# A New Approximate LU Factorization Scheme for the Reynolds-Averaged Navier-Stokes Equations

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**A new approximate LU factorization scheme is developed to solve the steady-state Reynolds-averaged Navier-Stokes (NS) equations. Central differencing is used for both implicit and explicit operators, and special care is taken to obtain well-conditioned factors on the implicit side. The scheme is then analyzed and optimized according to a simple linear analysis. It is unconditionally stable for the model hyperbolic equation in both two and three dimensions. However, the requirement for well-conditioned factors has essentially limited the effective time step that the scheme can achieve. Supersonic and transonic 3-D flows past a hemisphere cylinder are computed to demonstrate the convergence characterstics of the scheme. A good convergence rate is achieved in the inviscid case. Finally, an explicit eigenvector annihilation procedure is employed successfully to remove the stiffness caused by the fine grid spacing for viscous flows.**

## I. Introduction

THE use of implicit methods to solve steady-state Reynolds-averaged NS equations has been increasing in recent years. For multidimensional problems, the most popular scheme is the Beam and Warming approximate factorization scheme.[1] This scheme factors the implicit operator into two or three 1-D factors according to the spatial dimensions of the problem. This factorization is very similar to the Alternating Direction Implicit (ADI) method originally developed for second-order diffusion equations. Because of this, it is often (and will be herein) referred to as an ADI scheme. The solution requires the inversion of a block banded matrix along the grid lines for each factor. This represents a considerable amount of work, especially for 3-D problems where three factors are formed and three sweeps through the domain are necessary. Also, a linear von Neumann analysis shows that the ADI scheme is unconditionally stable for 2-D problems, but it is unconditionally *unstable* for 3-D problems due to the extra factor for the third dimension.[2]

One possible alternative to the ADI scheme is an approximate LU factorization scheme that produces two implicit factors, independent of the spatial dimensions of the problem. Such schemes can be constructed to obtain linear unconditional stability (in the relaxation sense) in both 2-D and 3-D problems. The two factors are composed of 1) a lower ($L$) block triangular matrix and 2) an upper ($U$) block triangular matrix; hence the name LU. Since classical LU decomposition is not always practical for multidimensional problems, an approximate LU factorization is chosen that provides only an approximation of the original unfactored implicit operator. With carefully constructed LU factors, the inversion of such a scheme can be very easy and efficient since only one explicit point by point sweep is necessary for each LU factor. In this sense, an approximate LU factorization scheme resembles the Symmetric Successive Over Relaxation (SSOR) method[3] originally designed for second-order elliptic equations.

Several approximate LU factorization schemes have been proposed in the past. For example, Steger[4] suggested that the flux-split scheme can be used to construct LU factors. Jameson and Turkel[5] proposed an implicit LU decomposition scheme for model hyperbolic equations. Buratynski and Caughey[6] applied this scheme to solve the 2-D Euler equations for cascade flows. A similar version of this scheme with a multigrid method was used by Jameson and Yoon.[7] Obayashi and Kuwahara[8] solved the 2-D NS equations by splitting the 1-D ADI factors into L and U factors using the flux-split concept. Although it has a similar stability boundary as the ADI scheme, a straightforward extension of this scheme to 3-D problems was reported by Obayashi and Fujii.[9] Walters et al.[10] applied a variation of the Strongly Implicit Procedure of Stone[11] to the 2-D NS equations and to 3-D model hyperbolic equations. Also, MacCormack[12] applied the Gauss-Seidel relaxation method to a flux-split scheme for solving the 2-D Euler equations.

Different LU schemes employ different strategies to obtain well-conditioned (defined in Sec. 5) LU factors. Each LU factor needs to be well-conditioned; otherwise, the inversion process will encounter serious numerical instability. This is true even when the product of LU factors as a whole shows unconditional stability. In the flux-split LU scheme, well-conditioned LU factors are obtained by one-sided upwind differencing. In Jameson and Turkel's scheme,[5] well-conditioned LU factors are obtained by constructing special 3-point one-sided difference operators whose product resembles the effect of a 3-point central difference operator plus a dissipation-like operator.

In the present study, a new approximate LU factorization scheme is developed for the 3-D NS equations. Central differencing is used for both implicit and explicit operators. The

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diagonal term in each LU factor is carefully constructed to ensure the required well-conditioning. The scheme is then analyzed and optimized according to a simple linear analysis. The results show an unconditional stability for the model hyperbolic equations regardless of the spatial dimensions of the problem. However, the requirement for well-conditioned LU factors has essentially limited the maximum CFL number the scheme can achieve. To test this new scheme, 3-D supersonic and transonic flows past a hemisphere cylinder are computed for both inviscid and viscous cases. Results are compared with those obtained by the ADI scheme[13] and excellent agreement is obtained. A good convergence rate is achieved for the inviscid case, but it deteriorates for the viscous case. Finally, an explicit eigenvector annihilation procedure[14] is successfully applied to the scheme to remove the stiffness caused by the fine grid spacing needed for the viscous flows.

## II. Mathematical Model

The divergence form of the Reynolds-averaged NS equations in the generalized coordinates $(\xi,\eta,\zeta)$ and time $(\tau)$ can be written as

$$\partial_\tau q = -[\partial_\xi(E-E_\nu)+\partial_\eta(F-F_\nu)+\partial_\zeta(G-G_\nu)]$$
$$= -\text{Div(flux)} \tag{1}$$

where $q$ is solution vector, $(E,E_\nu)$, $(F,F_\nu)$, and $(G,G_\nu)$ are (inviscid, viscous) flux vectors in each coordinate direction, and $\partial$ represents either an analytical differential or a numerical difference operator. This system of equations is hyperbolic in nature (convection dominated) and the strong conservation law form permits the capture of weak solutions. If only the steady-state solution is of interest, a suitable choice for time marching is the backward Euler scheme. In the delta-law form, it can be written (after local linearization)

$$(I+\Delta\tau M)\Delta q^n = -\Delta\tau \text{Div(flux)}^n \tag{2a}$$

$$q^{n+1} = q^n + \Delta q^n \tag{2b}$$

$$M = \partial_\xi(A-A_\nu)+\partial_\eta(B-B_\nu)+\partial_\zeta(C-C_\nu) \tag{2c}$$

where $I$ is identity matrix, $\Delta\tau$ is time increment, and $(A,A_\nu)$, $(B,B_\nu)$, and $(C,C_\nu)$ are the flux Jacobians evaluated at time level $n$. Each local flux Jacobian is a $4\times4$ matrix for 2-D problems and a $5\times5$ matrix for 3-D problems. The actual expressions of these vectors and matrices may be found in many references, e.g., Ref. 13.

The inviscid flux vectors are homogenous functions of degree one in $q$ for a perfect gas. It follows for inviscid flows

$$E=Aq,\ F=Bq,\ G=Cq,\quad \text{Div(flux)}=Mq$$

and hence

$$(I+\Delta\tau M)\Delta q^n = -\Delta\tau M q^n$$

in Eq. (2). For viscous flux vectors such relationships do not exist and Div (flux) $=Mq$ is valid only for certain model equations. The direct inversion of Eq. (2) is still prohibitive at the present time mainly due to the large memory requirement and large amount of arithmetic required for the Gaussian elimination for large, banded matrices.

## III. The ADI Scheme

The left-hand side (LHS) operator is factored into two or three 1-D factors according to the spatial dimensions of the problem. For 3-D problems we have

$$[I+\Delta\tau\partial_\xi(A-A_\nu)][I+\Delta\tau\partial_\eta(B-B_\nu)]$$
$$[I+\Delta\tau\partial_\zeta(C-C_\nu)]\Delta q^n = -\Delta\tau\,\text{Div(flux)}^n \tag{3}$$

Application of each factor corresponds to a sweep through the domain, inverting a block banded matrix along the grid lines. This represents a considerable amount of work, especially for 3-D problems in which three sweeps are necessary.

Efforts have been made to reduce the computational work of the ADI scheme. For inviscid flows, the LHS flux Jacobians of the ADI scheme can be diagonalized[15] by similarity transformations such that the solution requires inverting scalar banded matrices only. Although strictly speaking this diagonal algorithm is valid only for inviscid flows, it has been used and found to be stable[16,17] for many high Reynolds number flow calculations with the LHS viscous flux Jacobians completely neglected. A matrix reduction method[18] can also be applied to the inviscid flux Jacobians to reduce the computational work. All of the these efforts are successful in that they have greatly simplified the inversion process for the implicit operators; however, a linear von Neumann analysis shows that the ADI scheme is unconditionally unstable for 3-D problems. This instability occurs because ADI factorization in three dimensions produces an error term proportional to $\Delta\tau^3$. To address this 3-D instability, Ying[2] suggested a partial ADI factorization that produces only two factors, one 1-D and the other 2-D, and, therefore, retains the 2-D unconditional stability. Upwind differencing in one of the two dimensions of the 2-D operator is needed in order to reduce the bandwidth of the 2-D operator to achieve an efficient inversion process.

## IV. The Basic LU Factorization Scheme

First, because of their accuracy and simplicity, central difference operators are used for spatial derivatives on both the LHS and the RHS of the backward Euler scheme [Eq. (2)]. Since the delta-law form is enforced, the RHS operator alone decides the spatial accuracy of the steady-state solution. The operator $M$ is then split into a strictly lower $(M_l)$ triangular part and a strictly upper $(M_u)$ triangular part without any regard to the spatial dimensions of the problem. Together with the identity matrix $I$, the LHS operator is then factored into

$$(I+\Delta\tau M_l)(I+\Delta\tau M_u)\Delta q^n = (L)(U)\Delta q^n = -\Delta\tau\,\text{Div(flux)}^n$$

or equivalently since $M=M_l+M_u$

$$[I+\Delta\tau M+\Delta\tau^2 M_l M_u]\Delta q^n = -\Delta\tau\,\text{Div(flux)}^n$$

where $M_l M_u$ is the product of $M_l$ and $M_u$. Clearly, an error term $\Delta\tau^2 M_l M_u \Delta q^n$ is introduced by the factorization procedure. This is still first-order time accurate, since the error term is of order $\Delta\tau^2$. Note that if $\Delta\tau/2$ is used on the LHS, the scheme then corresponds to using Trapezoidal Rule time marching in Eq. (1). In this case it becomes second-order accurate in time.

To investigate the stability of this basic scheme, we employ the usual assumptions necessary for a linear von Neumann-type analysis. First, the equation to be solved is considered to be a linear model hyperbolic equation with $M=\partial_\xi+\partial_\eta+\partial_\zeta$. This allows Div(flux) $=Mq$ in Eq. (2). Second, all the operators involved are assumed to commute and, therefore, they can be simultaneously diagonalized. Third, either a periodic boundary condition or a known Dirichlet boundary condition is assumed such that the effects of boundary points can be neglected. Under these assumptions, we then can write the scheme as

$$(I+\Delta\tau M_l)(I+\Delta\tau M_u)\Delta q^n = -\Delta\tau M q^n \tag{4a}$$

$$q^{n+1} = q^n + \Delta q^n \tag{4b}$$

and the amplification factor $\sigma$ for a particular eigenmode as

$$\sigma = \frac{q^{n+1}}{q^n} = \frac{1+\Delta\tau^2\lambda_{M_l M_u}}{1+\Delta\tau\lambda_M+\Delta\tau^2\lambda_{M_l M_u}} \tag{5}$$

where $\lambda_{(*)}$ represents the eigenvalue of operator (*). The numerator of Eq. (5) can be combined into one eigenvalue $\lambda_{(I+\Delta\tau^2 M_l M_u)}$, if so desired. Recall that central differencing was used for $M$. Citing a 1-D case as an example, with a 3-point central difference operator we have

$$M=\frac{1}{2\Delta\xi}\mathbf{B}(-1,0,1), \qquad M_l=\frac{1}{2\Delta\xi}\mathbf{B}(-1,0,0)$$

$$M_u=\frac{1}{2\Delta\xi}\mathbf{B}(0,0,1), \qquad M_l M_u=\frac{1}{4\Delta\xi^2}\mathbf{B}(0,-1,0)$$

where $\mathbf{B}(a,b,c)$ represents a banded matrix with $b$ as the diagonal entries, $a$ and $c$ as the off-diagonal entries, and the first diagonal element of $M_l M_u$ is actually 0, not $-1$, making $M_l M_u$ degenerate. For a periodic $M$, one or two more entries at the boundary rows or columns should be added to these matrices, but this will not change the results of the analysis.

Note that $M$ is an antisymmetric matrix. Furthermore, $M_l M_u$ is a degenerate but symmetric matrix since $M_l=-M_u^T$ where $M^T$ represents the transpose of $M$. We immediately recognize that $\lambda_M$ is a pure imaginary number, while $\lambda_{M_l M_u}$ and $\lambda_{(I+\Delta\tau^2 M_l M_u)}$ are pure real numbers. This implies that the absolute value of the amplification factor $|\sigma|$ is always less than or equal to unity and, hence, the scheme is unconditionally stable. Note that the LU factorization procedure deals with the LHS operator without any regard to the spatial dimensions of the problem. For 2-D and 3-D problems, it is easy to verify that $M$ is still antisymmetric, $M_l M_u$ is still degenerate but symmetric and, hence, the scheme is still unconditionally stable. If 5-point central difference operators were used for $M$, the same conclusion would still apply.

The above analysis is, of course, oversimplified. We know, for example, that $M$ and $M_l M_u$ do not commute and, hence, cannot be simultaneously diagonalized even for the model equation. Furthermore, the analysis is performed for a model hyperbolic equation, not for a mixed hyperbolic-parabolic equation. The fact that $M_l=-M_u^T$ for an antisymmetric $M$ gives the linear unconditional stability for the model hyperbolic equation. Although it is true that the scheme is also unconditionally stable for a model diffusion equation, it is not true for the mixed-type equations. For the model diffusion equation, $M$ is symmetric and yields real positive eigenvalues on the LHS and real negative eigenvalues on the RHS of the backward Euler scheme. The splitting of $M$ can be done to give $M=M_l+M_u$ as well as $M_l=M_u^T$. Then, one can easily verify that $|\sigma|\leq 1$ is true regardless of the dimensions of the problem. However, if $M$ is composed of mixed-type operators, then the symmetry property of $M_l M_u$ and, hence, the unconditional stability, may be lost after the factorization procedure. Fortunately, the NS equations in high Reynolds number flows are convection-dominant and, hence, hyperbolic in nature. It was hoped, and later numerically confirmed, that the analysis done for the model hyperbolic equation could be carried over to the high Reynolds number NS equations.

If the Trapezoidal Rule were used in Eq. (1), then the following $\sigma$ would be the result:

$$\sigma=\frac{q^{n+1}}{q^n}=\frac{1-(\Delta\tau/2)\lambda_M+(\Delta\tau/2)^2\lambda_{M_l M_u}}{1+(\Delta\tau/2)\lambda_M+(\Delta\tau/2)^2\lambda_{M_l M_u}} \tag{6}$$

This $\sigma$ has an absolute value of one as long as $M$ is antisymmetric. The scheme is then neutrally stable for model hyperbolic equations.

## V. Well-Conditioned LU Factors

We define a well-conditioned LU factor one whose inverse has elements that can be numerically computed by a particular computer. This definition is necessary because a computer has only limited significant digits and, hence, a number may not be numerically computable even when analytically finite. This situation can occur in the inversion process of an "unconditionally stable" LU factorization scheme. We can demonstrate this fact by considering the inverse of a model lower triangular banded matrix $P=\mathbf{B}(a,b,c,0,0)_{m\times m}$ with $c$ as diagonal entry, $a$ and $b$ as off-diagonal entries, and $m$ as the order of $P$. It is easy to verify the following relations:

$$P^{-1}=\mathbf{B}(x_m,x_{m-1},\ldots,x_2,x_1,0,\ldots,0)_{m\times m}$$

$$x_i=\frac{1}{\sqrt{b^2-4ac}}(r_+^i-r_-^i), \qquad i=1\sim m$$

$$r_\pm=\frac{1}{2c}(-b\pm\sqrt{b^2-4ac})$$

$$|r|=|r\pm|_{\max}\geq 1, \quad \text{if } -ac\geq c^2-|c|\,|b|$$

where $x_1$ is the diagonal entry and the remaining $x$'s are the off-diagonal entries of $P^{-1}$. The elements of $P^{-1}$ grow like $|r|^m$, if $|r|$ is greater than one. Unless the computer has an infinite number of significant digits, $P^{-1}$ cannot be numerically computed when $|r|^m$ is excessively large. In other words, although $P^{-1}$ is analytically known, its numerical evaluation is not always possible for arbitrarily large $m$ and $|r|$. This instability is purely due to the accumulation of round-off errors. Since $m$ is usually large for multidimensional flow problems, $|r|$ must be limited such that $x_m$ can be numerically computed. The sufficient condition, is of course,

$$|r|\leq 1 \tag{7}$$

although it can be relaxed in actual computations. The actual upper limit of $|r|$ depends on the order $m$ of the problem as well as the number of significant digits of the computer used. Since a model upper triangular matrix is the transpose of $P$, that is, $P^T=\mathbf{B}(0,0,c,b,a)_{m\times m}$, it is subjected to the same sufficient condition of Eq. (7) for well-conditioning.

It should be emphasized that the sufficient condition Eq. (7) does not require diagonal dominance, although a diagonally dominant $P$ is well-conditioned. By definition, a diagonally dominant $P$ satisfies

$$c^2-|c|\,|b|=|c|(|c|-|b|)\geq|c|\,|a|\geq(-ca)$$

and, hence, is well-conditioned. On the other hand, it is easy to verify that the following matrices satisfy the marginally sufficient condition $|r|=1$:

$$\mathbf{B}(0,-1,1,0,0), \quad \mathbf{B}(0,-1,-1,0,0) \tag{8}$$

$$\mathbf{B}(1,-4,3,0,0), \quad \mathbf{B}(1,-4,-5,0,0) \tag{9}$$

$$\mathbf{B}(1,-8,7,0,0), \quad \mathbf{B}(1,-8,-9,0,0) \tag{10}$$

but the upwind operator $\mathbf{B}(1,-4,3,0,0)$, for example, is not diagonally dominant.

It is clear now that although the previous basic LU factorization scheme offers "unconditional stability," $\Delta\tau$ still must be limited to a small number in order to complete the inversion process. As previously mentioned, different LU factorization schemes use different methods to obtain the required well-conditioned LU factors. In the flux-split LU schemes, one-sided upwind differencing is used and matrices shown in Eqs. (8) or (9) result. In Jameson and Turkel's scheme, a dissipation-like operator is carefully included in the decomposition procedure resulting in well-conditioned LU factors. In the present scheme, instead of limiting $\Delta\tau$, the remedy is to construct a new diagonal operator in each LU factor and then attempt to optimize it.

## VI. The Proposed LU Factorization Scheme

Replacing the identity matrix $I$ in each factor with a new operator $D$, the scheme now becomes

$$(D+\Delta\tau M_l)(D+\Delta\tau M_u)\Delta q^n = -\Delta\tau M q^n$$

or equivalently

$$(D^2+\Delta\tau DM+\Delta\tau^2 M_l M_u)\Delta q^n = -\Delta\tau M q^n$$

This gives the amplification factor

$$\sigma = \frac{q^{n+1}}{q^n} = \frac{\lambda_D^2 + \Delta\tau(\lambda_D - 1)\lambda_M + \Delta\tau^2\lambda_{M_l M_u}}{\lambda_D^2 + \Delta\tau\lambda_D\lambda_M + \Delta\tau^2\lambda_{M_l M_u}}$$

This scheme is still unconditionally stable if we require $\lambda_D$ to be real and $|\lambda_D| \geq 1/2$. But, for the best convergence rate, or equivalently for the smallest $|\sigma|$, we need to eliminate the imaginary part of the numerator. This can be done by preconditioning the RHS as

$$(D+\Delta\tau M_l)(D+\Delta\tau M_u)\Delta q^n = -\Delta\tau DMq^n$$

$$q^{n+1} = q^n + \Delta q^n \tag{11}$$

that yields

$$\sigma = \frac{q^{n+1}}{q^n} = \frac{\lambda_D^2 + \Delta\tau^2\lambda_{M_l M_u}}{\lambda_D^2 + \Delta\tau\lambda_D\lambda_M + \Delta\tau^2\lambda_{M_l M_u}}$$

This is an unconditionally stable scheme as long as $\lambda_D$ is real. The remaining problem is then to construct $D$ such that each LU factor is well-conditioned.

For the model scalar problem, the choice of $D$ in 1-D is obviously $1/2\ (\Delta\tau/\Delta\xi)$ for a 3-point central differencing and $3/4\ (\Delta\tau/\Delta\xi)$ for a 5-point central differencing. These choices can be easily verified by examining matrices in Eq. (8) and (9). Note that the choice of $D$ must make both $L$ and $U$ well-conditioned. Hence, if two different $D$'s satisfy the sufficient condition for $L$ and $U$, respectively, the one with greater absolute value must be chosen. For 2-D and 3-D problems, the inverse of a model matrix should be analytically derived such that $D$ can be chosen accordingly. However, the mathematics is very complicated and, hence, we simply extend the 1-D choice to 2-D and 3-D problems. The test results shown later confirmed this choice.

For the Euler equations, in addition to nonlinearity, more complications arise because $M_l$ and $M_u$ are composed of the flux Jacobians. If 3-point central difference operators are used for $M$, the elements of $M_l$ and $M_u$ are either $(-A/2\Delta\xi, -B/2\Delta\eta, -C/2\Delta\zeta)$ or $(A/2\Delta\xi, B/2\Delta\eta, C/2\Delta\zeta)$. Taking a 1-D case, for example, we have

$$M_l = \mathbf{B}\left(\frac{-A}{2\Delta\xi},0,0\right), M_u = \mathbf{B}\left(0,0,\frac{A}{2\Delta\xi}\right)$$

where $A$ is a $3\times 3$ matrix. An obvious but risky choice is to treat $A$ as if it were a nonzero scalar, which gives

$$D = \Delta\tau\cdot\mathbf{B}\left(0,\frac{A}{2\Delta\xi},0\right)$$

This $D$ and Eq. (11) were used successfully to solve the quasi-1-D Euler equations for some model supersonic and transonic nozzle flows. Furthermore, it was found that for numerical efficiency we can replace $A$ by its spectral radius $|\lambda_A|_{\max}$ without losing the required unconditional stability. Hence, we construct the clock element of $D$ at a point $i$ as

$$D_i = \Delta\tau\cdot\text{MAX}\left\{\frac{|\lambda_A|}{2\Delta\xi}\right\}_i \cdot I$$

A similar choice is carried over to 2-D and 3-D Euler equations. In 3-D the block element of $D$ at a point $(i,j,k)$ is a $5\times 5$ scalar diagonal matrix

$$D_{i,j,k} = \Delta\tau\cdot\text{MAX}\left\{\frac{|\lambda_A|}{2\Delta\xi},\frac{|\lambda_B|}{2\Delta\eta},\frac{|\lambda_C|}{2\Delta\zeta}\right\}_{i,j,k}\cdot I$$

Recall that the constant 1/2 in $D$ is predetermined by the choice of 3-point central differencing. If a 5-point central differencing were used instead, the constant would be 3/4.

For the NS equations, the block element is still a $5\times 5$ scalar diagonal matrix

$$D_{i,j,k} = \Delta\tau\cdot\text{MAX}\left\{\frac{1}{2\Delta\xi}|\lambda_{(A-A_v)}|, \frac{1}{2\Delta\eta}|\lambda_{(B-B_v)}|,\frac{1}{2\Delta\zeta}|\lambda_{(C-C_v)}|,\right\}_{i,j,k}\cdot I$$

But, as mentioned before, neglecting the LHS viscous flux Jacobians in high Reynolds number flows seems not to alter the stability of an ADI scheme.[16] We expect the same behavior in a LU factorization scheme. Therefore, we chose to use the same $D$ for both the Euler and the NS equations. Results shown later confirmed this choice.

## VII. Effective Time Step

In the basic LU factorization scheme $\Delta\tau$ is an input parameter. Solutions advance forward one time increment $\Delta\tau$ after one iteration. If we could finish the inversion process without any numerical instability, that is, if the computer had an infinite number of significant digits, $\Delta\tau$ could be arbitrarily large or small. In this sense, the basic scheme is first-order time accurate and "unconditionally stable." However, we have shown that $\Delta\tau$ must be limited to a small number in the basic LU factorization scheme. The proposed LU factorization scheme is not time accurate since the added operator $D$ is a point function and depends on the local spectral radius of the flux Jacobians. In fact, $\Delta\tau$ is no longer a true time increment because $D$ is now proportional to $\Delta\tau$. For simplicity, let's write

$$D_{i,j,k} = \Delta\tau|\lambda|_{\max}$$

Then, locally at a point $(i,j,k)$, we have

$$(\Delta\tau^2|\lambda|^2_{\max} + \Delta\tau^2|\lambda|_{\max}M + \Delta\tau^2 M_l M_u)\Delta q^n = -\Delta\tau^2|\lambda|_{\max}Mq^n$$

or equivalently

$$q^{n+1} = q^n - \frac{1}{|\lambda|_{\max}}Mq^{n+1} - \frac{1}{|\lambda|^2_{\max}}M_l M_u\Delta q^n$$

This is a backward Euler scheme with a local effective time step $1/|\lambda|_{\max}$ and an error term proportional to $1/|\lambda|^2_{\max}$. Furthermore, the local CFL number is always 2 since $|\lambda|_{\max}$ is actually half of the maximum spectral radius of the flux Jacobians. The constant 2 is due to the choice of 3-point central differencing for $M$. If a 5-point central differencing were used instead, the local CFL number would be 4/3. Thus, it is clear that the requirement for well-conditioned LU factors has in effect put an upper limit on the CFL number that the scheme can achieve. This upper limit can be determined by the sufficient condition of Eq. (7).

It should be pointed out that as long as central difference operators are used for $M$ on both the LHS and the RHS, a maximum CFL number is set for a LU factorization scheme. This results because a central difference operator has no diagonal term. An "error" diagonal term proportional to $\Delta\tau$

and the spectral radius of off-diagonals must be added to obtain well-conditioning for the inversion process. This is equivalent to limiting the ratio of the off-diagonals to the diagonals of the resulting factor, which is a measure of the "true" CFL number. Furthermore, carefully designed "error" off-diagonal terms can also be used to obtain well-conditioning, provided that the sufficient condition of Eq. (7) is satisfied. In particular, the overall "error" terms added to the scheme can be designed to simulate the effects of a dissipation operator. The exceptions may be the classical LU decomposition method and the flux-split scheme. In the latter scheme, proper upwind difference operators are chosen based on the sign of eigenvalues of the local flux Jacobians. Well-conditioned factors are a natural result of upwind differencing and, hence, there is no need for an added operator $D$.

One may try to construct a LU scheme that seems to preserve the true time step. But, care must be taken to evaluate such a scheme. For example, the following "unconditionally stable" scheme

$$(I+\Delta\tau D+\Delta\tau M_l)(I+\Delta\tau D+\Delta\tau M_u)\Delta q^n = -(I+\Delta\tau D)\Delta\tau M q^n \tag{12}$$

or, equivalently

$$q^{n+1}=q^n-\Delta\tau M q^{n+1} - \Delta\tau^2 DMq^{n+1}-2\Delta\tau D\Delta q^n-\Delta\tau^2[D^2+M_lM_u]\Delta q^n \tag{13}$$

seems to have preserved a true time step $\Delta\tau$, if terms other than the first three of Eq. (13) are considered to be error terms. But, in order to achieve well-conditioning, for the 1-D Euler equation we must require

$$|1+\Delta\tau\lambda_D|\geq\frac{\Delta\tau|\lambda_A|}{2\Delta\xi}$$

where the constant 1/2 is due to the 3-point central differencing. This means that the error terms associated with $D$ are no longer small and cannot be left out when we evaluate the effective time step for the scheme. That is, Eq. (13) must be normalized by its diagonal term as

$$q^{n+1}=q^n-\frac{\Delta\tau M}{(I+\Delta\tau D)}q^{n+1}-\frac{\Delta\tau^2 M_lM_u}{(I+\Delta\tau D)^2}\Delta q^n$$

This is equivalent to having a CFL number

$$\mathbf{CFL}=\frac{\Delta\tau\lambda_A}{(1+\Delta\tau\lambda_D)\Delta\xi}$$

that has a maximum of 2 when $\Delta\tau$ approaches infinity.

Of course, Eq. (12) is a valid scheme. It has a $\Delta\tau$ that can be varied between zero and infinity, while the corresponding CFL number varies only between zero and 2. It has been our experience that in this range of CFL number, using a higher CFL number results in a better convergence rate. In general, the maximum CFL number depends on the minimum $|\lambda_D|$ chosen and, hence, is determined by the sufficient condition of Eq. (7).

## VIII. Implementation of the New LU Factorization Scheme

For time accurate computations, the basic scheme of Eq. (4) should be used with a CFL number limited to 2. If $\Delta\tau/2$ is used on the LHS, the scheme becomes second-order time accurate and the maximum CFL number can be doubled to 4. For steady-state solutions, the proposed scheme of Eq. (11) that has a uniform CFL number throughout the grid should be used. In all cases the RHS should always use Div(flux) instead of $Mq$. Two sweeps are necessasry to invert the LHS factors. For Eq. (11) they are: forward sweep

$$\text{RHS}_{i,j,k}=-\Delta\tau D_{i,j,k}[\text{Div}(\text{flux})]_{i,j,k}$$

$$\Delta q^*_{i,j,k}=D^{-1}_{i,j,k}\Big[\text{RHS}_{i,j,k}+\frac{\Delta\tau}{2\Delta\zeta}C_{i,j,k-1}\cdot\text{RHS}_{i,j,k-1} + \frac{\Delta\tau}{2\Delta\eta}B_{i,j-1,k}\cdot\text{RHS}_{i,j-1,k}+\frac{\Delta\tau}{2\Delta\xi}A_{i-1,j,k}\cdot\text{RHS}_{i-1,j,k}\Big]$$

and backward sweep

$$\Delta q_{i,j,k}=D^{-1}_{i,j,k}\Big[\Delta q^*_{i,j,k}-\frac{\Delta\tau}{2\Delta\zeta}C_{i,j,k+1}\cdot\Delta q^*_{i,j,k+1} - \frac{\Delta\tau}{2\Delta\eta}B_{i,j+1,k}\cdot\Delta q^*_{i,j+1,k}-\frac{\Delta\tau}{2\Delta\xi}A_{i+1,j,k}\cdot\Delta q^*_{i+1,j,k}\Big]$$

$$q^{n+1}_{i,j,k}=q^n_{i,j,k}+\Delta q^n_{i,j,k}$$

Note that $\Delta\tau$ can be eliminated from Eq. (11); it is kept here for consistency. This scheme is similar to the SSOR method[3] originally designed for second-order elliptic equations. In this case $D$ corresponds to the relaxation parameter, and it has been optimized for the NS equations that are hyperbolic in nature. Both sweeps have at least one recursive index, say $i$, which indexes the innermost diagonal. The inversion of the innermost matrix in each LU factor is the only inversion work that is difficult to vectorize. This situation may be resolved by using the checkboard indexing in the innermost direction. Since $D$ is a scalar diagonal matrix, no banded matrix inversion of any kind is required in each sweep. However, $A$, $B$, and $C$ need to be computed twice, once for each sweep, since normally the computer does not have enough memory to store them.

No special care is needed for boundary points. Bear in mind that the LU factorization is applied to the full 3-D LHS operator after it is formed. Any implicit or explicit boundary point treatment needed for the problem should be included in the full 3-D formulation before the factorization is applied. In the test case shown later, boundary point values are all computed explicitly. For example, the supersonic outflow condition is done by a first-order extrapolation, the surface pressure on the cylinder is done by satisfying the equation of zero normal momentum flux, etc. A full description of boundary point treatment for the testing case may be found in Refs. 13, 16, and 17.

Implicit and explicit artificial dissipation are sometimes necessary when the flow field varies greatly, e.g., near a shock. Any explicit dissipation operator can be easily added to the RHS of the new scheme. The implicit dissipation operator is split into two parts just as we split the central difference operator. For example, a second-order dissipation operator has coefficients $\mathbf{B}(0,-1,2,-1,0)$. It can be split into $\mathbf{B}(0,-1,1,0,0)$ for the lower part and $\mathbf{B}(0,0,1,-1,0)$ for the upper part. A fourth-order dissipation operator has coefficients $\mathbf{B}(1,-4,6,-4,1)$. It can be split into $\mathbf{B}(1,-4,3,0,0)$ for the lower part and $\mathbf{B}(0,0,3,-4,1)$ for the upper part. However, caution must be used in splitting the dissipation operators. As mentioned in Sec. 4, the interactions among symmetric and antisymmetric operations on the LHS may cause some instability. In this case the diagonal term of the dissipation operator may need a larger coefficient, say $\mathbf{B}(1,-4,4,0,0)$ and $\mathbf{B}(0,0,4,-4,1)$ for the fourth-order dissipation. In the test case shown later both second-order and fourth-order dissipation is used. The second-order dissipation is switched on only when the flow field experiences a great change. A full description of this nonlinear switching can be found in Ref. 19.

## IX. Explicit Eigenvector Annihilation

An explicit eigenvector annihilation procedure[14] is adopted by the new scheme. The motivation is to remove the stiffness caused by the fine grid spacing required for viscous flows. Since the CFL number is limited to 2, the LU factorization scheme is inherently slow for viscous flow calculations. Basically, the procedure uses several levels of $\Delta q$ to estimate the dominant eigenvalue of the resulting system of a particular numerical scheme. It then applies an explicit Richardson annihilation step based on the estimated eigenvalue. When the estimation is accurate, the error component corresponding to the dominant eigenvalue will be annihilated. The procedure allows some instabilities to occur for other eigenvalues, as long as they can be quickly suppressed by subsequent iterations. The whole process is done in real arithmetic even when the dominant eigenvalue is complex. In the latter case, a dominant pair of complex eigenvalues is estimated, and the two corresponding complex annihilation steps are analytically combined such that all the computations can be performed in real arithmetic. A full description of this procedure may be found in Ref. 14.

## X. Test Results

A 3-D supersonic flow past a hemisphere cylinder at a high angle of attack is chosen as the first test case. The freestream Mach number is 1.2 and the angle of attack is 19 deg. The Reynolds number based on the freestream and the radius of the hemisphere is 222500. Both inviscid and laminar viscous flow is computed. Although the full NS equations pose no problem for the new scheme, the thin-layer NS equations that neglect $A_v$ and $B_v$ are solved for the viscous case. Since the flowfield contains a bow shock in front of the cylinder, a subsequent acceleration from subsonic flow to supersonic outflow, and a massive separation on the leeward side of the cylinder, this is a serious test for any new numerical scheme.

A research program ARC3D created by Pulliam and Steger[13] is used as the base program to implement the new scheme. ARC3D employs the ADI scheme with a diagonalized LHS. A local time step scaled by the metric Jacobians is used to accelerate the convergence. Nonlinear second- and fourth-order dissipation is added explicitly and implicitly. To implement the new scheme, the LHS ADI factors of ARC3D are replaced by the new LU factors, and the inversion process is modified accordingly. Since the delta-law form is enforced, no modification on the RHS is necessary. Although the fourth-order differencing poses no trouble for the new scheme, a 3-point second-order differencing is chosen for its higher CFL number.

The grid system is shown in Fig. 1. A moderate $40 \times 23 \times 30$ grid with bilateral symmetry in $\eta$ is used. Figure 2 shows the surface pressure along the leeward symmetry plane computed by ARC3D and the present scheme at different iterations (NC). Since both schemes have the same RHS, almost identical results for both schemes are to be expected. Figure 3 shows the density comparison. Note that the pressure converges long before the density, suggesting that density is a better criterion for convergence. The initial condition is an impulsive start, and the initial $l_2$ residual is about $0.2 \times 10^{-3}$. This suggests that for plotting purposes a drop of four orders of magnitude in $l_2$ residual is a good indication of a converged solution. Although not shown here, all essential flow phenomena such as the bow shock, the crossflow reversal and the massive separation on the leeward side, are captured by the new scheme and are in excellent agreement with those computed by ARC3D. Figure 4 is an example of particle paths computed by the new scheme.

Figure 5 is the convergence history of the inviscid calculation. The $l_2$ residual has dropped four orders of magnitude within 500 iterations and to machine zero within 1300 iterations. Note that this is an iteration by iteration plot, and no oscillatory nature is present. Figure 6 is the convergence history for viscous calculations. The deterioration of the convergence rate is obvious for the LU scheme since it has three distinct slopes. A drop of three orders of magnitude is achieved at around 1000 iterations, and after that the scheme slows down considerably. Because the convergence follows the invisid case for the first 300 iterations, the subsequent slowing

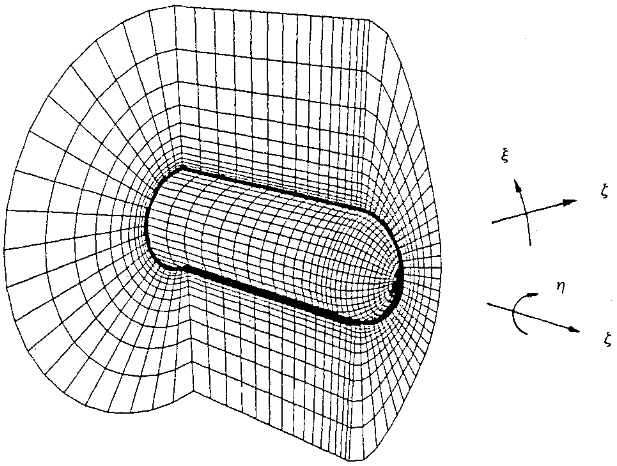

Fig. 1 Grid system for the hemisphere cylinder.

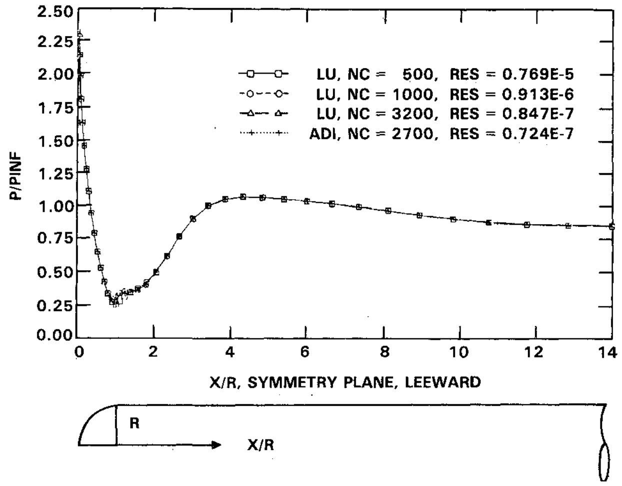


Fig. 2 Surface pressure on the leeward symmetry plane of the hemisphere cylinder, laminar viscous ($M_\infty = 1.2$, $\alpha = 19$ deg, $Re_r = 222500.$, PINF = 0.714).

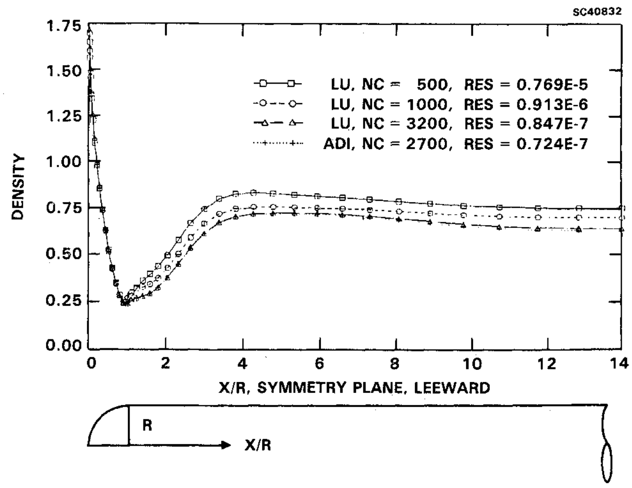


Fig. 3 Surface density on the leeward symmetry plane of the hemisphere cylinder, laminar viscous ($M_\infty = 1.2$, $\alpha = 19$ deg, $Re_r = 222500.$, $\rho_\infty = 1$).

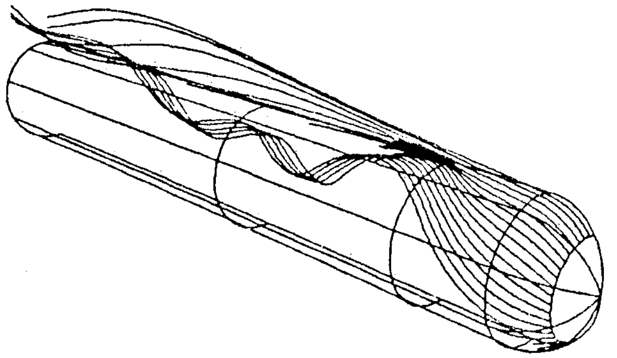

Fig. 4 Particle traces showing leeward side separation of the hemisphere cylinder, LU scheme, laminar vicous, ($M_\infty = 1.2$, $\alpha = 19$ deg, $Re_r = 222500$).

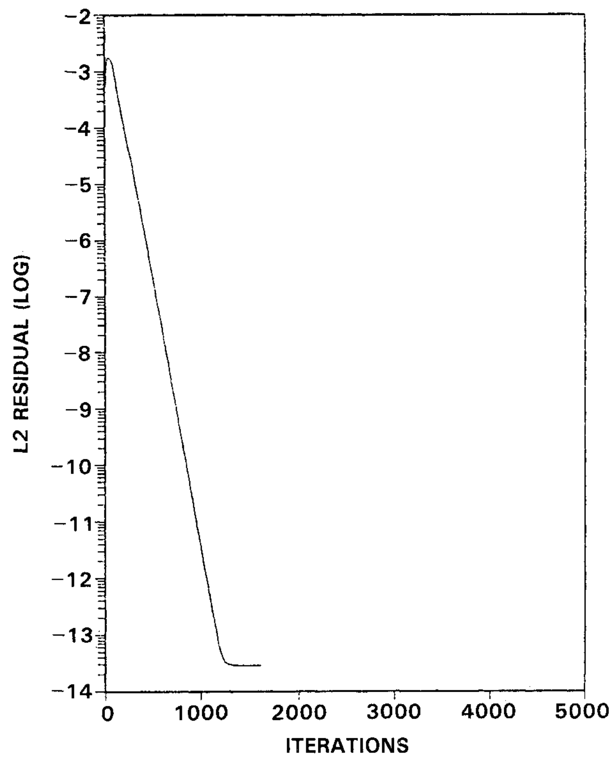


Fig. 5 Convergence history for the inviscid supersonic computation, hemisphere cylinder, LU scheme ($M_\infty = 1.2$, $\alpha = 19$ deg).

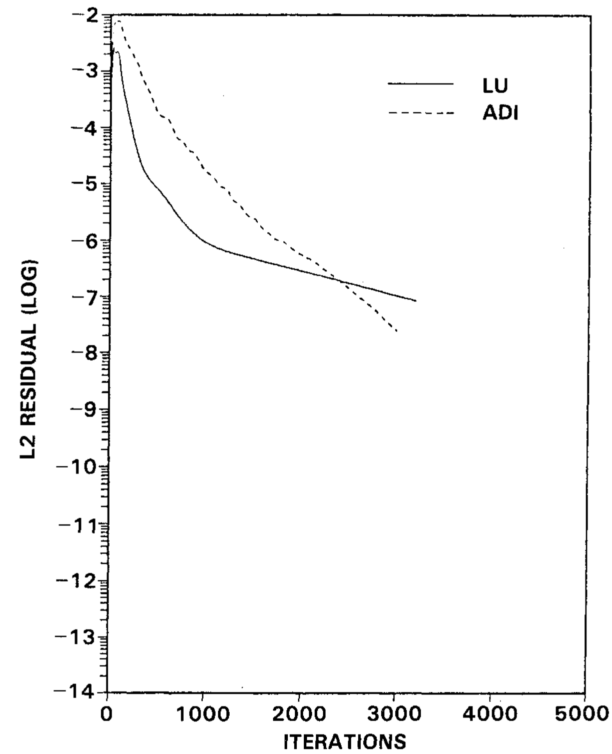


Fig. 6 Convergence history for the viscous supersonic computations, hemisphere cylinder, LU and ADI scheme ($M_\infty = 1.2$, $\alpha = 19$ deg, $Re_r = 222500$).

down is mainly due to the fine grid spacing required for the viscous case. The fine grid spacing is necessary in order to resolve the viscous effect within the boundary layer. Here the ratio of the finest grid spacing between the viscous and the inviscid calculation is 1:100.

The convergence history for the ADI scheme is also included in Fig. 6. This may not be the best convergence rate that the ADI scheme could achieve because no serious attempt has been made to optimize the parameters used in the scheme. For the current plot, the parameters used were chosen by experience. The maximum local CFL number based on the eigenvalues of the inviscid flux Jacobians is of order 10. A drop of four orders of magnitude in $l_2$ residual is achieved at around 2000 iterations. Local oscillations in the convergence can be easily observed, which are in contrast to the monotonic decrease observed for the LU factorization scheme.

As we have mentioned, an explicit eigenvector annihilation procedure is adopted by the new scheme in order to remove the stiffness caused by the fine grid spacing. It is motivated by the observation of the monotonic decrease of $l_2$ residual. Although it may vary from problem to problem, the observed monotonicity suggests that the dominant eigenvalue of the resulting system of the new scheme is probably real, which is in contrast to the dominant complex eigenvalue of the ADI scheme. If this speculation is true, then the dominant eigenvalue of the system can be easily estimated and, hence, annihilated by a Richardson annihilation step. Figure 7 shows the result. The sudden jumps in the $l_2$ residual indicate the applications of Richardson annihilation steps. The convergence is disturbed, but then the instability is quickly suppressed. Note that this procedure is applied at a very early stage of the convergence. It is applied after the first 150 iterations in order to maintain the fast convergence of the early stage. A drop of five orders of magnitude in $l_2$ residual is achieved within 1000 steps, indicating the success of the annihilation procedure. It should be mentioned here that because we use IMSL subroutines in the annihilation program, it requires some extra memory to load the code. As a result, the grid size must be reduced to $32 \times 23 \times 30$ for the current run. Since the finest grid spacing is kept at the same value to maintain stiffness, the reduced $\xi$ grid size should have no effect on our conclusion. No extra memory would be needed if we wrote the entire annihilation subroutine.

The second test is a transonic flow past the same hemisphere cylinder. The flow has a freestream Mach number of 0.9, an angle of attack of 19 deg and a Reynolds number of 212500. The flow is assumed laminar. Figure 8 shows the convergence history for both the ADI scheme and the present scheme with and without annihilation. This flow is more difficult for both schemes to converge, presumably due to the more elliptic nature of the flow. It takes 3000 steps for the ADI scheme to drop three orders of magnitude in $l_2$ residual, while it takes 1000 steps for the LU scheme without annihilation. The maximum CFL number is about 15 for the ADI scheme, and again this may not be the optimal value. The annihilation attempt is still successful, but not as successful as for the supersonic test. One possible explanation is that the disturbances introduced by the annihilation steps may have persisted inside the elliptic domain of the flow. The oscillatory nature in the early stage of convergence suggests that the eigensystem in this case may be

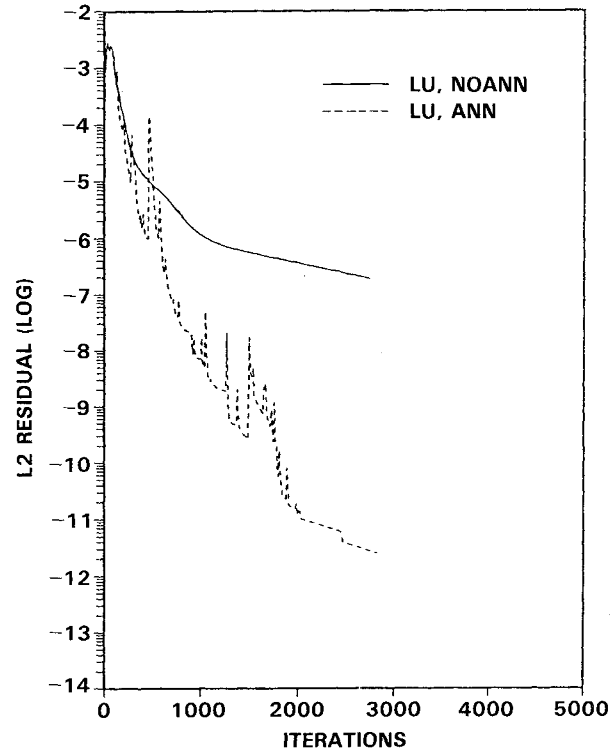


**Fig. 7 Convergence history for the viscous supersonic computations, hemisphere cylinder, LU with and without annihilation ($M_\infty = 1.2$, $\alpha = 19$ deg, $Re_r = 2225000$).**

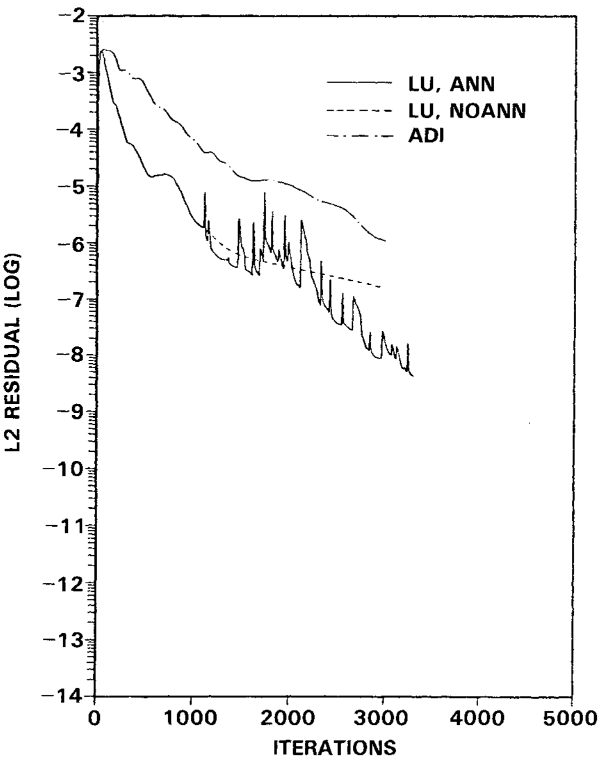


**Fig. 8 Convergence history for the viscous transonic computations, hemisphere cylinder, ADI, LU with and without annihilation ($M_\infty = 0.9$, $\alpha = 19$ deg, $Re_r = 212500$).**

complex dominant. An early start of annihilation has been tried, but the result is about the same as the current figure.

The final note concerns numerical efficiency. As previously indicated, the inversion of LU factors of the new scheme is very easy and efficient. Since $D$ is a scalar diagonal matrix, it costs almost nothing to invert. Only matrix-vector multiplication and vector addition are necessary in the solution process. The real cost of the new scheme is the evaluation of the flux Jacobians. Since it requires too much memory to store them, the flux Jacobians are computed twice, once for each sweep, in each iteration. Although it depends on the computational vector length of the problem, the CPU time per iteration for the new LU scheme with annihilation is slightly less than that for the ADI scheme. The actual ratio is about 0.9 for the results presented here. In the ADI scheme, the numerical efficiency is improved by a diagonalized LHS.

## XI. Conclusions

A new approximate LU factorization scheme has been developed and implemented for the steady-state Reynolds-averaged NS equations. The scheme is analyzed and optimized according to a simple linear analysis. It is unconditionally stable for the model hyperbolic equation regardless of the spatial dimensions of the problem. However, the requirement for well-conditioned factors has essentially limited the effective time step that the scheme can achieve. The new scheme is very easy and efficient to implement since only matrix-vector multiplication and vector addition are necessary in the solution process. Any appropriate boundary point treatment can be readily adopted, and artificial dissipation can be easily added. The two explicit sweeps of the solution process resemble the SSOR method originally designed for second-order elliptic equations. Supersonic and transonic 3-D flows past a hemisphere cylinder at a high angle of attack are successfully computed by the new scheme. A good convergence rate is achieved for the inviscid flow, and it can be maintained for the viscous case with the help of an explicit eigenvector annihilation procedure.

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