AIAA JOURNAL
Vol. 31, No. 1, January 1993

# Nonlinear Relaxation/Quasi-Newton Algorithm for the Compressible Navier-Stokes Equations

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**An efficient implicit method for the computation of steady, two-dimensional compressible Navier-Stokes flowfields is presented. The discretization of the governing equations is hybrid in nature, with flux-vector splitting used in the streamwise direction and central differences with flux-limited artificial dissipation used for the transverse fluxes. Line Jacobi relaxation is used to provide a suitable initial guess for a new nonlinear iteration strategy based on line Gauss-Seidel sweeps. The applicability of quasi-Newton methods as convergence accelerators for this and other line relaxation algorithms is examined, and efficient implementations of such techniques are presented. Convergence histories and comparisons with experimental data are presented for a high-speed compression corner interaction. Results indicate a marked improvement in computational efficiency over more conventional upwind relaxation strategies, particularly for flowfields containing large pockets of streamwise subsonic flow.**

## Introduction

THE development of high-resolution upwind methods for the Navier-Stokes equations has led to corresponding advancements in implicit solution algorithms. In particular, the more diagonally dominant linearizations afforded by upwind discretizations allow the use of point, line, and planar Gauss-Seidel matrix splittings that preserve the ease of invertibility of alternating direction implicit (ADI) methods while often sustaining a much higher time step. The works of Thomas and Walters[1] and MacCormack,[2] among others, illustrate the benefits of symmetric line Gauss-Seidel (SLGS) "relaxation" techniques as applied to the computation of two-dimensional, predominantly streamwise supersonic flowfields. For such problems, one forward line Gauss-Seidel sweep is very nearly a direct inversion of the system Jacobian, and a high rate of linear convergence can often be achieved.

The factorization error of commonly used line Gauss-Seidel methods is, however, directly proportional to the amount of upstream influence allowed by the discretization.[3] As a result, the presence of large regions of streamwise elliptic flow will tend to degrade the asymptotic convergence rate of SLGS methods, especially when fine grids are employed. Some researchers, notably Taylor et al.,[4] have alleviated the problem somewhat by using multiple sweeps of SLGS performed at a given time level to reduce the factorization error. Such techniques, as well as related concepts involving preconditioned conjugate gradient-like methods, seek to solve the linear problem more exactly, thus approaching a Newton method for an exact linearization.

The purpose of the present study is to develop alternative, SLGS-based methods that eliminate many of the convergence problems of standard line relaxation strategies without resorting to the aforementioned "inexact" Newton framework. One approach toward reducing asymptotic convergence degradation is to encourage a faster, more nonlinear propagation of information throughout the computational domain. In this regard, an iteration strategy based on a stable sequence of SLGS relaxation sweeps is considered. Residual updating after each forward or backward sweep is used to promote information transfer, but in contrast with a similar method presented in Ref. 1, full coupling between sweeps and between nonlinear iteration levels is achieved. A marked improvement over more conventional line Gauss-Seidel strategies is demonstrated.

Further acceleration of convergence can be achieved by the use of quasi-Newton techniques, which may provide locally superlinear convergence if applied correctly. The Sherman-Morrison-Woodbury formula[5] allows the methods to be implemented very efficiently provided that an initial solution update (obtained from an SLGS sweep) is available. Reference 3 illustrates a successful application of Broyden's quasi-Newton update[6] as a convergence accelerator for a conventional SLGS method. In the present study, another more stable quasi-Newton update is considered, and a combined nonlinear relaxation/quasi-Newton methodology is presented.

The flowfields in question are governed by the steady, compressible Navier-Stokes equations written in a generalized coordinate system. The discretization of the equation set is hybrid in nature, with Van Leer's MUSCL upwind scheme used for the streamwise inviscid fluxes and a central difference approach with flux-limited artificial dissipation implemented in the transverse direction. Such an approach allows a consistent second-order linearization (except for the dissipation operator) while requiring only block tridiagonal inversions and providing a measure of diagonal dominance. The viscous fluxes are central differenced, and no thin-layer assumption is invoked. Further details about the discretization can be found in Ref. 7.

To illustrate the benefits of the combined nonlinear relaxation/quasi-Newton technique, the algorithm is applied to a compression corner interaction at Mach 4.[8] The results include comparisons with experimental data and convergence history comparisons between the new method and other SLGS approaches.

## Relaxation Procedure

The residual vector $\mathcal{R}$ is formed from a natural ordering of the discretized approximation to the steady Navier-Stokes set over the mesh nodes. At a given grid point, the backward

Received Sept. 18, 1991; presented as Paper 92-2643 at the AIAA 10th Applied Aerodynamics Conference, Palo Alto, CA, June 22-24, 1992; revision received July 6, 1992; accepted for publication July 7, 1992. 

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Euler time discretization/linearization of the difference approximations yields a vector equation of the form

$$\left(\frac{M}{\Delta t}+\hat{A}\right)\delta W_{i,j}+\hat{B}\delta W_{i+1,j}+\hat{C}\delta W_{i-1,j}+\hat{D}\delta W_{i,j+1}+\hat{E}\delta W_{i,j-1}+\hat{F}\delta W_{i+2,j}+\hat{G}\delta W_{i-2,j}=-\mathcal{R}_{i,j} \tag{1}$$

Where $M=\partial\hat{U}/\partial W$, $\delta W$ is the update vector $W^{n+1}-W^n$, and the matrices $\hat{A}$–$\hat{G}$ are functions of the flux Jacobians and the dissipation model linearization.[7] The vector $W$ is composed of the primitive variables $\rho$, $u$, $v$, and $e$, and $\hat{U}$ is the conservative-variable vector.

Ordered columnwise over the grid nodes, Eq. (1) yields a large, sparse, linear system, hitherto denoted as $\bar{A}$. Direct factorization procedures for $\bar{A}$ are impractical for large problems, and matrix splittings corresponding to line relaxation methods provide a more efficient alternative. As background for the presentation of the new algorithm, a brief review of other line relaxation approaches is appropriate.

A line-based partioning of $\bar{A}$ can be defined by denoting the block tridiagonal system $\{\hat{E},\ [(M/\Delta t)+\hat{A}],\ \hat{D}\}$ by $D$ and letting $L$ and $U$ be block triangular matrices composed of $[\hat{C},\ \hat{G}]$ and $[\hat{B},\ \hat{F}]$, respectively. Considering a backward-forward relaxation process in the streamwise direction (identified with the $i$ index of the grid) and evaluating all matrices at time level $n$, the symmetric Gauss-Seidel algorithm suggested by MacCormack[2] and implemented by Taylor et al.[4] is given as

$$\begin{aligned}(D+U)\delta W^{n+1}_{(l+\frac{1}{2})}&=-\mathcal{R}(W^n)-L\delta W^{n+1}_{(l)}\\(D+L)\delta W^{n+1}_{(l+1)}&=-\mathcal{R}(W^n)-U\delta W^{n+1}_{(l+\frac{1}{2})}\end{aligned} \tag{2}$$

The index $l$ defines a sequence of "inner iterations" designed to solve the linear system more exactly at a given time level. This process can be expensive, as the sweeps are not fully vectorizable. A simpler approximation, useful for computing predominately streamwise supersonic flowfields, is the following[3]:

$$(D+U)D^{-1}(D+L)\delta W^{n+1}=-\mathcal{R}(W^n) \tag{3}$$

This splitting is equivalent to Eq. (2) when $\delta W^{n+1}_{(l)}$ is set to zero and only one backward and one forward sweep is taken per time level. The factorization error for the preceding SLGS method is directly proportional to the number of nonzero elements of matrix $U$, a measure of the amount of upstream influence allowed by the discretization. As a result, the presence of large pockets of streamwise subsonic flow will tend to degrade the convergence rate of algorithm (3), especially when fine grids are employed.

Only the convergence rate for the nonlinear problem is really of interest, so it seems logical to consider relaxation schemes that allow a higher degree of *nonlinear* information propagation. In Ref. 1, Thomas and Walters present the following algorithm:

$$\begin{aligned}(D+U)\delta W^{n+\frac{1}{2}}&=-\mathcal{R}(W^n)\\(D+L)\delta W^{n+1}&=-\mathcal{R}(W^{n+\frac{1}{2}})\end{aligned} \tag{4}$$

The solution and residual vector are updated after the completion of each backward or forward sweep. In this approach, the sweeps are essentially decoupled, in contrast to the fully coupled approach (for the linear problem) illustrated by Eq. (2). The algorithm proposed in this work combines the best features of the techniques outlined in Eqs. (2) and (4). An SLGS sweep sequence is constructed that is similar to Eq. (2) except that full coupling between sweeps is achieved through the use of previously computed *nonlinear* corrections $\delta W$ rather than corrections to the linear problem $\delta W_l$. The solution and the residual for the nonlinear problem are updated after each sweep, further enhancing the information transfer. At time level $n$, the algorithm is given by

$$\begin{aligned}(D+U)\delta W^{n+\frac{1}{2}}&=-\mathcal{R}(W^n)-\omega_f L\delta W^n\\W^{n+\frac{1}{2}}&=W^n+\omega_b\delta W^{n+\frac{1}{2}}\\(D+L)\delta W^{n+1}&=-\mathcal{R}(W^{n+\frac{1}{2}})-\omega_b U\delta W^{n+\frac{1}{2}}\\W^{n+1}&=W^{n+\frac{1}{2}}+\omega_f\delta W^{n+1}\end{aligned} \tag{5}$$

Computational experiments have shown that under-relaxation of the sweeps is required to insure stability at arbitrary time steps. For the test cases considered, under-relaxation parameters of $\omega_f=1.0$ and $\omega_b=0.7$ were used. Note that the update vector $\delta W$ must be set to zero only before the first iteration. Otherwise, the previous update is used as a "forcing function" for the next sweep. Convergence comparisons between the new technique and methods (3) and (4) will be presented later in this article.

## Quasi-Newton Acceleration

The convergence characteristics of SLGS algorithms can be further improved by using quasi-Newton updating procedures. Quasi-Newton techniques are a generalization of the secant method for one-variable nonlinear equations to nonlinear systems, and most involve the updating of an approximation to the system Jacobian (denoted by $N$) by a rank-one matrix at each iteration:

$$N_{n+1}=N_n+\frac{\mathcal{R}(W^{n+1})z^T}{z^T\delta W^{n+1}} \tag{6}$$

The choice of the vector $z$ delineates particular quasi-Newton updates, all of which satisfy the "secant" equation given next:

$$N_{n+1}\delta W^{n+1}=\mathcal{R}(W^{n+1})+N_n\delta W^{n+1} \tag{7}$$

Superlinear convergence $[(\|\mathcal{R}^n\|_2/\|\mathcal{R}^{n-1}\|_2)\Rightarrow 0$ as $n\Rightarrow\infty]$ can be proven for a class of these methods, with the governing factors being the closeness of the current solution $W$ to the steady-state answer, the closeness of the initial value for $N$ to the steady-state Jacobian, and the satisfaction of the secant condition.[6,9] Implemented as written in Eq. (6), the quasi-Newton procedure is at least as computationally intensive as Newton's method. By the use of the Sherman-Morrison-Woodbury theorem,[5] however, the updating process can be performed on the *inverse* of $N$, thus eliminating both matrix factorization and matrix computation requirements. Consider the following inverse form of Eq. (6):

$$N^{-1}_{n+1}=(I-\theta_n\psi_n^T)N_n^{-1} \tag{8}$$

where

$$\psi_n=\frac{z}{z^T\delta W^{n+1}} \tag{9}$$

$$\theta_n=\frac{N_n^{-1}\mathcal{R}(W^{n+1})}{1+\psi_n^T N_n^{-1}\mathcal{R}(W^{n+1})} \tag{10}$$

and $I$ is the identity matrix. By multiplying Eq. (8) by the updated residual $-\mathcal{R}(W^{n+1})$, one arrives at a recursion relation for the new step vector $\delta W^{n+2}$ that requires only vector operations provided that an initial step approximation $-N_1^{-1}\mathcal{R}(W^{n+1})$ is available. This vector is obtained by the application of the SLGS matrix splitting (3). The quasi-Newton procedure, then, can be viewed as a mechanism by which

an SLGS correction is "improved" so that faster convergence to the steady state is realized. At a current iterate $n$, a "pseudocode" procedure for applying a $k$-step quasi-Newton algorithm is a follows:

0) Define

$$W_{QN} = W^n$$

$$\delta W_{QN} = \delta W^{n+1} \tag{11}$$

$$N = (D + U)D^{-1}(D + L)$$

1) For $i = 1, k$,

update

$$W_{QN} = W_{QN} + \delta W_{QN}$$

compute

$$\mathcal{R}(W_{QN})$$

$$\delta W_{GS} = -N^{-1}\mathcal{R}(W_{QN})$$

2) For $j = 1, i-1$, compute

$$\delta W_{GS} = \delta W_{GS} + \theta_j \psi_j^T \delta W_{GS}$$

3) Form and store

$$\psi_i = \frac{z_i}{z_i^T \delta W_{QN}}$$

$$\theta_i = \frac{\delta W_{GS}}{1 - \psi_i^T \delta W_{GS}}$$

4) Compute the new update vector

$$\delta W_{QN} = \delta W_{GS} + \theta_i \psi_i^T \delta W_{GS}$$

5) Return to step 1.

In the previous expressions, $k$ is the number of allowable quasi-Newton steps (six in this investigation), and the superscript T denotes the matrix transpose operator. Although the implementation is computationally efficient, the recursive process in step 2 requires the storage of $2k$ vectors for $\theta$ and $\psi$ (or $z$).

The most popular quasi-Newton method is that due to Broyden,[6] for which $z$ in Eq. (11) is given by $\delta W_{QN}$. A related algorithm of Gay and Schnabel,[9] referred to as the "projected" Broyden update, is considered in this article. The projected Broyden method is designed to satisfy the secant equation

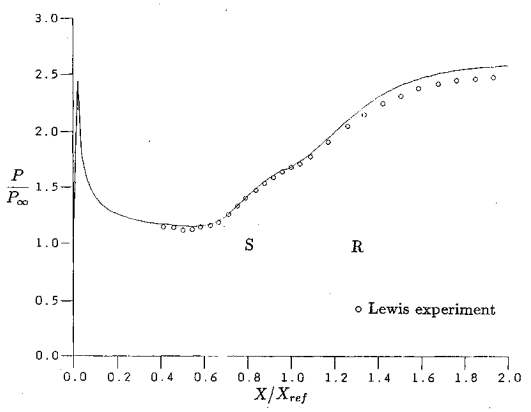


**Fig. 1 Surface pressure for Mach 4.0 case.[8]**

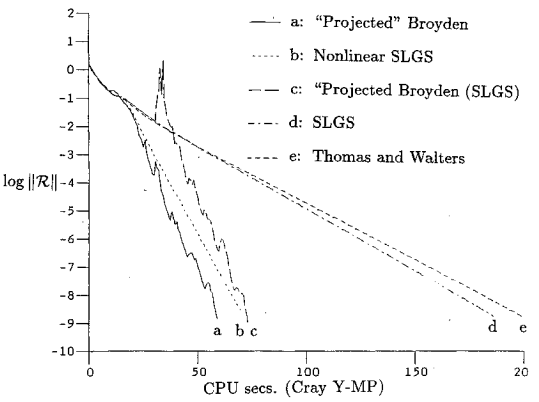


**Fig. 2 Convergence histories for Mach 4.0 case.[8]**

$$N_{n+1}\delta W^{m+1} = \mathcal{R}(W^{m+1}) + N_m \delta W^{m+1} \tag{12}$$

for *all* $m \leq n$ by defining the vector $z$ to be the projection of $\delta W^{n+1}$ perpendicular to all $\delta W^{m+1}$, $m < n$. In the notation of Eq. (11),

$$z_i = \delta W_{QN} - \sum_{j=1}^{i-1} z_j \frac{z_j^T \delta W_{QN}}{z_j^T z_j} \tag{13}$$

Quasi-Newton acceleration is integrated into the relaxation algorithm by first defining a starting location (a two order-of-magnitude residual reduction usually suffices). From this point, the quasi-Newton process is initiated, with four relaxation iterates performed between each six-step application of Eq. (11) until convergence is reached.

## Results and Discussion

The test case considered in this article corresponds to an experiment by Lewis et al.[8] and involves laminar flow over a flat plate – 10-deg wedge apparatus at the following conditions: $M_\infty = 4.0$, $T_\infty = 50.21$ K, adiabatic wall. A reference length of 6.35 cm, corresponding to the distance between the flat plate leading edge and the wedge apex, is used, and the resulting Reynolds number is $6.8 \times 10^4$. Other test cases are discussed in Ref. 7. A $101 \times 101$ mesh was used in the simulation, and a comparison between the computed wall pressure distribution and the data of Ref. 8 is shown in Fig. 1. Good agreement is indicated, particularly in the large region of reversed flow downstream of the wedge apex ($X/X_{\text{ref}} = 1.0$). Separation (S) and reattachment (R) points are shown in the figure for clarity.

Steady-state convergence characteristics of various SLGS-based algorithms for this problem are illustrated by the plots of residual $\mathcal{L}_2$ norm vs Cray Y-MP CPU time shown in Fig. 2. Fifty iterations of a fully vectorizable line Jacobi method were used to provide a suitable initial guess, and each computation was then allowed to proceed until a nine-order-of-magnitude residual reduction had been achieved. Curves *d* and *e* are the results obtained from the baseline SLGS algorithm (3) and the more nonlinear approach of Thomas and Walters, Eq. (4), respectively. Although the Thomas and Walters approach converged in fewer iterations, the overall time is greater than that of algorithm (3) due to the expense of the extra residual evaluation. Curve *b* shows that the nonlinear relaxation algorithm (5) provides significant improvement, converging approximately 2.7 times faster than methods (3) and (4). Convergence histories for "projected" Broyden accelerations of the nonlinear algorithm (5) and the baseline approach (3) are presented as curves *a* and *c*. Only a small improvement is evidenced for the nonlinear case (curve *a*), although significant acceleration of the baseline SLGS technique occurs.

Curves *a* and *c* also illustrate the need for the alternating quasi-Newton/relaxation strategy mentioned earlier. When implemented in limited-storage inverse form, quasi-Newton methods tend to accelerate the computation by reducing low-frequency error responsible for asymptotic convergence degradation. During the process, however, high-frequency error components may be increased, causing jumps in the nonlinear residual norm. The application of a number of relaxation steps following a quasi-Newton sequence appears to smooth the high-frequency errors while propagating the quasi-Newton "corrections" to the low-frequency spectrum.

## Conclusions

The development of a rapidly converging implicit algorithm for the steady, two-dimensional compressible Navier-Stokes equations has been described. Based on a nonlinear line Gauss-Seidel iteration strategy, the new algorithm has been shown to eliminate much of the convergence degradation experienced by more conventional line relaxation techniques when applied to flows with large subsonic regions and/or strong shock formation. A basic discussion of quasi-Newton techniques and their implementation as convergence accelerators for line relaxation algorithms has been presented, and the methods have been shown to result in significant computational savings when applied properly. For the compression-corner interactions considered in this investigation, a hybrid upwind/central difference discretization of the steady Navier-Stokes set has been shown to yield good comparisons with available experimental data.

## Acknowledgments

This work was supported by the Graduate Training and Research Program in Hypersonic Aerodynamics Grant NAGW-1072, funded jointly by NASA, the Air Force Office of Scientific Research, and the Office of Naval Research. The first author would like to thank C. T. Kelley of the Department of Mathematics at North Carolina State University for introducing him to the subject of quasi-Newton techniques and for many helpful discussions on their implementation. Thanks is also extended to the North Carolina Supercomputing Center for the use of its facilities.

## References

[1]Thomas, J. L., and Walters, R. W., "Upwind Relaxation Algorithm for the Navier-Stokes Equations," *AIAA Journal*, Vol. 25, No. 4, 1987, pp. 527–534.

[2]MacCormack, R. W., "Current Status of Numerical Solutions of the Navier-Stokes Equations," AIAA Paper 85-0032, Jan. 1985.

[3]Edwards, J. R., and McRae, D. S., "An Efficient Solution Technique for Shockwave-Boundary Layer Interactions with Flow Separation and Slot Suction Effects," AIAA Paper 91-0652, Jan. 1991.

[4]Taylor, A. C., Ng, W. F., and Walters, R. W., "Upwind Relaxation Algorithms for the Navier-Stokes Equations Using Inner Iterations," AIAA Paper 89-1954, June 1989.

[5]Hager, W. W., "Updating the Inverse of a Matrix," *SIAM Review*, Vol. 31, No. 6, 1989, pp. 221–239.

[6]Broyden, C. G., "A Class of Methods for Solving Nonlinear Simultaneous Equations," *Mathematics of Computation*, Vol. 19, 1965, pp. 577–593.

[7]Edwards, J. R., and McRae, D. S., "A Nonlinear Relaxation/Quasi-Newton Algorithm for the Compressible Navier-Stokes Equations," AIAA Paper 92-2643, June 1992.

[8]Lewis, J. E., Kubota, T., and Lees, L., "Experimental Investigation of Supersonic Laminar Two-Dimensional Boundary-Layer Separation in a Compression Corner with and without Cooling," *AIAA Journal*, Vol. 6, No. 1, 1968, pp. 7–14.

[9]Gay, D. M., and Schnabel, R. B., "Solving Systems of Nonlinear Equations by Broyden's Method with Projected Updates," *Nonlinear Programming 3: Proceedings of the Symposium of Special Interest Group Mathematics Programming*, Academic Press, New York, 1978, pp. 245–281.