\mu(\theta) = \mu_1(\theta)^{\nu_1} + \left[1 - \mu_1(\theta)^{\nu_1}\right]L_1(\theta)^{-1}\mu_2(\theta)^{\nu_2}L_1(\theta)$, so in scalar cases $\bar{\mu} < \bar{\mu}_1^{\nu_1} + \bar{\mu}_2^{\nu_2}$ | Not tried |
<table>
<thead>
<tr>
<th>Difficulty</th>
<th>Possible Solutions</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Smoothing for special CFD systems</td>
<td>$M = \text{distribution operator}$</td>
<td>(1) TME demonstrated [BD], [Dinar]</td>
</tr>
<tr>
<td></td>
<td>$P = \text{preconditioner}$</td>
<td>(2) TME validated [T6]</td>
</tr>
<tr>
<td>• Cauchy Riemann on staggered grid</td>
<td>$L = \begin{pmatrix} \partial_x &amp; \partial_y \ \partial_y &amp; -\partial_x \end{pmatrix}$</td>
<td></td>
</tr>
<tr>
<td>• Stokes on staggered grid</td>
<td>$L = \begin{pmatrix} -\Delta &amp; 0 &amp; \partial_x \ 0 &amp; -\Delta &amp; \partial_y \ \partial_x &amp; \partial_y &amp; 0 \end{pmatrix}$</td>
<td>(1) $M = L$, $P = I$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) $P = L$, $M = I$</td>
</tr>
<tr>
<td>• Stokes, non-staggered</td>
<td>$L = \begin{pmatrix} -\Delta &amp; 0 &amp; \partial_x^{2h} \ 0 &amp; -\Delta &amp; \partial_y^{2h} \ \partial_x^{2h} &amp; \partial_y^{2h} &amp; 0 \end{pmatrix}$</td>
<td>(1) $M = \begin{pmatrix} 1 &amp; 0 &amp; -\partial_x \ 0 &amp; 1 &amp; -\partial_y \ 0 &amp; 0 &amp; -\Delta \end{pmatrix}$</td>
</tr>
<tr>
<td>(1) Quasi-elliptic discretization</td>
<td></td>
<td>(1) TME demonstrated [BD], [Dinar]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) $P = \begin{pmatrix} 1 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 \ \partial_x &amp; \partial_y &amp; -\Delta \end{pmatrix}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) TME validated [T6]</td>
</tr>
<tr>
<td>(2) $h$-elliptic discretization, e.g.</td>
<td>Analogous to the staggered case:</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(1) In a quasi-elliptic approach, TME demonstrated [G84, §18.6], [quasi]</td>
</tr>
<tr>
<td></td>
<td>$M = \begin{pmatrix} 1 &amp; 0 &amp; -\partial_x^{2h} \ 0 &amp; 1 &amp; -\partial_y^{2h} \ 0 &amp; 0 &amp; -\Delta \end{pmatrix}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>No modifications of the FMG algorithm is required, even in the quasi-elliptic case (as explained in [G84, §18.6]). In generalization to NS, pressure averaging is required of coarse-level results before their interpolation to the next finer level (whenever the coarse-level employs the quasi-elliptic discretization)</td>
<td></td>
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<tr>
<td>Difficulty</td>
<td>Possible Solutions</td>
<td>Status</td>
</tr>
<tr>
<td>------------</td>
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</tr>
<tr>
<td>Non-conservative incompressible Euler</td>
<td>(1) Employ cycle index $\gamma = 2^p$, where $p$ is the order of discretization</td>
<td>(1) TME for first-order discretization using $W$ cycles shown in [BD], [Dinar]</td>
</tr>
<tr>
<td></td>
<td>$L = \begin{pmatrix} u \cdot \nabla &amp; 0 &amp; \partial_x \ 0 &amp; u \cdot \nabla &amp; \partial_y \ \partial_x &amp; \partial_y &amp; 0 \end{pmatrix}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(similarly 3D) on staggered grid, second (or higher) order discretization</td>
<td>(2) TME demonstrated for 2D entering flows with second-order discretization [BY2] and for recirculating flows with first-order discretization [BY3]</td>
</tr>
<tr>
<td>Low-Reynolds Incompressible NS, staggered or not</td>
<td>(2) Use canonical variable $(u, v, P)$ on staggered grid, where $P = (u^2 + v^2)/2 + p$. Upwind only $P$, use central discretization for $(u, v)$. Relaxation is marching for $P$, and weighted (preconditioning) for $(u, v)$</td>
<td>(3) TME in [T1-T3]</td>
</tr>
<tr>
<td>High-Reynolds Incompressible NS, staggered or not</td>
<td>Fully analogous to Incompressible Euler (outside boundary layers: see discussion on such layers below): just replace $u \cdot \nabla$ everywhere with $Q$</td>
<td>TME demonstrated 1978 [BD], [Dinar]</td>
</tr>
<tr>
<td></td>
<td>Fully analogous to Stokes solvers: just replace $\Delta$ in $L$ by $Q = -R^{-1}\Delta + u \cdot \nabla$</td>
<td>TME demonstrated for first-order discretization on staggered ([BD], [Dinar] and non-staggered grids [G84, §19.5], and for second-order staggered discretization [BY2]</td>
</tr>
</tbody>
</table>
Difficulty

- **Compressible Euler**, non-conservative, on staggered grid:
The subprincipal operator on \((u_1, u_2, u_3, \rho, \varepsilon, p)\) is

\[
L = \begin{pmatrix}
\rho u \cdot \nabla & 0 & 0 & 0 & 0 & \partial_1 \\
0 & \rho u \cdot \nabla & 0 & 0 & 0 & \partial_2 \\
0 & 0 & \rho u \cdot \nabla & 0 & 0 & \partial_3 \\
\rho^2 \partial_1 & \rho^2 \partial_2 & \rho^2 \partial_3 & \rho u \cdot \nabla & 0 & 0 \\
p \partial_1 & p \partial_2 & p \partial_3 & 0 & \rho u \cdot \nabla & 0 \\
0 & 0 & 0 & -\partial p/\partial \rho & -\partial p/\partial \varepsilon & 1 \\
\end{pmatrix}
\]

\[
\det L = \rho^5 (u \cdot \nabla)^3 ((u \cdot \nabla)^2 - a^2 \Delta)
\]

\[
a^2 = \frac{\partial p}{\partial \rho} + \frac{p}{\rho^2} \frac{\partial p}{\partial \varepsilon}, \quad M_0 = |u|/a
\]

\(\rho, \varepsilon, p\) defined at cell centers,

\(u_i\) - at center of cell faces perpendicular to the \(i\)-th coordinate

- **2D Compressible Euler**, nonconservative and conservative, staggered grid, using canonical variables \((u, v, S, H)\). Structured and unstructured grids

- **2D/3D incompressible and compressible Euler**: Canonical variables in which velocities are replaced by vector potential representation. Nonstaggered structured and unstructured grid

Possible Solutions

\[
M = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & -\rho(u \cdot \nabla)\partial_1 \\
0 & 1 & 0 & 0 & 0 & -\rho(u \cdot \nabla)\partial_2 \\
0 & 0 & 1 & 0 & 0 & -\rho(u \cdot \nabla)\partial_3 \\
0 & 0 & 0 & 1 & 0 & -\rho^2 \Delta \\
0 & 0 & 0 & 0 & 1 & -p\Delta \\
0 & 0 & 0 & 0 & 0 & \rho^2 (u \cdot \nabla)^2 \\
\end{pmatrix}
\]

The advection and full-potential operators are each relaxed by one of the approaches described for them below. (The *semi* coarsening described there would then be used as an *inner* multigrid cycle for *relaxing* one factor of the determinant, to be distinguished from the *outer* multigrid cycle, which can use *full* coarsening.)

Use \((u, v)\) at cell edges, \(H\) at middle of cell, \(S\) at vertices. Upwind only \(S\) at momentum equations. Relax \(S, H\) by marching. \((u, v)\) by a weighting relaxation. Crocco’s form is used here to define relaxation

All variables at cell nodes. Relax hyperbolic quantities using marching. Relax vector potential using point Gauss-Seidel

Status

Not tried

TME in \([T2-T5]\)

TME achieved (unpublished) for interior and exterior flows in 2D, interior in 3D
**Difficulty**

- *Compressible Navier-Stokes*, non-conservative.

The subprincipal operator on \((u_1, u_2, u_3, \rho, \varepsilon, p)\) is

\[
L_s = \begin{pmatrix}
Q_\mu - \bar{\lambda} \partial_{11} & -\bar{\lambda} \partial_{12} & -\bar{\lambda} \partial_{13} & 0 & 0 & \partial_1 \\
-\bar{\lambda} \partial_{21} & Q_\mu - \bar{\lambda} \partial_{22} & -\bar{\lambda} \partial_{23} & 0 & 0 & \partial_2 \\
-\bar{\lambda} \partial_{31} & -\bar{\lambda} \partial_{32} & Q_\mu - \bar{\lambda} \partial_{33} & 0 & 0 & \partial_3 \\
\rho^2 \partial_1 & \rho^2 \partial_2 & \rho^2 \partial_3 & Q_0 & 0 & 0 \\
p \partial_1 & p \partial_2 & p \partial_3 & 0 & Q_\kappa & 0 \\
0 & 0 & 0 & -\partial p / \partial \rho & -\partial p / \partial \varepsilon & 1
\end{pmatrix}
\]

where \(Q_\alpha = -\alpha \Delta + \rho u \cdot \nabla, \quad \bar{\lambda} = \lambda + \mu, \quad \lambda = \frac{2}{3} \mu, \quad \kappa = k/c_v \) (coefficient of thermal conductivity divided by the specific heat at constant volume),

\[
\det L_s = Q_\mu^2 \det L_c,
\]

where \(L_c\) is the "core operator"

\[
L_c = \begin{pmatrix}
Q_0 & 0 & -\rho^2 \Delta \\
0 & Q_\kappa & -\rho \Delta \\
-\partial p / \partial \rho & -\partial p / \partial \varepsilon & Q_{\mu + \bar{\lambda}}
\end{pmatrix}
\]

At standard conditions of laminar air flow the Prandtl number \(\gamma \mu / \kappa \approx 0.72\); for turbulence \(\gamma \mu / \kappa \approx 0.9\), with \(\gamma = c_p / c_v = 1.4\).

**Possible Solutions**

1. Where \(\bar{\lambda}, \mu, \kappa \ll \rho h |u|\) relax as in Euler above

2. Otherwise use

\[
M = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & -\partial_1 \\
0 & 1 & 0 & 0 & 0 & -\partial_2 \\
0 & 0 & 1 & 0 & 0 & -\partial_3 \\
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
\bar{\lambda} \partial_1 & \bar{\lambda} \partial_2 & \bar{\lambda} \partial_3 & 0 & 0 & Q_{\mu + \bar{\lambda}}
\end{pmatrix}
\]

relaxing each \(Q_\mu\) by one of the approaches described for the advection-diffusion below, and \(L_c\) by procedures discussed for it below (in the chapter on non-elliptic operators)
<table>
<thead>
<tr>
<th>Difficulty</th>
<th>Possible Solutions</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Non-conservative <em>not staggered</em> Euler and NS</td>
<td>(1) Probably similar to the staggered (cf. transition from staggered to non-stag-</td>
<td>TME demonstrated for 2D incompressible Euler [RSS] in the cases of channel (with bump) and airfoil flows</td>
</tr>
<tr>
<td>Difficulty</td>
<td>Possible Solutions</td>
<td>Status</td>
</tr>
<tr>
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</tr>
<tr>
<td><strong>Non-elliptic operators</strong>, or more precisely: small ellipticity measures at some (e.g., large) scales. The main operators of interest here are</td>
<td>The DGS relaxation of the full flow equations allows a specific individual treatment for each of these cases, taking into account its particular set of characteristic</td>
<td>TME demonstrated in many cases</td>
</tr>
</tbody>
</table>
| (1) The advection operator (or, similarly, the convection-diffusion operator at large Reynolds numbers). 
(2) The near-sonic full-potential operator or more generally the core operator $L_C$. 
(See below a separate discussion of anisotropies caused by the discretization) | | |
| • Grid *aligned* with the characteristics | Block (e.g., line or plane) or ILU relaxation schemes and/or semi-coarsening, possibly in alternating directions, guided by mode analyses [B77], [Stages] | |
| • Distinguishing different regimes (open vs. closed characteristics) | Running separately the relaxation subroutine of a given non-elliptic factor can 
(1) Separately check its convergence properties 
(2) Produce a scalar $\sigma \approx 1$ at regions of open characteristics and $\sigma \ll 1$ on closed characteristics (such as separated flow zones) | |
### Difficulty

- **Non-aligned** grids, with open characteristics (e.g., entering flow): The main difficulty is the shorter distance (along the characteristics) for which a coarser grid still approximates some smooth solution components (characteristic components with intermediate cross-characteristic smoothness) [NESP], [BY1]

### Possible Solutions

Three possible approaches, all guided by half-space two-level FMG mode analysis, using for simplicity the first Differential Approximation (FDA) to the discrete operator [NESP], [G, §7.5]:

1. **Downstream-ordered relaxation marching**
   [R88, §2.3]. (Suitable only for the advection factor, sometimes still requires \( W \) cycles, and not very good for massively parallel processing). In the case of an \( O(h^p) \) discretization which is not purely upstreamed, relaxation should involve a predictor-corrector downstream marching. If the predictor order is \( q \), the corrector should be applied at least \( p/q \) times.

2. **Semi-coarsening** (especially for the near-sonic full-potential operator). Better suits massive parallel processing.

3. **Cycle index** \( = 2^p/n \), where \( p \) is the order of discretization and \( m \) is the order of the differential factor. (Suitable actually only for the advection operator, for which \( m = 1 \); especially attractive \( p = 2 \) in 3D; not requiring ordered relaxation, but still disadvantageous for massively parallel processing because of the high cycle index)

### Status

1. TME demonstrated in [BY2], and in Ruge's recent calculations, both for the advection operator by itself and as part of the incompressible Euler system.

2. TME has been shown for the sonic full-potential operator [sonic]

3. For \( p = 1 \), TME has been shown on various occasions. For \( p = 2 \), should be tried.
<table>
<thead>
<tr>
<th>Difficulty</th>
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<tbody>
<tr>
<td>• The mixed convection-diffusion operator with order $p$ approximation, having natural viscosity $\nu$ and artificial viscosity $\alpha h^p$</td>
<td>Treatment as elliptic operator on levels where $\nu \gtrsim (2^p \cdot 4 - 5) \alpha h^p$ and as the non-elliptic advection operator otherwise. Using the above-mentioned scalar $\sigma$, form a $\sigma$-dependent convergence test, to tell between slowness of open and closed characteristics (and possibly ignore the latter). Also based on $\sigma$, at recirculation regions use uniform (explicit) $O(h)$ numerical viscosity, with continuation from large to small viscosity integrated into the FMG algorithm. The cycles can employ one of the following 3 options. (1) DCW method (using Defect Corrections within $W$ cycles), with suitable over-weighting of residuals [BY3]. Suitable only for $O(h)$ discretizations. (2) Effectively downstream relaxation ordering (using alternate-direction sweeps) and doubling of transferred residuals (for $O(h)$ discretization) [YVB]. (3) Semicoarsening, generally similar to [sonic].</td>
<td>Not precisely tried</td>
</tr>
<tr>
<td>• Closed characteristics (recirculating flows). Here uniformity of viscosity (including numerical viscosity) is important for accuracy. The size of viscosity is less important here (except at resolved boundary layers, discussed below). In fact, a uniform $O(h)$ artificial viscosity can yield higher order approximations. Full convergence may also be less important here (steady state may take exceedingly long to be attained in reality, if at all)</td>
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<tr>
<td>• Full-potential operator $(u \cdot \nabla)^2 - a^2 \Delta$, $M_0 =</td>
<td>u</td>
<td>/a \lesssim .7$ (uniformly elliptic)</td>
</tr>
<tr>
<td><strong>Difficulty</strong></td>
<td><strong>Possible Solutions</strong></td>
<td><strong>Status</strong></td>
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<tr>
<td>• Full potential $0.7 \leq M_0 \leq 1.4$</td>
<td>Relaxation marching downstream (for transition to the supersonic case below) together with semicoarsening in the characteristic (cross-stream) direction</td>
<td>TME shown for the case $M = 1$ [Sonic]. Other cases have not yet been implemented</td>
</tr>
<tr>
<td>• Full potential $1.4 \leq M_0$ (uniformly hyperbolic, with the stream as the time-like direction, and with $O(1)$ “Courant number”.)</td>
<td>Marching in the stream direction, possibly with a predictor-corrector procedure. For full massive parallelization, however, wave methods (extending standing wave methods [Irj]) should be used</td>
<td>Not yet tried?</td>
</tr>
</tbody>
</table>
The "core operator"

\[ L_c = \begin{bmatrix} Q_0 & 0 & -\rho^2 \Delta \\ 0 & Q_\kappa & -p \Delta \\ -\partial \rho/\partial \rho & -\partial \rho/\partial \varepsilon & Q_{\mu+\lambda} \end{bmatrix} \]

should be relaxed as part of relaxing the compressible NS system, in the case that \( \rho |u|h \lesssim \max(\lambda, \mu, \kappa) \).

In the case of alignment between the grid and the flow, with meshsize \( h_1 \) and \( h_2 \) in the stream and cross-stream directions, respectively, and \( h_2 \leq h_1 \) (e.g., in boundary layers), the case where \( L_c \) need be relaxed is when \( \rho |u|h_2^2 \lesssim h_1 \max(\lambda, \mu, \kappa) \).

In aerodynamics, \( \lambda, \mu \) and \( \kappa \) are comparable, so the case of interest is \( |u|h_2^2 \leq \nu h_1 \), where \( \nu = \mu/\rho \).

Best relaxation scheme depends on the flow parameters. For example:

1. If \( \kappa \ll \rho |u|h \), then \( Q_\kappa \approx Q_0 \) (in principal terms) and one can use DGS with

\[
M = \begin{pmatrix} 1 & 0 & \rho^2 \Delta \\ 0 & 1 & p \Delta \\ 0 & 0 & Q_0 \end{pmatrix}
\]

resulting in the need to relax the first two equations each on an advection operator (see methods above), and the third equation on the operator \( Q_0 Q_{\mu+\lambda} - \rho^2 a^2 \Delta \).

In the case of interest the principal part of the latter is \( [(\mu + \lambda)Q_0 + \rho^2 a^2] \Delta \), so it can be relaxed by the general method for relaxing a product operator (see \( L = L_2 L_1 \) above).

2. In the aerodynamics and aligned case of interest, the term \( Q_{\mu+\lambda} \) in \( L_c \) is not principal. Therefore relaxation can easily be conducted with the weighting (preconditioning) matrix

\[
P = \begin{pmatrix} 1 & 0 & 0 \\ -p & \rho^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}
\]

and the distribution matrix

\[
M = \begin{pmatrix} 0 & 1 & 0 \\ 0 & -p\rho/p\varepsilon & 1 \\ 1 & 0 & 0 \end{pmatrix}
\]

yielding PLM whose principal part is its main diagonal, on which separately appear the Laplace operator \( \Delta \), the convection-diffusion operator \( Q_\kappa \) where \( \kappa = p\rho \rho^2/(2p\varepsilon) = 1.25\kappa \) (for air), and a free function.

[Difficulty]

[Possible Solutions]

[Status]
<table>
<thead>
<tr>
<th>Difficulty</th>
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<tr>
<td>FDA factorizability question: The decomposition of a system relaxation into its scalar factors depends on the equality of the different occurrences of the advection-diffusion operator ( Q ) (or ( Q_{\mu+\lambda} )) appearing in PL, the prefactoring by ( P ) of a conservative discretization ( L ). However, in relaxing a non-elliptic discrete operator, important is not only the differential operator it approximates, but also its First Differential Approximation (FDA) terms in non-characteristic directions; e.g., the cross-stream numerical viscosity of ( Q ). This may not be the same in the different occurrences of ( Q ), putting the factorization into question.</td>
<td>(1) Examining several examples of conservative discretization of transsonic flows, the FDA terms in various occurrences of ( Q_{\mu+\lambda} ) turn out sufficiently close to each other (e.g., only (4% discrepancy) to allow full efficiency of the proposed relaxation schemes.</td>
<td>Further examination is needed.</td>
</tr>
<tr>
<td>High order discretization (away from shocks)</td>
<td>(2) Conservative schemes may be designed so that the various FDAs of ( Q_{\mu+\lambda} ) are identical, or at least so that the scheme is still factorizable.</td>
<td>Some “genuinely multidimensional upwind” schemes turn out to yield factorizable schemes, e.g., in the subsonic case in the control-volume structured-grid context [DS2]. Further studies are in progress.</td>
</tr>
<tr>
<td>“Double discretization” schemes: Use high-order only in calculating residuals transferred to the coarse grid, not in relaxation (unless the high order scheme is preferable also for h-f modes).</td>
<td>(1) “Double discretization” schemes: Use high-order only in calculating residuals transferred to the coarse grid, not in relaxation (unless the high order scheme is preferable also for h-f modes).</td>
<td>Introduced 1978 [BD]. Successfully implemented in various elliptic cases (see description and refs in [G, §10.2]). Methods for non-elliptic have not been tested beyond second order.</td>
</tr>
<tr>
<td>However, in relaxing non-elliptic factors (e.g., downstream relaxation marching for convection operator) the high order must be used (e.g., by a predictor-corrector downstream relaxation)</td>
<td></td>
<td>Comment: High order approximations on unstructured grids are very expensive.</td>
</tr>
</tbody>
</table>
(1) A set of $N$ continuity equations, volume is large compared with $\max(h^{-2}D_i, h^{-1}p_i|u|)$, for a simple model

<table>
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<tr>
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<tbody>
<tr>
<td>Shocks</td>
<td>Obtained by a conservative fine-to-coarse residual transfer plus local post-relaxation passes near the shock</td>
<td>Full efficiency shown [DS]</td>
</tr>
<tr>
<td>Shock displacements associated with corrections from a coarse grid that does not resolve the shock</td>
<td>Construction of new, genuinely multidimensional upwind schemes</td>
<td>Developed in the context of unstructured triangular grids [DS1]</td>
</tr>
<tr>
<td>Poor $h$-ellipticity of high-resolution schemes</td>
<td>Switching to general robust schemes (e.g., box Kacmarz), adding extra local passes (c.f. relaxation near boundaries)</td>
<td>Not tried?</td>
</tr>
<tr>
<td>Relaxation near strong shocks</td>
<td></td>
<td></td>
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</table>
**Difficulty**

- Relaxation at and near Boundaries:
  
  **Difficulties:**
  
  1. There is no smoothing analysis in case the boundaries are not aligned with the grid.
  2. The fine-to-coarse residual weighting near boundaries is generally very imprecise, hence the residuals should be reduced there more than in the interior.
  3. Larger residuals are created near polations.

- Boundary layers (in the case that they need be resolved). (See also grid adaptation below.)

**Possible Solutions**

A general-type robust relaxation scheme, e.g., box Kacmarz, throughout several-meshsize-wide zone near the boundary. Boxes size in each direction should be several meshsizes and the boxes should have substantial overlap. One can afford several passes of such a relaxation per each full interior sweep since the zone width is \( O(h^{1-\varepsilon}) \), with \( 0 \leq \varepsilon < 1 \). In particular, add near-boundary relaxation passes after the FMG interpolation (allowing the latter to be of lower order near the boundary).

Resolved by boundary-fitted local grid patches, with local semi refinements: finer levels, in narrower layers near the boundary, have smaller cross-layer meshsizes, allowing the physical cross-stream viscosity to dominate over the numerical one. Additional terms in the governing equations (NS instead of Euler, or turbulent modelling, etc.) may be used in these patches. Downstream Marching relaxation and cross-stream semi coarsening in the multigrid cycles, employed in a "\( \lambda \)-FMG" kind of algorithm [G, §9.6], so that coarse FMG stages already include local semi-refinements at the boundary, thus effectively incorporating continuation in \( R_e \) into the FMG stages.

**Status**

For uniformly elliptic equations it has been proved [RLMA], [RQMA] and demonstrated computationally (for cases of reentrant corners [Bai]) that the interior efficiency as predicted by mode analysis (implying TME) can always be obtained. TME demonstrated (by Ruge & Brandt) for incompressible Euler on staggered cartesian cartesian grids.

Description in [R88, §2.4]; not implemented. The local refinement techniques for Poisson equation, with TME, are demonstrated in [Bai].
<table>
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<tbody>
<tr>
<td>Far-field artificial boundary conditions: requiring in some cases non-local absorbing boundary conditions (ABC) for some wave factor. [Has any MPer had experience with this difficulty?]</td>
<td>Increasingly coarser grids covering increasingly larger domains. The size of each domain is based on accuracy-to-work. Optimization criteria (similar to those in [B77, §8], [G, §9.5], implying also a natural criterion for the largest needed domain. On interior boundaries (boundaries of a grid residing in the interior of the next coarser grid) the solution is interpolated from the coarser grid. On such boundaries, if ABC is at all needed, only high-frequency components need be absorbed, for which the ABC are local, and can be enforced as part of the relaxation process (of the corresponding wave factor)</td>
<td>Details of the algorithm have been worked out, and TME (or its equivalent accuracy-to-work relation) has recently been demonstrated (by Brandt &amp; Danowitz) for the 2D Poisson equation in the unbounded plane. Techniques for non-elliptic or indefinite cases have not been systematically studied.</td>
</tr>
<tr>
<td>Small-scale singularities invisible on the next coarser grid, such as small “islands” or “holes” in the domain (e.g., an airplane smaller than the meshsize of some coarser grid) or small BC features (e.g., small regions of Neumann BC in otherwise Dirichlet BC)</td>
<td>Local relaxation passes around the singularities after return from the next coarser grid, together with either one of the following three devices: (a) Enlarging the singularity on the coarser grid. (b) Modifying the interior coarse-grid equation near the singularity. (c) If the coarse grid equations are not modified, convergence is slow, but slow to converge are just few very special components. Hence slowness can be eliminated by recombining iterants.</td>
<td>TME shown in elliptic cases [Rec]</td>
</tr>
</tbody>
</table>
Grid-induced slow convergence

- Large aspect ratios
  - Either one of the following:
    1. Block (part-line or part-plane) relaxation, analyzed by mode analysis [B77].
    2. Semi coarsening [Arl], [Stages, §3.2] (often natural, since the large aspect ratio is in the first place created by semi refinements) with relaxation “semi smoothing” analysis [Stages, §2.1], [G, §3.3].
    3. Combinations of block relaxation in some directions and semi coarsening in others
  - Relaxation marching in the direction of increasing meshsize; or distributive relaxation [Njm, §6]

TME has been shown in a variety of elliptic cases
<table>
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<tr>
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<tbody>
<tr>
<td>Grid adaptation</td>
<td>Use local multigrid levels in creating any desired local refinement, aspect ratio, boundary fitting or even flow fitting (see [R88, §2.7]). Base refinement criteria on the fine-to-coarse multigrid correction ($\tau$). Adaptation can be integrated into the $\lambda$-FMG algorithm together with proper (e.g., Reynolds-number) continuations.</td>
<td>Introduced in [B77] and [G], but tried only for Poisson equation near singularities [Bai]</td>
</tr>
<tr>
<td>Stagnation point (causing an instability in the coarse-grid corrections)</td>
<td>Coarse-grid numerical viscosity depending on the average (e.g., “full-weighting”) of the fine-grid numerical viscosity (not on its injected value) [BY3, §4.5]</td>
<td>TME shown in an example [BY3]</td>
</tr>
</tbody>
</table>
References


Either [G82] or [G84].


Brandt, A. and Diskin, B., Multigrid solvers for the non-aligned sonic flow: the constant coefficient case. To appear in Computer and Fluids.


Ta’asan, S., Lectures on numerical solution of PDE (unpublished).

Barriers to Achieving Textbook Multigrid Efficiency (TME) in CFD

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“Textbook multigrid efficiency” (TME) means solving a discrete PDE problem in a computational work which is only a small (less than 10) multiple of the operation count in the discretized system of equations itself. As a guide to attaining this optimal performance for general CFD problems, the table below lists every foreseen kind of computational difficulty for achieving that goal, together with the possible ways for resolving that difficulty, their current state of development, and references.

Included in the table are staggered and nonstaggered, conservative and nonconservative discretizations 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 listing of associated computational barriers involves: non-alignment of streamlines or sonic characteristics with the grids; 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 adaption.

Subject Terms: cfd, multigrid, Euler equations, Navier-Stokes equations, incompressible flows, transonic flows, algebraic turbulence, reacting flows, non-alignment, recirculating flows, stagnation point, shocks, far-field boundary conditions, boundary layer, grid adaption

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