Appendix E

Numerical Treatment of Subgrid Transport Equations

In the Appendix D, the subgrid momentum, scalar, turbulent kinetic energy and dissipation rate equations were derived. Each of the subgrid transport equations can be written in the following generic form:

$$\frac{\rho U}{\sqrt{g_{11}}}\left(\frac{\partial \phi}{\partial \xi}\right)^* + \frac{\rho V}{\sqrt{g_{22}}}\left(\frac{\partial \phi}{\partial \eta}\right)^* + \frac{\rho W}{\sqrt{g_{33}}}\left(\frac{\partial \phi}{\partial \zeta}\right)^* = \frac{1}{J}\frac{\partial}{\partial \zeta}\left(Jg^{33}\Gamma\frac{\partial \phi}{\partial \zeta}\right) + C \tag{E.1}$$

where ϕ denotes one of the subgrid parameters: U, V, k or $\tilde{\varepsilon}$, Γ is the diffusivity and the source term, C, includes all geometry-related source terms and the pressure gradient in the momentum equations. Following the finite-volume method, the subgrid transport equations are discretized and integrated over subgrid control volumes which have physical dimensions ($J\Delta\xi\Delta\eta\Delta\zeta$) where, in the present treatment, it is assumed that the ξ-axis is parallel to east-west, η-axis north-south and ζ-axis top-bottom (the wall-normal direction). Using the same method as used previously for the UMIST-N wall function, gradients appearing in diffusion and source terms are calculated using central differencing while convective terms are discretized using upwind differencing.

E.1 1-D Diffusion

Considering only diffusion and the source term, the generic subgrid transport equation can be written:

$$\frac{1}{J}\frac{\partial}{\partial \zeta}\left(Jg^{33}\Gamma\frac{\partial \phi}{\partial \zeta}\right) + C = 0 \tag{E.2}$$

which is discretized:

$$\frac{1}{\Delta\zeta_{tb}}\left(\frac{1}{J}\right)_P\left[\left(Jg^{33}\Gamma\frac{\partial \phi}{\partial \zeta}\right)_t - \left(Jg^{33}\Gamma\frac{\partial \phi}{\partial \zeta}\right)_b\right] + (C)_P = 0 \tag{E.3}$$

and integrated over the control volume (where $\Delta Vol = J\Delta\xi_{ew}\Delta\eta_{ns}\Delta\zeta_{tb}$):

$$\left[\left(Jg^{33}\Gamma\right)_t \frac{(\phi_T - \phi_P)}{\Delta\zeta_{TP}} - \left(Jg^{33}\Gamma\right)_b \frac{(\phi_P - \phi_B)}{\Delta\zeta_{PB}}\right] \Delta\xi_{ew}\Delta\eta_{ns} + (C)_P \Delta Vol \tag{E.4}$$

where subscripts T, P, and B refer to the top, current and bottom nodes respectively, t and b denote values at the top and bottom boundaries of the subgrid cell, respectively. Equation (E.4) can be rearranged into:

$$D_t(\phi_T - \phi_P) - D_b(\phi_P - \phi_B) + (C)_P \Delta Vol = 0 \tag{E.5}$$

where:

$$D_t = \left(Jg^{33}\Gamma\right)_t \frac{\Delta\xi_{ew}\Delta\eta_{ew}}{\Delta\zeta_{TP}} \tag{E.6}$$

$$D_b = \left(Jg^{33}\Gamma\right)_b \frac{\Delta\xi_{ew}\Delta\eta_{ns}}{\Delta\zeta_{PB}} \tag{E.7}$$

Grouping coefficients of ϕ_P, Equation (E.5) becomes:

$$D_t\phi_T + D_b\phi_B + (C)_P \Delta Vol = (D_t + D_b)\,\phi_P \tag{E.8}$$

This can be expressed as:

$$a_P\phi_P = a_T\phi_T + a_B\phi_B + S \tag{E.9}$$

where:

$$a_T = D_t = \left(Jg^{33}\Gamma\right)_t \frac{\Delta\xi_{ew}\Delta\eta_{ew}}{\Delta\zeta_{TP}} \tag{E.10}$$

$$a_B = D_b = \left(Jg^{33}\Gamma\right)_b \frac{\Delta\xi_{ew}\Delta\eta_{ns}}{\Delta\zeta_{PB}} \tag{E.11}$$

$$a_P = a_T + a_B \tag{E.12}$$

$$S = (C)_P \Delta Vol \tag{E.13}$$

It is assumed that the cells have unit dimensions in curvilinear coordinates, i.e.:

$$\Delta\xi_{ew} = \Delta\eta_{ns} = \Delta\zeta_{tb} = 1 \tag{E.14}$$

Additionally, the distances between adjacent nodes are assumed to be unity so that, for example:

$$\Delta\xi_{EP} = 1 \tag{E.15}$$

In the subgrid cells adjacent to boundaries the distance from the node to the boundary is half a cell width. For example, the subgrid cell adjacent to bottom boundary shown in Figure E.1 has $\Delta\zeta_{PB} = 0.5$. The covariant metric tensor $(g_{33})_b$ at the bottom boundary of the near-wall cell is given by:

$$(g_{33})_b = \frac{\partial z}{\partial \zeta}\frac{\partial z}{\partial \zeta} = \left(\frac{z_P - z_B}{\Delta\zeta_{PB}}\right)^2 = \left(\frac{\Delta z_{PB}}{0.5}\right)^2 \tag{E.16}$$

the Jacobian, J, at the bottom boundary is calculated from:

$$(J)_b = (\sqrt{g_{11}g_{22}g_{33}})_b = 2\Delta x_{ew}\Delta y_{ns}\Delta z_{PB} \tag{E.17}$$

and the contravariant metric tensor $\left(g^{33}\right)_b$ is given by:

$$\left(g^{33}\right)_b = \frac{1}{J^2}g_{11}g_{22} = \frac{(\Delta x_{ew}\Delta y_{ns})^2}{4\left(\Delta x_{ew}\Delta y_{ns}\Delta z_{PB}\right)^2} = \frac{1}{4\left(\Delta z_{PB}\right)^2} \tag{E.18}$$

Substituting these expressions into Equation (E.11) for the diffusion coefficient at the bottom boundary:

$$\begin{aligned} a_B &= \left(Jg^{33}\Gamma\right)_b \frac{\Delta\xi_{ew}\Delta\eta_{ns}}{\Delta\zeta_{PB}} \\ &= 2\Delta x_{ew}\Delta y_{ns}\Delta z_{PB}\frac{1}{4\left(\Delta z_{PB}\right)^2}\Gamma_b\frac{1}{0.5} \\ &= \frac{\Delta x_{ew}\Delta y_{ns}\Gamma_b}{\Delta z_{PB}} \end{aligned} \tag{E.19}$$

This is exactly the same form as would be expected in a standard Cartesian discretization of the diffusion term. The coefficients are in the form ($a_B = \Gamma_b A/L$), where A is the cross-sectional area of the cell and L is the distance between the near-wall node and the node on the boundary.

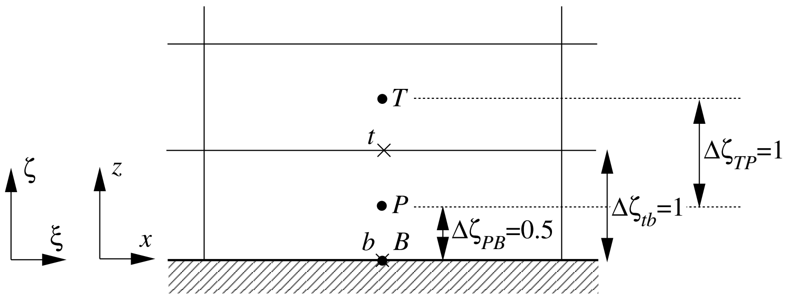

Figure E.1: Near-wall subgrid arrangement showing the location of the nodes and the computational cell widths.

E.2 Convection Parallel to the Wall

Convection of scalar ϕ in the ξ-direction is integrated over the subgrid cell volume (ΔVol) and added into the discretized equation source term, S, as follows:

$$S = -\int_{\Delta Vol} \frac{\rho U}{\sqrt{g_{11}}} \frac{\partial \phi}{\partial \xi} \mathrm{d}Vol \tag{E.20}$$

where the minus sign is introduced since the convection term is moved from the left- to the right-hand-side of the transport equation (Equation E.1). Using an upwind scheme, the convective ξ-direction source term is given by:

$$S = -\left(\frac{\rho U}{\sqrt{g_{11}}}\right)_P \frac{(\phi_P - \phi_W)}{\Delta \xi_{PW}} \Delta Vol \qquad \text{for} \quad U_P > 0 \tag{E.21}$$

$$S = -\left(\frac{\rho U}{\sqrt{g_{11}}}\right)_P \frac{(\phi_E - \phi_P)}{\Delta \xi_{EP}} \Delta Vol \qquad \text{for} \quad U_P < 0 \tag{E.22}$$

Rearranging these expressions in terms of coefficients of ϕ_P, ϕ_E and ϕ_W and splitting the source S into s_U and s_P terms (as described in Chapter 3) one obtains the following expressions:

$$\left.\begin{aligned} s_U &= \left(\frac{\rho U}{\sqrt{g_{11}}}\right)_P \frac{\phi_W}{\Delta \xi_{PW}} \Delta Vol \\ s_P &= -\left(\frac{\rho U}{\sqrt{g_{11}}}\right)_P \frac{1}{\Delta \xi_{PW}} \Delta Vol \end{aligned}\right\} \qquad \text{for} \quad U_P > 0 \tag{E.23}$$

$$\left.\begin{aligned} s_U &= -\left(\frac{\rho U}{\sqrt{g_{11}}}\right)_P \frac{\phi_E}{\Delta \xi_{EP}} \Delta Vol \\ s_P &= \left(\frac{\rho U}{\sqrt{g_{11}}}\right)_P \frac{1}{\Delta \xi_{EP}} \Delta Vol \end{aligned}\right\} \qquad \text{for} \quad U_P < 0 \tag{E.24}$$

where the discretized equation is given by:

$$(a_P - s_P)\,\phi_P = a_T \phi_T + a_B \phi_B + s_U \tag{E.25}$$

Using a similar approach one can show that the convective flux in the wall-parallel η-direction results in the following source terms:

$$\left.\begin{aligned} s_U &= \left(\frac{\rho V_P}{\sqrt{g_{22}}}\right)_P \frac{\phi_S}{\Delta \eta_{PS}} \Delta Vol \\ s_P &= -\left(\frac{\rho V_P}{\sqrt{g_{22}}}\right)_P \frac{1}{\Delta \eta_{PS}} \Delta Vol \end{aligned}\right\} \qquad \text{for} \quad V_P > 0 \tag{E.26}$$

$$\left.\begin{aligned} s_U &= -\left(\frac{\rho V_P}{\sqrt{g_{22}}}\right)_P \frac{\phi_N}{\Delta\eta_{NP}}\Delta Vol \\ s_P &= \left(\frac{\rho V_P}{\sqrt{g_{22}}}\right)_P \frac{1}{\Delta\eta_{NP}}\Delta Vol \end{aligned}\right\} \quad \text{for} \quad V_P < 0 \tag{E.27}$$

E.3 Convection Normal to the Wall

Convection of scalar ϕ in the ζ-direction is integrated over the subgrid cell volume and added into the discretized equation source term, S, as follows:

$$S = -\int_{\Delta Vol} \frac{\rho W}{\sqrt{g_{33}}}\frac{\partial \phi}{\partial \zeta}\mathrm{d}Vol \tag{E.28}$$

where the W-velocity is obtained from subgrid continuity with additional scaling to satisfy the boundary conditions, as described in Section E.7. Using an upwind scheme, the convective ζ-direction source term is given by:

$$S = -\left(\frac{\rho W}{\sqrt{g_{33}}}\right)_P \frac{(\phi_P - \phi_B)}{\Delta\zeta_{PB}}\Delta Vol \qquad \text{for} \quad W_P > 0 \tag{E.29}$$

$$S = -\left(\frac{\rho W}{\sqrt{g_{33}}}\right)_P \frac{(\phi_T - \phi_P)}{\Delta\zeta_{TP}}\Delta Vol \qquad \text{for} \quad W_P < 0 \tag{E.30}$$

The above source terms can be rearranged in terms of coefficients of the nodal terms ϕ_N, ϕ_P and ϕ_S and then split into contributions for the source term s_P and the coefficients a_T and a_B, as follows:

$$\left.\begin{aligned} s_P &= -\left(\frac{\rho W}{\sqrt{g_{33}}}\right)_P \frac{1}{\Delta\zeta_{PB}}\Delta Vol \\ a_T &= 0 \\ a_B &= \left(\frac{\rho W}{\sqrt{g_{33}}}\right)_P \frac{1}{\Delta\zeta_{PB}}\Delta Vol \end{aligned}\right\} \quad \text{for} \quad W_P > 0 \tag{E.31}$$

$$\left.\begin{aligned} s_P &= \left(\frac{\rho W}{\sqrt{g_{33}}}\right)_P \frac{1}{\Delta\zeta_{TP}}\Delta Vol \\ a_T &= -\left(\frac{\rho W}{\sqrt{g_{33}}}\right)_P \frac{1}{\Delta\zeta_{TP}}\Delta Vol \\ a_B &= 0 \end{aligned}\right\} \quad \text{for} \quad W_P < 0 \tag{E.32}$$

E.4 Summary of Discretized Convection Terms

The following equations summarize the terms arising in the discretized subgrid transport equations due to convection parallel and normal to the wall:

$$\begin{aligned} s_U &= \left(\frac{\rho}{\sqrt{g_{11}}}\right)_P \frac{\max\left(U_P,0\right)\phi_W}{\Delta\xi_{PW}}\Delta Vol + \left(\frac{\rho}{\sqrt{g_{11}}}\right)_P \frac{\max\left(-U_P,0\right)\phi_E}{\Delta\xi_{EP}}\Delta Vol \\ &+ \left(\frac{\rho}{\sqrt{g_{22}}}\right)_P \frac{\max\left(V_P,0\right)\phi_S}{\Delta\eta_{PS}}\Delta Vol + \left(\frac{\rho}{\sqrt{g_{22}}}\right)_P \frac{\max\left(-V_P,0\right)\phi_N}{\Delta\eta_{NP}}\Delta Vol \end{aligned} \tag{E.33}$$

$$\begin{aligned} s_P &= \left(\frac{\rho}{\sqrt{g_{11}}}\right)_P \frac{\min\left(-U_P,0\right)}{\Delta\xi_{PW}}\Delta Vol + \left(\frac{\rho}{\sqrt{g_{11}}}\right)_P \frac{\min\left(U_P,0\right)}{\Delta\xi_{EP}}\Delta Vol \\ &+ \left(\frac{\rho}{\sqrt{g_{22}}}\right)_P \frac{\min\left(-V_P,0\right)}{\Delta\eta_{PS}}\Delta Vol + \left(\frac{\rho}{\sqrt{g_{22}}}\right)_P \frac{\min\left(V_P,0\right)}{\Delta\eta_{NP}}\Delta Vol \\ &+ \left(\frac{\rho}{\sqrt{g_{33}}}\right)_P \frac{\min\left(-W_P,0\right)}{\Delta\zeta_{PB}}\Delta Vol + \left(\frac{\rho}{\sqrt{g_{33}}}\right)_P \frac{\min\left(W_P,0\right)}{\Delta\zeta_{TP}}\Delta Vol \end{aligned} \tag{E.34}$$

$$a_T = \left(\frac{\rho}{\sqrt{g_{33}}}\right)_P \frac{\max\left(-W_P,0\right)}{\Delta\zeta_{TP}}\Delta Vol \tag{E.35}$$

$$a_B = \left(\frac{\rho}{\sqrt{g_{33}}}\right)_P \frac{\max\left(W_P,0\right)}{\Delta\zeta_{PB}}\Delta Vol \tag{E.36}$$

Convection of momentum follows the same approach as described above for scalar ϕ once the upstream velocity has been transformed from the coordinate system used in the upstream cell into the coordinate system of the current cell.

E.5 Source Terms

The following sections identify the source terms for the subgrid momentum, turbulent kinetic energy and dissipation rate equations in addition to those derived above from convection.

E.5.1 U-Momentum

Using the linear $k-\varepsilon$ model, the source term S_U^1 in the subgrid wall-parallel U-momentum equation is given by:

$$\begin{aligned} S_U^1 &= -g^{1j}\sqrt{g_{11}}\frac{\partial P'}{\partial \xi^j} - \tau^{1j}\frac{\Gamma_{1j}^m g_{1m}}{\sqrt{g_{11}}} + \tau^{mj}\Gamma_{mj}^1\sqrt{g_{11}} \\ &+ \frac{1}{J}\frac{\partial}{\partial\zeta}\left[J\mu_{eff}g^{33}\left(U^{(m)}\frac{\sqrt{g_{11}}}{\sqrt{g_{mm}}}\Gamma_{m3}^1 - U\frac{g_{1m}}{g_{11}}\Gamma_{13}^m\right)\right] \end{aligned} \tag{E.37}$$

The four terms in S_U^1 are expanded as follows:

$$-g^{1j}\sqrt{g_{11}}\frac{\partial P^{'}}{\partial \xi^j} = -\sqrt{g_{11}}\left(g^{11}\frac{\partial P^{'}}{\partial \xi} + g^{12}\frac{\partial P^{'}}{\partial \eta} + g^{13}\frac{\partial P^{'}}{\partial \zeta}\right) \tag{E.38}$$

$$\begin{aligned}
-\tau^{1j}\frac{\Gamma_{1j}^{m} g_{1m}}{\sqrt{g_{11}}} \quad = \quad & -\frac{\tau^{11}}{\sqrt{g_{11}}}\left(\Gamma_{11}^{1} g_{11} + \Gamma_{11}^{2} g_{12} + \Gamma_{11}^{3} g_{13}\right) \\
& -\frac{\tau^{12}}{\sqrt{g_{11}}}\left(\Gamma_{12}^{1} g_{11} + \Gamma_{12}^{2} g_{12} + \Gamma_{12}^{3} g_{13}\right) \\
& -\frac{\tau^{13}}{\sqrt{g_{11}}}\left(\Gamma_{13}^{1} g_{11} + \Gamma_{13}^{2} g_{12} + \Gamma_{13}^{3} g_{13}\right)
\end{aligned} \tag{E.39}$$

$$\begin{aligned}
\tau^{mj}\Gamma_{mj}^{1}\sqrt{g_{11}} \quad = \quad & \sqrt{g_{11}}\left(\tau^{11}\Gamma_{11}^{1} + \tau^{21}\Gamma_{21}^{1} + \tau^{31}\Gamma_{31}^{1}\right) \\
& + \sqrt{g_{11}}\left(\tau^{12}\Gamma_{12}^{1} + \tau^{22}\Gamma_{22}^{1} + \tau^{32}\Gamma_{32}^{1}\right) \\
& + \sqrt{g_{11}}\left(\tau^{13}\Gamma_{13}^{1} + \tau^{23}\Gamma_{23}^{1} + \tau^{33}\Gamma_{33}^{1}\right)
\end{aligned} \tag{E.40}$$

$$\begin{aligned}
& \frac{1}{J}\frac{\partial}{\partial \zeta}\left[J\mu_{eff} g^{33}\left(U^{(m)}\frac{\sqrt{g_{11}}}{\sqrt{g_{mm}}}\Gamma_{m3}^{1} - U\frac{g_{1m}}{g_{11}}\Gamma_{13}^{m}\right)\right] \\
& = \frac{1}{J}\frac{\partial}{\partial \zeta}\left[J\mu_{eff} g^{33}\left(U\frac{\sqrt{g_{11}}}{\sqrt{g_{11}}}\Gamma_{13}^{1} + V\frac{\sqrt{g_{11}}}{\sqrt{g_{22}}}\Gamma_{23}^{1} + W\frac{\sqrt{g_{11}}}{\sqrt{g_{33}}}\Gamma_{33}^{1}\right)\right. \\
& \left. - \left(U\frac{g_{11}}{g_{11}}\Gamma_{13}^{1} + U\frac{g_{12}}{g_{11}}\Gamma_{13}^{2} + U\frac{g_{13}}{g_{11}}\Gamma_{13}^{3}\right)\right]
\end{aligned} \tag{E.41}$$

The above source terms are integrated over the subgrid cell and included in the discretized U-momentum equation source term, s_U, as follows:

$$s_U = \int_{\Delta Vol} \left(S_U^1\right)_P \mathrm{d}Vol \tag{E.42}$$

where $(\Delta Vol = J\Delta\xi\Delta\eta\Delta\zeta)$ is the volume of the subgrid cell and $()_P$ denotes the value obtained at the current node P. The wall-parallel components of the pressure-gradient term ($\partial P^{'}/\partial\xi$ and $\partial P^{'}/\partial\eta$) are calculated from the main-grid node pressure values. The calculation of the pressure profile across the subgrid in order to find $\partial P^{'}/\partial\zeta$ is discussed in Section E.9.

E.5.2 V-Momentum

The source term S_U^2 in the subgrid wall-parallel V-momentum equation is given by:

$$\begin{aligned} S_U^2 &= -g^{2j}\sqrt{g_{22}}\frac{\partial P'}{\partial \xi^j} - \tau^{2j}\frac{\Gamma_{2j}^m g_{2m}}{\sqrt{g_{22}}} + \tau^{mj}\Gamma_{mj}^2\sqrt{g_{22}} \\ &+\frac{1}{J}\frac{\partial}{\partial \zeta}\left[J\mu_{eff}g^{33}\left(U^{(m)}\frac{\sqrt{g_{22}}}{\sqrt{g_{mm}}}\Gamma_{m3}^2 - V\frac{g_{2m}}{g_{22}}\Gamma_{23}^m\right)\right] \end{aligned} \quad \text{(E.43)}$$

The four terms in S_U^2 are expanded:

$$-g^{2j}\sqrt{g_{22}}\frac{\partial P}{\partial \xi^j} = -\sqrt{g_{22}}\left(g^{21}\frac{\partial P}{\partial \xi} + g^{22}\frac{\partial P}{\partial \eta} + g^{23}\frac{\partial P}{\partial \zeta}\right) \quad \text{(E.44)}$$

$$\begin{aligned} \tau^{2j}\frac{\Gamma_{2j}^m g_{2m}}{\sqrt{g_{22}}} &= -\frac{\tau^{21}}{\sqrt{g_{22}}}\left(\Gamma_{21}^1 g_{21} + \Gamma_{21}^2 g_{22} + \Gamma_{21}^3 g_{23}\right) \\ &-\frac{\tau^{22}}{\sqrt{g_{22}}}\left(\Gamma_{22}^1 g_{21} + \Gamma_{22}^2 g_{22} + \Gamma_{22}^3 g_{23}\right) \\ &-\frac{\tau^{23}}{\sqrt{g_{22}}}\left(\Gamma_{23}^1 g_{21} + \Gamma_{23}^2 g_{22} + \Gamma_{23}^3 g_{23}\right) \end{aligned} \quad \text{(E.45)}$$

$$\begin{aligned} \tau^{mj}\Gamma_{mj}^2\sqrt{g_{22}} &= \sqrt{g_{22}}\left(\tau^{11}\Gamma_{11}^2 + \tau^{21}\Gamma_{21}^2 + \tau^{31}\Gamma_{31}^2\right) \\ &+\sqrt{g_{22}}\left(\tau^{12}\Gamma_{12}^2 + \tau^{22}\Gamma_{22}^2 + \tau^{32}\Gamma_{32}^2\right) \\ &+\sqrt{g_{22}}\left(\tau^{13}\Gamma_{13}^2 + \tau^{23}\Gamma_{23}^2 + \tau^{33}\Gamma_{33}^2\right) \end{aligned} \quad \text{(E.46)}$$

$$\begin{aligned} &\frac{1}{J}\frac{\partial}{\partial \zeta}\left[J\mu_{eff}g^{33}\left(U^{(m)}\frac{\sqrt{g_{22}}}{\sqrt{g_{mm}}}\Gamma_{m3}^2 - V\frac{g_{2m}}{g_{22}}\Gamma_{23}^m\right)\right] \\ &= \frac{1}{J}\frac{\partial}{\partial \zeta}\left[J\mu_{eff}g^{33}\left(U\frac{\sqrt{g_{22}}}{\sqrt{g_{11}}}\Gamma_{13}^2 + V\frac{\sqrt{g_{22}}}{\sqrt{g_{22}}}\Gamma_{23}^2 + W\frac{\sqrt{g_{22}}}{\sqrt{g_{33}}}\Gamma_{33}^2\right)\right. \\ &\left. -\left(V\frac{g_{21}}{g_{22}}\Gamma_{23}^1 + V\frac{g_{22}}{g_{22}}\Gamma_{23}^2 + V\frac{g_{23}}{g_{22}}\Gamma_{23}^3\right)\right] \end{aligned} \quad \text{(E.47)}$$

These source terms are integrated over the subgrid cell and included in the discretized V-momentum equation source term in the same manner as described above for the U-momentum equation.

E.5.3 Turbulent Kinetic Energy, k

The kinetic energy equation in non-orthogonal curvilinear coordinates is given by:

$$\frac{\rho U}{\sqrt{g_{11}}}\frac{\partial k}{\partial \xi} + \frac{\rho V}{\sqrt{g_{22}}}\frac{\partial k}{\partial \eta} + \frac{\rho W}{\sqrt{g_{33}}}\frac{\partial k}{\partial \zeta} = \frac{1}{J}\frac{\partial}{\partial \zeta}\left[Jg^{33}\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial \zeta}\right] + G - \rho\varepsilon \quad \text{(E.48)}$$

where the production term, G (given by Equation D.21) and the dissipation term, ε (given by Equation D.22) are grouped together into the source term, S:

$$S = G - \rho\varepsilon \tag{E.49}$$

In order to maximize stability, the integrated source term split into components s_U and s_P as follows:

$$s_U = \max\left[\left(G - \rho\tilde{\varepsilon}\right), 0\right]_P \Delta Vol \tag{E.50}$$

$$s_P = \frac{1}{k_P}\left\{\max\left[\left(G - \rho\tilde{\varepsilon}\right), 0\right] - \rho\hat{\varepsilon}\right\}_P \Delta Vol \tag{E.51}$$

where:

$$\hat{\varepsilon} = 2\nu g^{33}\left(\frac{\partial k^{1/2}}{\partial\zeta}\right)\left(\frac{\partial k^{1/2}}{\partial\zeta}\right) \tag{E.52}$$

E.5.4 Dissipation Rate, $\tilde{\varepsilon}$

The dissipation rate equation in non-orthogonal curvilinear coordinates is given by:

$$\begin{aligned}\frac{\rho U}{\sqrt{g_{11}}}\frac{\partial\tilde{\varepsilon}}{\partial\xi} + \frac{\rho V}{\sqrt{g_{22}}}\frac{\partial\tilde{\varepsilon}}{\partial\eta} + \frac{\rho W}{\sqrt{g_{33}}}\frac{\partial\tilde{\varepsilon}}{\partial\zeta} &= \frac{1}{J}\frac{\partial}{\partial\zeta}\left[Jg^{33}\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial\tilde{\varepsilon}}{\partial\zeta}\right] \\ &+ c_{\varepsilon1}f_1G\frac{\tilde{\varepsilon}}{k} - c_{\varepsilon2}f_2\rho\frac{\tilde{\varepsilon}^2}{k} + \rho Y_c + P_{\varepsilon3}\end{aligned} \tag{E.53}$$

where the gradient production term $P_{\varepsilon3}$ is given in Equation (D.27). The source term, S, is as follows:

$$S = c_{\varepsilon1}f_1G\frac{\tilde{\varepsilon}}{k} - c_{\varepsilon2}f_2\rho\frac{\tilde{\varepsilon}^2}{k} + \rho Y_c + P_{\varepsilon3} \tag{E.54}$$

which is integrated over the subgrid control volume and split into components s_U and s_P, given by:

$$s_U = \left\{\max\left[\left(c_{\varepsilon1}f_1G\frac{\tilde{\varepsilon}}{k} - c_{\varepsilon2}f_2\rho\frac{\tilde{\varepsilon}^2}{k}\right), 0\right] + \rho Y_c + P_{\varepsilon3}\right\}_P \Delta Vol \tag{E.55}$$

$$s_P = \frac{1}{\tilde{\varepsilon}_P}\left\{\min\left[\left(c_{\varepsilon1}f_1G\frac{\tilde{\varepsilon}}{k} - c_{\varepsilon2}f_2\rho\frac{\tilde{\varepsilon}^2}{k}\right), 0\right]\right\}_P \Delta Vol \tag{E.56}$$

E.5.5 Main-Grid $P_{\varepsilon3}$ Source Term

A low-Reynolds-number turbulence model is used in the main-grid domain, when the UMIST-N wall function is used, so that arbitrarily small near-wall cells can be employed. In the low-Re Launder-Sharma and Craft *et al.* models, the main-grid $\tilde{\varepsilon}$-equation includes a damping term known as the gradient production, $P_{\varepsilon3}$. Care must be taken in evaluating the $P_{\varepsilon3}$ at the main-grid node adjacent to the near-wall node (node P in Figure E.2)[1]. The treatment of the

[1] In the near-wall main-grid cell (with node S in Figure E.2), the subgrid average $\overline{P_{\varepsilon3}}$ is used in the main-grid calculation.

main-grid $P_{\varepsilon 3}$ term in the TEAM and STREAM codes is discussed below.

The gradient production term involves double-derivatives of the velocity components and is written in Cartesian coordinates as follows:

$$P_{\varepsilon 3} = 2\mu\nu_t \left(\frac{\partial^2 U_i}{\partial x_j \partial x_k}\right)^2 \tag{E.57}$$

To determine a double derivative, such as $\partial^2 U/\partial y^2$, the strain-rate at the cell faces are first calculated, $(\partial U/\partial y)_n$ and $(\partial U/\partial y)_s$, and then the gradient of the strain-rate across the cell are calculated as follows:

$$\frac{\partial^2 U}{\partial y^2} = \frac{[(\partial U/\partial y)_n - (\partial U/\partial y)_s]}{\Delta y_{ns}} \tag{E.58}$$

where n and s denote the north and south cell faces, respectively. In the TEAM code the strain-rate at cell faces is evaluated from the difference in velocity between neighbouring nodal values, e.g. $(\partial U/\partial y)_n = (U_N - U_P)/\Delta y_{NP}$. The STREAM code, however, evaluates the strain-rates at the cell face by interpolating between strain-rates evaluated at the cell centres, e.g. $(\partial U/\partial y)_n = 0.5\,[(\partial U/\partial y)_N + (\partial U/\partial y)_S]$. These two methods are shown in Figure E.2.

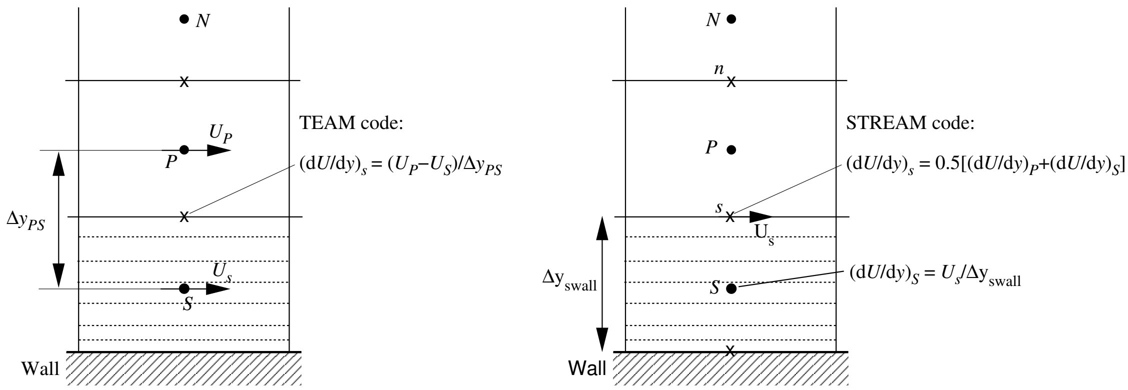

Figure E.2: Schematics of the near-wall grid arrangement showing the main-grid strain-rate $(\partial U/\partial y)_s$ as calculated by the TEAM code (left(and the STREAM code (right).

In the approach adopted by STREAM, the strain-rate at the southern cell boundary, s, shown in Figure E.2, is not calculated accurately when the near-wall node is outside the viscous sublayer (say $y^+ \approx 30$). This is because the main-grid strain-rate at the near wall node, $(\partial U/\partial y)_S$, is calculated assuming a linear velocity profile across the near-wall main-grid cell (whereas the actual velocity profile is closer to logarithmic for a plane channel flow). In the approach adopted by TEAM, this problem does not occur since it only uses the velocity at the main-grid nodes P and S to evaluate the gradient at the cell face.

To obtain a more accurate value for the main-grid strain-rate at the cell boundary with the STREAM code, one could use the strain-rate in the subgrid cell adjacent to the boundary (i.e. in the subgrid cell next to position s in Figure E.2). However, the transformation of the second-order strain-rate tensor from contravariant subgrid components to Cartesian main-grid components is costly, as the tensor expression involves three dummy indices for each of the 9 independent strain-rate components (for details see Section E.8):

$$\underbrace{V^{p,q}}_{Cartesian} = g^{jk} \frac{\partial x^p}{\partial \xi^i} \frac{\partial x^q}{\partial \xi^k} \underbrace{U^i_{,j}}_{contravariant} \tag{E.59}$$

An alternative and more computationally efficient approach is simply to scale the main-grid $P_{\varepsilon 3}$ term so that it only becomes active when a relatively fine near-wall grid is used, in which case the assumed linear velocity profile across the main-grid near-wall cell is an adequate approximation. The following function was tested in the Ahmed body flow:

$$f_{P\varepsilon 3} = \exp\left(-\frac{\tilde{R}_t}{55}\right)^4 \tag{E.60}$$

where $\tilde{R}_t$ is the turbulence Reynolds number. The above $f_{P\varepsilon 3}$ function rapidly decreases from $f_{P\varepsilon 3} = 0.92$ at $\tilde{R}_t = 30$ to $f_{P\varepsilon 3} = 0.07$ at $\tilde{R}_t = 70$. Using this function, the linear $k - \varepsilon$ model main-grid $P_{\varepsilon 3}$ term becomes:

$$P_{\varepsilon 3} = 2 f_{P\varepsilon 3} \mu \nu_t \left(\frac{\partial^2 U_i}{\partial x_j \partial x_k}\right)^2 \tag{E.61}$$

E.6 Grid Generation and Geometric Parameters

A number of geometric parameters are involved in the subgrid transport equations in non-orthogonal curvilinear coordinates such as metric tensors (g_{ij}) and Christoffel symbols $\left(\Gamma^i_{jk}\right)$. Table E.1 gives a list of these parameters and where they are evaluated (at the subgrid node or at the subgrid cell face). To calculate and store each of these parameters at each subgrid node along the length of the wall would entail huge storage costs. Instead, efficient interpolation routines are employed. Values of the particular geometric parameter are stored at the top and bottom subgrid domain boundaries together with a few interpolation constants and, at each iteration, values of the parameter within the subgrid are interpolated.

The following sections firstly discuss grid generation and the calculation of grid parameters s and Δs, which denote the position and thickness of the subgrid cells, respectively. A description of the interpolation practices used for calculating the covariant metric tensors, g_{ij}, is then given. This is followed by a presentation of the equations used to calculate the Jacobian, the contravariant metric tensors and the Christoffel symbols.

Geometric Parameter	Node/ Boundary	Term in which the parameter appears	See Equations
J	Node	ΔVol in convection and source terms	(E.33–E.36), (E.50), (E.51), (E.42) etc.
	Boundary	$P_{\varepsilon 3}$ and Diffusion	(D.27), (E.4)
Γ^i_{jk}	Node	Momentum equation source terms, strain-rate for G	(D.21), (D.12)
	Boundary	Strain-rate for $P_{\varepsilon 3}$, $\left(\partial\tau^{13}/\partial\zeta\right)$	(D.27), (D.12)
g^{ij}	Node	Pressure gradient, ε, G	(D.21), (D.22), (D.12)
	Boundary	$P_{\varepsilon 3}$	(D.27)
g_{ij}	Node	Convection, source terms, G	(D.21), (E.33–E.36), (E.50), (E.51) etc.
	Boundary	$\left(\partial\tau^{13}/\partial\zeta\right)$	(D.12)

Table E.1: Geometric parameters employed in the subgrid transport equations in non-orthogonal curvilinear coordinates and where the parameter is required (at the node or boundary).

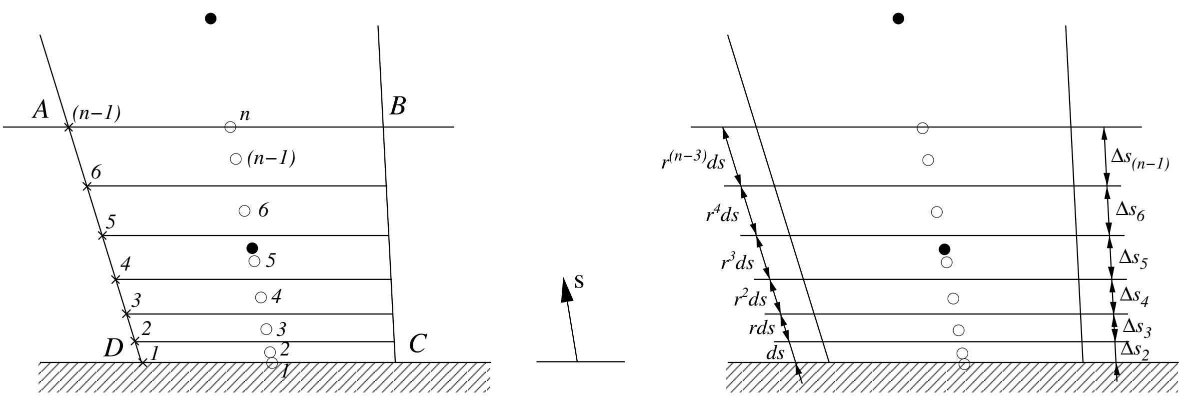

Figure E.3: Subgrid arrangement showing node and vertex notation and cell thicknesses. Distances indicated on the right are in the measured parallel to the s-axis (the physical equivalent of the ζ-axis).

E.6.1 Generating the Subgrid Mesh

Figure E.3 shows a typical curvilinear grid arrangement where the subgrid mesh is embedded within the near-wall cell which has corners $ABCD$. Subgrid vertices on the AD line are numbered from 1 to $(n-1)$ and subgrid nodes from 1 to n. The position of the main-grid vertex at corner A is denoted with upper-case (XV_A, YV_A, ZV_A) and the position of the subgrid nodes with lower-case (x_i, y_i, z_i). The positions of the first and last subgrid nodes are given by:

$$x_1 = \frac{1}{2}(XV_C + XV_D) \;\; ; \;\; y_1 = \frac{1}{2}(YV_C + YV_D) \;\; ; \;\; z_1 = \frac{1}{2}(ZV_C + ZV_D) \tag{E.62}$$

$$x_n = \frac{1}{2}(XV_A + XV_B) \;\; ; \;\; y_n = \frac{1}{2}(YV_A + YV_B) \;\; ; \;\; z_n = \frac{1}{2}(ZV_A + ZV_B) \tag{E.63}$$

Between the first and last subgrid nodes the subgrid is algebraically generated, expanding with a given ratio from the wall to the outer edge of the domain, according to:

$$\Delta s_i = r \Delta s_{i-1} \tag{E.64}$$

where r is the expansion ratio and Δs_i is the cell width for node i, measured in the s-direction (parallel to the curvilinear ζ-axis). The distance between the bottom and top subgrid domain boundary locations, s_1 and s_n, consists of the sum of the control volume widths:

$$s_n - s_1 = t\, ds \tag{E.65}$$

where:

$$t = \sum_{m=0}^{(n-3)} r^m = \left(1 + r + r^2 + ... + r^{(n-3)}\right) \tag{E.66}$$

The thickness of the smallest control volume (adjacent to the wall) is then given by:

$$ds = \frac{(s_n - s_1)}{t} \tag{E.67}$$

The thickness of a subgrid cell, Δs_i, is as follows:

$$\begin{aligned} \Delta s_i &= r^{(i-2)} ds \\ &= \frac{r^{(i-2)}}{t}(s_n - s_1) \end{aligned} \tag{E.68}$$

This can also be expressed as:

$$c_i = \frac{\Delta s_i}{(s_n - s_1)} = \frac{r^{(i-2)}}{\sum_{m=0}^{(n-3)} r^m} \tag{E.69}$$

where c_i is the ratio of the size of the subgrid cell, Δs_i, to the thickness of the subgrid domain $(s_n - s_1)$. This ratio is only dependent upon the given expansion ratio, r, and the number of nodes, n. The ratio $\Delta s_i / (s_n - s_1)$ is stored for each wall (only requiring an array with n values, where n is the number of subgrid nodes across a given main-grid cell) and the thickness of a particular subgrid cell is obtained from the product of this ratio and the width of the main-grid near-wall cell $(s_n - s_1)$. One can calculate the thickness of cell i in Cartesian coordinates as follows:

$$(\Delta x_{tb})_i = c_i (x_n - x_1) \tag{E.70}$$

$$(\Delta y_{tb})_i = c_i (y_n - y_1) \tag{E.71}$$

$$(\Delta z_{tb})_i = c_i (z_n - z_1) \tag{E.72}$$

where:

$$\Delta s_i^2 = (\Delta x_{tb})_i^2 + (\Delta y_{tb})_i^2 + (\Delta z_{tb})_i^2 \tag{E.73}$$

and:

$$(s_n - s_1)^2 = (x_n - x_1)^2 + (y_n - y_1)^2 + (z_n - z_1)^2 \tag{E.74}$$

Subscript tb refers to the distance from the top to the bottom of cell i (for cell notation see also Figure E.7). The location of the subgrid nodes in terms of distance s is determined from:

$$s_i = s_1 + \frac{1}{2}\Delta s_i + \sum_{j=2}^{(i-1)} \Delta s_j \tag{E.75}$$

so that, for instance, the location of node 4 in Figure E.3 is given by:

$$s_4 = s_1 + \Delta s_2 + \Delta s_3 + \frac{1}{2}\Delta s_4 \tag{E.76}$$

where s_1 is the location of the wall. Substituting Equation (E.69) into (E.75):

$$\begin{aligned} s_i - s_1 &= \frac{1}{2}c_i (s_n - s_1) + \sum_{j=2}^{(i-1)} [c_j (s_n - s_1)] \\ &= (s_n - s_1)\left(\frac{1}{2}c_i + \sum_{j=2}^{(i-1)} c_j\right) \\ &= (s_n - s_1)\, d_i \end{aligned} \tag{E.77}$$

which states that the position of the subgrid node relative to the wall $(s_i - s_1)$ is a function of the thickness of the main-grid cell $(s_n - s_1)$ and parameter d_i. Parameter d_i is only a function of c_i which was shown above to have storage requirements limited to a one-dimensional array with n entries.

The location of the top boundary of subgrid cell i, denoted s_i^t, is calculated as follows:

$$s_i^t = s_1 + \sum_{j=2}^{i} \Delta s_j \tag{E.78}$$

Rearranging this, using Equation (E.69), one obtains:

$$\begin{aligned} s_i^t - s_1 &= \sum_{j=2}^{i} \left[c_j \left(s_n - s_1 \right) \right] \\ &= \left(s_n - s_1 \right) \left(\sum_{j=2}^{i} c_j \right) \\ &= \left(s_n - s_1 \right) e_i \end{aligned} \tag{E.79}$$

where e_i depends only upon c_i and hence can be stored in a one-dimensional array with n entries. The parameter e_i is used to interpolate values to the top and bottom faces of the subgrid cells.

To summarize the above discussion, the subgrid is generated by specifying the number of subgrid nodes n (which includes nodes on the top and bottom boundaries) and the expansion ratio r, for which $(r > 1)$ leads to smaller cells near the wall than the outer boundary of the subgrid. The thickness each subgrid cell, Δs_i, is obtained from:

$$\boxed{\Delta s_i = c_i \left(s_n - s_1 \right)} \tag{E.80}$$

where:

$$c_i = \frac{r^{(i-2)}}{\sum_{m=0}^{(n-3)} r^m} \tag{E.81}$$

and the position of each subgrid node s_i relative to the wall boundary node, s_1, is given by:

$$\boxed{s_i - s_1 = \left(s_n - s_1 \right) d_i} \tag{E.82}$$

where:

$$d_i = \left(\frac{1}{2} c_i + \sum_{j=2}^{(i-1)} c_j \right) \tag{E.83}$$

The position of the subgrid top boundary for cell i is also calculated from

$$\boxed{s_i^t - s_1 = \left(s_n - s_1 \right) e_i} \tag{E.84}$$

where:

$$e_i = \sum_{j=2}^{i} c_j \tag{E.85}$$

E.6.2 Interpolation to Subgrid Cell Boundaries

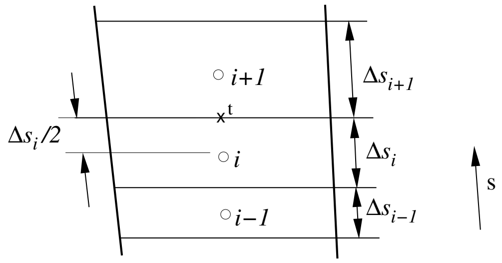

Figure E.4: Subgrid cells showing position of nodes within the cells

In order to assemble the diffusion terms in the coefficient matrix it is necessary to interpolate to find the eddy-viscosity at subgrid cell boundaries. The subgrid nodes are positioned in the centre of the subgrid cells (as defined by the calculation of d_i, see Equation E.77), and linear interpolation of parameter ϕ to the top boundary (position t in Figure E.4) is achieved using the function f_i:

$$\boxed{\phi_t = \phi_i + f_i\left(\phi_{i+1} - \phi_i\right)} \tag{E.86}$$

where:

$$f_i = \frac{\Delta s_i}{\left(\Delta s_{i+1} + \Delta s_i\right)} \tag{E.87}$$

Using Equation (E.80), this can be written:

$$f_i = \frac{c_i\left(s_n - s_1\right)}{\left[c_{i+1}\left(s_n - s_1\right) + c_i\left(s_n - s_1\right)\right]} = \frac{c_i}{\left(c_{i+1} + c_i\right)} \tag{E.88}$$

For an entire wall, the interpolation function can therefore be stored in a single one-dimensional array with n entries (where n is the number of subgrid cells in the wall-normal direction).

In addition to interpolating values at the top and bottom subgrid cell faces, it is necessary to find east, west, north and south subgrid cell face values. These are used, for example, in the calculation of the subgrid W-velocity. The value of ϕ at the eastern subgrid cell boundary is given by:

$$\phi_e = \phi_P + f_j^e\left(\phi_E - \phi_P\right) \tag{E.89}$$

where:

$$f_j^e = \frac{1}{2}\frac{\sqrt{\left(g_{11}\right)_P}}{\sqrt{\left(g_{11}\right)_e}} \tag{E.90}$$

and likewise:

$$\phi_w = \phi_W + f_j^w\left(\phi_P - \phi_W\right) \quad ; \quad f_j^w = \frac{1}{2}\frac{\sqrt{\left(g_{11}\right)_W}}{\sqrt{\left(g_{11}\right)_w}} \tag{E.91}$$

$$\phi_n = \phi_P + f_k^n\left(\phi_N - \phi_P\right) \quad ; \quad f_k^n = \frac{1}{2}\frac{\sqrt{\left(g_{22}\right)_P}}{\sqrt{\left(g_{22}\right)_n}} \tag{E.92}$$

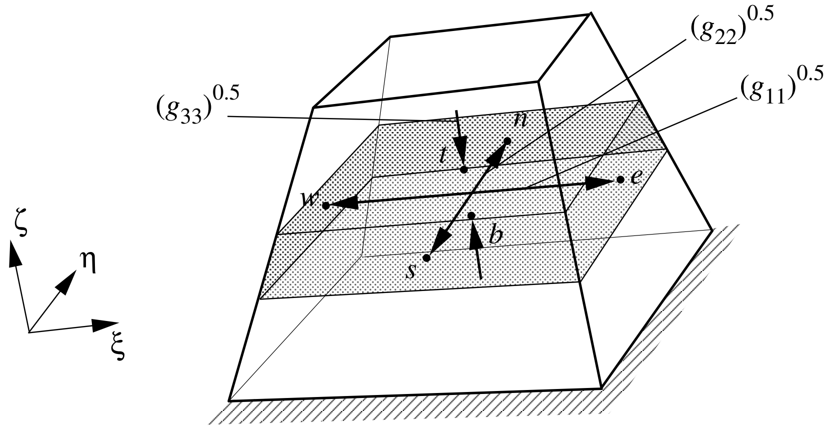

Figure E.5: Three-dimensional near-wall cell showing subgrid volume (shaded). The square-root of the metric tensors $\sqrt{g_{11}}$, $\sqrt{g_{22}}$ and $\sqrt{g_{33}}$ represent the physical distances between the east-west, north-south and top-bottom faces, respectively.

$$\phi_s = \phi_S + f_j^s \left(\phi_P - \phi_S\right) \quad ; \quad f_k^s = \frac{1}{2} \frac{\sqrt{(g_{22})_S}}{\sqrt{(g_{22})_s}} \tag{E.93}$$

where upper case E, W, N, S refer to nodal values and lower case e, w, n, s refer for cell face values in the east, west, north and south directions respectively.

E.6.3 Covariant Metric Tensor, g_{ij}

The covariant metric tensor, g_{ij}, is calculated from:

$$g_{ij} = \sum_{k=1}^{3} \frac{\partial x^k}{\partial \xi^i} \frac{\partial x^k}{\partial \xi^j} = \frac{\partial x}{\partial \xi^i} \frac{\partial x}{\partial \xi^j} + \frac{\partial y}{\partial \xi^i} \frac{\partial y}{\partial \xi^j} + \frac{\partial z}{\partial \xi^i} \frac{\partial z}{\partial \xi^j} \tag{E.94}$$

So, for example, g_{12} is given by:

$$g_{12} = x_\xi x_\eta + y_\xi y_\eta + z_\xi z_\eta \tag{E.95}$$

where, for example:

$$x_\xi \equiv \frac{\partial x}{\partial \xi} = \frac{x_e - x_w}{\Delta \xi_{ew}} = x_e - x_w \tag{E.96}$$

The g_{ij} components are given by:

$$\begin{aligned}
[g_{ij}] &= \begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{bmatrix} \\
&= \begin{bmatrix} \left(x_\xi^2 + y_\xi^2 + z_\xi^2\right) & (x_\xi x_\eta + y_\xi y_\eta + z_\xi z_\eta) & (x_\xi x_\zeta + y_\xi y_\zeta + z_\xi z_\zeta) \\ (x_\xi x_\eta + y_\xi y_\eta + z_\xi z_\eta) & \left(x_\eta^2 + y_\eta^2 + z_\eta^2\right) & (x_\eta x_\zeta + y_\eta y_\zeta + z_\eta z_\zeta) \\ (x_\xi x_\zeta + y_\xi y_\zeta + z_\xi z_\zeta) & (x_\eta x_\zeta + y_\eta y_\zeta + z_\eta z_\zeta) & \left(x_\zeta^2 + y_\zeta^2 + z_\zeta^2\right) \end{bmatrix}
\end{aligned} \tag{E.97}$$

Since the metric tensor is symmetric ($g_{ij} = g_{ji}$), only 6 independent quantities need to be calculated.

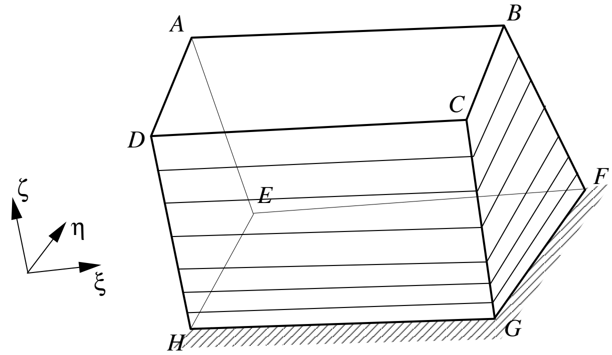

Figure E.6: Three-dimensional view of subgrid block. The top surface $ABCD$ is assumed to be parallel to the wall surface $EFGH$. Both planes are parallel to the subgrid $\xi - \eta$ plane.

In the UMIST-N wall function, rather than store all 6 components of the metric tensor for each of the subgrid cells all the way along the wall, values of the metric tensors are stored at the subgrid domain boundaries (top and bottom) together with a few interpolation constants. At the beginning of each subgrid iteration, values of the metric tensor within the subgrid are interpolated. The interpolation functions are derived below for each of the metric tensors. Figure E.6 shows the general arrangement for a subgrid, where it is assumed that the top and bottom surfaces of the subgrid cells are parallel to the wall surface.

The simplest interpolation functions are for the metric tensors g_{11} and g_{22}. Figure E.7 shows a typical subgrid cell and the distance between the east and west cell faces, Δr_{ew}. The metric tensor, g_{11} is given by:

$$\begin{aligned}
g_{11} &= x_\xi^2 + y_\xi^2 + z_\xi^2 \\
&= (x_e - x_w)^2 + (y_e - y_w)^2 + (z_e - z_w)^2 \\
&= \Delta r_{ew}^2
\end{aligned} \tag{E.98}$$

Distance Δr_{ew} is a linear function of the physical wall-normal distance. The metric tensor

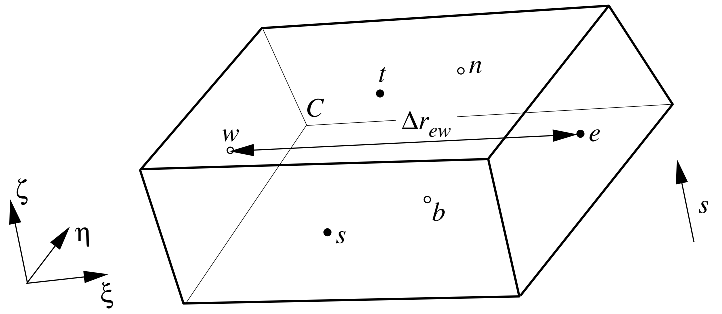

Figure E.7: Three-dimensional subgrid cell showing the distance from the east to the west face, Δr_{ew} . The physical wall-normal distance in the ζ-direction is denoted s.

g_{11} can therefore be interpolating from values at the top and bottom of the subgrid block, as follows:

$$\sqrt{g_{11}} = \frac{\left(\sqrt{(g_{11})_T} - \sqrt{(g_{11})_B}\right)}{(s_n - s_1)} (s - s_1) + \sqrt{(g_{11})_B} \tag{E.99}$$

where s_1 is the position of the subgrid node on the wall surface, $(s_n - s_1)$ is the total height of the subgrid domain, and upper-case T and B refer to values at the top and bottom of the subgrid domain (at the same positions as subgrid nodes 1 and n, shown in Figure E.3). Using Equation (E.82), this expression can be written:

$$\sqrt{g_{11}} = \sqrt{(g_{11})_B} + \left(\sqrt{(g_{11})_T} - \sqrt{(g_{11})_B}\right) d_i \tag{E.100}$$

A similar result can be obtained for the g_{22} metric, which is equivalent to the square of the distance from the north to the south faces of the subgrid cell, $(\Delta r_{ns})^2$. The metric tensor g_{33} is given by:

$$\begin{aligned} g_{33} &= x_\zeta^2 + y_\zeta^2 + z_\zeta^2 \\ &= (x_t - x_b)^2 + (y_t - y_b)^2 + (z_t - z_b)^2 \\ &= \Delta s^2 \end{aligned} \tag{E.101}$$

where Δs is the thickness of the subgrid cell, from top to bottom.

The metric tensor g_{12} is given by:

$$\begin{aligned} g_{12} &= (x_\xi x_\eta + y_\xi y_\eta + z_\xi z_\eta) \\ &= (x_e - x_w)(x_n - x_s) + (y_e - y_w)(y_n - y_s) + (z_e - z_w)(z_n - z_s) \end{aligned} \tag{E.102}$$

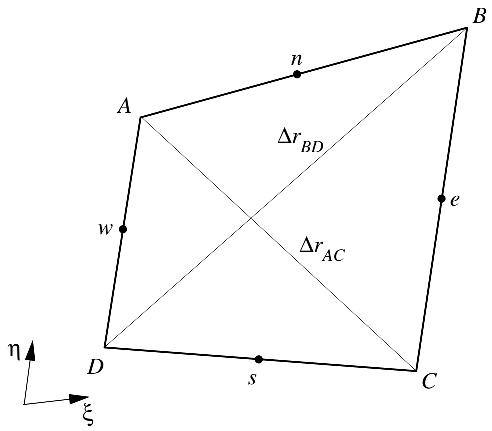

Figure E.8: 2-D plane in the $\xi - \eta$ axis used to calculate the metric tensor g_{12}. The four sides of the trapezoid $ABCD$ are (in general) non-parallel and the lengths of the diagonal elements are denoted Δr_{BD} and Δr_{AC}.

The x-axis term can be expanded:

$$\begin{aligned}(x_e - x_w)(x_n - x_s) &= \frac{1}{4}(x_B + x_C - x_A - x_D)(x_A + x_B - x_C - x_D) \\ &= \frac{1}{4}\left[\left(x_B^2 - 2x_Bx_D - x_D^2\right) - \left(x_A^2 - 2x_Ax_C - x_C^2\right)\right] \\ &= \frac{1}{4}\left[(x_B - x_D)^2 - (x_A - x_C)^2\right] \qquad \text{(E.103)}\end{aligned}$$

where subscripts A, B, C and D refer to corners of the quadrilateral element in the $\xi - \eta$ plane, as shown in Figure E.8. Performing similar manipulations of the y and z terms, the metric tensor g_{12} can be written:

$$\begin{aligned}g_{12} &= \frac{1}{4}\left[(x_B - x_D)^2 - (x_A - x_C)^2\right. \\ &\quad + (y_B - y_D)^2 - (y_A - y_C)^2 \\ &\quad \left. + (z_B - z_D)^2 - (z_A - z_C)^2\right] \\ &= \frac{1}{4}\left(\Delta r_{BD}^2 - \Delta r_{AC}^2\right) \qquad \text{(E.104)}\end{aligned}$$

where Δr_{BD} is the length of the diagonal from corners B to D, and Δr_{AC} from corners A to C. The two diagonals lie in the $\xi - \eta$ plane parallel to the wall[2]. Both Δr_{BD} and Δr_{AC} are linear functions of the distance along the ζ-axis, denoted s. The metric tensor g_{12} can therefore be interpolated from:

$$\Delta r_{BD} = \Delta r_{BD}^B + \left(\Delta r_{BD}^T - \Delta r_{BD}^B\right) d_i \qquad \text{(E.105)}$$

[2]N.B. if the cell is orthogonal in the $\xi - \eta$ plane, the two diagonal lines Δr_{BD} and Δr_{AC} will be equal in length and hence g_{12} will be zero.

$$\Delta r_{AC} = \Delta r^B_{AC} + \left(\Delta r^T_{AC} - \Delta r^B_{AC}\right) d_i \tag{E.106}$$

where:

$$g_{12} = \frac{1}{4}\left(\Delta r^2_{BD} - \Delta r^2_{AC}\right) \tag{E.107}$$

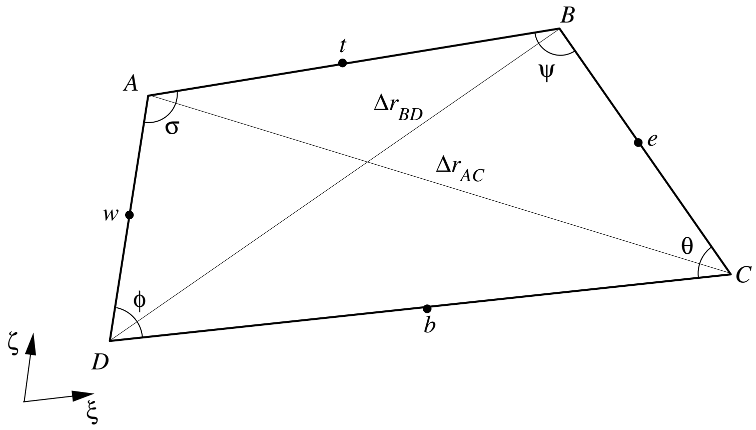

Figure E.9: 2-D plane parallel to the $\xi - \zeta$ axis used to calculate the metric tensor g_{13}. Sides AB and CD of the trapezoid $ABCD$ are both parallel to the wall while sides BC and DA are (in general) non-parallel.

The interpolation of the g_{13} and g_{23} covariant metric tensors is slightly more complex than g_{12} as the diagonal lengths (shown in Figure E.9 as Δr_{BD} and Δr_{AC}) are no longer a linear function of the distance from the wall since the subgrid cells have non-uniform thickness (assuming that cells are clustered towards the wall). The following derivation proves that the metric tensor g_{13} is proportional to $\sqrt{g_{11}g_{33}}$. Since expressions for the interpolation of g_{11} and g_{33} are already known, this proportionality expression provides an efficient route to interpolating g_{13}.

Using the cosine rule one can express the square of the length Δr_{BD} in terms of the lengths of the sides of the triangle ABD or triangle BCD:

$$\Delta r^2_{BD} = \Delta r^2_{BC} + \Delta r^2_{CD} - \frac{1}{2}\Delta r_{BC}\Delta r_{CD}\cos\theta \tag{E.108}$$

or:

$$\Delta r^2_{BD} = \Delta r^2_{AB} + \Delta r^2_{AD} - \frac{1}{2}\Delta r_{AB}\Delta r_{AD}\cos\sigma \tag{E.109}$$

Combining these two expressions:

$$\Delta r^2_{BD} = \frac{1}{2}\left(\Delta r^2_{BC} + \Delta r^2_{CD} + \Delta r^2_{AB} + \Delta r^2_{AD}\right) - \frac{1}{4}\left(\Delta r_{BC}\Delta r_{CD}\cos\theta + \Delta r_{AB}\Delta r_{AD}\cos\sigma\right) \tag{E.110}$$

Similarly, for the diagonal length Δr_{AC} one can write:

$$\Delta r_{AC}^2 = \frac{1}{2}\left(\Delta r_{AB}^2 + \Delta r_{BC}^2 + \Delta r_{AD}^2 + \Delta r_{CD}^2\right) - \frac{1}{4}\left(\Delta r_{AB}\Delta r_{BC}\cos\psi + \Delta r_{AD}\Delta r_{CD}\cos\phi\right) \tag{E.111}$$

From Equation (E.104), the covariant metric g_{13} can be written:

$$\begin{aligned} g_{13} &= \frac{1}{4}\left(\Delta r_{BD}^2 - \Delta r_{AC}^2\right) \\ &= \frac{1}{16}\left(\Delta r_{AB}\Delta r_{BC}\cos\psi + \Delta r_{AD}\Delta r_{CD}\cos\phi\right. \\ &\quad \left. - \Delta r_{BC}\Delta r_{CD}\cos\theta - \Delta r_{AB}\Delta r_{AD}\cos\sigma\right) \end{aligned} \tag{E.112}$$

It is assumed that the top and bottom faces of the subgrid cell are parallel and therefore the sum of the internal angles $(\sigma + \phi) = 180^o$ and $(\psi + \theta) = 180^o$, hence:

$$\cos\sigma = \cos\left(180^o - \phi\right) = -\cos\phi \tag{E.113}$$

$$\cos\theta = \cos\left(180^o - \psi\right) = -\cos\psi \tag{E.114}$$

The metric tensor g_{13} can therefore be written:

$$\begin{aligned} g_{13} &= \frac{1}{16}\left(\Delta r_{AB}\Delta r_{BC}\cos\psi + \Delta r_{AD}\Delta r_{CD}\cos\phi + \Delta r_{BC}\Delta r_{CD}\cos\psi + \Delta r_{AB}\Delta r_{AD}\cos\phi\right) \\ &= \frac{1}{16}\left[\left(\Delta r_{AB}\Delta r_{BC} + \Delta r_{BC}\Delta r_{CD}\right)\cos\psi + \left(\Delta r_{AD}\Delta r_{CD} + \Delta r_{AB}\Delta r_{AD}\right)\cos\phi\right] \\ &= \frac{1}{16}\left[\left(\Delta r_{AB} + \Delta r_{CD}\right)\left(\Delta r_{BC}\cos\psi + \Delta r_{AD}\cos\phi\right)\right] \end{aligned} \tag{E.115}$$

Earlier it was shown that the covariant metric tensor g_{11} is given by:

$$g_{11} = \frac{1}{2}\left(\Delta r_{AB} + \Delta r_{CD}\right) \tag{E.116}$$

which is a linear function of the distance from the wall. The lengths of the sides Δr_{BC} and Δr_{AD} are also proportional to the thickness of the subgrid cell, Δs, and the angles ψ and ϕ are constant for a particular near-wall main-grid cell. Therefore, using Equation (E.101) one can write:

$$g_{13} \propto \sqrt{g_{11}g_{33}} \tag{E.117}$$

The metric g_{13} can then be linearly interpolated as follows,

$$g_{13} = \left(g_{13}\right)_B + \frac{\left[\left(g_{13}\right)_T - \left(g_{13}\right)_B\right]}{\left[\sqrt{\left(g_{11}g_{33}\right)_T} - \sqrt{\left(g_{11}g_{33}\right)_B}\right]}\left[\sqrt{g_{11}g_{33}} - \sqrt{\left(g_{11}g_{33}\right)_B}\right] \tag{E.118}$$

or, more simply:

$$g_{13} = a\sqrt{g_{11}g_{33}} + b \tag{E.119}$$

where the metric tensors g_{11} and g_{33} are evaluated using Equations (E.99) and (E.101) respectively, and constants a and b are given by:

$$a = \frac{[(g_{13})_T - (g_{13})_B]}{[\sqrt{(g_{11}g_{33})_T} - \sqrt{(g_{11}g_{33})_B}]} \quad ; \quad b = (g_{13})_B - \frac{\sqrt{(g_{11}g_{33})_B}\,[(g_{13})_T - (g_{13})_B]}{(\sqrt{(g_{11}g_{33})_T} - \sqrt{(g_{11}g_{33})_B})} \tag{E.120}$$

Note that in Equations (E.118) and (E.120), subscripts T and B do not refer to values at the top and bottom of the subgrid domain. Instead these subscripts refer to values at the neighbouring cells $(n-1)$ and 2, shown in Figure E.3. This is because one needs to have a finite cell thickness ($\Delta s_i \neq 0$) in order to calculate g_{13}. Constants a and b are calculated once and stored in computer memory to reduce computing time. Values of $(g_{13})_T$ and $(g_{13})_B$ can be calculated from:

$$g_{13} = (x_e - x_w)(x_t - x_b) + (y_e - y_w)(y_t - y_b) + (z_e - z_w)(z_t - z_b) \tag{E.121}$$

An analogous solution can be obtained for the g_{23} metric tensor, where the trapezoid $ABCD$ is located in the $\eta - \zeta$ plane.

E.6.4 Jacobian, J

The Jacobian, J, is evaluated from the determinant of the covariant metric tensor matrix, g. Once one has calculated all the g_{ij} components across the subgrid, one can evaluate J from Equations (B.58) and (B.95), as follows:

$$\begin{aligned} J &= \sqrt{g} \\ &= [g_{11}(g_{22}g_{33} - g_{23}g_{23}) - g_{12}(g_{21}g_{33} - g_{23}g_{31}) + g_{13}(g_{21}g_{32} - g_{22}g_{31})]^{0.5} \end{aligned} \tag{E.122}$$

E.6.5 Contravariant Metric Tensor, g^{ij}

The contravariant metric tensor, g^{ij}, is evaluated by inverting of the covariant metric tensor matrix:

$$g^{ij} = \frac{1}{g} G_{ij} \tag{E.123}$$

where g is the determinant and G_{ij} is the matrix of cofactors of covariant metric tensor matrix. The contravariant metric tensor is thus given by:

$$\begin{aligned} g^{ij} &= \frac{1}{g}\begin{bmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{bmatrix} \\ &= \frac{1}{J^2}\begin{bmatrix} (g_{22}g_{33} - g_{23}g_{32}) & -(g_{12}g_{33} - g_{13}g_{32}) & (g_{12}g_{23} - g_{13}g_{22}) \\ -(g_{21}g_{33} - g_{23}g_{31}) & (g_{11}g_{33} - g_{13}g_{31}) & -(g_{11}g_{23} - g_{13}g_{21}) \\ (g_{21}g_{32} - g_{22}g_{31}) & -(g_{11}g_{32} - g_{12}g_{31}) & (g_{11}g_{22} - g_{12}g_{21}) \end{bmatrix} \end{aligned} \tag{E.124}$$

where $g_{ij} = g_{ji}$ and $G_{ij} = G_{ji}$, hence only 6 independent cofactors need to be calculated.

The leading diagonal terms in the cofactor matrix (G_{11}, G_{22} and G_{33}) are equivalent to the square of the ratio of the cell face areas to the cell volume. This can be deduced from the definition of the contravariant metric tensor (Equation B.31), as follows:

$$\begin{aligned} g^{33} &= \mathbf{g}^3 \cdot \mathbf{g}^3 \\ &= \frac{1}{\Delta Vol}(\mathbf{g}_1 \times \mathbf{g}_2) \cdot \frac{1}{\Delta Vol}(\mathbf{g}_1 \times \mathbf{g}_2) \\ &= \left(\frac{A_{12}}{\Delta Vol}\right)^2 \end{aligned} \tag{E.125}$$

where A_{12} is the area of the cell face in the $\xi - \eta$ plane and ΔVol is the cell volume. The above equation can be used to determine the wall-normal distance from $\Delta Vol/A_{12}$, where A_{12} is the area of the cell face on the wall.

Interpreting a physical meaning for the off-diagonal contravariant metric tensors is slightly more difficult. The g^{12} metric tensor is expanded as follows:

$$g^{12} = \mathbf{g}^1 \cdot \mathbf{g}^2 = \frac{1}{\Delta Vol}(\mathbf{g}_2 \times \mathbf{g}_3) \cdot \frac{1}{\Delta Vol}(\mathbf{g}_1 \times \mathbf{g}_3) \equiv \frac{\mathbf{A}_{23} \cdot \mathbf{A}_{13}}{\Delta Vol^2} \tag{E.126}$$

where, from the definition of the cross-product, the vector $\mathbf{A}_{23}$ is the area formed by vectors $\mathbf{g}_2$ and $\mathbf{g}_3$ with direction normal to both $\mathbf{g}_2$ and $\mathbf{g}_3$ (i.e. in the direction of $\mathbf{g}^1$). If the base vectors $\mathbf{g}^1$ and $\mathbf{g}^2$ are orthogonal the g^{12} metric tensor will be zero.

E.6.6 Christoffel Symbol, Γ^i_{jk}

The Christoffel symbol of the second kind is calculated from:

$$\Gamma^k_{ij} = \frac{1}{2} g^{kl}\left(\frac{\partial g_{jl}}{\partial \xi^i} + \frac{\partial g_{il}}{\partial \xi^j} - \frac{\partial g_{ij}}{\partial \xi^l}\right) \tag{E.127}$$

For example, Γ^3_{12} is given by:

$$\Gamma^3_{12} = \frac{1}{2}\left[g^{31}\left(\frac{\partial g_{21}}{\partial \xi} + \frac{\partial g_{11}}{\partial \eta} - \frac{\partial g_{12}}{\partial \xi}\right) + g^{32}\left(\frac{\partial g_{22}}{\partial \xi} + \frac{\partial g_{12}}{\partial \eta} - \frac{\partial g_{12}}{\partial \eta}\right) + g^{33}\left(\frac{\partial g_{23}}{\partial \xi} + \frac{\partial g_{13}}{\partial \eta} - \frac{\partial g_{12}}{\partial \zeta}\right)\right] \tag{E.128}$$

where $\xi^1 \equiv \xi$, $\xi^2 \equiv \eta$ and $\xi^3 \equiv \zeta$. Since the metric tensor is symmetric ($g_{ij} = g_{ji}$), this can be simplified:

$$\Gamma^3_{12} = \frac{1}{2}\left[g^{31}\frac{\partial g_{11}}{\partial \eta} + g^{32}\frac{\partial g_{22}}{\partial \xi} + g^{33}\left(\frac{\partial g_{23}}{\partial \xi} + \frac{\partial g_{13}}{\partial \eta} - \frac{\partial g_{12}}{\partial \zeta}\right)\right] \tag{E.129}$$

To calculate the gradients of the covariant metric tensor, g_{ij}, it is necessary to evaluate g_{ij} at cell boundaries. The subscripts of the Christoffel symbol are interchangeable ($\Gamma^k_{ij} = \Gamma^k_{ji}$) and therefore there are only 18 independent terms, which are summarized below:

$$\begin{aligned}\Gamma^1_{11} &= \frac{1}{2}g^{1l}\left(2\frac{\partial g_{1l}}{\partial \xi} - \frac{\partial g_{11}}{\partial \xi^l}\right)\\ &= \frac{1}{2}\left[g^{11}\left(\frac{\partial g_{11}}{\partial \xi}\right) + g^{12}\left(2\frac{\partial g_{12}}{\partial \xi} - \frac{\partial g_{11}}{\partial \eta}\right) + g^{13}\left(2\frac{\partial g_{13}}{\partial \xi} - \frac{\partial g_{11}}{\partial \zeta}\right)\right]\end{aligned} \tag{E.130}$$

$$\begin{aligned}\Gamma^1_{22} &= \frac{1}{2}g^{1l}\left(2\frac{\partial g_{2l}}{\partial \eta} - \frac{\partial g_{22}}{\partial \xi^l}\right)\\ &= \frac{1}{2}\left[g^{11}\left(2\frac{\partial g_{21}}{\partial \eta} - \frac{\partial g_{22}}{\partial \xi}\right) + g^{12}\left(\frac{\partial g_{22}}{\partial \eta}\right) + g^{13}\left(2\frac{\partial g_{23}}{\partial \eta} - \frac{\partial g_{22}}{\partial \zeta}\right)\right]\end{aligned} \tag{E.131}$$

$$\begin{aligned}\Gamma^1_{33} &= \frac{1}{2}g^{1l}\left(2\frac{\partial g_{3l}}{\partial \zeta} - \frac{\partial g_{33}}{\partial \xi^l}\right)\\ &= \frac{1}{2}\left[g^{11}\left(2\frac{\partial g_{31}}{\partial \zeta} - \frac{\partial g_{33}}{\partial \xi}\right) + g^{12}\left(2\frac{\partial g_{32}}{\partial \zeta} - \frac{\partial g_{33}}{\partial \eta}\right) + g^{13}\left(\frac{\partial g_{33}}{\partial \zeta}\right)\right]\end{aligned} \tag{E.132}$$

$$\begin{aligned}\Gamma^1_{12} = \Gamma^1_{21} &= \frac{1}{2}g^{1l}\left(\frac{\partial g_{2l}}{\partial \xi} + \frac{\partial g_{1l}}{\partial \eta} - \frac{\partial g_{12}}{\partial \xi^l}\right)\\ &= \frac{1}{2}\left[g^{11}\left(\frac{\partial g_{11}}{\partial \eta}\right) + g^{12}\left(\frac{\partial g_{22}}{\partial \xi}\right) + g^{13}\left(\frac{\partial g_{23}}{\partial \xi} + \frac{\partial g_{13}}{\partial \eta} - \frac{\partial g_{12}}{\partial \zeta}\right)\right]\end{aligned} \tag{E.133}$$

$$\begin{aligned}\Gamma^1_{13} = \Gamma^1_{31} &= \frac{1}{2}g^{1l}\left(\frac{\partial g_{3l}}{\partial \xi} + \frac{\partial g_{1l}}{\partial \zeta} - \frac{\partial g_{13}}{\partial \xi^l}\right)\\ &= \frac{1}{2}\left[g^{11}\left(\frac{\partial g_{11}}{\partial \zeta}\right) + g^{12}\left(\frac{\partial g_{32}}{\partial \xi} + \frac{\partial g_{12}}{\partial \zeta} - \frac{\partial g_{13}}{\partial \eta}\right) + g^{13}\left(\frac{\partial g_{33}}{\partial \xi}\right)\right]\end{aligned} \tag{E.134}$$

$$\Gamma^1_{23} = \Gamma^1_{32} = \frac{1}{2} g^{1l} \left(\frac{\partial g_{3l}}{\partial \eta} + \frac{\partial g_{2l}}{\partial \zeta} - \frac{\partial g_{23}}{\partial \xi^l} \right)$$
$$= \frac{1}{2} \left[g^{11} \left(\frac{\partial g_{31}}{\partial \eta} + \frac{\partial g_{21}}{\partial \zeta} - \frac{\partial g_{23}}{\partial \xi} \right) + g^{12} \left(\frac{\partial g_{22}}{\partial \zeta} \right) + g^{13} \left(\frac{\partial g_{33}}{\partial \eta} \right) \right] \quad \text{(E.135)}$$

$$\Gamma^2_{11} = \frac{1}{2} \left[g^{21} \left(\frac{\partial g_{11}}{\partial \xi} \right) + g^{22} \left(2\frac{\partial g_{12}}{\partial \xi} - \frac{\partial g_{11}}{\partial \eta} \right) + g^{23} \left(2\frac{\partial g_{13}}{\partial \xi} - \frac{\partial g_{11}}{\partial \zeta} \right) \right] \quad \text{(E.136)}$$

$$\Gamma^2_{22} = \frac{1}{2} \left[g^{21} \left(2\frac{\partial g_{21}}{\partial \eta} - \frac{\partial g_{22}}{\partial \xi} \right) + g^{22} \left(\frac{\partial g_{22}}{\partial \eta} \right) + g^{23} \left(2\frac{\partial g_{23}}{\partial \eta} - \frac{\partial g_{22}}{\partial \zeta} \right) \right] \quad \text{(E.137)}$$

$$\Gamma^2_{33} = \frac{1}{2} \left[g^{21} \left(2\frac{\partial g_{31}}{\partial \zeta} - \frac{\partial g_{33}}{\partial \xi} \right) + g^{22} \left(2\frac{\partial g_{32}}{\partial \zeta} - \frac{\partial g_{33}}{\partial \eta} \right) + g^{23} \left(\frac{\partial g_{33}}{\partial \zeta} \right) \right] \quad \text{(E.138)}$$

$$\Gamma^2_{12} = \Gamma^2_{21} = \frac{1}{2} \left[g^{21} \left(\frac{\partial g_{11}}{\partial \eta} \right) + g^{22} \left(\frac{\partial g_{22}}{\partial \xi} \right) + g^{23} \left(\frac{\partial g_{23}}{\partial \xi} + \frac{\partial g_{13}}{\partial \eta} - \frac{\partial g_{12}}{\partial \zeta} \right) \right] \quad \text{(E.139)}$$

$$\Gamma^2_{13} = \Gamma^2_{31} = \frac{1}{2} \left[g^{21} \left(\frac{\partial g_{11}}{\partial \zeta} \right) + g^{22} \left(\frac{\partial g_{32}}{\partial \xi} + \frac{\partial g_{12}}{\partial \zeta} - \frac{\partial g_{13}}{\partial \eta} \right) + g^{23} \left(\frac{\partial g_{33}}{\partial \xi} \right) \right] \quad \text{(E.140)}$$

$$\Gamma^2_{23} = \Gamma^2_{32} = \frac{1}{2} \left[g^{21} \left(\frac{\partial g_{31}}{\partial \eta} + \frac{\partial g_{21}}{\partial \zeta} - \frac{\partial g_{23}}{\partial \xi} \right) + g^{22} \left(\frac{\partial g_{22}}{\partial \zeta} \right) + g^{23} \left(\frac{\partial g_{33}}{\partial \eta} \right) \right] \quad \text{(E.141)}$$

$$\Gamma^3_{11} = \frac{1}{2} \left[g^{31} \left(\frac{\partial g_{11}}{\partial \xi} \right) + g^{32} \left(2\frac{\partial g_{12}}{\partial \xi} - \frac{\partial g_{11}}{\partial \eta} \right) + g^{33} \left(2\frac{\partial g_{13}}{\partial \xi} - \frac{\partial g_{11}}{\partial \zeta} \right) \right] \quad \text{(E.142)}$$

$$\Gamma^3_{22} = \frac{1}{2} \left[g^{31} \left(2\frac{\partial g_{21}}{\partial \eta} - \frac{\partial g_{22}}{\partial \xi} \right) + g^{32} \left(\frac{\partial g_{22}}{\partial \eta} \right) + g^{33} \left(2\frac{\partial g_{23}}{\partial \eta} - \frac{\partial g_{22}}{\partial \zeta} \right) \right] \quad \text{(E.143)}$$

$$\Gamma^3_{33} = \frac{1}{2} \left[g^{31} \left(2\frac{\partial g_{31}}{\partial \zeta} - \frac{\partial g_{33}}{\partial \xi} \right) + g^{32} \left(2\frac{\partial g_{32}}{\partial \zeta} - \frac{\partial g_{33}}{\partial \eta} \right) + g^{33} \left(\frac{\partial g_{33}}{\partial \zeta} \right) \right] \quad \text{(E.144)}$$

$$\Gamma^3_{12} = \Gamma^3_{21} = \frac{1}{2} \left[g^{31} \left(\frac{\partial g_{11}}{\partial \eta} \right) + g^{32} \left(\frac{\partial g_{22}}{\partial \xi} \right) + g^{33} \left(\frac{\partial g_{23}}{\partial \xi} + \frac{\partial g_{13}}{\partial \eta} - \frac{\partial g_{12}}{\partial \zeta} \right) \right] \quad \text{(E.145)}$$

$$\Gamma^3_{13} = \Gamma^3_{31} = \frac{1}{2}\left[g^{31}\left(\frac{\partial g_{11}}{\partial \zeta}\right) + g^{32}\left(\frac{\partial g_{32}}{\partial \xi} + \frac{\partial g_{12}}{\partial \zeta} - \frac{\partial g_{13}}{\partial \eta}\right) + g^{33}\left(\frac{\partial g_{33}}{\partial \xi}\right)\right] \quad \text{(E.146)}$$

$$\Gamma^3_{23} = \Gamma^3_{32} = \frac{1}{2}\left[g^{31}\left(\frac{\partial g_{31}}{\partial \eta} + \frac{\partial g_{21}}{\partial \zeta} - \frac{\partial g_{23}}{\partial \xi}\right) + g^{32}\left(\frac{\partial g_{22}}{\partial \zeta}\right) + g^{33}\left(\frac{\partial g_{33}}{\partial \eta}\right)\right] \quad \text{(E.147)}$$

E.7 Calculation of Wall-Normal Velocity

The subgrid velocity in the ζ-direction is calculated from continuity and scaled, as described in Section 4.3.1. The continuity equation in curvilinear coordinates is given by:

$$\frac{\partial \rho}{\partial t} + \frac{1}{J}\frac{\partial}{\partial \xi}\left(\frac{J}{\sqrt{g_{11}}}\rho U\right) + \frac{1}{J}\frac{\partial}{\partial \eta}\left(\frac{J}{\sqrt{g_{22}}}\rho V\right) + \frac{1}{J}\frac{\partial}{\partial \zeta}\left(\frac{J}{\sqrt{g_{33}}}\rho W\right) = 0 \quad \text{(E.148)}$$

where, U, V and W denote the physical velocity components in the direction of the base vector components ξ, η and ζ respectively. For a steady, incompressible flow this expression integrated over a subgrid cell with volume ($\Delta Vol = J\Delta\xi_{ew}\Delta\eta_{ns}\Delta\zeta_{tb}$) gives:

$$\underbrace{\left(\frac{J}{\sqrt{g_{11}}}U\right)_e - \left(\frac{J}{\sqrt{g_{11}}}U\right)_w}_{flux_{ew}} + \underbrace{\left(\frac{J}{\sqrt{g_{22}}}V\right)_n - \left(\frac{J}{\sqrt{g_{22}}}V\right)_s}_{flux_{ns}}$$
$$+ \left(\frac{J}{\sqrt{g_{33}}}W\right)_t - \underbrace{\left(\frac{J}{\sqrt{g_{33}}}W\right)_b}_{flux_b} = 0 \quad \text{(E.149)}$$

where, for instance, $flux_{ew}$ is the sum of the flux through the east and west subgrid cell faces. This can be rearranged in terms of the velocity at the top subgrid cell face, W_t, as follows:

$$W_t = (flux_b - flux_{ew} - flux_{ns})\left(\frac{\sqrt{g_{33}}}{J}\right)_t \quad \text{(E.150)}$$

The calculation procedure for the subgrid W-velocity starts from the wall surface where, for a non-porous wall, it is assumed that the flux through the bottom wall is zero ($flux_b = 0$). In the wall-adjacent subgrid cell one can therefore calculate the W-velocity through the top cell face (W_t) from Equation (E.150). This calculation is repeated sequentially for each subgrid cell, moving steadily up the subgrid towards the top boundary. The W-velocity at the subgrid nodes (W_P) is then simply the mean of the top and bottom face values. Once all the W-velocity is known at all the subgrid nodes a scaling is applied as followed:

$$W = \alpha W_P^* \quad \text{(E.151)}$$

where:

$$\alpha = \frac{W_t'}{(W_t^* \pm tiny)} \qquad -3 < \alpha < 3 \tag{E.152}$$

Subscript t denotes the position at outer edge of the subgrid domain (i.e. top of the main-grid cell), superscript $*$ denotes the value calculated from continuity and the prime ($'$) denotes the main-grid value or boundary condition (see also Section 4.3.1).

E.8 Conversion between Contravariant and Cartesian Components

E.8.1 Vector Quantities

The velocity vector, $\mathbf{v}$, can be expressed in terms of the Cartesian base vectors, $\mathbf{e}_i$, or the non-orthogonal curvilinear base vectors, $\mathbf{g}_j$, as follows:

$$\mathbf{v} = u^i \mathbf{e}_i = v^j \mathbf{g}_j \tag{E.153}$$

where u^i and v^j are the Cartesian and non-physical curvilinear components, respectively. One can similarly write an expression for the position vector $\mathbf{r}$:

$$\mathbf{r} = x^i \mathbf{e}_i = \xi^j \mathbf{g}_j \tag{E.154}$$

Rearranging this expression using the chain rule:

$$\mathbf{e}_i = \frac{\partial \mathbf{r}}{\partial x^i} = \frac{\partial \mathbf{r}}{\partial \xi^j}\frac{\partial \xi^j}{\partial x^i} = \mathbf{g}_j \frac{\partial \xi^j}{\partial x^i} \tag{E.155}$$

and substituting for the Cartesian base vector, one obtains:

$$\mathbf{v} = u^i \mathbf{e}_i = u^i \frac{\partial \xi^j}{\partial x^i} \mathbf{g}_j \tag{E.156}$$

Comparing Equations (E.153) and (E.156), the curvilinear velocity components $\left(v^j\right)$ must be equivalent to components $\left(u^i \partial \xi^j / \partial x^i\right)$:

$$v^j = u^i \frac{\partial \xi^j}{\partial x^i} \tag{E.157}$$

This can be expanded:

$$v^1 = u^1 \xi_x + u^2 \xi_y + u^3 \xi_z \tag{E.158}$$

$$v^2 = u^1 \eta_x + u^2 \eta_y + u^3 \eta_z \tag{E.159}$$

$$v^3 = u^1 \zeta_x + u^2 \zeta_y + u^3 \zeta_z \tag{E.160}$$

and written in matrix form, using the physical velocity components $v^{(j)}$, where $v^j = v^{(j)}/\sqrt{g_{jj}}$:

$$\underbrace{\begin{bmatrix} v^{(1)}/\sqrt{g_{11}} \\ v^{(2)}/\sqrt{g_{22}} \\ v^{(3)}/\sqrt{g_{33}} \end{bmatrix}}_{curvilinear} = \underbrace{\begin{bmatrix} \xi_x & \xi_y & \xi_z \\ \eta_x & \eta_y & \eta_z \\ \zeta_x & \zeta_y & \zeta_z \end{bmatrix}}_{[J]^{-1}} \underbrace{\begin{bmatrix} u^1 \\ u^2 \\ u^3 \end{bmatrix}}_{Cartesian} \tag{E.161}$$

where the 3×3 matrix in the above expression is equivalent to the inverse of the Jacobian matrix $[J]^{-1}$. The conversion factor $\partial\xi^j/\partial x^i$ is sometimes given the symbol β_i^j.

To reverse the above function and obtain Cartesian velocity components from the curvilinear one needs to express the curvilinear base vectors in terms of the Cartesian vectors, as follows:

$$\mathbf{g}_j = \frac{\partial \mathbf{r}}{\partial \xi^j} = \frac{\partial \mathbf{r}}{\partial x^i}\frac{\partial x^i}{\partial \xi^j} = \mathbf{e}_i \frac{\partial x^i}{\partial \xi^j} \tag{E.162}$$

The velocity vector can thus be written:

$$\mathbf{v} = u^i \mathbf{e}_i = v^j \mathbf{g}_j = v^j \frac{\partial x^i}{\partial \xi^j}\mathbf{e}_i \tag{E.163}$$

and so the in Cartesian velocity components $\left(u^i\right)$ are given by:

$$u^i = v^j \frac{\partial x^i}{\partial \xi^j} \tag{E.164}$$

In matrix form using physical contravariant velocity components, this can be written:

$$\underbrace{\begin{bmatrix} u^1 \\ u^2 \\ u^3 \end{bmatrix}}_{Cartesian} = \underbrace{\begin{bmatrix} x_\xi & x_\eta & x_\zeta \\ y_\xi & y_\eta & y_\zeta \\ z_\xi & z_\eta & z_\zeta \end{bmatrix}}_{[J]} \underbrace{\begin{bmatrix} v^{(1)}/\sqrt{g_{11}} \\ v^{(2)}/\sqrt{g_{22}} \\ v^{(3)}/\sqrt{g_{33}} \end{bmatrix}}_{curvilinear} \tag{E.165}$$

where the 3×3 matrix in the above expression is simply the Jacobian matrix, $[J]$.

The inverse Jacobian matrix $[J]^{-1}$ is found from:

$$[J]^{-1} = \frac{1}{J}\left[\mathrm{cof}\,(J)\right]^T \tag{E.166}$$

where J is the determinant, $\mathrm{cof}(J)$ is the matrix of cofactors and $\left[\mathrm{cof}\,(J)\right]^T$ is the adjoint of the $[J]$ matrix. This is expanded as follows:

$$\begin{aligned}
[J]^{-1} &= \frac{1}{J}\left[\operatorname{cof}(J)\right]^T \\
&= \frac{1}{J}\begin{bmatrix} (y_\eta z_\zeta - y_\zeta z_\eta) & -(x_\eta z_\zeta - x_\zeta z_\eta) & (x_\eta y_\zeta - x_\zeta y_\eta) \\ -(y_\xi z_\zeta - z_\zeta y_\xi) & (x_\xi z_\zeta - x_\zeta z_\xi) & -(x_\xi y_\zeta - x_\zeta y_\xi) \\ (y_\xi z_\eta - y_\eta z_\xi) & -(x_\xi z_\eta - x_\eta z_\xi) & (x_\xi y_\eta - x_\eta y_\xi) \end{bmatrix}
\end{aligned} \tag{E.167}$$

where the Jacobian, J, is given by:

$$J = x_\xi (y_\eta z_\zeta - y_\zeta z_\eta) - x_\eta (y_\xi z_\zeta - z_\zeta y_\xi) + x_\zeta (y_\xi z_\eta - y_\eta z_\xi) \tag{E.168}$$

E.8.2 Second-Order Tensors

A second-order tensor, such as the Reynolds stress, is expressed in contravariant and Cartesian coordinates as follows:

$$\mathbf{T} = \tau^{ij}\mathbf{g}_i \otimes \mathbf{g}_j = t_{ij}\mathbf{e}_i \otimes \mathbf{e}_j \tag{E.169}$$

Earlier it was show that the covariant base vector, $\mathbf{g}_j$, can be written in terms of the Cartesian unit vector $\mathbf{e}_i$:

$$\mathbf{g}_j = \frac{\partial \mathbf{r}}{\partial \xi^j} = \frac{\partial \mathbf{r}}{\partial x^i}\frac{\partial x^i}{\partial \xi^j} = \frac{\partial x^i}{\partial \xi^j}\mathbf{e}_i \tag{E.170}$$

Substituting this into Equation (E.169):

$$\mathbf{T} = \tau^{ij}\left(\frac{\partial x^p}{\partial \xi^i}\mathbf{e}_p\right) \otimes \left(\frac{\partial x^q}{\partial \xi^j}\mathbf{e}_q\right) \tag{E.171}$$

which can be rearranged:

$$\underbrace{t^{pq}}_{Cartesian} = \frac{\partial x^p}{\partial \xi^i}\frac{\partial x^q}{\partial \xi^j}\underbrace{\tau^{ij}}_{contravariant} \tag{E.172}$$

The above equation can be used to convert the Reynolds stress tensor, $\overline{u^i u^j}$ from contravariant to Cartesian coordinates.

The mean strain-rate tensor, $U^i_{,j}$, is a mixed contravariant and covariant tensor, having both a raised and a lowered index. To satisfy the summation convention of repeated upper and lower indices, the subgrid strain-rate tensor must be converted into a fully contravariant second-order tensor before it is transformed into into Cartesian coordinates, i.e.:

$$V^{p,q} = U^{i,k}\frac{\partial x^p}{\partial \xi^i}\frac{\partial x^q}{\partial \xi^k} = g^{jk}U^i_{,j}\frac{\partial x^p}{\partial \xi^i}\frac{\partial x^q}{\partial \xi^k} \tag{E.173}$$

where $V^{p,q}$ is the Cartesian strain-rate tensor and the contravariant strain-rate tensor is calculated from Equation (C.96):

$$U^i_{,j} = \frac{\partial}{\partial \xi^j}\left(\frac{U^{(i)}}{\sqrt{g_{ii}}}\right) + \frac{U^{(m)}}{\sqrt{g_{mm}}}\Gamma^i_{mj} \tag{E.174}$$

E.9 Calculation of Pressure Gradient, $\partial P/\partial\zeta$

In Section 4.2.2 it was discussed that the subgrid pressure gradient in the ζ-direction ($\partial P/\partial\zeta$) appears in the wall-parallel momentum equations when the near-wall grid is skewed in the plane normal to the wall. This is because the gradient of the pressure in the ζ-direction has a component which is parallel to the wall (since the ζ-axis is not perpendicular to the wall). The subgrid pressure gradient in the ζ-direction is calculated from the following expression:

$$\nabla P \cdot \hat{\mathbf{n}} + (\nabla \cdot \rho\overline{\mathbf{u} \otimes \mathbf{u}}) \cdot \hat{\mathbf{n}} = 0 \tag{E.175}$$

This states that the sum of the projection of the pressure gradient and the projection of the divergence of the Reynolds stress tensor in the wall-normal direction is zero. The ∇P and $(\nabla \cdot \overline{\mathbf{u} \otimes \mathbf{u}})$ terms are expanded as follows:

$$\nabla P = \frac{\partial P}{\partial \xi^j}\beta^j_i \mathbf{e}_i \tag{E.176}$$

$$\begin{aligned} \nabla \cdot \overline{\mathbf{u} \otimes \mathbf{u}} &= \mathbf{g}^k \cdot \frac{\partial}{\partial \xi^k}\left(\overline{u^i u^j}\mathbf{e}_i \otimes \mathbf{e}_j\right) \\ &= \frac{\partial \overline{u^i u^j}}{\partial \xi^k}\beta^k_j \mathbf{e}_i \end{aligned} \tag{E.177}$$

where the Reynolds stress components $\overline{u^i u^j}$ are in Cartesian coordinates. To convert from contravariant to Cartesian components, the conversion factor β^i_k is introduced which can be shown to be equivalent to the inverse Jacobian matrix, $[J]^{-1}$, as follows:

$$\beta^k_j = \mathbf{e}_j \cdot \mathbf{g}^k = \frac{\partial \xi^m}{\partial x^j}\mathbf{g}_m \cdot \mathbf{g}^k = \frac{\partial \xi^m}{\partial x^j}\delta^k_m = \underbrace{\frac{\partial \xi^k}{\partial x^j}}_{[J]^{-1}} \tag{E.178}$$

The pressure gradient, ∇P, is expanded further as follows:

$$\begin{aligned}\nabla P = \frac{\partial P}{\partial \xi^j}\beta_i^j \mathbf{e}_i \quad = \quad & \left(\underbrace{\frac{\partial P}{\partial \xi}\beta_1^1 + \frac{\partial P}{\partial \eta}\beta_1^2}_{P_x^{\xi\eta}} + \frac{\partial P}{\partial \zeta}\beta_1^3\right)\mathbf{e}_1 \\ & + \left(\underbrace{\frac{\partial P}{\partial \xi}\beta_2^1 + \frac{\partial P}{\partial \eta}\beta_2^2}_{P_y^{\xi\eta}} + \frac{\partial P}{\partial \zeta}\beta_2^3\right)\mathbf{e}_2 \\ & + \left(\underbrace{\frac{\partial P}{\partial \xi}\beta_3^1 + \frac{\partial P}{\partial \eta}\beta_3^2}_{P_z^{\xi\eta}} + \frac{\partial P}{\partial \zeta}\beta_3^3\right)\mathbf{e}_3 \end{aligned} \tag{E.179}$$

and the projection of the pressure gradient in the wall-normal direction is given by:

$$\nabla P \cdot \hat{\mathbf{n}} = \left(P_x^{\xi\eta} + \frac{\partial P}{\partial \zeta}\beta_1^3\right) n_x + \left(P_y^{\xi\eta} + \frac{\partial P}{\partial \zeta}\beta_2^3\right) n_y + \left(P_z^{\xi\eta} + \frac{\partial P}{\partial \zeta}\beta_3^3\right) n_z \tag{E.180}$$

where the wall-normal unit vector is given by:

$$\hat{\mathbf{n}} = n_x\mathbf{e}_1 + n_y\mathbf{e}_2 + n_z\mathbf{e}_3 \tag{E.181}$$

The divergence of the Reynolds stress tensor is expanded:

$$
\begin{aligned}
\frac{\partial \overline{u^i u^j}}{\partial \xi^m}\beta_j^m \mathbf{e}_i = & \underbrace{\left(\frac{\partial \overline{uu}}{\partial \xi}\beta_1^1 + \frac{\partial \overline{uu}}{\partial \eta}\beta_1^2 + \frac{\partial \overline{uu}}{\partial \zeta}\beta_1^3 + \frac{\partial \overline{uv}}{\partial \xi}\beta_2^1 + \frac{\partial \overline{uv}}{\partial \eta}\beta_2^2 + \frac{\partial \overline{uv}}{\partial \zeta}\beta_2^3 + \frac{\partial \overline{uw}}{\partial \xi}\beta_3^1 + \frac{\partial \overline{uw}}{\partial \eta}\beta_3^2 + \frac{\partial \overline{uw}}{\partial \zeta}\beta_3^3\right)}_{S_x}\mathbf{e}_1 \\
& + \underbrace{\left(\frac{\partial \overline{vu}}{\partial \xi}\beta_1^1 + \frac{\partial \overline{vu}}{\partial \eta}\beta_1^2 + \frac{\partial \overline{vu}}{\partial \zeta}\beta_1^3 + \frac{\partial \overline{vv}}{\partial \xi}\beta_2^1 + \frac{\partial \overline{vv}}{\partial \eta}\beta_2^2 + \frac{\partial \overline{vv}}{\partial \zeta}\beta_2^3 + \frac{\partial \overline{vw}}{\partial \xi}\beta_3^1 + \frac{\partial \overline{vw}}{\partial \eta}\beta_3^2 + \frac{\partial \overline{vw}}{\partial \zeta}\beta_3^3\right)}_{S_y}\mathbf{e}_2 \\
& + \underbrace{\left(\frac{\partial \overline{wu}}{\partial \xi}\beta_1^1 + \frac{\partial \overline{wu}}{\partial \eta}\beta_1^2 + \frac{\partial \overline{wu}}{\partial \zeta}\beta_1^3 + \frac{\partial \overline{wv}}{\partial \xi}\beta_2^1 + \frac{\partial \overline{wv}}{\partial \eta}\beta_2^2 + \frac{\partial \overline{wv}}{\partial \zeta}\beta_2^3 + \frac{\partial \overline{ww}}{\partial \xi}\beta_3^1 + \frac{\partial \overline{ww}}{\partial \eta}\beta_3^2 + \frac{\partial \overline{ww}}{\partial \zeta}\beta_3^3\right)}_{S_z}\mathbf{e}_3
\end{aligned}
\tag{E.182}
$$

and its projection in the wall-normal direction is given by:

$$
\begin{aligned}
(\nabla \cdot \overline{\mathbf{u} \otimes \mathbf{u}}) \cdot \hat{\mathbf{n}} &= (S_x \mathbf{e}_1 + S_y \mathbf{e}_2 + S_z \mathbf{e}_3) \cdot (n_x \mathbf{e}_1 + n_y \mathbf{e}_2 + n_z \mathbf{e}_3) \\
&= S_x n_x + S_y n_y + S_z n_z
\end{aligned}
\tag{E.183}
$$

Finally, Equation (E.175) can be rearranged in terms of $\partial P / \partial \zeta$:

$$
\frac{\partial P}{\partial \zeta} = -\left[\frac{(S_x n_x + S_y n_y + S_z n_z) + \left(P_x^{\xi\eta} n_x + P_y^{\xi\eta} n_y + P_z^{\xi\eta} n_z\right)}{\left(\beta_1^3 n_x + \beta_2^3 n_y + \beta_3^3 n_z\right)}\right]
\tag{E.184}
$$

Since one needs to find gradients of the Reynolds stress components across the subgrid cells, the above method requires the subgrid Reynolds stress in Cartesian coordinates to be stored. A similar method to that described above is used to determine the main-grid pressure on the wall surface in the STREAM code (see Section 3.3.5).

E.10 Calculation of Wall Shear Stress, τ_{wall}

The wall shear stress, τ_{wall}, is calculated using the non-physical contravariant subgrid velocity components and then transformed into Cartesian coordinates. The two wall shear stress components, τ^{ξ}_{wall} and τ^{η}_{wall}, in the grid-aligned ξ- and η-directions are calculated from:

$$\tau^{\xi}_{wall} = \mu \frac{\partial U}{\partial n} = \mu \frac{\left[\left(U/\sqrt{g_{11}} \right)_P - \left(U/\sqrt{g_{11}} \right)_{wall} \right]}{\Delta n} \tag{E.185}$$

$$\tau^{\eta}_{wall} = \mu \frac{\partial V}{\partial n} = \mu \frac{\left[\left(V/\sqrt{g_{22}} \right)_P - \left(V/\sqrt{g_{22}} \right)_{wall} \right]}{\Delta n} \tag{E.186}$$

where $\left(U/\sqrt{g_{11}} \right)_P$ and $\left(V/\sqrt{g_{22}} \right)_P$ are the non-physical contravariant velocity components at the near-wall subgrid node, U_{wall} and V_{wall} are assumed to be zero, and Δn is the perpendicular distance from the wall to the adjacent subgrid node[3]. This distance, Δn, is calculated from the contravariant metric tensor, g^{33}, in the near-wall control volume. It was shown in Section E.6.5 that this metric tensor has the physical meaning:

$$g^{33} = \left(\frac{A_{12}}{\Delta Vol} \right)^2 \tag{E.187}$$

where A_{12} is the cell face area in the $\xi - \eta$ plane through the midpoint of the cell, and Vol is the cell volume. Assuming that the top and bottom (wall) faces of the near-wall cell are parallel, the volume is given by the product of area A_{12} and the wall-normal distance. The distance from the node (halfway down the cell) to the wall is therefore given by:

$$\Delta n = \frac{1}{2} \frac{\Delta Vol}{A_{12}} = \frac{1}{2\sqrt{g^{33}}} \tag{E.188}$$

The wall shear stress is then transformed into Cartesian components using Equation (E.165):

$$\begin{bmatrix} \tau^{x}_{wall} \\ \tau^{y}_{wall} \\ \tau^{z}_{wall} \end{bmatrix} = \underbrace{\begin{bmatrix} x_\xi & x_\eta & x_\zeta \\ y_\xi & y_\eta & y_\zeta \\ z_\xi & z_\eta & z_\zeta \end{bmatrix}}_{[J]} \begin{bmatrix} \tau^{\xi}_{wall} \\ \tau^{\eta}_{wall} \\ 0 \end{bmatrix} \tag{E.189}$$

[3]Non-physical components must be used here since the wall shear stress is subsequently converted into Cartesian coordinates using the Jacobian matrix, $[J]$. It was shown in Section (E.8) that this Jacobian matrix converts from non-physical contravariant into Cartesian components.