# Diagonal Inversion of Lower-Upper Implicit Schemes

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**A new diagonally inverted lower-upper (LU) implicit scheme is developed for the three-dimensional Euler equations. The matrix systems that are to be inverted in the scheme are treated by local diagonalizing transformations that decouple them into systems of scalar equations. Unlike the diagonalized alternating direction implicit method, the time accuracy of the LU scheme is not reduced since the diagonalizing procedure does not destroy time conservation. Furthermore, this diagonalization reduces the computational effort required to solve the implicit approximation and therefore transforms it into a more efficient method of numerically solving the three-dimensional Euler equations.**

INCREASINGLY, attention is being directed towards implicit schemes as the need to develop more efficient numerical methods becomes apparent. An implicit approximation is an attractive way to increase the efficiency of the time-marching technique because implicit schemes permit much larger time steps than most explicit methods normally allow. The drawback of most implicit schemes is that they are computationally more expensive, per time step, than explicit methods. As a result, interest is being focused upon decreasing the computational effort required to solve the implicit approximation. Examples of schemes that address this issue are Chaussee and Pulliam's diagonalized alternating direction implicit (ADI) scheme[1] and Obayashi and Fujii's lower-upper (LU) alternating direction implicit scheme.[2]

The Euler equations can be discretized into an implicit approximation that, when written in delta form, produces a large block-banded matrix system that is impractical to solve without first being approximately factored. In the present work, the LU implicit multigrid algorithm developed by Yokota and Caughey[3] for the three-dimensional Euler equations has been made more efficient through a local diagonalizing procedure that reduces the computational effort required to solve the LU approximation. The LU factorization produces two block triangular operators (one upper and one lower) which, through back substitution, can be solved by effectively explicit sweeps that require matrix inversions at every mesh cell in the domain. The efficiency of this LU scheme can be increased by reducing the computational costs associated with these matrix inversions. This reduction can be achieved by a local diagonalizing transformation that decouples the matrix systems into scalar equations. Time conservation and stability remain unaltered by the decoupling since the LU scheme's differencing operators are unaffected by the diagonalizing transformations. This result is unlike the diagonalized ADI method, which is produced at the expense of time accuracy.

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The Euler equations for the generalized coordinate system $(\xi,\eta,\zeta)$ can be written

$$\frac{\partial W}{\partial t}+\frac{\partial F}{\partial \xi}+\frac{\partial G}{\partial \eta}+\frac{\partial H}{\partial \zeta}=0 \tag{1}$$

where $W=(\rho D,\rho Du,\rho Dv,\rho Dw,\rho DE)^T$; $F$, $G$, and $H$ are the flux vectors; $\rho$ and $P$ are the fluid density and pressure; $(u,v,w)$ are the Cartesian velocity components; and $E$ is the total energy per unit volume. The Jacobians of the coordinate transformation are as follows:

$$J=\begin{pmatrix} x_\xi & x_\eta & x_\zeta \\ y_\xi & y_\eta & y_\zeta \\ z_\xi & z_\eta & z_\zeta \end{pmatrix} \qquad J^{-1}=\begin{pmatrix} \xi_x & \xi_y & \xi_z \\ \eta_x & \eta_y & \eta_z \\ \zeta_x & \zeta_y & \zeta_z \end{pmatrix}$$

where $D$ is the determinant of the matrix $J$ and contravariant velocities are defined as $(U,V,W)^T=J^{-1}(u,v,w)^T$.

The Euler equations can be discretized into a finite-volume implicit approximation[4]:

$$[I+\mu\Delta t(\delta_\xi A+\delta_\eta B+\delta_\zeta C)]\Delta W^n_{ijk}=-\Delta t(\bar\delta_\xi F+\bar\delta_\eta G+\bar\delta_\zeta H)^n_{ijk} \tag{2}$$

where $\Delta W^n=W^{n+1}-W^n$; $\Delta t$ is the time step size; $0\le\mu\le 1$ is a parameter governing the degree of implicitness; $\delta$ and $\bar\delta$ are cell- and face-centered central differences; $I$ is the identity matrix; and $A$, $B$, and $C$ are the flux Jacobian matrices relative to the vectors $F$, $G$, and $H$. This finite-volume formulation reduces to a central-difference approximation on a uniform grid and therefore requires the addition of explicit artificial dissipation terms to suppress possible odd and even point oscillations and shock overshoots. Following the works of Jameson[5] and Pulliam,[6] fourth difference terms are added throughout the flowfield to prevent odd-even decoupling, and second difference terms are used to stabilize the flow calculation near shocks.

The LU factorization, which is based on one-sided, implicit, spatial differences, can be written as follows:

$$[I+\mu\Delta t(\delta_\xi^- A_1+\delta_\eta^- B_1+\delta_\zeta^- C_1)]\cdot[I+\mu\Delta t(\delta_\xi^+ A_2+\delta_\eta^+ B_2 + \delta_\zeta^+ C_2)]\Delta W^n_{ijk}=-\Delta t(\bar\delta_\xi F+\bar\delta_\eta G+\bar\delta_\zeta H+T)^n_{ijk} \tag{3}$$

where $\delta^+$ and $\delta^-$ are cell-centered forward and backward first differences and $T$ is the explicitly added artificial dissipation. The flux Jacobian matrices are split and reconstructed as $A_1 = 0.5\ (A + \beta|A|I)$ and $A_2 = 0.5\ (A - \beta|A|I)$, where $|A| = \max(|\lambda_A|)$ is the maximum absolute-valued eigenvalue of the flux Jacobian matrix $A$, $\beta \approx 1$ is a scalar constant governing the amount of implicit dissipation produced by the matrix reconstructions,[3] and $I$ is the identity matrix. This implicit system of equations is solved in the following two steps:

1) Lower sweep:

$$[I + \mu\Delta t(\delta_\xi^- A_1 + \delta_\eta^- B_1 + \delta_\zeta^- C_1)]\Delta Y_{ijk}^n = -\Delta t(\bar{\delta}_\xi \boldsymbol{F} + \bar{\delta}_\eta \boldsymbol{G} + \bar{\delta}_\zeta \boldsymbol{H} + \boldsymbol{T})_{ijk}^n \tag{4}$$

2) Upper sweep:

$$[I + \mu\Delta t(\delta_\xi^+ A_2 + \delta_\eta^+ B_2 + \delta_\zeta^+ C_2)]\Delta W_{ijk}^n = \Delta Y_{ijk}^n \tag{5}$$

which, through back substitution, can be reduced to simple $5 \times 5$ matrix systems at every mesh cell. These reduced systems can now be written as

1) Lower sweep:

$$[I + \mu\Delta t(A_1 + B_1 + C_1)]\Delta Y_{ijk}^n = -\Delta t(\bar{\delta}_\xi \boldsymbol{F} + \bar{\delta}_\eta \boldsymbol{G} + \bar{\delta}_\zeta \boldsymbol{H} + \boldsymbol{T})_{ijk}^n + \mu\Delta t(A_1\Delta Y_{i-1,j,k}^n + B_1\Delta Y_{i,j-1,k}^n + C_1\Delta Y_{i,j,k-1}^n) \tag{6}$$

2) Upper sweep:

$$[I + \mu\Delta t(A_2 + B_2 + C_2)]\Delta W_{ijk}^n = \Delta Y_{ijk}^n + \mu\Delta t(A_2\Delta W_{i+1,j,k}^n + B_2\Delta W_{i,j+1,k}^n + C_2\Delta W_{i,j,k+1}^n) \tag{7}$$

The solution of the LU factorization can be made more efficient by treating these $5 \times 5$ matrix systems with the diagonalizing tranformation[3]:

$$Q^{-1}(A + B + C)Q = \Lambda$$

which can be derived from the Warming et al.[7] transforms and has the elements

$$Q_{11} = \hat{l}_1 \qquad Q_{21} = u\hat{l}_1 \qquad Q_{31} = v\hat{l}_1 + \rho\hat{l}_3$$

$$Q_{12} = \hat{l}_2 \qquad Q_{22} = u\hat{l}_2 - \rho\hat{l}_3 \qquad Q_{32} = v\hat{l}_2$$

$$Q_{13} = \hat{l}_3 \qquad Q_{23} = u\hat{l}_3 + \rho\hat{l}_2 \qquad Q_{33} = v\hat{l}_3 - \rho\hat{l}_1$$

$$Q_{14} = \frac{\rho}{\sqrt{2}c} \qquad Q_{24} = \frac{\rho u}{\sqrt{2}c} + \frac{\rho\hat{l}_1}{\sqrt{2}} \qquad Q_{34} = \frac{\rho v}{\sqrt{2}c} + \frac{\rho\hat{l}_2}{\sqrt{2}}$$

$$Q_{15} = \frac{\rho}{\sqrt{2}c} \qquad Q_{25} = \frac{\rho u}{\sqrt{2}c} - \frac{\rho\hat{l}_1}{\sqrt{2}} \qquad Q_{35} = \frac{\rho v}{\sqrt{2}c} - \frac{\rho\hat{l}_2}{\sqrt{2}}$$

$$Q_{41} = w\hat{l}_1 - \rho\hat{l}_2 \qquad Q_{51} = \frac{q^2}{2}\hat{l}_1 + \rho v\hat{l}_3 - \rho w\hat{l}_2$$

$$Q_{42} = w\hat{l}_2 + \rho\hat{l} \qquad Q_{52} = \frac{q^2}{2}\hat{l}_2 - \rho u\hat{l}_3 + \rho w\hat{l}_1$$

$$Q_{43} = w\hat{l}_3 \qquad Q_{53} = \frac{q^2}{2}\hat{l}_3 + \rho u\hat{l}_2 - \rho v\hat{l}_1$$

$$Q_{44} = \frac{\rho w}{\sqrt{2}c} + \frac{\rho\hat{l}_3}{\sqrt{2}} \qquad Q_{54} = \frac{\rho q^2}{2\sqrt{2}c} + \frac{\rho u\hat{l}_1}{\sqrt{2}} + \frac{\rho v\hat{l}_2}{\sqrt{2}} + \frac{\rho w\hat{l}_3}{\sqrt{2}} + \frac{\rho c}{\sqrt{2}(\gamma - 1)}$$

$$Q_{45} = \frac{\rho w}{\sqrt{2}c} - \frac{\rho\hat{l}_3}{\sqrt{2}} \qquad Q_{55} = \frac{\rho q^2}{2\sqrt{2}c} - \frac{\rho u\hat{l}_1}{\sqrt{2}} - \frac{\rho v\hat{l}_2}{\sqrt{2}} - \frac{\rho w\hat{l}_3}{\sqrt{2}} + \frac{\rho c}{\sqrt{2}(\gamma - 1)}$$

$$Q_{11}^{-1} = \hat{l}_1 - \frac{v\hat{l}_3}{\rho} + \frac{w\hat{l}_2}{\rho} - \frac{(\gamma - 1)q^2\hat{l}_1}{2c^2} \qquad Q_{21}^{-1} = \hat{l}_2 + \frac{u\hat{l}_3}{\rho} - \frac{w\hat{l}_1}{\rho} - \frac{(\gamma - 1)q^2\hat{l}_2}{2c^2}$$

$$Q_{12}^{-1} = \frac{(\gamma - 1)u\hat{l}_1}{c^2} \qquad Q_{22}^{-1} = -\frac{\hat{l}_3}{\rho} + \frac{(\gamma - 1)u\hat{l}_2}{c^2}$$

$$Q_{13}^{-1} = \frac{\hat{l}_3}{\rho} + \frac{(\gamma - 1)v\hat{l}_1}{c^2} \qquad Q_{23}^{-1} = \frac{(\gamma - 1)v\hat{l}_2}{c^2}$$

$$Q_{14}^{-1} = \frac{\hat{l}_2}{\rho} + \frac{(\gamma - 1)w\hat{l}_1}{c^2} \qquad Q_{24}^{-1} = \frac{\hat{l}_1}{\rho} + \frac{(\gamma - 1)w\hat{l}_2}{c^2}$$

$$Q_{15}^{-1} = -\frac{(\gamma - 1)\hat{l}_1}{c^2} \qquad Q_{25}^{-1} = -\frac{(\gamma - 1)\hat{l}_2}{c^2}$$

$$Q_{31}^{-1} = \hat{l}_3 - \frac{u\hat{l}_2}{\rho} + \frac{v\hat{l}_1}{\rho} - \frac{(\gamma - 1)q^2\hat{l}_3}{2c^2} \qquad Q_{41}^{-1} = -\frac{u\hat{l}_1}{\sqrt{2}\rho} - \frac{v\hat{l}_2}{\sqrt{2}\rho} - \frac{w\hat{l}_3}{\sqrt{2}\rho} + \frac{(\gamma - 1)q^2}{2\sqrt{2}\rho c}$$

$$Q_{32}^{-1} = \frac{\hat{l}_2}{\rho} + \frac{(\gamma - 1)u\hat{l}_3}{c^2} \qquad Q_{42}^{-1} = \frac{\hat{l}_1}{\sqrt{2}\rho} - \frac{(\gamma - 1)u}{\sqrt{2}\rho c}$$

$$Q_{33}^{-1} = -\frac{\hat{l}_1}{\rho} + \frac{(\gamma - 1)v\hat{l}_3}{c^2} \qquad Q_{43}^{-1} = \frac{\hat{l}_2}{\sqrt{2}\rho} - \frac{(\gamma - 1)v}{\sqrt{2}\rho c}$$

$$Q_{34}^{-1} = \frac{(\gamma - 1)w\hat{l}_3}{c^2} \qquad Q_{44}^{-1} = \frac{\hat{l}_3}{\sqrt{2}\rho} - \frac{(\gamma - 1)w}{\sqrt{2}\rho c}$$

$$Q_{35}^{-1} = -\frac{(\gamma - 1)\hat{l}_3}{2c^2} \qquad Q_{45}^{-1} = \frac{(\gamma - 1)}{\sqrt{2}\rho c}$$

$$Q_{51}^{-1} = \frac{u\hat{l}_1}{\sqrt{2}\rho} + \frac{v\hat{l}_2}{\sqrt{2}\rho} + \frac{w\hat{l}_3}{\sqrt{2}\rho} + \frac{(\gamma-1)q^2}{2\sqrt{2}\rho c} \qquad q^2 = u^2 + v^2 + w^2$$

$$l_1 = \xi_x + \eta_x + \zeta_x$$

$$Q_{52}^{-1} = -\frac{\hat{l}_1}{\sqrt{2}\rho} - \frac{(\gamma-1)u}{\sqrt{2}\rho c} \qquad l_2 = \xi_y + \eta_y + \zeta_y$$

$$l_3 = \xi_z + \eta_z + \zeta_z$$

$$Q_{53}^{-1} = -\frac{\hat{l}_2}{\sqrt{2}\rho} - \frac{(\gamma-1)v}{\sqrt{2}\rho c} \qquad \hat{l}_1 = \frac{l_1}{\sqrt{l_1^2 + l_2^2 + l_3^2}}$$

$$Q_{54}^{-1} = -\frac{\hat{l}_3}{\sqrt{2}\rho} - \frac{(\gamma-1)w}{\sqrt{2}\rho c} \qquad \hat{l}_2 = \frac{l_2}{\sqrt{l_1^2 + l_2^2 + l_3^2}}$$

$$Q_{55}^{-1} = \frac{(\gamma-1)}{\sqrt{2}\rho c} \qquad \hat{l}_3 = \frac{l_3}{\sqrt{l_1^2 + l_2^2 + l_3^2}}$$

and $\Lambda$ has elements

$$\lambda_{11} = \lambda_{22} = \lambda_{33} = U + V + W$$

$$\lambda_{44} = U + V + W + c\sqrt{l_1^2 + l_2^2 + l_3^2}$$

$$\lambda_{55} = U + V + W - c\sqrt{l_1^2 + l_2^2 + l_3^2}$$

$$\lambda_{ij} = 0 \qquad \text{when} \qquad i \neq j$$

where $c$ is the local speed of sound. Applying this local diagonalizing transformation to the lower and upper sweeps produces the following scalar systems:

1) Lower sweep:

$$\left\{I + \frac{\mu\Delta t}{2}[\Lambda + \beta(|A| + |B| + |C|)]\right\} Q^{-1}\Delta Y_{ijk}^n = -\Delta t Q_{ijk}^{-1}[(\bar{\delta}_\xi F + \bar{\delta}_\eta G + \bar{\delta}_\zeta H + T)_{ijk}^n - \mu(A_1\Delta Y_{i-1,j,k}^n + B_1\Delta Y_{i,j-1,k}^n + C_1\Delta Y_{i,j,k-1}^n)] \quad (8)$$

2) Upper sweep:

$$\left\{I - \frac{\mu\Delta t}{2}[\Lambda - \beta(|A| + |B| + |C|)I]\right\} Q^{-1}\Delta W_{ijk}^n = Q_{ijk}^{-1}[\Delta Y_{ijk}^n - \mu\Delta t(A_2\Delta W_{i+1,j,k}^n + B_2\Delta W_{i,j+1,k}^n + C_2\Delta W_{i,j,k+1}^n)] \quad (9)$$

whose time conservation is unaltered by the decoupling process because the diagonalizing transformations are not factored out of the implicit spatial differences. Each of these equations can now be inverted by a single scalar division, and thus the construction and solution of Eqs. (8) and (9) require less computational effort than the original sweeps, Eqs. (6) and (7).

For steady-state calculations, further simplifications can be achieved by defining a local time step

$$\Delta t = \frac{Cn}{(|A| + |B| + |C|)}$$

where $Cn$ is the Courant number. By writing the vector components ($m = 1,\ldots,5$) of the lower and upper sweeps as

1) Lower sweep:

$$(Q^{-1}\Delta Y_{ijk}^n)_m = \frac{\left(-\Delta t Q_{ijk}^{-1}[(\bar{\delta}_\xi F + \bar{\delta}_\eta G + \bar{\delta}_\zeta H + T)_{ijk}^n - \mu(A_1 Q Q^{-1}\Delta Y_{i-1,j,k}^n + B_1 Q Q^{-1}\Delta Y_{i,j-1,k}^n + C_1 Q Q^{-1}\Delta Y_{i,j,k-1}^n)]\right)_m}{\left[\left(1 + \frac{\mu\beta Cn}{2}\right)I + \frac{\mu\Delta t}{2}\Lambda\right]_m} \quad (10)$$

2) Upper sweep:

$$(Q^{-1}\Delta W_{ijk}^n)_m = \frac{\left(Q_{ijk}^{-1}[\Delta Y_{ijk}^n - \mu\Delta t(A_2 Q Q^{-1}\Delta W_{i+1,j,k}^n + B_2 Q Q^{-1}\Delta W_{i,j+1,k}^n + C_2 Q Q^{-1}\Delta W_{i,j,k+1}^n)]\right)_m}{\left[\left(1 + \frac{\mu\beta Cn}{2}\right)I - \frac{\mu\Delta t}{2}\Lambda\right]_m} \quad (11)$$

and then by approximating these equations with

1) Lower sweep:

$$(Q^{-1}\Delta Y_{ijk}^n)_m = \frac{\left(-\Delta t[Q^{-1}(\bar{\delta}_\xi F + \bar{\delta}_\eta G + \bar{\delta}_\zeta H + T)_{ijk}^n - \mu(\tilde{D}_{a_1} Q^{-1}\Delta Y_{i-1,j,k}^n + \tilde{D}_{b_1} Q^{-1}\Delta Y_{i,j-1,k}^n + \tilde{D}_{c_1} Q^{-1}\Delta Y_{i,j,k-1}^n)]\right)_m}{\left[\left(1 + \frac{\mu\beta Cn}{2}\right)I + \frac{\mu\Delta t}{2}\Lambda\right]_m} \quad (12)$$

2) Upper sweep:

$$(Q^{-1}\Delta W_{ijk}^n)_m = \frac{\left([Q^{-1}\Delta Y_{ijk}^n - \mu\Delta t(\tilde{D}_{a_2} Q^{-1}\Delta W_{i+1,j,k}^n + \tilde{D}_{b_2} Q^{-1}\Delta W_{i,j+1,k}^n + \tilde{D}_{c_2} Q^{-1}\Delta W_{i,j,k+1}^n)]\right)_m}{\left[\left(1 + \frac{\mu\beta Cn}{2}\right)I - \frac{\mu\Delta t}{2}\Lambda\right]_m} \quad (13)$$

where $\tilde{D}_{a_1} = 0.5\,(\tilde{D}_a + \beta|A|I)$; $\tilde{D}_{a_2} = 0.5\,(\tilde{D}_a - \beta|A|I)$; and $\tilde{D}_a$ contains only the diagonal elements of the symmetric matrix $Q^{-1}AQ$[i.e., $\tilde{d}_{a_{11}} = \tilde{d}_{a_{22}} = \tilde{d}_{a_{33}} = U$; $\tilde{d}_{a_{44}} = U + c(\xi_x l_1 + \xi_y l_2 + \xi_z l_3)$; and $\tilde{d}_{a_{55}} = U - c(\xi_x l_1 + \xi_y l_2 + \xi_z l_3)$, with similar terms for $\tilde{D}_{b_1}$, $\tilde{D}_{b_2}$, $\tilde{D}_{c_1}$, and $\tilde{D}_{c_2}$].

The computational savings produce by this treatment can be quantified as follows. The two undiagonalized sweeps, Eqs. (6) and (7), each require the construction and summation of three flux Jacobian matrices to produce the full matrix systems which are then inverted, typically by Gaussian elimination. These sweeps can be represented by

$$A_l X_i = -R_i + B_l X_{i-1}$$

$$A_u Y_i = X_i - B_u Y_{i+1}$$

where $A_l$, $A_u$, $B_l$, and $B_u$ are full $5 \times 5$ matrices and $R$, $X$, and $Y$ are the residual and correction-type vectors. In the diagonally inverted sweeps, only one matrix multiplication is needed in the lower sweep, Eq. (12), to produce a scalar system, while the upper sweep, Eq. (13), is an uncoupled system by definition. Thus the equations in both sweeps are inverted by single scalar divisions. These sweeps can be reduced to

$$\Lambda_l \hat{X}_i = -Q^{-1} R_i + \hat{\Lambda}_l \hat{X}_{i-1}$$

$$\Lambda_u \hat{Y}_i = \hat{X}_i - \hat{\Lambda}_u \hat{Y}_{i+1}$$

where $\Lambda_l$, $\Lambda_u$, $\hat{\Lambda}_l$, and $\hat{\Lambda}_u$ are diagonal matrices; $Q^{-1}$ is a full $5 \times 5$ matrix; and $\hat{X}$ and $\hat{Y}$ are correction-type vectors. Numerical results from the diagonally inverted LU scheme, developed within the framework of the multigrid method, can be found in Ref. 4.

A new diagonally inverted LU implicit scheme has been developed for the three-dimensional Euler equations. The matrix systems that are normally inverted in the LU scheme are treated by local diagonalizing transformations that decouple them, without a loss of time conservation, into systems of scalar equations. This decoupling reduces the computational effort required to solve the LU approximation and can be used for both the steady and unsteady equations.

## References


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