APPENDIX F

Generalized Coordinates

F.1 Navier-Stokes Equations in Cartesian Coordinates

The compressible three-dimensional Navier-Stokes equations, excluding body forces and external heat sources, in Cartesian coordinates are

\[
\frac{\partial Q}{\partial t} + \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} + \frac{\partial h}{\partial z} = 0
\]  

(F-1)

where

\[
Q = \begin{bmatrix}
\rho \\
\rho u \\
\rho v \\
\rho w \\
e
\end{bmatrix}
\]

(F-2)

\[
f = \begin{bmatrix}
\rho u \\
\rho u^2 + p - \tau_{xx} \\
\rho uv - \tau_{xy} \\
\rho uw - \tau_{xz} \\
(e + p)u - u\tau_{xx} - v\tau_{xy} - w\tau_{xz} + q_x
\end{bmatrix}
\]

(F-3)

\[
g = \begin{bmatrix}
\rho v \\
\rho uv - \tau_{xy} \\
\rho v^2 + p - \tau_{yy} \\
\rho vw - \tau_{yz} \\
(e + p)v - u\tau_{xy} - v\tau_{yy} - w\tau_{yz} + q_y
\end{bmatrix}
\]

(F-4)
$$h = \begin{bmatrix} \rho w \\ \rho u w - \tau_{xz} \\ \rho v w - \tau_{yz} \\ \rho v^2 + p - \tau_{zz} \\ (e + p) w - u \tau_{xz} - v \tau_{yz} - w \tau_{zz} + q_z \end{bmatrix}$$ (F-5)

and

$$\tau_{xx} = \frac{2}{3} \mu \left(2 \frac{\partial u}{\partial x} \frac{\partial v}{\partial y} - \frac{\partial w}{\partial z}\right)$$ (F-6)

$$\tau_{yy} = \frac{2}{3} \mu \left(2 \frac{\partial v}{\partial y} \frac{\partial u}{\partial x} - \frac{\partial w}{\partial z}\right)$$ (F-7)

$$\tau_{zz} = \frac{2}{3} \mu \left(2 \frac{\partial w}{\partial z} - \frac{\partial u}{\partial x} \frac{\partial v}{\partial y}\right)$$ (F-8)

$$\tau_{xy} = \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) = \tau_{yx}$$ (F-9)

$$\tau_{xz} = \mu \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z}\right) = \tau_{zx}$$ (F-10)

$$\tau_{yz} = \mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right) = \tau_{zy}$$ (F-11)

The pressure is defined by the equation of state for an ideal gas:

$$p = (\gamma - 1) \left[ e - \frac{\rho}{2} (u^2 + v^2 + w^2) \right]$$ (F-12)

### F.2 Transformation to Generalized Coordinates

Now apply the generalized coordinate transformation

$$\xi = \xi(x, y, z, t)$$

$$\eta = \eta(x, y, z, t)$$ (F-13)

$$\zeta = \zeta(x, y, z, t)$$

From the chain-rule for a function of multiple variables,
\[ \frac{\partial}{\partial x} = \xi_x \frac{\partial}{\partial \xi} + \eta_x \frac{\partial}{\partial \eta} + \zeta_x \frac{\partial}{\partial \zeta} + t_x \frac{\partial}{\partial t} \]
\[ \frac{\partial}{\partial y} = \xi_y \frac{\partial}{\partial \xi} + \eta_y \frac{\partial}{\partial \eta} + \zeta_y \frac{\partial}{\partial \zeta} + t_y \frac{\partial}{\partial t} \]
\[ \frac{\partial}{\partial z} = \xi_z \frac{\partial}{\partial \xi} + \eta_z \frac{\partial}{\partial \eta} + \zeta_z \frac{\partial}{\partial \zeta} + t_z \frac{\partial}{\partial t} \]
\[ \frac{\partial}{\partial t} = \xi_t \frac{\partial}{\partial \xi} + \eta_t \frac{\partial}{\partial \eta} + \zeta_t \frac{\partial}{\partial \zeta} + t_t \frac{\partial}{\partial t} \]

where $\xi_x$, $\eta_x$, $\xi_y$, $\eta_y$, $\xi_z$, $\eta_z$, $\xi_t$, $\eta_t$, $\zeta_t$ are the metrics.

**F.2.1 Obtaining the Metrics**

The metrics are determined as follows. (For a description of the geometrical evaluation of the metrics, see “Geometrical Evaluation of the Metrics” on page 263.) The derivatives of the generalized coordinates can be written

\[ d\xi = \xi_x dx + \xi_y dy + \xi_z dz + \xi_t dt \]
\[ d\eta = \eta_x dx + \eta_y dy + \eta_z dz + \eta_t dt \]
\[ d\zeta = \zeta_x dx + \zeta_y dy + \zeta_z dz + \zeta_t dt \]
\[ dt = t_x dx + t_y dy + t_z dz + t_t dt \]

or, in matrix form (noting that $t_x = t_y = t_z = 0$ and $t_t = 1$),

\[
\begin{bmatrix}
    d\xi \\
    d\eta \\
    d\zeta \\
    dt
\end{bmatrix} =
\begin{bmatrix}
    \xi_x & \xi_y & \xi_z & \xi_t \\
    \eta_x & \eta_y & \eta_z & \eta_t \\
    \zeta_x & \zeta_y & \zeta_z & \zeta_t \\
    0 & 0 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
    dx \\
    dy \\
    dz \\
    dt
\end{bmatrix}
\]

(F-16)

Similarly, the derivatives of the Cartesian coordinates can be written

\[
\begin{bmatrix}
    dx \\
    dy \\
    dz \\
    dt
\end{bmatrix} =
\begin{bmatrix}
    x_\xi & x_\eta & x_\zeta & x_t \\
    y_\xi & y_\eta & y_\zeta & y_t \\
    z_\xi & z_\eta & z_\zeta & z_t \\
    0 & 0 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
    d\xi \\
    d\eta \\
    d\zeta \\
    dt
\end{bmatrix}
\]

(F-17)

Therefore, it is evident that
The Jacobian of the transformation is defined to be

\[
\begin{bmatrix}
\xi_x & \xi_y & \xi_z & \xi_t \\
\eta_x & \eta_y & \eta_z & \eta_t \\
\zeta_x & \zeta_y & \zeta_z & \zeta_t \\
0 & 0 & 0 & 1
\end{bmatrix}
= \begin{bmatrix} x_x & x_y & x_z & x_t \\ y_x & y_y & y_z & y_t \\ z_x & z_y & z_z & z_t \\ 0 & 0 & 0 & 1 \end{bmatrix}^{-1} \tag{F-18}
\]

To determine the inverse matrix represented on the right-hand side of Equation (F-18), first the cofactor matrix is found to be:

\[
\begin{bmatrix}
(y_\eta z_\zeta - y_\zeta z_\eta) & -(y_\xi z_\zeta - y_\zeta z_\xi) & (y_\xi z_\eta - y_\eta z_\xi) & 0 \\
-(x_\eta z_\zeta - x_\zeta z_\eta) & (x_\xi z_\zeta - x_\zeta z_\xi) & -(x_\xi z_\eta - x_\eta z_\xi) & 0 \\
(x_\eta y_\zeta - x_\zeta y_\eta) & -(x_\xi y_\zeta - x_\zeta y_\xi) & (x_\xi y_\eta - x_\eta y_\xi) & 0 \\
0 & -C F_{41} & -C F_{42} & -C F_{43} \end{bmatrix} \tag{F-19}
\]

where

\[
C F_{41} = -x_t (y_\eta z_\zeta - y_\zeta z_\eta) - y_t (x_\xi z_\eta - x_\eta z_\xi) - z_t (x_\eta y_\xi - x_\xi y_\eta) \\
C F_{42} = x_t (y_\xi z_\zeta - y_\zeta z_\xi) + y_t (x_\xi z_\eta - x_\eta z_\xi) + z_t (x_\xi y_\eta - x_\eta y_\xi) \tag{F-20} \\
C F_{43} = -x_t (y_\xi z_\zeta - y_\zeta z_\xi) - y_t (x_\xi z_\eta - x_\eta z_\xi) - z_t (x_\xi y_\eta - x_\eta y_\xi) \\
C F_{44} = x_t (y_\eta z_\zeta - y_\zeta z_\eta) + x_t (y_\xi z_\eta - y_\zeta z_\xi) + x_t (y_\xi z_\eta - y_\zeta z_\xi)
\]

The transpose of the cofactor matrix (i.e. the adjoint matrix) is

\[
\begin{bmatrix}
(y_\eta z_\zeta - y_\zeta z_\eta) & -(x_\eta z_\zeta - x_\zeta z_\eta) & (x_\eta y_\zeta - x_\zeta y_\eta) & CF_{41} \\
-(y_\xi z_\zeta - y_\zeta z_\xi) & (x_\xi z_\zeta - x_\zeta z_\xi) & -(x_\xi y_\zeta - x_\zeta y_\xi) & CF_{42} \\
(x_\eta y_\zeta - x_\zeta y_\eta) & -(x_\xi y_\zeta - x_\zeta y_\xi) & (x_\xi y_\eta - x_\eta y_\xi) & CF_{43} \\
0 & 0 & 0 & 0 & CF_{44} \end{bmatrix} \tag{F-21}
\]

The determinant of the inverse matrix represented on the right-hand side of Equation (F-18) is

\[
\begin{vmatrix}
x_x & x_y & x_z & x_t \\
y_x & y_y & y_z & y_t \\
z_x & z_y & z_z & z_t \\
0 & 0 & 0 & 1
\end{vmatrix} = x_\xi (y_\eta z_\zeta - y_\zeta z_\eta) - x_\eta (y_\xi z_\zeta - y_\zeta z_\xi) + x_\zeta (y_\xi z_\eta - y_\eta z_\xi) \tag{F-22}
\]

The Jacobian of the transformation is defined to be
Therefore,

\[ J = \frac{\partial (\xi, \eta, \zeta, t)}{\partial (x, y, z, t)} = \begin{vmatrix} \xi_x & \xi_y & \xi_z & \xi_t \\ \eta_x & \eta_y & \eta_z & \eta_t \\ \zeta_x & \zeta_y & \zeta_z & \zeta_t \\ 0 & 0 & 0 & 1 \end{vmatrix} \quad (F-23) \]

Note that \( CF_{44} = 1/J \). Now, from the property of an invertible matrix \( D \),

\[ D^{-1} = \frac{1}{\det(D)} \text{adj}(D) \quad (F-25) \]

let

\[
D = \begin{bmatrix} x_\xi & x_\eta & x_\zeta & x_t \\ y_\xi & y_\eta & y_\zeta & y_t \\ z_\xi & z_\eta & z_\zeta & z_t \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad (F-26)
\]

It follows from Equation (F-18) that

\[
D^{-1} = J^{-1} = \begin{bmatrix} (y_\eta \zeta - y_\zeta \eta) & (x_\eta \zeta - x_\zeta \eta) & (x_\eta y_\zeta - x_\zeta y_\eta) & CF_{41} \\ -(y_\eta \zeta - y_\zeta \eta) & (x_\eta \zeta - x_\zeta \eta) & (x_\eta y_\zeta - x_\zeta y_\eta) & CF_{42} \\ (y_\xi \eta - y_\eta \xi) & -(x_\xi \eta - x_\eta \xi) & (x_\xi y_\eta - x_\eta y_\xi) & CF_{43} \\ 0 & 0 & 0 & 1/J \end{bmatrix} \quad (F-27)
\]

Therefore, the metrics are
\[ \xi_x = J(y_\eta z_\zeta - y_\zeta z_\eta) \]
\[ \xi_y = J(x_\zeta z_\eta - x_\eta z_\zeta) \]
\[ \xi_z = J(x_\eta y_\zeta - x_\zeta y_\eta) \]
\[ \xi_t = -x_t \xi_x - y_t \xi_y - z_t \xi_z \]
\[ \eta_x = J(y_\zeta z_\xi - y_\xi z_\zeta) \]
\[ \eta_y = J(x_\xi z_\eta - x_\eta z_\xi) \]
\[ \eta_z = J(x_\eta y_\xi - x_\xi y_\eta) \]
\[ \eta_t = -x_t \eta_x - y_t \eta_y - z_t \eta_z \]
\[ \zeta_x = J(y_\xi z_\eta - y_\eta z_\xi) \]
\[ \zeta_y = J(x_\eta z_\xi - x_\xi z_\eta) \]
\[ \zeta_z = J(x_\xi y_\eta - x_\eta y_\xi) \]
\[ \zeta_t = -x_t \zeta_x - y_t \zeta_y - z_t \zeta_z \]

\[ (F-28) \]

**F.2.2 Applying the Transformation**

Now, to apply the transformation to the Navier-Stokes equations represented in Equation (F-1), substitute Equation (F-14) into Equation (F-1) and multiply by \(1/J\):

\[
\frac{1}{J} \frac{\partial}{\partial t} Q + \frac{\partial}{\partial \xi_x} \left( \frac{f}{J} \frac{\xi_x}{J} \right) + \frac{\partial}{\partial \xi_y} \left( \frac{g}{J} \frac{\xi_y}{J} \right) + \frac{\partial}{\partial \xi_z} \left( \frac{h}{J} \frac{\xi_z}{J} \right) + \frac{\partial}{\partial \eta_t} \left( \frac{f}{J} \frac{\eta_t}{J} \right) + \frac{\partial}{\partial \eta_x} \left( \frac{f}{J} \frac{\eta_x}{J} \right) + \frac{\partial}{\partial \eta_y} \left( \frac{g}{J} \frac{\eta_y}{J} \right) + \frac{\partial}{\partial \eta_z} \left( \frac{h}{J} \frac{\eta_z}{J} \right) + \frac{\partial}{\partial \zeta_t} \left( \frac{f}{J} \frac{\zeta_t}{J} \right) + \frac{\partial}{\partial \zeta_x} \left( \frac{f}{J} \frac{\zeta_x}{J} \right) + \frac{\partial}{\partial \zeta_y} \left( \frac{g}{J} \frac{\zeta_y}{J} \right) + \frac{\partial}{\partial \zeta_z} \left( \frac{h}{J} \frac{\zeta_z}{J} \right) = 0
\]

(Remember, however, that \(t_x = t_y = t_z = 0\)). Since

\[
\frac{\partial}{\partial \xi} \left( \frac{f}{J} \frac{\xi_x}{J} \right) = \frac{\partial}{\partial \xi} \left( \frac{f}{J} \right) \frac{\xi_x}{J} + \frac{\xi_x}{J} \frac{\partial}{\partial \xi} \left( \frac{f}{J} \right)
\]

(F-30)

Then,

\[
\frac{\xi_x}{J} \frac{\partial}{\partial \xi} \left( \frac{f}{J} \frac{\xi_x}{J} \right) = \frac{\partial}{\partial \xi} \left( \frac{f}{J} \frac{\xi_x}{J} \right) - \left( \frac{\xi_x}{J} \frac{\partial}{\partial \xi} \left( \frac{f}{J} \right) \right)
\]

(F-31)

So, Equation (F-29) becomes
Consider the fifth major term in Equation (F-33):

$$\frac{\partial}{\partial t} \left( \frac{Q}{J} \right) + \frac{\partial}{\partial \xi} \left[ f \xi_x + g \xi_y + h \xi_z + Q \xi_t \right] = 0$$

The summation of the terms in Equation (F-34) is zero. The same can be shown for the sixth, seventh and eighth major terms in Equation (F-33). Therefore, Equation (F-33) can be written
\[
\frac{\partial}{\partial t}(Q) + \frac{\partial}{\partial \xi_x} \int J (f \xi_x + g \xi_y + h \xi_z + Q \xi_i) \right]
+ \frac{\partial}{\partial \eta} \int J (f \eta_x + g \eta_y + h \eta_z + Q \eta_i) \right]
+ \frac{\partial}{\partial \zeta} \int J (f \zeta_x + g \zeta_y + h \zeta_z + Q \zeta_i) \right] = 0
\]

When summed, the expression in the second major term in Equation (F-35) can be written

\[
f \xi_x + g \xi_y + h \xi_z + Q \xi_i = \begin{bmatrix}
\rho U \\
\rho Uu + p \xi_x \\
\rho Uv + p \xi_y \\
\rho Uw + p \xi_z \\
(e + p)U - \xi_i \rho
\end{bmatrix} - \begin{bmatrix}
0 \\
\xi_x \tau_{xx} + \xi_y \tau_{xy} + \xi_z \tau_{xz} \\
\xi_x \tau_{xy} + \xi_y \tau_{yy} + \xi_z \tau_{yz} \\
\xi_x \tau_{xz} + \xi_y \tau_{yz} + \xi_z \tau_{zz} \\
\xi_x b_x + \xi_y b_y + \xi_z b_z
\end{bmatrix}
\]

where

\[
U = \xi_x u + \xi_y v + \xi_z w + \xi_i
\]

\[
b_x = u \tau_{xx} + v \tau_{xy} + w \tau_{xz} + \dot{q}_x
\]

\[
b_y = u \tau_{xy} + v \tau_{yy} + w \tau_{yz} + \dot{q}_y
\]

\[
b_z = u \tau_{xz} + v \tau_{yz} + w \tau_{zz} + \dot{q}_z
\]

Equation (F-38) can be written compactly using indicial notation as

\[
b_{xi} = u_j \tau_{xixj} - \dot{q}_{xi}
\]

with \(i = 1, 2, 3\) and \(j = 1, 2, 3\) where 1 indicates the x direction, 2 indicates the y direction, and 3 indicates the z direction.
F.3 Navier-Stokes Equation in Generalized Coordinates

Now, let

\[
\mathbf{F} = \begin{bmatrix}
\rho U \\
\rho Uu + p\xi_x \\
\rho Uv + p\xi_y \\
\rho Uw + p\xi_z \\
(e + p)U - \xi_ip
\end{bmatrix}, \quad \mathbf{F}_v = \begin{bmatrix}
0 \\
\xi_x \tau_{xx} + \xi_y \tau_{xy} + \xi_z \tau_{xz} \\
\xi_x \tau_{xy} + \xi_y \tau_{yy} + \xi_z \tau_{yz} \\
\xi_x \tau_{xz} + \xi_y \tau_{yz} + \xi_z \tau_{zz} \\
\xi_x b_x + \xi_y b_y + \xi_z b_z
\end{bmatrix}
\]  

(F-40)

Combining the other terms in a similar manner and letting \( \hat{\mathbf{Q}} = \mathbf{Q}/J, \hat{\mathbf{F}} = \mathbf{F}/J, \hat{\mathbf{F}}_v = \mathbf{F}_v/J, \hat{\mathbf{G}} = \mathbf{G}/J, \hat{\mathbf{G}}_v = \mathbf{G}_v/J, \hat{\mathbf{H}} = \mathbf{H}/J, \hat{\mathbf{H}}_v = \mathbf{H}_v/J \), Equation (F-35) can be written

\[
\frac{\partial \hat{\mathbf{Q}}}{\partial t} + \frac{\partial (\hat{\mathbf{F}} - \hat{\mathbf{F}}_v)}{\partial \xi} + \frac{\partial (\hat{\mathbf{G}} - \hat{\mathbf{G}}_v)}{\partial \eta} + \frac{\partial (\hat{\mathbf{H}} - \hat{\mathbf{H}}_v)}{\partial \zeta} = 0
\]  

(F-41)

The terms are as shown in Appendix A, Equations (A-3) through (A-14).

F.4 Geometrical Evaluation of the Metrics

By analogy with the integral form of the equations, a geometrical interpretation of the metric terms can be made. The vector \( \nabla k/J \) is the directed area of the cell interface normal to a \( k = \text{constant} \) coordinate direction (\( k = \xi, \eta, \) or \( \zeta \)). (See Figure F-1.) The unit vector \( (k_x, k_y, k_z)/|\nabla k| \) is composed of the direction cosines of the cell interface and \( |\nabla k|/J \) is the area of the cell interface. Note that

\[
\nabla k = k_x \hat{i} + k_y \hat{j} + k_z \hat{k}
\]

\[
|\nabla k| = \sqrt{k_x^2 + k_y^2 + k_z^2}
\]  

(F-42)

The directed areas are calculated as one-half the vector product of the two diagonal vectors connecting opposite vertex points of a cell face, taken such that the directed area is parallel to the direction of increasing \( k \).

Likewise, the normalized contravariant velocity, \( \mathbf{U} = U/|\nabla \xi| \), for example, represents the relative velocity normal to a \( \xi \) interface, where \( -\hat{\xi}_r = -\xi_r/|\nabla \xi| \) is the grid speed normal to the interface. The volume of the cell is \( 1/J \) and is determined by sum-
ming the volumes of the six pentahedra forming the hexagonal cell. Each pentahedron is defined by one of the six cell faces and the average point in the volume. The net effect is that the difference equations are satisfied identically when evaluated at free-stream conditions on arbitrary meshes.

In the code, the metric arrays are set up as follows using the $\xi$ direction as an example.

\[
\begin{align*}
si(j,k,i,1) &= \xi_x/|\nabla \xi| \equiv \hat{\xi}_x = x \text{ component of unit normal to } i \text{ face} \\
si(j,k,i,2) &= \xi_y/|\nabla \xi| \equiv \hat{\xi}_y = y \text{ component of unit normal to } i \text{ face} \\
si(j,k,i,3) &= \xi_z/|\nabla \xi| \equiv \hat{\xi}_z = z \text{ component of unit normal to } i \text{ face} \\
si(j,k,i,4) &= |\nabla \xi|/J = i \text{ face area} \\
si(j,k,i,5) &= -\xi_i/|\nabla \xi| = i \text{ face normal velocity}
\end{align*}
\]