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Appendix A The Shear Stress Transport Model of Menter

The details of the Shear Stress Transport Model of Menter[4] is outlined in this Appendix.

Dropping the primes and tilda's that donate mean quantities, the governing equations for general compressible turbulent flows as given by Wilcox[36] and Menter[37] can be summarised as:
Mass Conservation:

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_j}\left(\rho u_j\right)=0$$

Equation A-1

Momentum conservation:

$$\frac{\partial}{\partial t}\left(\rho u_i\right)+\frac{\partial}{\partial xj}\left(\rho u_j u_i\right)=-\frac{\partial p}{\partial x_i}+\frac{\partial \tau_{ji}}{\partial x_j}$$

Equation A-2

Mean energy conservation:

$$\frac{\partial}{\partial t}(\rho E)+\frac{\partial}{\partial x_j}\left(\rho u_j H\right)=\frac{\partial}{\partial x_j}\left[u_i \tau_{ij}+\left(\mu+\sigma_k \mu_T\right)\frac{\partial k_T}{\partial x_j}-q_j\right]$$

Equation A-3

Turbulent mixing energy:

$$\frac{\partial}{\partial t}\left(\rho k_T\right)+\frac{\partial}{\partial x_j}\left(\rho u_j k_T\right)=\tau_{ij}^T\frac{\partial u_i}{\partial x_j}-\beta^* \rho \omega k_T+\frac{\partial}{\partial x_j}\left[\left(\mu+\sigma_k \mu_T\right)\frac{\partial k_T}{\partial x_j}\right]$$

Equation A-4

Specific dissipation rate:

$$\frac{\partial}{\partial t}(\rho \omega)+\frac{\partial}{\partial x_j}\left(\rho u_j \omega\right)=\left(\frac{\gamma}{\upsilon_T}\right)\tau_{ij}^T\frac{\partial u_i}{\partial x_j}-\beta \rho \omega^2{}_T+\frac{\partial}{\partial x_j}\left[\left(\mu+\sigma_\omega \mu_T\right)\frac{\partial \omega}{\partial x_j}\right]$$
$$+2\left(1-F_1\right)\rho \sigma_{\omega 2}\frac{1}{\omega}\frac{\partial k}{\partial x_j}\frac{\partial \omega}{\partial x_j}$$

Equation A-5

Closure

The closure constants ϕ of this model are calculated from the constants of the k-ω (ϕ_1) and the k-ε (ϕ_2) models as follows:

$$\phi = F_1\phi_1 + (1-F_1)\phi_2$$

Equation A-6

where the constants ϕ_1 of the k-ω model are:

$\beta_1 = 0.0750$;	$\beta^* = 0.09$;	$\kappa = 0.41$;	$\sigma_{k1} = 0.85$;
$\sigma_{\omega 1} = 0.5$;	$\gamma_1 = \beta_1/\beta^* - \sigma_{\omega 1}\kappa^2/\sqrt{\beta^*}$;	$a_1=0.31$	

and the constants ϕ_2 of the k-ε model are:

$\beta_2 = 0.0828$;	$\beta^* = 0.09$;	$\kappa = 0.41$;	$\sigma_{k2} = 1.0$;
$\sigma_{\omega 2} = 0.856$;	$\gamma_2 = \beta_2/\beta^* - \sigma_{\omega 2}\kappa^2/\sqrt{\beta^*}$		

The eddy viscosity is defined as:

$$\nu_t = \frac{a_1 k}{\max(a_1\omega; \Omega F_2)}$$

Equation A-7

where $\Omega = |\delta u/\delta y|$ is the absolute value of vorticity. The blending function F_2 is given by:

$$F_2 = \tanh(\arg_2^2); \qquad \arg_2 = \max\left(2\frac{\sqrt{k}}{0.09\omega y}; \frac{500\nu}{y^2\omega}\right)$$

Equation A-8

The blending function F_1 is defined as:

$$F_1 = \tanh(\arg_1^4); \qquad \arg_1 = \min\left[\max\left(\frac{\sqrt{k}}{0.09\omega y}; \frac{500\nu}{y^2\omega}\right); \frac{4\rho\sigma_{\omega 2}k}{CD_{k\omega}y^2}\right]$$

Equation A-9

where y is the distance to the next surface point and $CD_{k\omega}$ is:

$$CD_{kw} = \max\left(2\rho\sigma_{\omega 2}\frac{1}{\omega}\frac{\partial k}{\partial x_j}\frac{\partial \omega}{\partial x_j}; 10^{-20}\right)$$

Equation A-10

The turbulent shear stress τ^T_{ij} is defined as: $\tau^T_{ij} = \tau_{ij} - \sigma_{ij}$

The total energy E is defined as: $E = e_i + k_T + u_i u_i/2$

The heat-flux vector q_j is approximated as: $q_i = -\left(\frac{\mu}{\Pr_L} + \frac{\mu_T}{\Pr_T}\right)\frac{\partial h}{\partial x_j}$

where h is the internal enthalpy defined as: $h = e + p/\rho$

Writing the governing equations in the special vector format all fluxes remain unchanged except for the viscous energy fluxes which become:

$$\tilde{\beta}_i = \tilde{u}_i\tilde{\tau}_{ij} + (\mu + \sigma_k\mu_T)\frac{\partial k_t}{\partial x_i} - q_i$$

Equation A-11

Although the SST method is more difficult to code, Menter claims that there is almost no loss in computational efficiency compared to the k-ω model.

<u>Boundary Conditions For Numerical Implementation of The TTS Model</u>

At the surface (y = 0) the following conditions must be specified:

No slip	:	$u_w = k_T = 0$
Wall temperature or heat flux	:	T_w/Q_w
Dissipation rate	:	ω_w
Smooth surface & no mass injection	:	$\omega_w = 10\frac{6\nu_w}{\beta_1(\Delta y_1)^2}$, where Δy_1 is the distance to the next point away from the wall
	:	$v_w = 0$
	:	$\Delta y_1^+ < 3$

Rough surface & no mass injection : $\omega_w = \frac{u_\tau^2}{\nu} S_R$ where $SR = \begin{cases} \left(\frac{50}{k_R^+}\right)^2, k_R^+ \langle 25 \\ \frac{100}{k_R^+}, k_R^+ \geq 25 \end{cases}$

$$k_R^+ = \frac{u_\tau k_R}{\nu}$$

$$u_\tau^2 = (\nu + \nu_T)\frac{\partial u}{\partial y} \quad ;$$

k_R = average height of sand grain roughness elements

Mass injection : $\omega = \frac{u_\tau^2}{v_w} S_B$ and v= v_w where,

$$S_B = \frac{20}{v_w^+ \left(1 + 5v_w^+\right)} \text{ and } v_w^+ = \frac{v_w}{u_\tau}$$

The following choice of free-stream values is recommended:

$\omega_\infty = (1 \rightarrow 10)U_\infty/L$; $\nu_{t\infty} = 10^{-(2\rightarrow 5)}\ \nu_\infty$; $k_\infty = \nu_{t\infty}\ \omega_\infty$

Appendix B The Flux Difference Splitting Method of ROE

The development of the numerical solver as used in the computational investigation of Chapter 3 is presented in this Appendix.

Implicit Algorithm

The algorithm for Roe's Flux Difference Splitting Method for the full 3D RANS equations is outlined in this section. A 2D thin layer version of Roe's method as described by Craig[28] was used as the basis for expansion. The thin layer algorithm was originally outlined by MacCormack[41]. A similar description is also given by Hirsch[48].

The Navier-Stokes equations as found in section 2.3.1 of the literature study can be written in 3D as:

$$\tilde{U}_t = \tilde{F}_{\varepsilon} + \tilde{G}_{\tau} + \tilde{H}_{\zeta} = 0$$

where

$$\tilde{U} = UV = UJ^{-1}$$

and

$$\tilde{F} = \tilde{F}_e + \tilde{F}_v; \quad \tilde{G} = \tilde{G}_e + \tilde{G}_v; \quad \tilde{H} = \tilde{H}_e + \tilde{H}_v$$

Equation B-1

The subscripts e denotes Euler fluxes and v viscous fluxes.

The implicit 3D algorithm which uses Roe's flux splitting is given as:

$$\left\{ \begin{array}{l} I + \dfrac{\Delta t}{V_{i,j,k}} \left(\dfrac{D_+}{\Delta\xi}\tilde{A}_- + \dfrac{D_-}{\Delta\xi}\tilde{A}_+ + \dfrac{D_+}{\Delta\eta}\tilde{B}_- + \dfrac{D_-}{\Delta\eta}\tilde{B}_+ + \dfrac{D_+}{\Delta\zeta}\tilde{C}_- + \dfrac{D_-}{\Delta\zeta}\tilde{C}_+ \right) \\ + \dfrac{\Delta t}{V_{i,j,k}} \left(\dfrac{D}{\Delta\xi}\tilde{F}_v + \dfrac{D}{\Delta\xi}\tilde{G}_v + \dfrac{D}{\Delta\xi}\tilde{H}_v \right) \end{array} \right\} \delta U_{i,j,k} = \Delta U_{i,j,k}$$

where the explicit driving term is:

$$\begin{aligned} \Delta U^n_{i,j,k} = & -\frac{\Delta t}{V_{i,j,k}} \left(\frac{D_+}{\Delta\xi}\tilde{F}_{e-} + \frac{D_-}{\Delta\xi}\tilde{F}_{e+} + \frac{D_+}{\Delta\eta}\tilde{G}_{e-} + \frac{D_-}{\Delta\eta}\tilde{G}_{e+} + \frac{D_+}{\Delta\zeta}\tilde{H}_{e-} + \frac{D_-}{\Delta\zeta}\tilde{H}_{e+} \right)^n_{i,j,k} \\ & + \frac{\Delta t}{V_{i,j,k}} \left(\frac{D_+}{\Delta\xi}\tilde{F}_{v-} + \frac{D_-}{\Delta\xi}\tilde{F}_{v+} + \frac{D_+}{\Delta\eta}\tilde{G}_{v-} + \frac{D_-}{\Delta\eta}\tilde{G}_{v+} + \frac{D_+}{\Delta\zeta}\tilde{H}_{v-} + \frac{D_-}{\Delta\zeta}\tilde{H}_{v+} \right)^n_{i,j,k} \end{aligned}$$

Equation B-2

As the algorithm is a pentadiagonal matrix which is expensive to invert, Gauss-Seidel Line relaxation is employed to convert the algorithm to a block-tri-diagonal matrix which can be solved efficiently. After line relaxation, descritizisation and the re-writing of the implicit viscous fluxes in terms of M-matrices (M-matrices are explained later in this appendix) the algorithm becomes:

$$\tilde{B}\delta U_{i,j+1,k} + \tilde{A}\delta U_{i,j,k} + \tilde{C}\delta U_{i,j-1,k} = \Delta U^n_{i,j,k} - \tilde{D}\delta U_{i+1,j,k} - \tilde{E}\delta U_{i-1,j,k} - \tilde{O}\delta U_{i,j,k+1} - \tilde{P}\delta U_{i,j,k-1}$$

Equation B-3

where matrices $\hat{A}, \hat{B}, \hat{C}, \hat{D}, \hat{E}, \hat{O}$ and $\hat{P}$ are defined as:

$$\hat{A} = I + \frac{\Delta t}{V_{i,j,k}}\left(\widetilde{A}_{+_{i+\frac{1}{2},j,k}} - \widetilde{A}_{-_{i-\frac{1}{2},j,k}} + \widetilde{B}_{+_{i,j+\frac{1}{2},k}} - \widetilde{B}_{-_{i,j-\frac{1}{2},k}} + \widetilde{C}_{+_{i,j,k+\frac{1}{2}}} - \widetilde{C}_{-_{i,j,k-\frac{1}{2}}}\right)$$
$$+ \frac{\Delta t}{V_{i,j,k}}\left(M^{11}_{i+\frac{1}{2}} N_{i,j,k} + M^{11}_{i-\frac{1}{2}} N_{i,j,k} + M^{22}_{j+\frac{1}{2}} N_{i,j,k} + M^{22}_{j-\frac{1}{2}} N_{i,j,k} + M^{33}_{k+\frac{1}{2}} N_{i,j,k} + M^{33}_{k-\frac{1}{2}} N_{i,j,k}\right)$$

$$\hat{B} = \frac{\Delta t}{V_{i,j,k}}\widetilde{B}_{-_{i,j+\frac{1}{2},k}} - \frac{\Delta t}{V_{i,j,k}}\begin{pmatrix} M^{22}_{j+\frac{1}{2}} N_{i,j+1,k} + \frac{1}{4} M^{12}_{i+\frac{1}{2}} N_{i,j+1,k} - \frac{1}{4} M^{12}_{i-\frac{1}{2}} N_{i,j+1,k} + \frac{1}{4} M^{32}_{k+\frac{1}{2}} N_{i,j+1,k} \\ -\frac{1}{4} M^{32}_{k-\frac{1}{2}} N_{i,j+1,k} \end{pmatrix}$$

$$\hat{C} = -\frac{\Delta t}{V_{i,j,k}}\widetilde{B}_{+_{i,j-\frac{1}{2},k}} - \frac{\Delta t}{V_{i,j,k}}\begin{pmatrix} M^{22}_{j-\frac{1}{2}} N_{i,j-1,k} - \frac{1}{4} M^{12}_{i+\frac{1}{2}} N_{i,j-1,k} + \frac{1}{4} M^{12}_{i-\frac{1}{2}} N_{i,j-1,k} + \frac{1}{4} M^{32}_{k+\frac{1}{2}} N_{i,j-1,k} \\ -\frac{1}{4} M^{32}_{k-\frac{1}{2}} N_{i,j-1,k} \end{pmatrix}$$

$$\hat{D} = \frac{\Delta t}{V_{i,j,k}}\widetilde{A}_{-_{i+\frac{1}{2},j,k}} - \frac{\Delta t}{V_{i,j,k}}\begin{pmatrix} \frac{1}{4} M^{21}_{j+\frac{1}{2}} N_{i+1,j-1,k} + \frac{1}{4} M^{21}_{j+\frac{1}{2}} N_{i+1,j,k} - \frac{1}{4} M^{21}_{j-\frac{1}{2}} N_{i+1,j,k} - \frac{1}{4} M^{21}_{j-\frac{1}{2}} N_{i+1,j-1,k} \\ -\frac{1}{4} M^{12}_{i+\frac{1}{2}} N_{i+1,j+1,k} - \frac{1}{4} M^{12}_{i+\frac{1}{2}} N_{i+1,j-1,k} + \frac{1}{4} M^{11}_{i+\frac{1}{2}} N_{i+1,j,k} + \frac{1}{4} M^{13}_{i+\frac{1}{2}} N_{i+1,j,k+1} \\ -\frac{1}{4} M^{13}_{k+\frac{1}{2}} N_{i+1,j,k-1} + \frac{1}{4} M^{31}_{k+\frac{1}{2}} N_{i+1,j,k} + \frac{1}{4} M^{31}_{k+\frac{1}{2}} N_{i+1,j,k+1} - \frac{1}{4} M^{31}_{k-\frac{1}{2}} N_{i+1,j,k} \\ -\frac{1}{4} M^{31}_{k-\frac{1}{2}} N_{i+1,j,k-1} \end{pmatrix}$$

$$\hat{E} = -\frac{\Delta t}{V_{i,j,k}}\widetilde{A}_{+_{i-\frac{1}{2},j,k}} - \frac{\Delta t}{V_{i,j,k}}\begin{pmatrix} -\frac{1}{4} M^{21}_{j+\frac{1}{2}} N_{i-1,j+1,k} - \frac{1}{4} M^{21}_{j+\frac{1}{2}} N_{i-1,j,k} + \frac{1}{4} M^{21}_{j-\frac{1}{2}} N_{i-1,j,k} + \frac{1}{4} M^{21}_{j-\frac{1}{2}} N_{i-1,j-1,k} \\ -\frac{1}{4} M^{12}_{i-\frac{1}{2}} N_{i-1,j+1,k} + \frac{1}{4} M^{12}_{i-\frac{1}{2}} N_{i-1,j-1,k} + \frac{1}{4} M^{11}_{i-\frac{1}{2}} N_{i-1,j,k} - \frac{1}{4} M^{13}_{i-\frac{1}{2}} N_{i-1,j,k+1} \\ +\frac{1}{4} M^{13}_{i-\frac{1}{2}} N_{i-1,j,k-1} - \frac{1}{4} M^{31}_{k+\frac{1}{2}} N_{i-1,j,k+1} - \frac{1}{4} M^{31}_{k+\frac{1}{2}} N_{i-1,j,k} + \frac{1}{4} M^{31}_{k-\frac{1}{2}} N_{i-1,j,k} \\ +\frac{1}{4} M^{31}_{k-\frac{1}{2}} N_{i-1,j,k-1} \end{pmatrix}$$

$$\hat{O} = \frac{\Delta t}{V_{i,j,k}}\widetilde{C}_{-_{i,j,k+\frac{1}{2}}} - \frac{\Delta t}{V_{i,j,k}}\begin{pmatrix} M^{33}_{k+\frac{1}{2}} N_{i,j,k+1} + \frac{1}{4} M^{13}_{k+\frac{1}{2}} N_{i,j,k+1} - \frac{1}{4} M^{13}_{i-\frac{1}{2}} N_{i,j,k+1} - \frac{1}{4} M^{23}_{j-\frac{1}{2}} N_{i,j,k+1} \\ +\frac{1}{4} M^{23}_{j+\frac{1}{2}} N_{i,j,k+1} + \frac{1}{4} M^{23}_{j+\frac{1}{2}} N_{i,j+1,k+1} - \frac{1}{4} M^{23}_{j-\frac{1}{2}} N_{i,j-1,k+1} + \frac{1}{4} M^{32}_{k+\frac{1}{2}} N_{i,j+1,k+1} \\ -\frac{1}{4} M^{32}_{k+\frac{1}{2}} N_{i,j-1,k+1} \end{pmatrix}$$

$$\hat{P} = -\frac{\Delta t}{V_{i,j,k}}\widetilde{C}_{+_{i,j,k-\frac{1}{2}}} - \frac{\Delta t}{V_{i,j,k}}\begin{pmatrix} M^{33}_{k-\frac{1}{2}} N_{i,j,k-1} - \frac{1}{4} M^{13}_{k+\frac{1}{2}} N_{i,j,k-1} + \frac{1}{4} M^{13}_{i-\frac{1}{2}} N_{i,j,k-1} - \frac{1}{4} M^{23}_{j+\frac{1}{2}} N_{i,j,k-1} \\ +\frac{1}{4} M^{23}_{j-\frac{1}{2}} N_{i,j,k-1} - \frac{1}{4} M^{23}_{j+\frac{1}{2}} N_{i,j+1,k-1} + \frac{1}{4} M^{23}_{j-\frac{1}{2}} N_{i,j-1,k-1} - \frac{1}{4} M^{32}_{k-\frac{1}{2}} N_{i,j+1,k-1} \\ +\frac{1}{4} M^{32}_{k-\frac{1}{2}} N_{i,j-1,k-1} \end{pmatrix}$$

Equation B-4

and the explicit driving term becomes:

$$\Delta U^{n}_{i,j,k} = \begin{bmatrix} -\frac{\Delta t}{V_{i,j,k}}\left(\widetilde{F}_{e_{i+\frac{1}{2}}} - \widetilde{F}_{e_{i-\frac{1}{2}}} + \widetilde{G}_{e_{j+\frac{1}{2}}} - \widetilde{G}_{e_{j-\frac{1}{2}}} + \widetilde{H}_{e_{k+\frac{1}{2}}} - \widetilde{H}_{e_{k-\frac{1}{2}}}\right) \\ +\frac{\Delta t}{V_{i,j,k}}\left(\widetilde{F}_{v_{i+\frac{1}{2}}} - \widetilde{F}_{v_{i-\frac{1}{2}}} + \widetilde{G}_{v_{j+\frac{1}{2}}} - \widetilde{G}_{v_{j-\frac{1}{2}}} + \widetilde{H}_{v_{k+\frac{1}{2}}} - \widetilde{H}_{v_{k-\frac{1}{2}}}\right) \end{bmatrix}^{n}_{i,j,k}$$

Equation B-5

Euler Fluxes

The geometric-averaged Jacobians $\hat{A}, \hat{B}$ and $\hat{C}$ are split through polarity of rotated eigen-values and are calculated as follows:

$$\hat{A}_{\pm} = S^{-1}R_A^{-1}C_A^{-1}\Lambda_{A_{\pm}}C_A R_A S; \quad \hat{B}_{\pm} = S^{-1}R_B^{-1}C_B^{-1}\Lambda_{B_{\pm}}C_B R_B S; \quad \hat{C}_{\pm} = S^{-1}R_C^{-1}C_C^{-1}\Lambda_{C_{\pm}}C_C R_C S;$$

$$\hat{A} = \hat{A}\left(\hat{U}\right);$$

$$\hat{\rho} = \sqrt{\rho_L}\sqrt{\rho_R}$$

$$\hat{u} = \frac{\left(\sqrt{\rho_L}u_L + \sqrt{\rho_R}u_R\right)}{\left(\sqrt{\rho_L} + \sqrt{\rho_R}\right)}$$

$$\hat{v} = \frac{\left(\sqrt{\rho_L}v_L + \sqrt{\rho_R}v_R\right)}{\left(\sqrt{\rho_L} + \sqrt{\rho_R}\right)}$$

$$\hat{w} = \frac{\left(\sqrt{\rho_L}w_L + \sqrt{\rho_R}w_R\right)}{\left(\sqrt{\rho_L} + \sqrt{\rho_R}\right)}$$

$$\hat{h} = \frac{\left(\sqrt{\rho_L}\dfrac{e_L + p_L}{\rho_L} + \sqrt{\rho_L}\dfrac{e_R + p_R}{\rho_R}\right)}{\left(\sqrt{\rho_L} + \sqrt{\rho_R}\right)}$$

$$\hat{c} = \sqrt{(\gamma - 1)\left(\hat{h} - \tfrac{1}{2}\left(\hat{u}^2 + \hat{v}^2 + \hat{w}^2\right)\right)}$$

Dropping the "^":

$$\Lambda_A = d_A \begin{bmatrix} u' & 0 & 0 & 0 & 0 \\ 0 & u'+c & 0 & 0 & 0 \\ 0 & 0 & u' & 0 & 0 \\ 0 & 0 & 0 & u' & 0 \\ 0 & 0 & 0 & 0 & u'-c \end{bmatrix}; \qquad \Lambda_B = d_B \begin{bmatrix} v' & 0 & 0 & 0 & 0 \\ 0 & v' & 0 & 0 & 0 \\ 0 & 0 & v'+c & 0 & 0 \\ 0 & 0 & 0 & v' & 0 \\ 0 & 0 & 0 & 0 & v'-c \end{bmatrix}$$

$$\Lambda_C = d_C \begin{bmatrix} w' & 0 & 0 & 0 & 0 \\ 0 & w' & 0 & 0 & 0 \\ 0 & 0 & w' & 0 & 0 \\ 0 & 0 & 0 & w'+c & 0 \\ 0 & 0 & 0 & 0 & w'-c \end{bmatrix}$$

$$\Lambda_+ = \frac{\Lambda + |\Lambda|}{2}; \qquad \Lambda_- = \frac{\Lambda - |\Lambda|}{2}$$

$$d_A = \sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}\Big|_{i+\frac{1}{2}}; \qquad d_B = \sqrt{\eta_x^2 + \eta_y^2 + \eta_z^2}\Big|_{j+\frac{1}{2}}; \qquad d_C = \sqrt{\zeta_x^2 + \zeta_y^2 + \zeta_z^2}\Big|_{k+\frac{1}{2}}$$

$$u' = \left(\xi_x u + \xi_y v + \xi_z w\right)/d_A; \qquad v' = \left(\eta_x u + \eta_y v + \eta_z w\right)/d_B; \qquad w' = \left(\zeta_x u + \zeta_y v + \zeta_z w\right)/d_C$$

Equation B-6

The metrics are used, at $i+\frac{1}{2}$ as listed in section 2.3.4 and the primitive metrics are

$$
\begin{aligned}
x_\eta &= \left(x_{i+1,j+1,k+1} - x_{i+1,j,k+1} + x_{i+1,j+1,k} - x_{i+1,j,k}\right)/2 \\
x_\zeta &= \left(x_{i+1,j,k+1} - x_{i+1,j,k} + x_{i+1,j+1,k+1} - x_{i+1,j+1,k}\right)/2 \\
y_\eta &= \left(y_{i+1,j+1,k+1} - y_{i+1,j,k+1} + y_{i+1,j+1,k} - y_{i+1,j,k}\right)/2 \\
y_\zeta &= \left(y_{i+1,j,k+1} - y_{i+1,j,k} + y_{i+1,j+1,k+1} - y_{i+1,j+1,k}\right)/2 \\
z_\eta &= \left(z_{i+1,j+1,k+1} - z_{i+1,j,k+1} + z_{i+1,j+1,k} - z_{i+1,j,k}\right)/2 \\
z_\zeta &= \left(z_{i+1,j,k+1} - z_{i+1,j,k} + z_{i+1,j+1,k+1} - z_{i+1,j+1,k}\right)/2
\end{aligned}
$$

Equation B-7

The metrics are used, at $j+\frac{1}{2}$ as listed in section 2.3.4 and the primitive metrics are:

$$
\begin{aligned}
x_\xi &= \left(x_{i+1,j+1,k+1} - x_{i,j+1,k+1} + x_{i+1,j+1,k} - x_{i,j+1,k}\right)/2 \\
x_\zeta &= \left(x_{i,j+1,k+1} - x_{i,j+1,k} + x_{i+1,j+1,k+1} - x_{i+1,j+1,k}\right)/2 \\
y_\xi &= \left(y_{i+1,j+1,k+1} - y_{i,j+1,k+1} + y_{i+1,j+1,k} - y_{i,j+1,k}\right)/2 \\
y_\zeta &= \left(y_{i,j+1,k+1} - y_{i,j+1,k} + y_{i+1,j+1,k+1} - y_{i+1,j+1,k}\right)/2 \\
z_\xi &= \left(z_{i+1,j+1,k+1} - z_{i,j+1,k+1} + z_{i+1,j+1,k} - z_{i,j+1,k}\right)/2 \\
z_\zeta &= \left(z_{i,j+1,k+1} - z_{i,j+1,k} + z_{i+1,j+1,k+1} - z_{i+1,j+1,k}\right)/2
\end{aligned}
$$

Equation B-8

The metrics are used, at $k+\frac{1}{2}$ as listed in section 2.3.4 and the primitive metrics are:

$$
\begin{aligned}
x_\xi &= \left(x_{i+1,j+1,k+1} - x_{i,j+1,k+1} + x_{i+1,j,k+1} - x_{i,j,k+1}\right)/2 \\
x_\eta &= \left(x_{i+1,j+1,k+1} - x_{i+1,j,k+1} + x_{i,j+1,k+1} - x_{i,j,k+1}\right)/2 \\
y_\xi &= \left(y_{i+1,j+1,k+1} - y_{i,j+1,k+1} + y_{i+1,j,k+1} - y_{i,j,k+1}\right)/2 \\
y_\eta &= \left(y_{i+1,j+1,k+1} - y_{i+1,j,k+1} + y_{i,j+1,k+1} - y_{i,j,k+1}\right)/2 \\
z_\xi &= \left(z_{i+1,j+1,k+1} - z_{i,j+1,k+1} + z_{i+1,j,k+1} - z_{i,j,k+1}\right)/2 \\
z_\eta &= \left(z_{i+1,j+1,k+1} - z_{i+1,j,k+1} + z_{i,j+1,k+1} - z_{i,j,k+1}\right)/2
\end{aligned}
$$

Equation B-9

Each cell volume can be made up of six tetrahedrons which are determined as follows:

Cell Volume = $Vol_1 + Vol_2 + Vol_3 + Vol_4 + Vol_5 + Vol_6$

where:

$$Vol_1 = \left\{ \begin{array}{l} x_{i,j,k+1}\left[y_{i,j,k}\left(z_{i+1,j,k} - z_{i,j+1,k}\right) - z_{i,j,k}\left(y_{i+1,j,k} - y_{i,j+1,k}\right) + \left(y_{i+1,j,k}z_{i,j+1,k} - z_{i+1,j,k}y_{i,j+1,k}\right)\right] \\ - y_{i,j,k+1}\left[x_{i,j,k}\left(z_{i+1,j,k} - z_{i,j+1,k}\right) - z_{i,j,k}\left(x_{i+1,j,k} - x_{i,j+1,k}\right) + \left(x_{i+1,j,k}z_{i,j+1,k} - x_{i,j+1,k}z_{i+1,j,k}\right)\right] \\ + z_{i,j,k+1}\left[x_{i,j,k}\left(y_{i+1,j,k} - y_{i,j+1,k}\right) - y_{i,j,k}\left(x_{i+1,j,k} - x_{i,j+1,k}\right) + \left(x_{i+1,j,k}y_{i,j+1,k} - y_{i+1,j,k}z_{i,j+1,k}\right)\right] \\ - \left[\begin{array}{l} x_{i,j,k}\left(y_{i+1,j,k}z_{i,j+1,k} - z_{i+1,j,k}y_{i,j+1,k}\right) - y_{i,j,k}\left(x_{i+1,j,k}z_{i,j+1,k} - z_{i+1,j,k}x_{i,j+1,k}\right) \\ + z_{i,j,k}\left(x_{i+1,j,k}y_{i,j+1,k} - y_{i+1,j,k}x_{i,j+1,k}\right) \end{array} \right] \end{array} \right\}$$

$$Vol_2 = \left\{ \begin{array}{l} x_{i,j,k+1}\left[y_{i+1,j,k}\left(z_{i+1,j+1,k} - z_{i,j+1,k}\right) - z_{i+1,j,k}\left(y_{i+1,j+1,k} - y_{i,j+1,k}\right) + \left(y_{i+1,j+1,k}z_{i,j+1,k} - z_{i+1,j+1,k}y_{i,j+1,k}\right)\right] \\ - y_{i,j,k+1}\left[x_{i+1,j,k}\left(z_{i+1,j+1,k} - z_{i,j+1,k}\right) - z_{i+1,j,k}\left(x_{i+1,j+1,k} - x_{i,j+1,k}\right) + \left(x_{i+1,j+1,k}z_{i,j+1,k} - x_{i,j+1,k}z_{i+1,j+1,k}\right)\right] \\ + z_{i,j,k+1}\left[x_{i+1,j,k}\left(y_{i+1,j+1,k} - y_{i,j+1,k}\right) - y_{i+1,j,k}\left(x_{i+1,j+1,k} - x_{i,j+1,k}\right) + \left(x_{i+1,j+1,k}y_{i,j+1,k} - y_{i+1,j+1,k}z_{i,j+1,k}\right)\right] \\ - \left[\begin{array}{l} x_{i+1,j,k}\left(y_{i+1,j+1,k}z_{i,j+1,k} - z_{i+1,j+1,k}y_{i,j+1,k}\right) - y_{i+1,j,k}\left(x_{i+1,j+1,k}z_{i,j+1,k} - z_{i+1,j+1,k}x_{i,j+1,k}\right) \\ + z_{i+1,j,k}\left(x_{i+1,j+1,k}y_{i,j+1,k} - y_{i+1,j+1,k}x_{i,j+1,k}\right) \end{array} \right] \end{array} \right\}$$

$$Vol_3 = \left\{ \begin{array}{l} x_{i,j,k+1}\left[\begin{array}{l} y_{i+1,j,k}\left(z_{i+1,j,k+1} - z_{i+1,j+1,k+1}\right) - z_{i+1,j,k}\left(y_{i+1,j,k+1} - y_{i+1,j+1,k+1}\right) \\ + \left(y_{i+1,j,k+1}z_{i+1,j+1,k+1} - z_{i+1,j,k+1}y_{i+1,j+1,k+1}\right) \end{array} \right] \\ - y_{i,j,k+1}\left[\begin{array}{l} x_{i+1,j,k}\left(z_{i+1,j,k+1} - z_{i+1,j+1,k+1}\right) - z_{i+1,j,k}\left(x_{i+1,j,k+1} - x_{i+1,j+1,k+1}\right) \\ + \left(x_{i+1,j,k+1}z_{i+1,j+1,k+1} - x_{i+1,j+1,k+1}z_{i+1,j,k+1}\right) \end{array} \right] \\ + z_{i,j,k+1}\left[\begin{array}{l} x_{i+1,j,k}\left(y_{i+1,j,k+1} - y_{i+1,j+1,k+1}\right) - y_{i+1,j,k}\left(x_{i+1,j,k+1} - x_{i+1,j+1,k+1}\right) \\ + \left(x_{i+1,j,k+1}y_{i+1,j+1,k+1} - y_{i+1,j,k+1}z_{i+1,j+1,k+1}\right) \end{array} \right] \\ - \left[\begin{array}{l} x_{i+1,j,k}\left(y_{i+1,j,k+1}z_{i+1,j+1,k+1} - z_{i+1,j,k+1}y_{i+1,j+1,k+1}\right) - y_{i+1,j,k}\left(x_{i+1,j,k+1}z_{i+1,j+1,k+1} - z_{i+1,j,k+1}x_{i+1,j+1,k+1}\right) \\ + z_{i+1,j,k}\left(x_{i+1,j,k+1}y_{i+1,j+1,k+1} - y_{i+1,j,k+1}x_{i+1,j+1,k+1}\right) \end{array} \right] \end{array} \right\}$$

$$Vol_4 = \left\{ \begin{array}{l} x_{i,j,k+1}\left[\begin{array}{l} y_{i+1,j,k}\left(z_{i+1,j+1,k+1} - z_{i+1,j+1,k}\right) - z_{i+1,j,k}\left(y_{i+1,j+1,k+1} - y_{i+1,j+1,k}\right) \\ + \left(y_{i+1,j+1,k+1}z_{i+1,j+1,k} - z_{i+1,j+1,k+1}y_{i+1,j+1,k}\right) \end{array} \right] \\ - y_{i,j,k+1}\left[\begin{array}{l} x_{i+1,j,k}\left(z_{i+1,j+1,k+1} - z_{i+1,j+1,k}\right) - z_{i+1,j,k}\left(x_{i+1,j+1,k+1} - x_{i+1,j+1,k}\right) \\ + \left(x_{i+1,j+1,k+1}z_{i+1,j+1,k} - x_{i+1,j+1,k}z_{i+1,j+1,k+1}\right) \end{array} \right] \\ + z_{i,j,k+1}\left[\begin{array}{l} x_{i+1,j,k}\left(y_{i+1,j+1,k+1} - y_{i+1,j+1,k}\right) - y_{i+1,j,k}\left(x_{i+1,j+1,k+1} - x_{i+1,j+1,k}\right) \\ + \left(x_{i+1,j+1,k+1}y_{i+1,j+1,k} - y_{i+1,j+1,k+1}z_{i+1,j+1,k}\right) \end{array} \right] \\ - \left[\begin{array}{l} x_{i+1,j,k}\left(y_{i+1,j+1,k+1}z_{i+1,j+1,k} - z_{i+1,j+1,k+1}y_{i+1,j+1,k}\right) - y_{i+1,j,k}\left(x_{i+1,j+1,k+1}z_{i+1,j+1,k} - z_{i+1,j+1,k+1}x_{i+1,j+1,k}\right) \\ + z_{i+1,j,k}\left(x_{i+1,j+1,k+1}y_{i+1,j+1,k} - y_{i+1,j+1,k+1}x_{i+1,j+1,k}\right) \end{array} \right] \end{array} \right\}$$

$$
Vol_5 = \left\{ \begin{array}{l}
x_{i,j,k+1}\left[\begin{array}{l} y_{i,j+1,k}\left(z_{i+1,j+1,k+1} - z_{i,j+1,k+1}\right) - z_{i,j+1,k}\left(y_{i+1,j+1,k+1} - y_{i,j+1,k+1}\right) \\ + \left(y_{i+1,j+1,k+1} z_{i,j+1,k+1} - z_{i+1,j+1,k+1} y_{i,j+1,k+1}\right) \end{array}\right] \\
- y_{i,j,k+1}\left[\begin{array}{l} x_{i,j+1,k}\left(z_{i+1,j+1,k+1} - z_{i,j+1,k+1}\right) - z_{i,j+1,k}\left(x_{i+1,j+1,k+1} - x_{i,j+1,k+1}\right) \\ + \left(x_{i+1,j+1,k+1} z_{i,j+1,k+1} - x_{i,j+1,k+1} z_{i+1,j+1,k+1}\right) \end{array}\right] \\
+ z_{i,j,k+1}\left[\begin{array}{l} x_{i,j+1,k}\left(y_{i+1,j+1,k+1} - y_{i,j+1,k+1}\right) - y_{i,j+1,k}\left(x_{i+1,j+1,k+1} - x_{i,j+1,k+1}\right) \\ + \left(x_{i+1,j+1,k+1} y_{i,j+1,k+1} - y_{i+1,j+1,k+1} z_{i,j+1,k+1}\right) \end{array}\right] \\
- \left[\begin{array}{l} x_{i,j+1,k}\left(y_{i+1,j+1,k+1} z_{i,j+1,k+1} - z_{i+1,j+1,k+1} y_{i,j+1,k+1}\right) - y_{i,j+1,k}\left(x_{i+1,j+1,k+1} z_{i,j+1,k+1} - z_{i+1,j+1,k+1} x_{i,j+1,k+1}\right) \\ + z_{i,j+1,k}\left(x_{i+1,j+1,k+1} y_{i,j+1,k+1} - y_{i+1,j+1,k+1} x_{i,j+1,k+1}\right) \end{array}\right]
\end{array} \right\}
$$

$$
Vol_6 = \left\{ \begin{array}{l}
x_{i,j,k+1}\left[\begin{array}{l} y_{i,j+1,k}\left(z_{i,j+1,k+1} - z_{i+1,j+1,k+1}\right) - z_{i,j+1,k}\left(y_{i,j+1,k+1} - y_{i+1,j+1,k+1}\right) \\ + \left(y_{i,j+1,k+1} z_{i+1,j+1,k+1} - z_{i,j+1,k+1} y_{i+1,j+1,k+1}\right) \end{array}\right] \\
- y_{i,j,k+1}\left[\begin{array}{l} x_{i,j+1,k}\left(z_{i,j+1,k+1} - z_{i+1,j+1,k+1}\right) - z_{i,j+1,k}\left(x_{i,j+1,k+1} - x_{i+1,j+1,k+1}\right) \\ + \left(x_{i,j+1,k+1} z_{i+1,j+1,k+1} - x_{i+1,j+1,k+1} z_{i,j+1,k+1}\right) \end{array}\right] \\
+ z_{i,j,k+1}\left[\begin{array}{l} x_{i,j+1,k}\left(y_{i,j+1,k+1} - y_{i+1,j+1,k+1}\right) - y_{i,j+1,k}\left(x_{i,j+1,k+1} - x_{i+1,j+1,k+1}\right) \\ + \left(x_{i,j+1,k+1} y_{i+1,j+1,k+1} - y_{i,j+1,k+1} z_{i+1,j+1,k+1}\right) \end{array}\right] \\
- \left[\begin{array}{l} x_{i,j+1,k}\left(y_{i,j+1,k+1} z_{i+1,j+1,k+1} - z_{i,j+1,k+1} y_{i+1,j+1,k+1}\right) - y_{i,j+1,k}\left(x_{i,j+1,k+1} z_{i+1,j+1,k+1} - z_{i,j+1,k+1} x_{i+1,j+1,k+1}\right) \\ + z_{i,j+1,k}\left(x_{i,j+1,k+1} y_{i+1,j+1,k+1} - y_{i,j+1,k+1} x_{i+1,j+1,k+1}\right) \end{array}\right]
\end{array} \right\}
$$

Equation B-10

The rotated Eigen-values are defined as:

$$
S = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -u\rho^{-1} & \rho^{-1} & 0 & 0 & 0 \\ -v\rho^{-1} & 0 & \rho^{-1} & 0 & 0 \\ -w\rho^{-1} & 0 & 0 & \rho^{-1} & 0 \\ \alpha\beta & -u\beta & -v\beta & -w\beta & \beta \end{pmatrix}; \quad S^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ u & \rho & 0 & 0 & 0 \\ v & 0 & \rho & 0 & 0 \\ w & 0 & 0 & \rho & 0 \\ \alpha & \rho u & \rho v & \rho w & \beta^{-1} \end{pmatrix}; \quad \begin{array}{l} \alpha = \frac{1}{2}\left(u^2 + v^2 + w^2\right); \\ \beta = \gamma - 1 \end{array}
$$

$$
C_A = \begin{pmatrix} 1 & 0 & 0 & 0 & -c^{-2} \\ 0 & \rho c & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & -\rho c & 0 & 0 & 1 \end{pmatrix}; \qquad C_A^{-1} = \begin{pmatrix} 1 & c^{-2}/2 & 0 & 0 & c^{-2}/2 \\ 0 & \rho^{-1}c^{-1}/2 & 0 & 0 & -\rho^{-1}c^{-1}/2 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1/2 & 0 & 0 & 1/2 \end{pmatrix}
$$

$$
C_B = \begin{pmatrix} 1 & 0 & 0 & 0 & -c^{-2} \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \rho c & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & -\rho c & 0 & 1 \end{pmatrix}; \qquad C_B^{-1} = \begin{pmatrix} 1 & 0 & c^{-2}/2 & 0 & c^{-2}/2 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \rho^{-1}c^{-1}/2 & 0 & -\rho^{-1}c^{-1}/2 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1/2 & 0 & 1/2 \end{pmatrix}
$$

$$
C_C = \begin{pmatrix} 1 & 0 & 0 & 0 & -c^{-2} \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \rho c & 1 \\ 0 & 0 & 0 & -\rho c & 1 \end{pmatrix}; \qquad C_C^{-1} = \begin{pmatrix} 1 & 0 & 0 & c^{-2}/2 & c^{-2}/2 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \rho^{-1}c^{-1}/2 & -\rho^{-1}c^{-1}/2 \\ 0 & 0 & 0 & 1/2 & 1/2 \end{pmatrix}
$$

and rotation matrices:

$$R_A = \frac{1}{d_A}\begin{pmatrix} d_A & 0 & 0 & 0 & 0 \\ 0 & \xi_x & \xi_y & \xi_z & 0 \\ 0 & -\xi_y & \xi_x & 0 & 0 \\ 0 & -\xi_z & 0 & \xi_x & 0 \\ 0 & 0 & 0 & 0 & d_A \end{pmatrix}; \qquad R_B = \frac{1}{d_B}\begin{pmatrix} d_B & 0 & 0 & 0 & 0 \\ 0 & \eta_y & -\eta_x & 0 & 0 \\ 0 & \eta_x & \eta_y & \eta_z & 0 \\ 0 & 0 & -\eta_z & \eta_y & 0 \\ 0 & 0 & 0 & 0 & d_B \end{pmatrix};$$

$$R_C = \frac{1}{d_C}\begin{pmatrix} d_C & 0 & 0 & 0 & 0 \\ 0 & \zeta_z & 0 & -\zeta_x & 0 \\ 0 & 0 & \zeta_z & -\zeta_y & 0 \\ 0 & \zeta_x & \zeta_y & \zeta_z & 0 \\ 0 & 0 & 0 & 0 & d_C \end{pmatrix}$$

where

$$R_A^{-1} = R_A^T; \qquad R_B^{-1} = R_B^T; \qquad R_C^{-1} = R_C^T;$$

Equation B-11

Explicit Euler Fluxes in the Driving Term

The explicit Euler Fluxes are calculated as follows:

$$\widetilde{F}_{e_{i+\frac{1}{2}}} = \frac{\widetilde{F}_{e_R} + \widetilde{F}_{e_L}}{2} - \tfrac{1}{2}\left(\hat{A}_+ - \hat{A}_-\right)\left(U_R - U_L\right)$$

$$\widetilde{G}_{e_{j+\frac{1}{2}}} = \frac{\widetilde{G}_{e_T} + \widetilde{G}_{e_B}}{2} - \tfrac{1}{2}\left(\hat{B}_+ - \hat{B}_-\right)\left(U_T - U_B\right)$$

$$\widetilde{H}_{e_{k+\frac{1}{2}}} = \frac{\widetilde{H}_{e_I} + \widetilde{H}_{e_O}}{2} - \tfrac{1}{2}\left(\hat{C}_+ - \hat{C}_-\right)\left(U_I - U_O\right)$$

R = Right, L = Left, T = Top, B = Bottom, I = In and O = Out

Equation B-12

The geometric Averaged Jacobians $\hat{A}$, $\hat{B}$ and $\hat{C}$ are calculated as defined earlier.

Dropping the subscript e, the transformed fluxes at the cell corners, $\widetilde{F}, \widetilde{G}$ *and* $\widetilde{H}$ (fluxes on RHS of the equations) are determined as follows:

$$\widetilde{F} = \xi_x F + \xi_y G + \xi_z H$$

$$\widetilde{G} = \eta_x F + \eta_y G + \eta_z H$$

$$\widetilde{H} = \zeta_x F + \zeta_y G + \zeta_z H$$

and

$$U = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ E \end{pmatrix}; \quad F = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ (E+p)u \end{pmatrix}; \quad G = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vw \\ (E+p)v \end{pmatrix}; \quad H = \begin{pmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ (E+p)w \end{pmatrix};$$

Equation B-13

Viscous Fluxes

The viscous fluxes can be written in terms of M-matrices as follows:

$$\left.\widetilde{F}_v\right|_{i+\frac{1}{2}} = \left.\left(M^{11}V_\xi + M^{12}V_\eta + M^{13}V_\zeta\right)\right|_{i+\frac{1}{2}}$$

$$\left.\widetilde{G}_v\right|_{j+\frac{1}{2}} = \left.\left(M^{21}V_\xi + M^{22}V_\eta + M^{23}V_\zeta\right)\right|_{j+\frac{1}{2}}$$

$$\left.\widetilde{H}_v\right|_{k+\frac{1}{2}} = \left.\left(M^{31}V_\xi + M^{32}V_\eta + M^{33}V_\zeta\right)\right|_{k+\frac{1}{2}}$$

where

$$V = \left(\rho \;\; u \;\; v \;\; w \;\; e\right)^T$$

Equation B-14

All the M-matrices have the same format i.e. zero and non-zero elements remain in the same positions:

$$M^{i,j} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & m_{22} & m_{23} & m_{24} & 0 \\ 0 & m_{32} & m_{33} & m_{34} & 0 \\ 0 & m_{42} & m_{43} & m_{44} & 0 \\ 0 & m_{52} & m_{53} & m_{54} & m_{55} \end{pmatrix}; \; i,j = 1 \rightarrow 3$$

Equation B-15

The viscous fluxes are only determined for use in the explicit driving term. The conserved variable vector V is discretisized as follows:

at the $i+1/2$ face

$$V_\xi = \begin{pmatrix} \rho_{i+1,j,k} - \rho_{i,j,k} \\ u_{i+1,j,k} - u_{i,j,k} \\ v_{i+1,j,k} - v_{i,j,k} \\ w_{i+1,j,k} - w_{i,j,k} \\ e_{i+1,j,k} - e_{i,j,k} \end{pmatrix}$$

$$V_\eta = \begin{pmatrix} \left[\begin{matrix} \rho_{i,j+1,k} - \rho_{i,j-1,k} \\ +\rho_{i+1,j+1,k} - \rho_{i+1,j-1,k} \end{matrix}\right] \Big/ 4 \\ \left[\begin{matrix} u_{i,j+1,k} - u_{i,j-1,k} \\ +u_{i+1,j+1,k} - u_{i+1,j-1,k} \end{matrix}\right] \Big/ 4 \\ \left[\begin{matrix} v_{i,j+1,k} - v_{i,j-1,k} \\ +v_{i+1,j+1,k} - v_{i+1,j-1,k} \end{matrix}\right] \Big/ 4 \\ \left[\begin{matrix} w_{i,j+1,k} - w_{i,j-1,k} \\ +w_{i+1,j+1,k} - w_{i+1,j-1,k} \end{matrix}\right] \Big/ 4 \\ \left[\begin{matrix} e_{i,j+1,k} - e_{i,j-1,k} \\ +e_{i+1,j+1,k} - e_{i+1,j-1,k} \end{matrix}\right] \Big/ 4 \end{pmatrix}$$

at the $j+1/2$ face

$$V_\xi = \begin{pmatrix} \left[\begin{matrix} \rho_{i+1,j,k} - \rho_{i-1,j,k} \\ +\rho_{i+1,j+1,k} - \rho_{i-1,j+1,k} \end{matrix}\right] \Big/ 4 \\ \left[\begin{matrix} u_{i+1,j,k} - u_{i-1,j,k} \\ +u_{i+1,j+1,k} - u_{i-1,j+1,k} \end{matrix}\right] \Big/ 4 \\ \left[\begin{matrix} v_{i+1,j,k} - v_{i-1,j,k} \\ +v_{i+1,j+1,k} - v_{i-1,j+1,k} \end{matrix}\right] \Big/ 4 \\ \left[\begin{matrix} w_{i+1,j,k} - w_{i-1,j,k} \\ +w_{i+1,j+1,k} - w_{i-1,j+1,k} \end{matrix}\right] \Big/ 4 \\ \left[\begin{matrix} e_{i+1,j,k} - e_{i-1,j,k} \\ +e_{i+1,j+1,k} - e_{i-1,j+1,k} \end{matrix}\right] \Big/ 4 \end{pmatrix}$$

$$V_\eta = \begin{pmatrix} \rho_{i,j+1,k} - \rho_{i,j,k} \\ u_{i,j+1,k} - u_{i,j,k} \\ v_{i,j+1,k} - v_{i,j,k} \\ w_{i,j+1,k} - w_{i,j,k} \\ e_{i,j+1,k} - e_{i,j,k} \end{pmatrix}$$

at the $k+1/2$ face

$$V_\xi = \begin{pmatrix} \left[\begin{matrix} \rho_{i+1,j,k} - \rho_{i-1,j,k} \\ +\rho_{i+1,j,k+1} - \rho_{i-1,j,k+1} \end{matrix}\right] \Big/ 4 \\ \left[\begin{matrix} u_{i+1,j,k} - u_{i-1,j,k} \\ +u_{i+1,j,k+1} - u_{i-1,j,k+1} \end{matrix}\right] \Big/ 4 \\ \left[\begin{matrix} v_{i+1,j,k} - v_{i-1,j,k} \\ +v_{i+1,j,k+1} - v_{i-1,j,k+1} \end{matrix}\right] \Big/ 4 \\ \left[\begin{matrix} w_{i+1,j,k} - w_{i-1,j,k} \\ +w_{i+1,j,k+1} - w_{i-1,j,k+1} \end{matrix}\right] \Big/ 4 \\ \left[\begin{matrix} e_{i+1,j,k} - e_{i-1,j,k} \\ +e_{i+1,j,k+1} - e_{i-1,j,k+1} \end{matrix}\right] \Big/ 4 \end{pmatrix}$$

$$V_\eta = \begin{pmatrix} \left[\begin{matrix} \rho_{i,j+1,k} - \rho_{i,j-1,k} \\ +\rho_{i,j+1,k+1} - \rho_{i,j-1,k+1} \end{matrix}\right] \Big/ 4 \\ \left[\begin{matrix} u_{i,j+1,k} - u_{i,j-1,k} \\ +u_{i,j+1,k+1} - u_{i,j-1,k+1} \end{matrix}\right] \Big/ 4 \\ \left[\begin{matrix} v_{i,j+1,k} - v_{i,j-1,k} \\ +v_{i,j+1,k+1} - v_{i,j-1,k+1} \end{matrix}\right] \Big/ 4 \\ \left[\begin{matrix} w_{i,j+1,k} - w_{i,j-1,k} \\ +w_{i,j+1,k+1} - w_{i,j-1,k+1} \end{matrix}\right] \Big/ 4 \\ \left[\begin{matrix} e_{i,j+1,k} - e_{i,j-1,k} \\ +e_{i,j+1,k+1} - e_{i,j-1,k+1} \end{matrix}\right] \Big/ 4 \end{pmatrix}$$

$$V_\zeta = \begin{pmatrix} \left[\begin{matrix}\rho_{i,j,k+1}-\rho_{i,j,k-1}\\ +\rho_{i+1,j,k+1}-\rho_{i+1,j,k-1}\end{matrix}\right]\Big/4 \\ \left[\begin{matrix}u_{i,j,k+1}-u_{i,j,k-1}\\ +u_{i+1,j,k+1}-u_{i+1,j,k-1}\end{matrix}\right]\Big/4 \\ \left[\begin{matrix}v_{i,j,k+1}-v_{i,j,k-1}\\ +v_{i+1,j,k+1}-v_{i+1,j,k-1}\end{matrix}\right]\Big/4 \\ \left[\begin{matrix}w_{i,j,k+1}-w_{i,j,k-1}\\ +w_{i+1,j,k+1}-w_{i+1,j,k-1}\end{matrix}\right]\Big/4 \\ \left[\begin{matrix}e_{i,j,k+1}-e_{i,j,k-1}\\ +e_{i+1,j,k+1}-e_{i+1,j,k-1}\end{matrix}\right]\Big/4 \end{pmatrix} \quad \Bigg| \quad V_\zeta = \begin{pmatrix} \left[\begin{matrix}\rho_{i,j,k+1}-\rho_{i,j,k-1}\\ +\rho_{i,j+1,k+1}-\rho_{i,j+1,k-1}\end{matrix}\right]\Big/4 \\ \left[\begin{matrix}u_{i,j,k+1}-u_{i,j,k-1}\\ +u_{i,j+1,k+1}-u_{i,j+1,k-1}\end{matrix}\right]\Big/4 \\ \left[\begin{matrix}v_{i,j,k+1}-v_{i,j,k-1}\\ +v_{i,j+1,k+1}-v_{i,j+1,k-1}\end{matrix}\right]\Big/4 \\ \left[\begin{matrix}w_{i,j,k+1}-w_{i,j,k-1}\\ +w_{i,j+1,k+1}-w_{i,j+1,k-1}\end{matrix}\right]\Big/4 \\ \left[\begin{matrix}e_{i,j,k+1}-e_{i,j,k-1}\\ +e_{i,j+1,k+1}-e_{i,j+1,k-1}\end{matrix}\right]\Big/4 \end{pmatrix} \quad \Bigg| \quad V_\zeta = \begin{pmatrix} \rho_{i,j,k+1}-\rho_{i,j,k} \\ u_{i,j,k+1}-u_{i,j,k} \\ v_{i,j,k+1}-v_{i,j,k} \\ w_{i,j,k+1}-w_{i,j,k} \\ e_{i,j,k+1}-e_{i,j,k} \end{pmatrix}$$

Equation B-16

$M^{1L}\Big|_{i+\frac{1}{2}};\ L = 1 \rightarrow 3$

$$m_{22}^{11} = (2\mu+\lambda)\xi_x^2 + \mu\xi_y^2 + \mu\xi_z^2$$
$$m_{23}^{11} = (\mu+\lambda)\xi_x\xi_y$$
$$m_{24}^{11} = (\mu+\lambda)\xi_x\xi_z$$
$$m_{32}^{11} = m_{23}^{11}$$
$$m_{33}^{11} = \mu\xi_x^2 + (2\mu+\lambda)\xi_y^2 + \mu\xi_z^2$$
$$m_{34}^{11} = (\mu+\lambda)\xi_y\xi_z$$
$$m_{42}^{11} = m_{24}^{11}$$
$$m_{43}^{11} = m_{34}^{11}$$
$$m_{44}^{11} = \mu\xi_x^2 + \mu\xi_y^2 + (2\mu+\lambda)\xi_z^2$$
$$m_{52}^{11} = \bar{u}m_{22}^{11} + \bar{v}m_{32}^{11} + \bar{w}m_{42}^{11}$$
$$m_{53}^{11} = \bar{u}m_{23}^{11} + \bar{v}m_{33}^{11} + \bar{w}m_{43}^{11}$$
$$m_{54}^{11} = \bar{u}m_{24}^{11} + \bar{v}m_{34}^{11} + \bar{w}m_{44}^{11}$$
$$m_{55}^{11} = \kappa\left(\xi_x^2 + \xi_y^2 + \xi_z^2\right)$$
$$m_{22}^{13} = (2\mu+\lambda)\xi_x\eta_x + \mu\xi_y\eta_y + \mu\xi_z\eta_z$$
$$m_{23}^{12} = \lambda\xi_x\eta_y + \mu\xi_y\eta_x$$
$$m_{24}^{12} = \lambda\xi_x\eta_z + \mu\xi_z\eta_x$$
$$m_{32}^{12} = \lambda\xi_x\eta_z + \mu\xi_z\eta_x$$
$$m_{33}^{12} = \mu\xi_x\eta_x + (2\mu+\lambda)\xi_y\eta_y + \mu\xi_z\eta_z$$
$$m_{34}^{13} = \lambda\xi_y\zeta_z + \mu\xi_z\zeta_y$$
$$m_{42}^{13} = \lambda\xi_z\zeta_y + \mu\xi_y\zeta_z$$
$$m_{43}^{13} = \lambda\xi_z\zeta_y + \mu\xi_y\zeta_z$$
$$m_{44}^{13} = \mu\xi_x\zeta_x + \mu\xi_y\zeta_y + (2\mu+\lambda)\xi_z\zeta_z$$
$$m_{52}^{11} = \bar{u}m_{22}^{11} + \bar{v}m_{32}^{11} + \bar{w}m_{42}^{11}$$
$$m_{53}^{11} = \bar{u}m_{23}^{11} + \bar{v}m_{33}^{11} + \bar{w}m_{43}^{11}$$
$$m_{54}^{11} = \bar{u}m_{24}^{11} + \bar{v}m_{34}^{11} + \bar{w}m_{44}^{11}$$
$$m_{55}^{11} = \kappa\left(\xi_x^2 + \xi_y^2 + \xi_z^2\right)$$

$$m_{22}^{12} = (2\mu+\lambda)\xi_x\eta_x + \mu\xi_y\eta_y + \mu\xi_z\eta_z$$
$$m_{23}^{12} = \lambda\xi_x\eta_y + \mu\xi_y\eta_x$$
$$m_{24}^{12} = \lambda\xi_x\eta_z + \mu\xi_z\eta_x$$
$$m_{32}^{12} = \lambda\xi_x\eta_z + \mu\xi_z\eta_x$$
$$m_{33}^{12} = \mu\xi_x\eta_x + (2\mu+\lambda)\xi_y\eta_y + \mu\xi_z\eta_z$$
$$m_{34}^{12} = \lambda\xi_y\eta_z + \mu\xi_z\eta_y$$
$$m_{42}^{12} = \lambda\xi_z\eta_x + \mu\xi_x\eta_z$$
$$m_{43}^{12} = \lambda\xi_z\eta_y + \mu\xi_y\eta_z$$
$$m_{44}^{12} = \mu\xi_x\eta_x + \mu\xi_y\eta_y + (2\mu+\lambda)\xi_z\eta_z$$
$$m_{52}^{12} = \bar{u}m_{22}^{12} + \bar{v}m_{32}^{12} + \bar{w}m_{42}^{12}$$
$$m_{53}^{12} = \bar{u}m_{23}^{12} + \bar{v}m_{33}^{12} + \bar{w}m_{43}^{12}$$
$$m_{54}^{12} = \bar{u}m_{24}^{12} + \bar{v}m_{34}^{12} + \bar{w}m_{44}^{12}$$
$$m_{55}^{12} = \kappa\left(\xi_x\eta_x + \xi_y\eta_y + \xi_z\eta_z\right)$$

$$\bar{u} = \frac{u_{i+1,j,k} + u_{i,j,k}}{2}$$
$$\bar{v} = \frac{v_{i+1,j,k} + v_{i,j,k}}{2}$$
$$\bar{w} = \frac{w_{i+1,j,k} + w_{i,j,k}}{2}$$
$$\mu = \mu\left(\frac{T_{i+1,j,k} + T_{i,j,k}}{2}\right)$$

with primitive metrics:

$$x_\xi = \begin{pmatrix} x_{i+2,j+1,k} - x_{i,j+1,k} + x_{i+2,j,k} - x_{i,j,k} \\ x_{i+2,j+1,k+1} - x_{i,j+1,k+1} + x_{i+2,j,k+1} - x_{i,j,k+1} \end{pmatrix} \Big/ 8$$

$$x_\eta = \left(x_{i+1,j+1,k+1} - x_{i+1,j,k+1} + x_{i+1,j+1,k} - x_{i+1,j,k} \right) / 2$$

$$x_\zeta = \left(x_{i+1,j,k+1} - x_{i+1,j,k} + x_{i+1,j+1,k+1} - x_{i+1,j+1,k} \right) / 2$$

$$y_\xi = \begin{pmatrix} y_{i+2,j+1,k} - y_{i,j+1,k} + y_{i+2,j,k} - y_{i,j,k} \\ y_{i+2,j+1,k+1} - y_{i,j+1,k+1} + y_{i+2,j,k+1} - y_{i,j,k+1} \end{pmatrix} \Big/ 8$$

$$y_\eta = \left(y_{i+1,j+1,k+1} - y_{i+1,j,k+1} + y_{i+1,j+1,k} - y_{i+1,j,k} \right) / 2$$

$$y_\zeta = \left(y_{i+1,j,k+1} - y_{i+1,j,k} + y_{i+1,j+1,k+1} - y_{i+1,j+1,k} \right) / 2$$

$$z_\xi = \begin{pmatrix} z_{i+2,j+1,k} - z_{i,j+1,k} + z_{i+2,j,k} - z_{i,j,k} \\ z_{i+2,j+1,k+1} - z_{i,j+1,k+1} + z_{i+2,j,k+1} - z_{i,j,k+1} \end{pmatrix} \Big/ 8$$

$$z_\eta = \left(z_{i+1,j+1,k+1} - z_{i+1,j,k+1} + z_{i+1,j+1,k} - z_{i+1,j,k} \right) / 2$$

$$z_\zeta = \left(z_{i+1,j,k+1} - z_{i+1,j,k} + z_{i+1,j+1,k+1} - z_{i+1,j+1,k} \right) / 2$$

$M^{2L}\Big|_{j+\frac{1}{2}}; \quad L = 1 \rightarrow 3$

$$m_{22}^{21} = (2\mu+\lambda)\xi_x\eta_x + \mu\xi_y\eta_y + \mu\xi_z\eta_z$$
$$m_{23}^{21} = \lambda\eta_x\xi_y + \mu\eta_y\xi_x$$
$$m_{24}^{21} = \lambda\eta_x\xi_z + \mu\eta_z\xi_x$$
$$m_{32}^{21} = \lambda\eta_y\xi_x + \mu\eta_x\xi_y$$
$$m_{33}^{21} = \mu\xi_x\eta_x + (2\mu+\lambda)\xi_y\eta_y + \mu\xi_z\eta_z$$
$$m_{34}^{21} = \lambda\eta_z\xi_y + \mu\eta_y\xi_z$$
$$m_{42}^{21} = \lambda\eta_x\xi_z + \mu\eta_z\xi_x$$
$$m_{43}^{21} = \lambda\eta_y\xi_z + \mu\eta_z\xi_y$$
$$m_{44}^{21} = \mu\xi_x\eta_x + \mu\xi_y\eta_y + (2\mu+\lambda)\xi_z\eta_z$$
$$m_{52}^{21} = \bar{u}m_{22}^{21} + \bar{v}m_{32}^{21} + \bar{w}m_{42}^{21}$$
$$m_{53}^{21} = \bar{u}m_{23}^{21} + \bar{v}m_{33}^{21} + \bar{w}m_{43}^{21}$$
$$m_{54}^{21} = \bar{u}m_{24}^{21} + \bar{v}m_{34}^{21} + \bar{w}m_{44}^{21}$$
$$m_{55}^{21} = \kappa\left(\xi_x\eta_x + \xi_y\eta_y + \xi_z\eta_z\right)$$

$$m_{22}^{22} = (2\mu+\lambda)\eta_x^2 + \mu\eta_y^2 + \mu\eta_z^2$$
$$m_{23}^{22} = (\mu+\lambda)\eta_x\eta_y$$
$$m_{24}^{22} = (\mu+\lambda)\eta_x\eta_z$$
$$m_{32}^{22} = m_{23}^{22}$$
$$m_{33}^{22} = \mu\eta_x^2 + (2\mu+\lambda)\eta_y^2 + \mu\eta_z^2$$
$$m_{34}^{22} = (\mu+\lambda)\eta_y\eta_z$$
$$m_{42}^{22} = m_{24}^{22}$$
$$m_{43}^{22} = m_{34}^{22}$$
$$m_{44}^{22} = \mu\eta_x^2 + \mu\eta_y^2 + (2\mu+\lambda)\eta_z^2$$
$$m_{52}^{22} = \bar{u}m_{22}^{22} + \bar{v}m_{32}^{22} + \bar{w}m_{42}^{22}$$
$$m_{53}^{22} = \bar{u}m_{23}^{22} + \bar{v}m_{33}^{22} + \bar{w}m_{43}^{22}$$
$$m_{54}^{22} = \bar{u}m_{24}^{22} + \bar{v}m_{34}^{22} + \bar{w}m_{44}^{22}$$
$$m_{55}^{22} = \kappa\left(\eta_x^2 + \eta_y^2 + \eta_z^2\right)$$

$$m_{22}^{23} = (2\mu + \lambda)\xi_x\zeta_x + \mu\xi_y\zeta_y + \mu\xi_z\zeta_z$$
$$m_{23}^{23} = \lambda\eta_x\zeta_y + \mu\eta_y\zeta_x$$
$$m_{24}^{23} = \lambda\eta_x\zeta_z + \mu\eta_z\zeta_x$$
$$m_{32}^{23} = \lambda\eta_y\zeta_x + \mu\eta_x\zeta_y$$
$$m_{33}^{23} = \mu\xi_x\zeta_x + (2\mu + \lambda)\xi_y\zeta_y + \mu\xi_z\zeta_z$$
$$m_{34}^{23} = \lambda\eta_y\zeta_z + \mu\eta_z\zeta_y$$
$$m_{42}^{23} = \lambda\eta_z\zeta_x + \mu\eta_x\zeta_z$$
$$m_{43}^{23} = \lambda\eta_z\zeta_y + \mu\eta_y\zeta_z$$
$$m_{44}^{23} = \mu\zeta_x\eta_x + \mu\zeta_y\eta_y + (2\mu + \lambda)\zeta_z\eta_z$$
$$m_{52}^{23} = \bar{u}m_{22}^{23} + \bar{v}m_{32}^{23} + \bar{w}m_{42}^{23}$$
$$m_{53}^{23} = \bar{u}m_{23}^{23} + \bar{v}m_{33}^{23} + \bar{w}m_{43}^{23}$$
$$m_{54}^{23} = \bar{u}m_{24}^{23} + \bar{v}m_{34}^{23} + \bar{w}m_{44}^{23}$$
$$m_{55}^{23} = \kappa\left(\zeta_x\eta_x + \zeta_y\eta_y + \zeta_z\eta_z\right)$$

$$\bar{u} = \frac{u_{i,j+1,k} + u_{i,j,k}}{2}$$
$$\bar{v} = \frac{v_{i,j+1,k} + v_{i,j,k}}{2}$$
$$\bar{w} = \frac{w_{i,j+1,k} + w_{i,j,k}}{2}$$
$$\mu = \mu\left(\frac{T_{i,j+1,k} + T_{i,j,k}}{2}\right)$$

with primitive metrics:

$$x_\xi = \left(x_{i+1,j+1,k+1} - x_{i,j+1,k+1} + x_{i+1,j+1,k} - x_{i,j+1,k}\right)/2$$
$$x_\eta = \left(\begin{matrix} x_{i,j+2,k+1} - x_{i,j,k+1} + x_{i,j+2,k} - x_{i,j,k} \\ x_{i+1,j+2,k+1} - x_{i+1,j,k+1} + x_{i+1,j+2,k} - x_{i+1,j,k} \end{matrix}\right)\Big/8$$
$$x_\zeta = \left(x_{i,j+1,k+1} - x_{i,j+1,k} + x_{i+1,j+1,k+1} - x_{i+1,j+1,k}\right)/2$$
$$y_\xi = \left(y_{i+1,j+1,k+1} - y_{i,j+1,k+1} + y_{i+1,j+1,k} - y_{i,j+1,k}\right)/2$$
$$y_\eta = \left(\begin{matrix} y_{i,j+2,k+1} - y_{i,j,k+1} + y_{i,j+2,k} - y_{i,j,k} \\ y_{i+1,j+2,k+1} - y_{i+1,j,k+1} + y_{i+1,j+2,k} - y_{i+1,j,k} \end{matrix}\right)\Big/8$$
$$y_\zeta = \left(y_{i,j+1,k+1} - y_{i,j+1,k} + y_{i+1,j+1,k+1} - y_{i+1,j+1,k}\right)/2$$
$$z_\xi = \left(z_{i+1,j+1,k+1} - z_{i,j+1,k+1} + z_{i+1,j+1,k} - z_{i,j+1,k}\right)/2$$
$$z_\eta = \left(\begin{matrix} z_{i,j+2,k+1} - z_{i,j,k+1} + z_{i,j+2,k} - z_{i,j,k} \\ z_{i+1,j+2,k+1} - z_{i+1,j,k+1} + z_{i+1,j+2,k} - z_{i+1,j,k} \end{matrix}\right)\Big/8$$
$$z_\zeta = \left(z_{i,j+1,k+1} - z_{i,j+1,k} + z_{i+1,j+1,k+1} - z_{i+1,j+1,k}\right)/2$$

$M^{3L}\Big|_{k+\frac{1}{2}}; \; L = 1 \rightarrow 3$

$$m_{22}^{31} = (2\mu+\lambda)\xi_x\zeta_x + \mu\xi_y\zeta_y + \mu\xi_z\zeta_z$$
$$m_{23}^{31} = \lambda\zeta_x\xi_y + \mu\zeta_y\xi_x$$
$$m_{24}^{31} = \lambda\zeta_x\xi_z + \mu\zeta_z\xi_x$$
$$m_{32}^{31} = \lambda\zeta_y\xi_x + \mu\zeta_x\xi_y$$
$$m_{33}^{31} = \mu\xi_x\zeta_x + (2\mu+\lambda)\xi_y\zeta_y + \mu\xi_z\zeta_z$$
$$m_{34}^{31} = \lambda\xi_z\zeta_y + \mu\xi_y\zeta_z$$
$$m_{42}^{31} = \lambda\zeta_z\xi_x + \mu\zeta_x\xi_z$$
$$m_{43}^{31} = \lambda\zeta_z\xi_y + \mu\zeta_y\xi_z$$
$$m_{44}^{31} = \mu\xi_x\zeta_x + \mu\xi_y\zeta_y + (2\mu+\lambda)\xi_z\zeta_z$$
$$m_{52}^{31} = \bar{u}m_{22}^{31} + \bar{v}m_{32}^{31} + \bar{w}m_{42}^{31}$$
$$m_{53}^{31} = \bar{u}m_{23}^{31} + \bar{v}m_{33}^{31} + \bar{w}m_{43}^{31}$$
$$m_{54}^{31} = \bar{u}m_{24}^{31} + \bar{v}m_{34}^{31} + \bar{w}m_{44}^{31}$$
$$m_{55}^{31} = \kappa\left(\xi_x\zeta_x + \xi_y\zeta_y + \xi_z\zeta_z\right)$$

$$m_{22}^{33} = (2\mu+\lambda)\zeta_x^2 + \zeta\eta_y^2 + \zeta\eta_z^2$$
$$m_{23}^{33} = (\mu+\lambda)\zeta_x\zeta_y$$
$$m_{24}^{33} = (\mu+\lambda)\zeta_x\zeta_z$$
$$m_{32}^{33} = m_{23}^{33}$$
$$m_{33}^{33} = \mu\zeta_x^2 + (2\mu+\lambda)\zeta_y^2 + \mu\zeta_z^2$$
$$m_{34}^{33} = (\mu+\lambda)\zeta_y\zeta_z$$
$$m_{42}^{33} = m_{24}^{33}$$
$$m_{43}^{33} = m_{34}^{33}$$
$$m_{44}^{33} = \mu\zeta_x^2 + \mu\zeta_y^2 + (2\mu+\lambda)\zeta_z^2$$
$$m_{52}^{33} = \bar{u}m_{22}^{33} + \bar{v}m_{32}^{33} + \bar{w}m_{42}^{33}$$
$$m_{53}^{33} = \bar{u}m_{23}^{33} + \bar{v}m_{33}^{33} + \bar{w}m_{43}^{33}$$
$$m_{54}^{33} = \bar{u}m_{24}^{33} + \bar{v}m_{34}^{33} + \bar{w}m_{44}^{33}$$
$$m_{55}^{33} = \kappa\left(\zeta_x^2 + \zeta_y^2 + \zeta_z^2\right)$$

$$m_{22}^{32} = (2\mu+\lambda)\eta_x\zeta_x + \mu\eta_y\zeta_y + \mu\eta_z\zeta_z$$
$$m_{23}^{32} = \lambda\zeta_x\eta_y + \mu\zeta_y\eta_x$$
$$m_{24}^{32} = \lambda\zeta_x\eta_z + \mu\zeta_z\eta_x$$
$$m_{32}^{32} = \lambda\zeta_z\eta_y + \mu\zeta_y\eta_z$$
$$m_{33}^{32} = \mu\eta_x\zeta_x + (2\mu+\lambda)\eta_y\zeta_y + \mu\eta_z\zeta_z$$
$$m_{34}^{32} = \lambda\eta_y\zeta_z + \mu\eta_z\zeta_y$$
$$m_{42}^{32} = \lambda\zeta_z\eta_x + \mu\zeta_x\eta_z$$
$$m_{43}^{32} = \lambda\zeta_z\eta_y + \mu\zeta_y\eta_z$$
$$m_{44}^{23} = \mu\zeta_x\eta_x + \mu\zeta_y\eta_y + (2\mu+\lambda)\zeta_z\eta_z$$
$$m_{52}^{32} = \bar{u}m_{22}^{32} + \bar{v}m_{32}^{32} + \bar{w}m_{42}^{32}$$
$$m_{53}^{32} = \bar{u}m_{23}^{32} + \bar{v}m_{33}^{32} + \bar{w}m_{43}^{32}$$
$$m_{54}^{32} = \bar{u}m_{24}^{32} + \bar{v}m_{34}^{32} + \bar{w}m_{44}^{32}$$
$$m_{55}^{32} = \kappa\left(\zeta_x\eta_x + \zeta_y\eta_y + \zeta_z\eta_z\right)$$

$$\bar{u} = \frac{u_{i,j,k+1} + u_{i,j,k}}{2}$$
$$\bar{v} = \frac{v_{i,j,k+1} + v_{i,j,k}}{2}$$
$$\bar{w} = \frac{w_{i,j,k+1} + w_{i,j,k}}{2}$$
$$\mu = \mu\left(\frac{T_{i,j,k+1} + T_{i,j,k}}{2}\right)$$

with primitive metrics:

$$x_\xi = \left(x_{i+1,j+1,k+1} - x_{i,j+1,k+1} + x_{i+1,j,k+1} - x_{i,j,k+1}\right)/2$$

$$x_\eta = \left(x_{i+1,j+1,k+1} - x_{i+1,j,k+1} + x_{i,j+1,k+1} - x_{i,j,k+1}\right)/2$$

$$x_\zeta = \left(\begin{matrix} x_{i,j+1,k+2} - x_{i,j+1,k} + x_{i,j,k+2} - x_{i,j,k} \\ x_{i+1,j+1,k+2} - x_{i+1,j+1,k} + x_{i+1,j,k+2} - x_{i+1,j,k} \end{matrix}\right) \Big/ 8$$

$$y_\xi = \left(y_{i+1,j+1,k+1} - y_{i,j+1,k+1} + y_{i+1,j,k+1} - y_{i,j,k+1}\right)/2$$

$$y_\eta = \left(y_{i+1,j+1,k+1} - y_{i+1,j,k+1} + y_{i,j+1,k+1} - y_{i,j,k+1}\right)/2$$

$$y_\zeta = \left(\begin{matrix} y_{i,j+1,k+2} - y_{i,j+1,k} + y_{i,j,k+2} - y_{i,j,k} \\ y_{i+1,j+1,k+2} - y_{i+1,j+1,k} + y_{i+1,j,k+2} - y_{i+1,j,k} \end{matrix}\right) \Big/ 8$$

$$z_\xi = \left(z_{i+1,j+1,k+1} - z_{i,j+1,k+1} + z_{i+1,j,k+1} - z_{i,j,k+1}\right)/2$$

$$z_\eta = \left(z_{i+1,j+1,k+1} - z_{i+1,j,k+1} + z_{i,j+1,k+1} - z_{i,j,k+1}\right)/2$$

$$z_\zeta = \left(\begin{matrix} z_{i,j+1,k+2} - z_{i,j+1,k} + z_{i,j,k+2} - z_{i,j,k} \\ z_{i+1,j+1,k+2} - z_{i+1,j+1,k} + z_{i+1,j,k+2} - z_{i+1,j,k} \end{matrix}\right) \Big/ 8$$

and

$$\kappa = \frac{\gamma\mu}{\Pr}; \; \lambda = -\frac{2}{3}\mu; \; e = c_v T$$

$$N = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -u\rho^{-1} & \rho^{-1} & 0 & 0 & 0 \\ -v\rho^{-1} & 0 & \rho^{-1} & 0 & 0 \\ -w\rho^{-1} & 0 & 0 & \rho^{-1} & 0 \\ (\alpha - e)\rho^{-1} & -u\rho^{-1} & -v\rho^{-1} & -w\rho^{-1} & \rho^{-1} \end{pmatrix}; \qquad \alpha = \frac{u^2 + v^2 + w^2}{2}$$

Equation B-17

Implementation

The algorithm is implemented in two sweeps:

sweep1: backward direction keeping k constant (decreasing i direction)
sweep2: forward direction keeping k constant (increasing i direction)

The process is now repeated incrementing k from 2 to *NZ-1*

Finally, the solution is updated and the time step is incremented.

Boundary Conditions

This method is an 3D extension of the Thin layer 2D Reynolds-averaged Navier-Stokes boundary conditions as described by Craig[28].

Impermeable Boundaries

The explicit and implicit boundary conditions are treated separately.

Explicit Euler boundary conditions:

$$U_m = R_o^{-1} T R_o U_n;$$

$$T = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & p & 0 & 0 \\ 0 & 0 & 0 & q & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad for \quad \begin{cases} J-\text{ surface: } p=-1; q=1; o=B \\ K-\text{surface: } p=1; q=-1; o=A \\ \text{lower boudary: } m=1; n=2 \\ \text{upper boundary: } \ m=NJ; n=NJ-1 \text{ on } J-\text{surface} \\ \qquad\qquad\qquad\quad m=NK; n=NK-1 \text{ on } K-\text{surface} \end{cases}$$

Equation B-18

$$\begin{aligned} \rho_m &= U_m(1) \\ u_m &= U_m(2)/U_m(1) \\ v_m &= U_m(3)/U_m(1) \\ w_m &= U_m(4)/U_m(1) \\ E_m &= U_m(5) \\ e_m &= U_m(5)/U_m(1) - \left(u_m^2 + v_m^2 + w_m^2\right)/2 \\ p_m &= (\gamma - 1) e_m \rho_m \\ c_m &= \sqrt{\frac{\gamma p_m}{\rho_m}} \end{aligned}$$

Explicit viscous boundary conditions:

$$\begin{aligned} \rho_m &= \rho_n \\ u_m &= -u_n + 2u_{wall} \\ v_m &= -v_n \\ w_m &= -w_n \\ e_m &= (1 - t_1) T_{wall} c_v + t_1 e_n \\ t_1 &= \begin{cases} 1 & adiabatic\ wall \\ -1 & isothermal\ wall \end{cases} \end{aligned}$$

Implicit viscous boundary conditions:

no slip boundary at $j=1\frac{1}{2}$

$$\hat{A}'_2 = \hat{A}_2 - \frac{\Delta t}{V_{i,2,k}} \widetilde{B}_{+_{i,1\frac{1}{2},k}} R_B^{-1} T R_B - \frac{\Delta t}{V_{i,2,k}} \begin{pmatrix} M^{22}_{i,1\frac{1}{2},k} E_l N_{i,2,k} - \frac{1}{4} M^{12}_{i+\frac{1}{2},j,k} E_l N_{i,2,k} + \frac{1}{4} M^{12}_{i-\frac{1}{2},j,k} E_l N_{i,2,k} + \frac{1}{4} M^{32}_{i,j,k+\frac{1}{2}} E_l N_{i,2,k} \\ -\frac{1}{4} M^{32}_{i,j,k-\frac{1}{2}} E_l N_{i,2,k} \end{pmatrix}$$

Equation B-19

no slip boundary at $j=NJ-½$

$$\hat{A}'_{NJ-1} = \hat{A}_{NJ-1} + \frac{\Delta t}{V_{i,NJ-1,k}} \widetilde{B}_{-_{i,NJ-\frac{1}{2},k}} R_B^{-1} T R_B - \frac{\Delta t}{V_{i,NJ-1,k}} \begin{pmatrix} M^{22}_{i,NJ-\frac{1}{2},k} E_l N_{i,NJ-1,k} + \frac{1}{4} M^{12}_{i+\frac{1}{2},NJ-\frac{1}{2},k} E_l N_{i,NJ-1,k} - \frac{1}{4} M^{12}_{i-\frac{1}{2},NJ-\frac{1}{2},k} E_l N_{i,NJ-1,k} \\ + \frac{1}{4} M^{32}_{i,NJ-\frac{1}{2},k+\frac{1}{2}} E_l N_{i,NJ-1,k} + \frac{1}{4} M^{32}_{i,NJ-\frac{1}{2},k-\frac{1}{2}} E_l N_{i,NJ-1,k} \end{pmatrix}$$

Equation B-20

no slip boundary at $k=1½$

$$\widetilde{A}'_2 = \widetilde{A}_2 - \frac{\Delta t}{V_{i,j,2}} \hat{C}_{+_{i,j,1\frac{1}{2}}} R_A^{-1} T R_A - \frac{\Delta t}{V_{i,j,2}} \begin{pmatrix} M^{33}_{i,j,1\frac{1}{2}} E_l N_{i,j,2} - \frac{1}{4} M^{13}_{i,j,1\frac{1}{2}} E_l N_{i,j,2} + \frac{1}{4} M^{13}_{i-\frac{1}{2},j,k} E_l N_{i,j,2} - \frac{1}{4} M^{23}_{i,j+\frac{1}{2},k} E_l N_{i,j,2} \\ + \frac{1}{4} M^{23}_{i,j-\frac{1}{2},k} E_l N_{i,j,2} - \frac{1}{4} M^{23}_{i,j+\frac{1}{2},k} E_l N_{i,j,2} + \frac{1}{4} M^{23}_{i,j-\frac{1}{2},k} E_l N_{i,j,2} - \frac{1}{4} M^{32}_{i,j,1\frac{1}{2}} E_l N_{i,j,2} \\ + \frac{1}{4} M^{32}_{i,j,1\frac{1}{2}} E_l N_{i,j,2} \end{pmatrix}$$

Equation B-21

no slip boundary at $k=NK-½$

$$\hat{A}'_{NK-1} = \widetilde{A}_{NK-1} \frac{\Delta t}{V_{i,j,NK-1}} \hat{C}_{-_{i,j,NJ-\frac{1}{2}}} R_A^{-1} T R_A - \frac{\Delta t}{V_{i,j,NK-1}} \begin{pmatrix} M^{33}_{i,j,NK-\frac{1}{2}} E_l N_{i,j,NK-1} + \frac{1}{4} M^{13}_{i,j,NK-\frac{1}{2}} E_l N_{i,j,NK-1} - \frac{1}{4} M^{13}_{i-\frac{1}{2},j,k-\frac{1}{2}} E_l N_{i,j,NK-1} \\ - \frac{1}{4} M^{23}_{i,j-\frac{1}{2},k-\frac{1}{2}} E_l N_{i,j,NK-1} + \frac{1}{4} M^{23}_{i,j+\frac{1}{2},NK-\frac{1}{2}} E_l N_{i,j,NK-1} + \frac{1}{4} M^{23}_{i,j+\frac{1}{2},NK-\frac{1}{2}} E_l N_{i,j,NK-1} \\ - \frac{1}{4} M^{23}_{i,j-\frac{1}{2},k-\frac{1}{2}} E_l N_{i,j,NK-1} + \frac{1}{4} M^{32}_{i,j,NK-\frac{1}{2}} E_l N_{i,j+1,NK-1} - \frac{1}{4} M^{32}_{i,j,NK-\frac{1}{2}} E_l N_{i,j-1,NK-1} \end{pmatrix}$$

Equation B-22

<u>Entrance Boundaries</u>

For 3D flow four independent external quantities have to be specified for subsonic entrance conditions. The following quantities were chosen:

p_t = Total ambient pressure [kPa]
T_t = Ambient temperature [K]
θ_v, θ_w = Entrance velocity angles

The entrance pressure and temperature can be expressed as a function of the flow velocity:

$$p = p_t \left[1 - \frac{\gamma - 1}{\gamma + 1} \left(1 + \tan^2 \theta_v + \tan^2 \theta_w \right) \frac{u^2}{a_*^2} \right]^{\frac{\gamma}{\gamma - 1}} = p(u)$$

$$T = T_t \left[1 - \frac{\gamma - 1}{\gamma + 1} \left(1 + \tan^2 \theta_v + \tan^2 \theta_w \right) \frac{u^2}{a_*^2} \right] = T(u)$$

$$v = u \tan\theta_v = v(u); \; w = u \tan\theta_w = w(u); \; a_*^2 = 2\gamma \frac{\gamma - 1}{\gamma + 1} c_v T_t$$

Equation B-23

The flow variables are updated as follows:

$$u_1^{n+1} = u_1^n + \delta u_1$$
$$v_1^{n+1} = u_1^{n+1} \tan\theta_v$$
$$w_1^{n+1} = u_1^{n+1} \tan\theta_w$$
$$p_1^{n+1} = p\left(u_1^{n+1}\right)$$
$$T_1^{n+1} = T\left(u_1^{n+1}\right)$$
$$\rho_1^{n+1} = \frac{p_1^{n+1}}{(\gamma-1)c_v T_1^{n+1}}$$
$$\alpha = \frac{\left(u_1^{n+1}\right)^2 + \left(v_1^{n+1}\right)^2 + \left(w_1^{n+1}\right)^2}{2}$$
$$E_1^{n+1} = \rho_1^{n+1}\left(c_v T_1^{n+1} + \alpha\right)$$

δu_1 is solved as follows:

$$\delta u_1 = \frac{R}{\left(\frac{\delta p}{\delta u}\right)_1 - \rho_1 c_1}$$

where

$$R = -\lambda_4\left(p_2 - p_1 - \rho_1 c_1 (u_2 - u_1)\right)$$
$$\lambda_4 = \frac{\lambda}{1-\lambda}$$
$$\lambda = \frac{(u_1 - c_1)\Delta t}{\Delta x}$$
$$\left(\frac{\delta p}{\partial u}\right)_1 = -\frac{p_t\left(1+\tan^2\theta_v + \tan^2\theta_w\right)u}{(\gamma-1)c_v T_t}\left[1 - \frac{\gamma-1}{\gamma+1}\left(1+\tan^2\theta_v + \tan^2\theta_w\right)\frac{u^2}{a_*^2}\right]^{\frac{1}{\gamma-1}}$$

Equation B-24

Exit Boundaries

For subsonic exit boundary conditions only one external variable needs to be specified. For super-sonic flows no external conditions need to be specified.

The flow variables are updated as follows:

$$
\begin{aligned}
\rho_{NI}^{n+1} &= \rho_{NI}^{n} + \delta\rho_{NI} \\
u_{NI}^{n+1} &= u_{NI}^{n} + \delta u_{NI} \\
v_{NI}^{n+1} &= v_{NI}^{n} + \delta v_{NI} \\
w_{NI}^{n+1} &= w_{NI}^{n} + \delta w_{NI} \\
p_{NI}^{n+1} &= p_{NI}^{n} + \delta p_{NI} \\
T_{NI}^{n+1} &= \frac{p_{NI}^{n+1}}{(\gamma-1)c_v\rho_{NI}^{n+1}} \\
\alpha &= \frac{\left(u_{NI}^{n+1}\right)^2 + \left(v_{NI}^{n+1}\right)^2 + \left(w_{NI}^{n+1}\right)^2}{2} \\
E_{NI}^{n+1} &= \rho_{NI}^{n+1}\left(c_v T_{NI}^{n+1} + \alpha\right)
\end{aligned}
$$

Equation B-25

The changes in the flow variables are defined as:

$$
\begin{aligned}
\delta p_{NI} &= \begin{cases} \dfrac{R_2 + R_5}{2} & \text{if } M_{NI-1} = \dfrac{u_{NI-1}}{c_{NI-1}} \geq 1 \\ \Delta t \dfrac{\delta p_e}{\delta t} = 0 & \text{if } M_{NI-1} = \dfrac{u_{NI-1}}{c_{NI-1}} < 1 \end{cases} \\
\delta\rho_{NI} &= R_1 + \frac{\delta p_{NI}}{c_{NI-1}^2} \\
\delta p_{NI} &= \frac{\left(R_2 - \delta p_{NI}\right)}{\rho_{NI-1}c_{NI-1}} \\
\delta v_{NI} &= R_3 \\
\delta w_{NI} &= R_4
\end{aligned}
$$

Equation B-26

where

$$
\begin{aligned}
R_1 &= -\lambda_1\left(\rho_{NI} - \rho_{NI-1} - \frac{1}{c_{NI-1}^2}\left(p_{NI} - p_{NI-1}\right)\right) \\
R_2 &= -\lambda_2\left(p_{NI} - p_{NI-1} + \rho_{NI-1}c_{NI-1}\left(u_{NI} - u_{NI-1}\right)\right) \\
R_3 &= -\lambda_1\left(v_{NI} - v_{NI-1}\right) \\
R_4 &= -\lambda_1\left(w_{NI} - w_{NI-1}\right) \\
R_5 &= -\lambda_4\left(p_{NI} - p_{NI-1} - \rho_{NI-1}c_{NI-1}\left(u_{NI} - u_{NI-1}\right)\right) \\
\lambda_i &= \frac{\lambda'_i}{1+\lambda'_i};\ i = 1,2,4 \\
\lambda'_1 &= \frac{u_{NI-1}\Delta t}{\Delta x};\quad \lambda'_2 = \frac{\left(u_{NI-1} + c_{NI-1}\right)\Delta t}{\Delta x};\quad \lambda'_4 = \frac{\left(u_{NI-1} - c_{NI-1}\right)\Delta t}{\Delta x}
\end{aligned}
$$