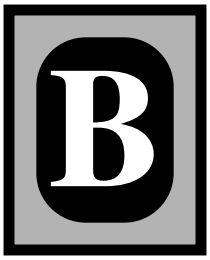

APPENDIX B

Time Advancement

For a nondeforming mesh, Equation (A-1) can be written as

$$\frac{1}{J}\frac{\partial \mathbf{Q}}{\partial t} = R(\mathbf{Q}) \tag{B-1}$$

where

$$R = -\left[\frac{\partial(\hat{\mathbf{F}} - \hat{\mathbf{F}}_v)}{\partial \xi} + \frac{\partial(\hat{\mathbf{G}} - \hat{\mathbf{G}}_v)}{\partial \eta} + \frac{\partial(\hat{\mathbf{H}} - \hat{\mathbf{H}}_v)}{\partial \zeta}\right] \tag{B-2}$$

The time term can be discretized with backward differencing:

$$\frac{(1+\phi)(\mathbf{Q}^{n+1} - \mathbf{Q}^n) - \phi(\mathbf{Q}^n - \mathbf{Q}^{n-1})}{J\Delta t} = R(\mathbf{Q}^{n+1}) \tag{B-3}$$

where the superscripts indicate time level. When $\phi = 0$ the method is first-order temporally accurate; when $\phi = 1/2$ the method is second-order accurate. This equation is implicit because the right-hand side is a function of the unknown flow variables at time level $n+1$.

The CFL3D code is advanced in time with an implicit approximate-factorization method. The implicit derivatives are written as spatially first-order accurate, which results in block-tridiagonal inversions for each sweep. However, for solutions that utilize FDS the block-tridiagonal inversions are usually further simplified with a diagonal algorithm (with a spectral radius scaling of the viscous terms).

Because of the method which the left-hand side is treated for computational efficiency in steady-state simulations (approximate factorization, first-order accuracy), second-order temporal accuracy is forfeited for unsteady computations. One method for recovering the desired accuracy is through the use of sub-iterations. Two different sub-iteration strategies have been implemented in CFL3D. The first method is termed "pseudo time sub-iteration (τ-TS)". The method is also often referred to as the "dual time stepping" method. The other method, termed "physical time sub-iteration (t-TS)," follows Pulliam.[28]

For the τ-TS method, a pseudo time term is added to the time-accurate Navier-Stokes equations.

$$\frac{1}{J}\frac{\partial \mathbf{Q}}{\partial \tau} + \frac{(1+\phi)(\mathbf{Q}^{n+1} - \mathbf{Q}^{n}) - \phi(\mathbf{Q}^{n} - \mathbf{Q}^{n-1})}{J\Delta t} = R(\mathbf{Q}^{n+1}) \tag{B-4}$$

This equation is then discretized and iterated in m, where m is the sub-iteration counter.

$$\frac{(1+\phi')(\mathbf{Q}^{m+1} - \mathbf{Q}^{m}) - \phi'(\mathbf{Q}^{m} - \mathbf{Q}^{m-1})}{J\Delta\tau} + \frac{(1+\phi)(\mathbf{Q}^{m+1} - \mathbf{Q}^{n}) - \phi(\mathbf{Q}^{n} - \mathbf{Q}^{n-1})}{J\Delta t} = R(\mathbf{Q}^{m+1}) \tag{B-5}$$

In Equation (B-5), ϕ and ϕ' govern the order of accuracy of the physical and pseudo time terms, respectively. In practice, the pseudo time term is treated as first order (i.e., $\phi' = 0$), but the general form is shown here for completeness. As $m \to \infty$, the pseudo time term vanishes if the sub-iterations converge and $\mathbf{Q}^{m+1} \to \mathbf{Q}^{n+1}$. If R is linearized with

$$R(\mathbf{Q}^{m+1}) \cong R(\mathbf{Q}^{m}) + \frac{\partial R}{\partial \mathbf{Q}}\Delta\mathbf{Q}^{m} \tag{B-6}$$

and the quantity $-(1+\phi)\mathbf{Q}^{m}/(J\Delta t)$ is added to both sides of Equation (B-5)), then Equation (B-5) becomes

$$\left[\left(\frac{1+\phi'}{J\Delta\tau} + \frac{1+\phi}{J\Delta t}\right)I + \delta_\xi \mathbf{A} + \delta_\eta \mathbf{B} + \delta_\zeta \mathbf{C}\right]\Delta\mathbf{Q}^{m} = \frac{\phi'\Delta\mathbf{Q}^{m-1}}{J\Delta\tau} + \frac{\phi\Delta\mathbf{Q}^{n-1}}{J\Delta t} - \frac{(1+\phi)(\mathbf{Q}^{m} - \mathbf{Q}^{n})}{J\Delta t} + R(\mathbf{Q}^{m}) \tag{B-7}$$

where

$$\Delta\mathbf{Q}^{m} = \mathbf{Q}^{m+1} - \mathbf{Q}^{m} \tag{B-8}$$

$$\mathbf{A} = \frac{\partial(\hat{\mathbf{F}} - \hat{\mathbf{F}}_v)}{\partial \mathbf{Q}} \tag{B-9}$$

$$\mathbf{B} = \frac{\partial(\hat{\mathbf{G}} - \hat{\mathbf{G}}_v)}{\partial \mathbf{Q}} \tag{B-10}$$

$$\mathbf{C} = \frac{\partial(\hat{\mathbf{H}} - \hat{\mathbf{H}}_v)}{\partial \mathbf{Q}} \tag{B-11}$$

Equation (B-7) is approximately factored and written in primitive variable form; it is solved as a series of sweeps in each coordinate direction as

$$\left[\left(\frac{(1+\phi')\mathbf{M}}{J\Delta\tau}+\frac{(1+\phi)\mathbf{M}}{J\Delta t}\right)+\delta_\xi\mathbf{A}^*\right]\Delta\mathbf{q}' = \frac{\phi'\mathbf{M}\Delta\mathbf{q}^{m-1}}{J\Delta\tau}+\frac{\phi\mathbf{M}\Delta\mathbf{q}^{n-1}}{J\Delta t}- \frac{(1+\phi)\mathbf{M}(\mathbf{q}^m-\mathbf{q}^n)}{J\Delta t}+R(\mathbf{q}^m) \tag{B-12}$$

$$\left[\left(\frac{(1+\phi')\mathbf{M}}{J\Delta\tau}+\frac{(1+\phi)\mathbf{M}}{J\Delta t}\right)+\delta_\eta\mathbf{B}^*\right]\Delta\mathbf{q}'' = \left(\frac{(1+\phi')\mathbf{M}}{J\Delta\tau}+\frac{(1+\phi)\mathbf{M}}{J\Delta t}\right)\Delta\mathbf{q}' \tag{B-13}$$

$$\left[\left(\frac{(1+\phi')\mathbf{M}}{J\Delta\tau}+\frac{(1+\phi)\mathbf{M}}{J\Delta t}\right)+\delta_\zeta\mathbf{C}^*\right]\Delta\mathbf{q}^m = \left(\frac{(1+\phi')\mathbf{M}}{J\Delta\tau}+\frac{(1+\phi)\mathbf{M}}{J\Delta t}\right)\Delta\mathbf{q}'' \tag{B-14}$$

$$\mathbf{q}^{m+1} = \mathbf{q}^m + \Delta\mathbf{q}^m \tag{B-15}$$

where the primitive variables are

$$\mathbf{q} = \begin{bmatrix}\rho\\ u\\ v\\ w\\ p\end{bmatrix} \tag{B-16}$$

$$\mathbf{M} = \frac{\partial\mathbf{Q}}{\partial\mathbf{q}} \tag{B-17}$$

$$\mathbf{A}^* = \frac{\partial(\hat{\mathbf{F}}-\hat{\mathbf{F}}_v)}{\partial\mathbf{q}} \tag{B-18}$$

$$\mathbf{B}^* = \frac{\partial(\hat{\mathbf{G}}-\hat{\mathbf{G}}_v)}{\partial\mathbf{q}} \tag{B-19}$$

$$\mathbf{C}^* = \frac{\partial(\hat{\mathbf{H}}-\hat{\mathbf{H}}_v)}{\partial\mathbf{q}} \tag{B-20}$$

The quantity $\Delta\tau$ is based on a constant CFL number set by the input parameter **cfl_tau** (See “LT5 - Time Step Parameters” on page 21). Multigrid is used to drive $\Delta\mathbf{q}^m$ to zero in a reasonable number of sub-iterations.

In the t-TS method, Equation (B-3) is merely iterated in m, where m is the sub-iteration counter:

$$\frac{(1+\phi)(\mathbf{Q}^{m+1}-\mathbf{Q}^{n})-\phi(\mathbf{Q}^{n}-\mathbf{Q}^{n-1})}{J\Delta t} = R(\mathbf{Q}^{m+1}) \tag{B-21}$$

The quantity $-(1+\phi)\mathbf{Q}^{m}/(J\Delta t)$ is added to both sides, the residual is linearized, and the equation is approximately factored and written in primitive variable form as

$$\left[\frac{(1+\phi)\mathbf{M}}{J\Delta t}+\delta_{\xi}\mathbf{A}^{*}\right]\Delta\mathbf{q}' = \frac{\phi\mathbf{M}\Delta\mathbf{q}^{n-1}}{J\Delta t}-\frac{(1+\phi)\mathbf{M}(\mathbf{q}^{m}-\mathbf{q}^{n})}{J\Delta t}+R(\mathbf{q}^{m}) \tag{B-22}$$

$$\left[\frac{(1+\phi)\mathbf{M}}{J\Delta t}+\delta_{\eta}\mathbf{B}^{*}\right]\Delta\mathbf{q}'' = \frac{(1+\phi)\mathbf{M}}{J\Delta t}\Delta\mathbf{q}' \tag{B-23}$$

$$\left[\frac{(1+\phi)\mathbf{M}}{J\Delta t}+\delta_{\zeta}\mathbf{C}^{*}\right]\Delta\mathbf{q}^{m} = \frac{(1+\phi)\mathbf{M}}{J\Delta t}\Delta\mathbf{q}'' \tag{B-24}$$

$$\mathbf{q}^{m+1} = \mathbf{q}^{m}+\Delta\mathbf{q}^{m} \tag{B-25}$$

As $m\to\infty$, $\mathbf{q}^{m+1}\to\mathbf{q}^{n+1}$. When only one series of sweeps is performed, $\mathbf{q}^{m} = \mathbf{q}^{n}$ and the standard time-accurate CFL3D scheme is recovered (i.e., no sub-iterations). Unlike the τ-TS method, this sub-iteration procedure (Equation (B-22) through Equation (B-25)) utilizes only one time step: the physical time step Δt (= constant).

Prior to the execution of Equation (B-25) in the code, the corrections are constrained in order to maintain the positivity of the thermodynamic variables ρ and p. For example, the update to pressure is taken as

$$p^{n+1} = p^{n}+\Delta p\left[1+\phi_{c}\left(\alpha_{c}+\left|\frac{\Delta p}{p^{n}}\right|\right)\right]^{-1} \tag{B-26}$$

whenever $\Delta p/p^{n}\le\alpha_{c}$. Currently, $\alpha_{c} = -0.2$ and $\phi_{c} = 2.0$.

In the limit of $\Delta p/p^{n}\to-\infty$, $p^{n+1}\to p^{n}/2$. This modification improves the robustness of the method by allowing it to proceed through local transients encountered during the convergence process which would otherwise terminate the calculation.

When running steady-state computations (**dt** < 0), the time step advanced locally in each cell is related to the input CFL number by

$$\Delta t = \frac{\mathrm{CFL}}{|\nabla\xi|t_{1}+|\nabla\eta|t_{2}+|\nabla\zeta|t_{3}} \tag{B-27}$$

where

$$t_1 = |\overline{U}| + a + 2|\nabla\xi|(\mu + \mu_T)\max\left(\frac{4}{3}, \frac{\gamma}{Pr}\right)\frac{M}{Re_{\tilde{L}_R}}\frac{1}{\rho}$$

$$t_2 = |\overline{V}| + a + 2|\nabla\eta|(\mu + \mu_T)\max\left(\frac{4}{3}, \frac{\gamma}{Pr}\right)\frac{M}{Re_{\tilde{L}_R}}\frac{1}{\rho} \qquad \textbf{(B-28)}$$

$$t_3 = |\overline{W}| + a + 2|\nabla\zeta|(\mu + \mu_T)\max\left(\frac{4}{3}, \frac{\gamma}{Pr}\right)\frac{M}{Re_{\tilde{L}_R}}\frac{1}{\rho}$$

where $\overline{U} = U/|\nabla\xi|$, $\overline{V} = V/|\nabla\eta|$, $\overline{W} = W/|\nabla\zeta|$ and U, V, and W are defined in Equation (A-7) in Appendix A. The viscous scaling terms (the last term in each equation of Equation (B-28)) are only used when the solution includes viscous terms. They arise from a spectral radius scaling (see Coakley[14]).