Chapter 2

Numerical Methods

1. Introduction

This chapter presents the fundamental equations and numerical methods involved in modeling turbulent boundary layer flows with heat transfer in cartesian coordinates. This requires adequate discretization of the governing equations, a stable time advancement scheme, and advanced turbulence modeling. The first part of the document presents the governing equations and derivation of the large-eddy simulation technique applied within a constant density framework. Of particular interest is the classical dynamic model proposed by Germano et al [1]. An extension to variable density framework is introduced for the governing equations as well as for the turbulence model showing that no additional terms need to be introduced in the subgrid scale model and that the inclusion of the density field in the model is a suitable update [3]. The fractional step "time-split" scheme applied to a low storage third order Runge Kutta method is presented in the discussion of time advancement "predictor-corrector" schemes. The finite difference discretization is introduced with respect to a modified staggered cell treatment where in addition to the spatial components the fields are also staggered in time. This leads a new representation of the governing discrete equations which follows a spatio-temporal cell convention. The primary focus of this work is the extension of an existing turbulent boundary layer code – LES3D-MP – to handle low Mach-number flows with heat transfer and density variations. The original code was provided by Keating and is described in detail in his PhD dissertation at the University of Queensland, Australia [2]. The extension of the code is based on the work by the late Charles Pierce and colleagues which is presented on his PhD dissertation at Stanford University, USA [3].

2. Governing Equations

The philosophy in large eddy simulation is to decompose the flow field into two regions. The large scale is called the 'resolved' scale and the small scale also known as the 'subgrid' or 'residual' part. This is achieved by applying a filtering operation in the domain Ω:

$$\bar{\boldsymbol{u}}(\boldsymbol{x},t) = \int_{\Omega} \boldsymbol{u}\,(\boldsymbol{x}-\boldsymbol{r},t)G(|\boldsymbol{r}|;\bar{\Delta})d\boldsymbol{r} \tag{1}$$

where $\bar{\boldsymbol{u}}(\boldsymbol{x},\boldsymbol{t})$ is the filtered velocity , and G is some arbitraty chosen filtering function.Then the quantity u may be described by $u = \bar{u} + u'$, where $\bar{u}$ is the resolved part and u' is the residual (subgrid) part. This may appear similar to the Reynolds decomposition however $\bar{u}$ refers to a random (and not mean) field, and the filtered residual may not be zero $\bar{u'} \neq 0$. The filtering function G by definition also satisfies the normalization condition $\int G\,(r,x)dr = 1$. In a finite difference approach the filter function is a simple top-hat filter, having a cut off frequency corresponding to the grid size iteself. Applying the filter operation to the equations of conservation of mass and momentum and scalar for an incompressible fluid, one can obtain the governing equations for the large scale variables, which can be written in dimensionless form as:

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0 \tag{2}$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \overline{u_i u_j}}{\partial x_j} = \frac{1}{Re}\frac{\partial}{\partial x_j}(2\overline{S}_{ij}) - \frac{\partial \bar{p}}{\partial x_i} \tag{3}$$

$$\frac{\partial \bar{Z}}{\partial t} + \frac{\partial \overline{Z u_j}}{\partial x_j} = \frac{1}{RePr}\frac{\partial^2 \bar{Z}}{\partial x_j \partial x_j} \tag{4}$$

where $\bar{u}_i$ is the resolved velocity, $\bar{p}$ is the pressure, Z is the mixture fraction scalar, Re is a typical Reynolds number of the flow and Pr is the Prandtl number of the fluid. S_{ij} is the rate deformation tensor, for a solenoidal field $\frac{\partial u_i}{\partial x_i} = 0$. This equation differs from the unfiltered NS equation because the filtered product $\overline{u_i u_j}$ is different than the product of the filtered

velocities $\bar{u}_i\bar{u}_j$. The difference is now defined as the residual stress tensor, $\tau_{ij}^R = \overline{u_i u_j} - \bar{u}_i\bar{u}_j$, which is analogous to the Reynolds stress tensor $< u_i u_j >=< u_i u_j > -< u_i >< u_j >$. The residual isotropic kinetic energy is $k_r = \frac{1}{2}\tau_{ii}^R$ and the anisotropic residual stress tensor is defined by $\tau_{ij}^r = \tau_{ij}^R - \frac{2}{3}k_r\delta_{ij}$. In terms of anisotropy tensors, the Reynolds stress tensor can be written as $\tau_{ij}^R = \tau_{ij}^r + \frac{2}{3}k_r\delta_{ij}$ leading to the following expression $\overline{u_i u_j} = \tau_{ij}^r + \frac{2}{3}k_r\delta_{ij} + \bar{u}_i\bar{u}_j$ that when substituted for the convective term in equation (3) defines a modified pressure as the sum of the filtered pressure and the isotropic residual stress $\bar{p} = \bar{p} + \frac{2}{3}\rho k_r$. It is only the anisotropic component τ_{ij}^r that is effective in transporting momentum. Substituting this into the filtered Navier Stokes and similarly for the scalar yields:

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j\frac{\partial \bar{u}_\iota}{\partial x_j} = \frac{1}{Re}\frac{\partial}{\partial x_j}(2\overline{S}_{ij}) - \frac{\partial \tau_{ij}^r}{\partial x_j} - \frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} \tag{5}$$

$$\frac{\partial \bar{Z}}{\partial t} + \frac{\partial \overline{Zu_j}}{\partial x_j} = \frac{1}{RePr}\frac{\partial^2 \bar{Z}}{\partial x_j \partial x_j} - \frac{\partial q_j}{\partial x_j} \tag{6}$$

where the subgrid-scale stress term τ_{ij}, and the subgrid-scale heat flux term q_j, contains the effects of the subgrid-scales on the resolved scales:

$$\tau_{ij} = \overline{u_i u_j} - \bar{u}_\iota\bar{u}_\jmath \tag{7}$$

$$q_j = \overline{Zu_j} - \bar{Z}\bar{u}_j \tag{8}$$

These terms contain quantities that cannot be explicitly obtained from the resolved fields and must be modeled. As in classical mechanics, the rate of strain tensor and characteristic rate of strain can be defined for the filtered variables as follows:

$$\overline{S}_{ij} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right) \tag{9}$$

$$|\overline{S}| = (2\overline{S}_{ij}\overline{S}_{ij})^{1/2} \tag{10}$$

2.1. Smagorinsky modeling

Using a classical Smagorinsky type model where one assumes isotropicity and homogeneity of the smallest eddies, τ_{ij}^{r} can be parametrized by an eddy viscosity model of the following form:

$$\tau_{ij}^{R} - \frac{\delta_{ij}}{3}\tau_{kk}^{R} = \tau_{ij}^{r} = -2\nu_t \bar{S}_{ij} = -2C_{ev}\,\Delta^2\,|\bar{S}_{ij}|\bar{S}_{ij} \tag{11}$$

where δ_{ij} is the Kronecker delta, ν_t is the edddy viscosity and $|\bar{S}_{ij}|$ is the magnitude of the large-scale strain rate tensor. Note that the trace of the subgrid scale stresses is incorporated in the pressure term as described earlier. Also, Δ is the filter width which reads for a finite difference discretization as $\Delta = (\Delta x\,\Delta y\,\Delta z)^{1/3}$. By analogy with what is normally done with the ensemble Reynolds equations, the subgrid scale tensors are in most of the cases expressed in terms of eddy viscosity and diffusivity coefficients in the form: $\tau_{ij}^{r} = \frac{\delta_{ij}}{3}\tau_{kk} - 2\nu_t\bar{S}_{ij}$, and for a scalar (i.e.,mixture fracion Z) a similar model can be used to parameterise the subgrid-scale heat flux:

$$q_j = \alpha_t \frac{\partial \bar{Z}}{\partial x_j} \tag{12}$$

where the subgrid scale eddy diffusivity is modeled similarly to the eddy viscosity with:

$$\alpha_t = C_\theta\,\Delta^2\,|\bar{S}| \tag{13}$$

Where C_θ can either be calculated using a subgrid-scale turbulent Prandtl number, $C_\theta = C_{ev}/Pr_t$, or by using a dynamic procedure. Then the LES equations for momentum and scalar transport become:

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j\frac{\partial \bar{u}_\iota}{\partial x_j} = \frac{\partial}{\partial x_j}\left[(\nu + \nu_t)\left(2\overline{S}_{ij}\right)\right] - \frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} \tag{14}$$

$$\frac{\partial \bar{Z}_i}{\partial t} + \frac{\partial(\bar{u}_j\bar{Z})}{\partial x_j} = \frac{\partial}{\partial x_j}\left[(\alpha + \alpha_t)\left(\frac{\partial \bar{Z}}{\partial x_j}\right)\right] \tag{15}$$

where as described earlier $\bar{p} = \bar{p} + \frac{1}{3}\rho\tau_{kk}$ is a modified pressure (macro pressure), which can

be determined with the aid of the filtered continuity equation[4].

2.2. Residual stress decomposition

A decomposition of the residual stresses will now be presented to introduce the commonly used three component stresses: Leonard,Cross and SGS Reynolds stresses. This is obtained beginning from the decomposition of $u = \bar{u} - u'$ to obtain $\tau^R = L_{ij} + C_{ij} + R_{ij}$

$$\tau_{ij}^R = \overline{u_i u_j} - \bar{u}_i \bar{u}_j \tag{16}$$

$$\tau_{ij}^R = (\bar{u}_i + u_i')(\bar{u}_j + u_j') \tag{17}$$

$$\tau_{ij}^R = \overline{\bar{u}_i \bar{u}_j + \bar{u}_i u_j' + u_i' \bar{u}_j + u_i' u_j'} \tag{18}$$

$$\tau_{ij}^R = \overline{\bar{u}_i \bar{u}_j} + \overline{\bar{u}_i u_j'} + \overline{u_i' \bar{u}_j} + \overline{u_i' u_j'} \tag{19}$$

$$\tau_{ij}^R = \underbrace{\overline{\bar{u}_i \bar{u}_j} - \bar{u}_i \bar{u}_j}_{} + \underbrace{\overline{\bar{u}_i u_j'} + \overline{u_i' \bar{u}_j}}_{} + \underbrace{\overline{u_i' u_j'}}_{} \tag{20}$$

$$\tau_{ij}^R = L_{ij} + C_{ij} + R_{ij} \tag{21}$$

The Leonard stress tensor is explicit since it is defined in terms of the filtered field, and it has been used in scale similarity models to provide information on subgrid stresses [4]. Leonard's stresses are also a major ingredient of the Germano's identity for the dynamic approach in physical space. The subgrid scale tensors and fluxes presented need of course to be modeled.

2.3. Dynamic modelling

The dynamic model provides a methodology to determine an appropriate local value for C_s to be used with a Smagorinsky type model. The underlying principle is to extract information via a double filtering operation in physical space [1]. Two grid filters are now introduced: the grid filter $\bar{\Delta}$ and the test filter $\widetilde{\Delta}$. The grid filter's width is usually taken to be that of the grid

spacing, h, or $2h$ for better resolution. The operation of grid filtering is denoted by an overbar, e.g.,

$$\overline{\boldsymbol{u}}(\boldsymbol{x},t) = \int \boldsymbol{u}\,(\boldsymbol{x}-\boldsymbol{r},t)G(|\boldsymbol{r}|;\overline{\Delta})d\boldsymbol{r} \tag{22}$$

The test filter, of larger width, is defined as $\widehat{\Delta}= \alpha\ \bar{\Delta}$ (for instance $\alpha = 2$).

$$\widehat{\boldsymbol{u}}(\boldsymbol{x},t) = \int \boldsymbol{u}\,(\boldsymbol{x}-\boldsymbol{r},t)G(|\boldsymbol{r}|;\widehat{\Delta})d\boldsymbol{r} \tag{23}$$

Since $\bar{u}(\boldsymbol{x},t)$ is unknown in a LES calculation, it is more relevant to consider the test filter applied to $\bar{u}$, to yield the doubly filtered quantity $\hat{\bar{u}}$. Thus, for both filters, the double-filtering operation can be written as

$$\widehat{\overline{\boldsymbol{u}}}(\boldsymbol{x},t) = \int \boldsymbol{u}\,(\boldsymbol{x}-\boldsymbol{r},t)G(|\boldsymbol{r}|;\widehat{\overline{\Delta}})d\boldsymbol{r} \tag{24}$$

Accordingly, the subtest-scale stresses and scalar flux appear which are parameterized as

$$T_{ij} = \widehat{\overline{u_\iota u_j}} - \hat{\bar{u}}_\iota \hat{\bar{u}}_j \tag{25}$$

$$Q_j = \widehat{\overline{Z u_j}} - \hat{\bar{Z}}\hat{\bar{u}}_j \tag{26}$$

In the dynamic SGS model, these are modeled in the same manner as the residual terms,

$$T_{ij} - \frac{\delta_{ij}}{3}T_{kk} = -2C_{ev}\ \widehat{\Delta}^2\ |\hat{\bar{S}}|\widehat{\bar{S}_{\iota J}} \tag{27}$$

$$Q_j = -\widehat{\alpha_t}\frac{\partial \hat{\bar{Z}}}{\partial x_j}, \qquad \widehat{\alpha_t} = C_\theta\ \widehat{\Delta^2}\ |\hat{\bar{S}}| \tag{28}$$

Test filtering the residual stress tensor $\widehat{\tau_{ij}^R} = \widehat{\overline{u_\iota u_j}} - \widehat{\bar{u}_\iota \bar{u}_j}$ and subtracting it from subtest-scale stress tensor defines what is known as the Germano's identity. It yields the known Leonard subtest scale stress also known as the resolved (turbulent) stress. Similarly, subtracting the filtered residual heat flux vector from the subtest-scale scalar flux yields,

$$L_{ij} = T_{ij} - \widehat{\tau_{ij}^R} = \widehat{\bar{u}_\iota \bar{u}_j} - \hat{\bar{u}}_\iota \hat{\bar{u}}_j \tag{29}$$

$$F_j = Q_j - \widehat{q_j} = \widehat{\bar{Z}\bar{u}_j} - \hat{\bar{Z}}\hat{\bar{u}}_j \tag{30}$$

Its main advantage is that it is known in terms of $\bar{u}$, whereas T_{ij}, τ_{ij}^{R}, q_j and Q_j are not. They are the contribution to the residual stress (and scalar flux) from the largest resolved motions (with respect to the test filter). By substituting the eddy viscosity and diffusivity models for L_{ij} and F_{ij}, one finds that the coefficient C_{ev} and C_{θ} are determined by relations,

$$Lij - \frac{\delta}{3}L_{kk} = -C_{ev}\,\Delta^2\,M_{ij}, \quad M_{ij} = -\left(2\,\bar{\Delta}^2\,\bar{\bar{S}}\bar{\bar{S}}_{ij} - 2\,\hat{\bar{\Delta}}^2\,\hat{\bar{S}}\hat{\bar{S}}_{ij}\right) \tag{31}$$

$$F_j = -C_{\theta}\,\Delta^2\,N_j, \quad N_j = -\left(\bar{\Delta}^2\,\bar{S}\frac{\widehat{\partial \bar{Z}}}{\partial x_j} - \hat{\bar{\Delta}}^2\,\hat{\bar{S}}\frac{\widehat{\partial \bar{Z}}}{\partial x_j}\right) \tag{32}$$

Similarly, the double filtered deformation tensor is defined $\widehat{\bar{S}_{ij}} = \frac{1}{2}\left(\frac{\partial \widehat{\bar{u}_i}}{\partial x_j} + \frac{\partial \widehat{\bar{u}_j}}{\partial x_i}\right)$ and its characteristic counter part also as $|\hat{\bar{S}}| = (2\widehat{\bar{S}_{ij}}\widehat{\bar{S}_{ij}})^{1/2}$. Further, taking C_{ev} to be uniform, a scale similar tensor M_{ij} was previously defined and can be confirmed by re-expressing the Leonards stress $L_{ij} = T_{ij} - \widehat{\tau_{ij}^{R}}$ and obtaining the following expression which contains M_{ij}: $L_{ij} = -2C_{ev}\,\hat{\bar{\Delta}}^2\,\widehat{|\bar{\bar{S}}|\bar{\bar{S}}_{ij}} + 2C_{ev}\,\bar{\Delta}^2\,\widehat{|\bar{\bar{S}}|\bar{\bar{S}}_{ij}}$, yielding the final relationship,

$$L_{ij} = C_{ev}M_{ij} \tag{33}$$

We may observe that both M_{ij} and L_{ij} are known in terms of $u(x,t)$, which can be used to determine C_{ev} for the present modelling technique. Also, a single coefficient C_{ev} cannot be chosen to match 5 independent equations. Therefore, a mean square error is minimized. Following Lilly et al [5], the square of the residual is required to be minimal and an equation for the local value of C_{ev} is:

$$C_{ev}(\boldsymbol{x},t) = -\frac{1}{2}\frac{< L_{ij}M_{ij} >_{avg}}{< M_{ij}M_{ij} >_{avg}} \tag{34}$$

Where the brackets $< >_{avg}$ indicate the type of averaging in the numerator and denominator used to overcome instabilities (Standard techniques used are line and plane spatial averaging or Lagrangian averaging for general inhomogeneous flows in which weighted averages are

formed backward in time along fluid-particle paths based on the filtered velocity field [4]). With this procedure the eddy viscosity tends to zero near the wall without the use of a Van Driest type of damping function. In addition, C_{ev} can take on negative values and apparently capture the effects of backscattering. Similarly, the eddy diffusivity model coefficient C_θ is now computed based on similar formulation,

$$C_\theta(\boldsymbol{x}, t) = -\frac{< F_j N_j >_{avg}}{< N_j N_j >_{avg}} \tag{35}$$

where the coefficient C_θ is computed through Lagrangian averaging and is limited to positive values.

3. Extension to variable density

This section includes the principles and methodology needed to account for the effects of variable density in the governing LES equations. The introduction of mass density weighted average, Favre averaging, is needed to satisfy the continuity equation while also retaining the standard form of the governing equations. The modeling corresponds to subsonic flows where the magnitude of the velocity is corresponds to the low-mach number regime. The LES modeling terms are introduced and it is shown that the inclusion of the filtered density field is a suitable update to the turbulence model. Recall that in this work, filtering is implicitly defined by the computational grid used for the large-scale equations and that it is not invoked explicitly. Quantities per unit volume are treated using the Reynold's decompositon,

$$\rho = \overline{\rho} + \rho'$$

while quantities per unit mass are best described by a Favre (density weighted) decomposition,

$$u = \tilde{u} + u''$$

where

$$\tilde{u} = \frac{\overline{\rho u}}{\overline{\rho}} = \frac{\int\int\int_{\Omega} G\,(|\boldsymbol{r}|;\widetilde{\Delta})\boldsymbol{\rho}((\boldsymbol{x}-\boldsymbol{r}),\boldsymbol{t})\boldsymbol{u}((\boldsymbol{x}-\boldsymbol{r}),\boldsymbol{t})\boldsymbol{dr}}{\int\int\int_{\Omega} G\,(|\boldsymbol{r}|;\widetilde{\Delta})\boldsymbol{\rho}((\boldsymbol{x}-\boldsymbol{r}),\boldsymbol{t})\boldsymbol{dr}}$$

3.1. Governing Equations and Filtering

With Favre decomposition, filtered variables represent "mixed mean" averages over subgrid volumes. This ensures that the filtering process does not alter the form of the conservation laws. Applying these procedures to the working equations, the Favre LES equations are now written as:

Continuity:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u_j}}{\partial x_j} \tag{36}$$

Momentum:

$$\frac{\partial \overline{\rho}\widetilde{u_\iota}}{\partial t} + \frac{\overline{\rho u_i u_j}}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial \overline{\sigma_{ij}}}{\partial x_j}$$

Using the decomposition $\overline{\rho u_i u_j} = \overline{\rho}\widetilde{u_\iota}\widetilde{u_j} + (\overline{\rho u_i u_j} - \overline{\rho}\widetilde{u_\iota}\widetilde{u_j})$, where the first term is the LES grid resolved convective flux and the second term the corresponding SGS contribution. The filtered viscous stress tensor is modeled as:

$$\overline{\sigma_{ij}} = 2\overline{\mu}\left(\widetilde{S_{\iota J}} - \frac{1}{3}\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}\right), \quad where \quad \overline{\mu} = \mu(\tilde{T})$$

$$= \mu_0\left(\frac{\tilde{T}}{T_0}^b\right), b = 0.76$$

where $\tilde{S}_{ij} = \frac{1}{2}(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i})$. It is also costumary (in the literature) to define the stress tensor as $\overline{\sigma_{ij}} = 2\overline{\mu}\left(\widetilde{S_{ij}^d}\right)$, where now the deviatoric deformation tensor is defined as $\tilde{S}_{ij}^d = \frac{1}{2}(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}) - \frac{1}{3}\nabla \cdot \tilde{u}_j \delta_{ij}$. Incorporating the decomposition yields the following momentum equations,

$$\frac{\partial \overline{\rho}\widetilde{u_\iota}}{\partial t} + \frac{\overline{\rho}\widetilde{u_i}\widetilde{u_j}}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(2\bar{\mu}\tilde{S}_{ij}^d\right) \tag{37}$$

where $\tau_{ij} = \overline{\rho}\left(\widetilde{u_\iota u_J} - \widetilde{u_\iota}\widetilde{u_J}\right)$ are the same terms that must be modeled.

Scalar Transport:

$$\frac{\partial \overline{\rho}\tilde{Z}}{\partial t} + \frac{\overline{\rho Z u_j}}{\partial x_j} = \frac{\partial}{\partial x_i}\left(\overline{\rho\alpha\frac{\partial Z}{\partial x_i}}\right)$$

Again, we can use the standard LES decomposition: $\overline{\rho Z u_j} = \overline{\rho}\tilde{Z}\widetilde{u_j} + (\overline{\rho Z u_j} - \overline{\rho}\tilde{Z}\widetilde{u_j})$, where the first term is the LES grid resolved convective scalar flux and the second term the corresponding SGS contribution. We approximate $\overline{\alpha \frac{\partial Z}{\partial x_i}} = \overline{\alpha}\frac{\partial \tilde{Z}}{\partial x_i}$, where $\overline{\alpha} = \overline{\alpha}(\tilde{T}) = \frac{\mu(\tilde{T})C_p}{Pr}$, which finally yields the following filtered LES, Favre equation:

$$\frac{\partial \overline{\rho}\tilde{Z}}{\partial t} + \frac{\overline{\rho}\tilde{Z}\widetilde{u_j}}{\partial x_j} = \frac{\partial}{\partial x_i}\left(\overline{\rho}\tilde{\alpha}\frac{\partial \tilde{Z}}{\partial x_i}\right) - \frac{\partial q_j}{\partial x_j} \tag{38}$$

where, $q_j = \bar{\rho}\left(\widetilde{Z u_j} - \tilde{Z}\widetilde{u_j}\right)$

State relation:

$$\overline{p} = \overline{\rho}\left(\frac{R}{M}\right)\tilde{T} \tag{39}$$

3.2. Dynamic Modeling

The extension to variable density of the SGS dynamic modeling is presented by inspection of the turbulent (and scalar flux) stress constituents

$$\tau_{ij} = \left(\tau_{ij} - \tau_{kk}\frac{\delta_{ij}}{3}\right) + \tau_{kk}\frac{\delta_{ij}}{3} = \tau_{ij}^A + \tau_{ij}^I \tag{40}$$

The anisotropic part is modeled based on a eddy-viscosity concept:

$$\tau_{ij}^A = -2\overline{\rho}\nu_\tau \tilde{S}_{ij} \tag{41}$$

Invoking the classical Smagorinsky model, where C_{ev} is the model coefficient that is dynamically computed from the LES solution

$$\nu_\tau = (C_{ev}\,\Delta)^2|\tilde{S}| \tag{42}$$

The anisotropic part is as follows,

$$\tau_{ij}^A = -2\overline{\rho}(C_{ev}\,\Delta)^2|\tilde{S}|\widetilde{S_{ij}^A} \tag{43}$$

Although not accounted for in the present work, previous researchers have additionally modeled the isotropic constituent of the SGS stress tensor based on the Yoshiwaza relation [6] from which $k_{sgs} = (C_I\ \Delta)^2|\tilde{S}|^2$, we have

$$\tau_{kk} = 2\overline{\rho}(C_I\ \Delta)^2|\tilde{S}|^2 \tag{44}$$

and the entire modeled term becomes

$$\tau_{ij} = -2\overline{\rho}(C_{ev}\ \Delta)^2|\tilde{S}|\widetilde{S_{ij}^A} + \frac{\delta_{ij}}{3}2\overline{\rho}(C_I\ \Delta)^2|\tilde{S}|^2 \tag{45}$$

where C_I is a model coefficient. Erlebacher et al [7] neglected the isotropic term on the grounds that it is negligible compared to the thermodynamic pressure. Similarly, Pierce et al also left this term out since he decoupled pressure from the thermodynamic variables as in done for low-mach number flows [3]. Currently, a Low-Mach number formulation is utilized which neglects acoustic interactions and compressibility effects. This present approach therefore leaves out the isotropic term and the modeling becomes:

$$\tau_{ij} = -2\overline{\rho}(C_{ev}\ \Delta)^2|\tilde{S}|\widetilde{S_{ij}} \tag{46}$$

In order to close the momentum equations, τ_{ij} must be modeled: (Using $\tilde{f} = \overline{\rho f}/\bar{\rho}$)

$$\tau_{ij} = \overline{\rho}\left(\widetilde{u_i u_j} - \tilde{u}_i\tilde{u}_j\right) \tag{47}$$

$$= \overline{\rho u_i u_j} - \left(\frac{\overline{\rho u_i}\ \overline{\rho u_j}}{\overline{\rho}}\right) \tag{48}$$

Utilization of the spectral data is performed with the introduction of the test filter in the resolved field. This has a larger width than the resolved grid filter, generating a region with larger scales which can be used dynamically. This width is denoted as $\widehat{\Delta}$. Therefore, the test filtered stresses T are defined as:

$$T_{ij} = \widehat{\overline{\rho u_i u_j}} - \frac{\left(\widehat{\overline{\rho u_i}}\ \widehat{\overline{\rho u_j}}\right)}{\hat{\overline{\rho}}} \tag{49}$$

Using Germano's identity, the Leonard stresses L_{ij} can be expressed in terms of T_{ij} and τ_{ij}

$$L_{ij} = T_{ij} - \hat{\tau}_{ij}$$

$$= \widehat{\overline{\rho}\widetilde{u_\iota}\widetilde{u_J}} - \frac{\left(\widehat{\overline{\rho}\widetilde{u_\iota}}\,\widehat{\overline{\rho}\widetilde{u_J}}\right)}{\hat{\overline{\rho}}} - \left(\widehat{\overline{\rho}\widetilde{u_\iota}\widetilde{u_J}} - \left(\frac{\widehat{\overline{\rho}\widetilde{u_\iota}}\,\widehat{\overline{\rho}\widetilde{u_J}}}{\overline{\rho}}\right)\right) \tag{50}$$

$$= \widehat{\overline{\rho}\widetilde{u}_\iota\widetilde{u}_J} - \frac{\widehat{\overline{\rho}\widetilde{u_\iota}}\,\widehat{\overline{\rho}\widetilde{u_J}}}{\hat{\overline{\rho}}}$$

$$= \widehat{\overline{\rho}\widetilde{u}_\iota\widetilde{u}_J} - \frac{\widehat{\overline{\rho}\widetilde{u}_\iota}\,\widehat{\overline{\rho}\widetilde{u}_J}}{\hat{\overline{\rho}}}$$

This identity is useful because it provides results (rhs) which can be obtained from the filtered variables. Knowing L_{ij} and re-expressing it in term of its modeled terms will yield a useful expression for the dynamic coefficient C_s. The anisotropic part of the Leonard stress tensor therefore becomes:

$$L_{ij} = T_{ij} - \hat{\tau}_{ij} \tag{51}$$

$$= 2(C_{ev}\,\overline{\Delta})^2\widetilde{\overline{\rho}|\tilde{S}|\tilde{S}_{\iota J}} - 2(C_{ev}\,\hat{\overline{\Delta}})^2\hat{\overline{\rho}}\widehat{\overline{\rho}|\tilde{S}|\tilde{S}_{\iota J}}$$

$$= C_{ev}^2\, M_{ij}$$

where

$$M_{ij} = \left(2\,\widetilde{\overline{\rho}|\tilde{S}|\tilde{S}_{\iota J}} - 2\left(\frac{\hat{\overline{\Delta}}}{\overline{\overline{\Delta}}}\right)^2 \hat{\overline{\rho}}\widehat{\overline{\rho}|\tilde{S}|\tilde{S}_{\iota J}}\right)\overline{\Delta}^2$$

This equation corresponds to 5 independent relations for C_{ev} making it overspecified. Therefore, the classical least squares approach is followed to calculate the model coefficients in analogy to the incompressible case.

$$C_{ev}(\boldsymbol{x}, t) = \frac{< L_{ij}M_{ij} >_{avg}}{< M_{ij}M_{ij} >_{avg}} \tag{52}$$

3.2.1. SGS scalar flux

A similar solution is obtained through the use of the eddy diffusivity concept to model the SGS heat flux, q_j.

$$q_j = -\overline{\rho} C_\theta \frac{\partial \tilde{T}}{\partial x_j} = -\frac{\overline{\rho}\,\overline{\Delta}^2\, C_{ev} \widetilde{|S|}}{Pr_t} \frac{\partial \tilde{T}}{\partial x_j} \tag{53}$$

where $C_\alpha = C_s/Pr_t$. Reynolds and Favre averaging yields the following model terms:

$$q_j = \overline{\rho u_j \phi} - \frac{\overline{\rho u_j}\,\overline{\rho \phi}}{\overline{\rho}} \tag{54}$$

The subtest scalar flux now takes the following form:

$$Q_j = \widehat{\overline{\rho u_j \phi}} - \frac{\widehat{\overline{\rho u_j}}\,\widehat{\overline{\rho \phi}}}{\hat{\overline{\rho}}} \tag{55}$$

Through the use of Germano's identity we obtain the scalar Leonards tensor K_{ij} and the modeling tensor T_j as:

$$K_j = \widehat{\overline{\rho}\widetilde{u_j}\tilde{\phi}} - \frac{\widehat{\overline{\rho}\widetilde{u_j}}\,\widehat{\overline{\rho}\tilde{\phi}}}{\hat{\overline{\rho}}} \tag{56}$$

$$T_j = \left(\widehat{\overline{\rho}|\tilde{S}|\frac{\partial \tilde{T}}{\partial x_j}} - \left(\frac{\hat{\overline{\Delta}}}{\hat{\overline{\Delta}}}\right)^2 \hat{\overline{\rho}}\widehat{|\tilde{S}|}\frac{\partial \hat{\tilde{T}}}{\partial x_j} \right) \overline{\Delta}^2 \tag{57}$$

Similarly, to the incompressible version we can solve this over-defined system through the least-squares method for C_θ,

$$C_\theta(\boldsymbol{x}, t) = \frac{< K_j T_j >_{avg}}{< T_j T_j >_{avg}} \tag{58}$$

4. Time Advancement

4.1. Runge Kutta

The three stage, Runge Kutta algorithm is now presented as applied to a fractional step method. An implicit second-order Crank-Nicholson method is used for wall normal diffusion while the other terms are advanced with the Runge Kutta method. The three steps (k=1,2,3) fractional step, time advancement is therefore:

$$\widehat{u_\iota} - \beta_k \Delta t M(\widehat{u_\iota}) = r_i^{k-1} \tag{59}$$

$$\frac{\partial^2(\delta p)}{\partial x_i \partial x_i} = \frac{1}{2\beta_k \Delta t} \frac{\partial \widehat{u_\iota}}{\partial x_i} \tag{60}$$

$$u_i^k = \widehat{u_\iota} - 2\beta_k \Delta t \frac{\partial \delta p}{\partial x_i} \tag{61}$$

$$p^k = p^{k-1} + \delta p \tag{62}$$

where the explicit terms, r_i^{k-1}, are

$$r_i^{k-1} = u_i^{k-1} + t\left(\beta_k M(u_i^{k-1}) + \gamma_k A(u_i^{k-1}) + \zeta_k A(u_i^{k-2}) - 2\beta_k \frac{\partial p^{k-1}}{\partial x_i}\right) \tag{63}$$

At the first substep, when k=1, $u^{k-1} = u^n$, and at the end of the third substep, the solution is $u^{n+1} = u^k$. The coefficients of the time advancement scheme are

$$\beta_1 = 4/15 \quad \beta_2 = 1/15 \quad \beta_3 = 1/6$$

$$\gamma_1 = 8/15 \quad \gamma_2 = 5/12 \quad \gamma_3 = 3/4$$

$$\zeta_1 = 0 \quad \zeta_2 = -17/60 \quad \zeta_3 = -5/12$$

The theoretical stability limit for this time advancement scheme is satisfied for the following conditions [2]: (Note that this limit is not satisfied for variable density flows)

$$\alpha = \Delta t \left(\frac{u_i}{\Delta x_i} \right) < \sqrt{3} \tag{64}$$

$$\beta = \left(\frac{4}{Re} \frac{\Delta t}{\Delta x_i^2} \right) < \sqrt{3} \tag{65}$$

where for $\alpha, i = 1,2,3$ and for $\beta, i = 1,3$. Equation (64) and (65) represent convective and diffusive stability condition limits. Note that the wall-normal component of the diffusive term is handled implicitly by the Crank-Nicholson scheme and is not included in equation (65). Also note, that when the LES cross terms are included, the limit on the timestep is lower.

4.2. Discrete Equation

The governing equations are discretized using a finite differences approach. Velocity components are staggered with respect to pressure in both space and time. The density is co-located at the pressure points. Thus, the calculation of the mass flux (momentum per unit volume) requires spatial interpolation and is given the symbol g_i. The density is staggered in time, so that effectively the density ρ^n is calculated at time $(n - 1/2)\,\Delta t$. Conversion between u_i and g_i is accomplished using the following

$$g_i = \overline{\overline{\rho}^{x_i}}^{t} u_i, \quad u_i = \frac{g_i}{\overline{\overline{\rho}^{x_i}}^{t}} \tag{66}$$

The fully discrete equations are now presented in the following form,

Continuity:

$$\frac{\partial \rho}{\partial t} + \frac{\partial g_j}{\partial x_j} = 0 \tag{67}$$

Momentum:

$$\frac{\partial}{\partial t}(g_i) + \frac{\partial}{\partial x_j}\left(\overline{\overline{g_j}^{x_i}}^{t}\,\overline{\overline{u_i}^{x_j}}^{t}\right) = -\frac{\partial}{\partial x_i}(p) + \frac{\partial}{\partial x_j}(\tau_{ij}) \tag{68}$$

$$\tau_{ij} = \begin{cases} \overline{\overline{\mu}^{x_i}}^{x_j}\left[\dfrac{\partial \overline{u_i}^{t}}{\partial x_j} + \dfrac{\partial \overline{u_j}^{t}}{\partial x_i}\right], & \text{if } i \neq j \\ 2\mu\left[\dfrac{\partial \overline{u_i}^{t}}{\partial x_j} - \dfrac{1}{3}\dfrac{\partial \overline{u_k}^{t}}{\partial \overline{x_k}^{t}}\delta_{ij}\right], & \text{if } i = j \end{cases}$$

Scalar Transport:

$$\frac{\partial}{\partial t}(\rho Z) + \frac{\partial}{\partial x_j}\left(g_j\,\overline{\overline{Z}^{x_j}}^{t}\right) = +\frac{\partial}{\partial x_j}\left[\overline{\overline{\rho\alpha}^{x_j}}^{t}\,\frac{\partial}{\partial x_j}(\overline{Z}^{t})\right] \tag{69}$$

For clarity the above compact notation can be expanded in more conventional form. For instance, the continuity equation in two dimensions for a staggered cell in time-space would expanded as,

$$\begin{aligned} &\frac{\rho_{i,j}^{n+1} - \rho_{i,j}^{n}}{\Delta t} + \frac{1}{4\,\Delta x}\left[(\rho_{i+1,j}^{n+1} + \rho_{i,j}^{n+1} + \rho_{i+1,j}^{n} + \rho_{i,j}^{n})u_{i,j}^{n+1}\right. \\ &\qquad \left. - (\rho_{i,j}^{n+1} + \rho_{i-1,j}^{n+1} + \rho_{i,j}^{n} + \rho_{i-1,j}^{n})u_{i-1,j}^{n+1}\right] \\ &+ \frac{1}{4\,\Delta y}\left[(\rho_{i,j+1}^{n+1} + \rho_{i,j}^{n+1} + \rho_{i,j+1}^{n} + \rho_{i,j}^{n})v_{i,j}^{n+1} - (\rho_{i,j}^{n+1} + \rho_{i,j-1}^{n+1} + \rho_{i,j}^{n} + \rho_{i,j-1}^{n})v_{i,j-1}^{n+1}\right] \end{aligned} \tag{70}$$

Next, discretization of each component of the streamwise momentum equation is shown in one dimension, the transient term becomes:

$$\frac{1}{4\,\Delta\,t}\begin{bmatrix} u_{i,j}^{n+1}\left(\rho_{i+1,j}^{n+1}+\rho_{i,j}^{n+1}+\rho_{i+1,j}^{n}+\rho_{i,j}^{n}\right) \\ -u_{i-1,j}^{n+1}\left(\rho_{i,j}^{n+1}+\rho_{i-1,j}^{n+1}+\rho_{i,j}^{n}+\rho_{i-1,j}^{n}\right)\end{bmatrix}$$

The convective terms are calculated by defining east and west components on the staggered grid and computing the following gradient:$(uuE-uuW)/dx$, where

uuE:

$$\frac{1}{4}\left(\frac{u_{i,j}^{n}+u_{i,j}^{n+1}}{2}+\frac{u_{i+1,j}^{n}+u_{i+1,j}^{n+1}}{2}\right)\begin{bmatrix} \frac{1}{8}\begin{Bmatrix} u_{i,j}^{n}\left(\rho_{i,j}^{n+1}+\rho_{i+1,j}^{n+1}+\rho_{i,j}^{n}+\rho_{i+1,j}^{n}\right)+ \\ u_{i,j}^{n+1}\left(\rho_{i,j}^{n+1}+\rho_{i+1,j}^{n+1}+\rho_{i,j}^{n}+\rho_{i+1,j}^{n}\right)\end{Bmatrix} \\ +\frac{1}{8}\begin{Bmatrix} u_{i+1,j}^{n}\left(\rho_{i+1,j}^{n+1}+\rho_{i+2,j}^{n+1}+\rho_{i+1,j}^{n}+\rho_{i+2,j}^{n}\right)+ \\ u_{i+1,j}^{n+1}\left(\rho_{i+1,j}^{n+1}+\rho_{i+2,j}^{n+1}+\rho_{i+1,j}^{n}+\rho_{i+2,j}^{n}\right)\end{Bmatrix}\end{bmatrix}$$

uuW:

$$\frac{1}{4}\left(\frac{u_{i,j}^{n}+u_{i,j}^{n+1}}{2}+\frac{u_{i-1,j}^{n}+u_{i-1,j}^{n+1}}{2}\right)\begin{bmatrix} \frac{1}{8}\begin{Bmatrix} u_{i,j}^{n}\left(\rho_{i,j}^{n+1}+\rho_{i+1,j}^{n+1}+\rho_{i,j}^{n}+\rho_{i+1,j}^{n}\right)+ \\ u_{i,j}^{n+1}\left(\rho_{i,j}^{n+1}+\rho_{i+1,j}^{n+1}+\rho_{i,j}^{n}+\rho_{i+1,j}^{n}\right)\end{Bmatrix} \\ +\frac{1}{8}\begin{Bmatrix} u_{i-1,j}^{n}\left(\rho_{i-1,j}^{n+1}+\rho_{i,j}^{n+1}+\rho_{i-1,j}^{n}+\rho_{i,j}^{n}\right)+ \\ u_{i-1,j}^{n+1}\left(\rho_{i-1,j}^{n+1}+\rho_{i,j}^{n+1}+\rho_{i-1,j}^{n}+\rho_{i,j}^{n}\right)\end{Bmatrix}\end{bmatrix}$$

The pressure and viscous terms are as follows:

$$-\left[\frac{P_{i+1,j}^{n}-P_{i,j}^{n+1}}{\Delta\,x_c}\right]+$$

$$2\left\{\begin{array}{l}\left[\frac{\mu_E}{\Delta x}\left(\frac{u_{i+1,j}^{n}+u_{i+1,j}^{n+1}}{2}-\frac{u_{i,j}^{n}+u_{i,j}^{n+1}}{2}\right)-\frac{\mu_W}{\Delta x}\left(\frac{u_{i,j}^{n}+u_{i,j}^{n+1}}{2}-\frac{u_{i-1,j}^{n}+u_{i-1,j}^{n+1}}{2}\right)\right]\frac{1}{\Delta x_c}\\ -\frac{1}{3}\left[\frac{\mu_E}{\Delta x}\left(\frac{u_{i+1,j}^{n}+u_{i+1,j}^{n+1}}{2}-\frac{u_{i,j}^{n}+u_{i,j}^{n+1}}{2}\right)-\frac{\mu_W}{\Delta x}\left(\frac{u_{i,j}^{n}+u_{i,j}^{n+1}}{2}-\frac{u_{i-1,j}^{n}+u_{i-1,j}^{n+1}}{2}\right)\right]\frac{1}{\Delta x_c}\end{array}\right\}$$

Generalizing the above equations for non-uniform grids (stretched), the interpolation and differencing operators are defined as,

$$\overline{u}^{x}_{i+1/2}=c_i u_{i+1}+(1-c_i)u_i,\qquad \frac{\partial}{\partial x}(u)_{i+1/2}=\frac{u_{i+1}-u_i}{x_{i+1}-x_i}$$

where c_i are the interpolation weights.These defenitions maintain formal second order accuracy of the interpolation operator, but they do not satisfy the discrete product rules exactly so that the secondary conservation is only approximately satisfied. For stability, we will use equally weighted interpolation (i.e. c=1/2).

5. Iterative Scheme

This section presents the density algorithm in seven subsequent steps. The initial time step is followed by the actual density iteration loop, the loop is contained within steps 2 through 7 where a specific density criteria (or number of iterations) have to be met in order to be density converged and advance to the next substep. The staggered spatio-temporal cells for the scalar and momentum equations are also presented at each stage of the description. Stage *rk* advances the solution from time $(n+a_{rk})$ to time $(n+a_{rk+1})$, with (a_1, a_2, a_3, a_4) = (0,8/15,2/3,1) (assuming *substeps* = 3)

STEP 1: INITIALIZATION (before start of iterative loop)

In this step we choose the predictors through initial guess for the variables at the current sub-step time levels. The density estimate for the three stage Runge-Kutta time advancement scheme has two components corresponding to the first and subsequent time steps.

- Initial guess (*iter* = 0) of mass density:

  If *rk* = 1,

$$(\rho^{n+a_{rk+1}})^{iter=0} = \frac{t(n+a_{rk+1})-t(n-1+a_{substeps})}{t(n+a_{rk})-t(n-1+a_{substeps})}\rho^{n+a_{rk}} - \frac{t(n+a_{rk+1})-t(n+a_{rk})}{t(n+a_{rk})-t(n-1+a_{substeps})}\rho^{n-1+a_{substeps}}$$

  or $(\rho^{n+a_{rk+1}})^{iter=0} = \frac{bk(rk)+bk(substeps)}{bk(substeps)}\rho^{n+a_{rk}} - \frac{bk(rk)}{bk(substeps)}\rho^{n-1+a_{substeps}}$

  If *rk* > 1,

$$(\rho^{n+a_{rk+1}})^{iter=0} = \frac{t(n+a_{rk+1})-t(n+a_{rk-1})}{t(n+a_{rk})-t(n+a_{rk-1})}\rho^{n+a_{rk}} - \frac{t(n+a_{rk+1})-t(n+a_{rk})}{t(n+a_{rk})-t(n+a_{rk-1})}\rho^{n+a_{rk-1}}$$

  or $(\rho^{n+a_{rk+1}})^{iter=0} = \frac{bk(rk)+bk(rk-1)}{bk(rk-1)}\rho^{n+a_{rk}} - \frac{bk(rk)}{bk(rk-1)}\rho^{n+a_{rk-1}}$

- Store previous values of various quantities required for advancing the solution: $\phi^{n+a_{rk}}$,

$D_\phi^{n+a_{rk}}$, RHS_ϕ^{rk-1}, $u_j^{n+a_{rk}}$, $g_j^{n+a_{rk}} = (\overline{\overline{\rho}^{x_j}}^{t} u_j)^{n+a_{rk}}$, $RHS_{u_j}^{rk-1}$

STEP 2: SCALAR EQUATIONS (start of iterative loop, from (*iter*-1) to *iter*)

New to the formulation of this scheme is the advancement of the scalar equations prior to the momentum equation. The reason for the early advancement is due to the momentum equation convective term requirement of a mass flux, g_i, a priori. The following figure shows the location of the density fields, scalar fields and mass flux in the staggered spatio-temporal cell,

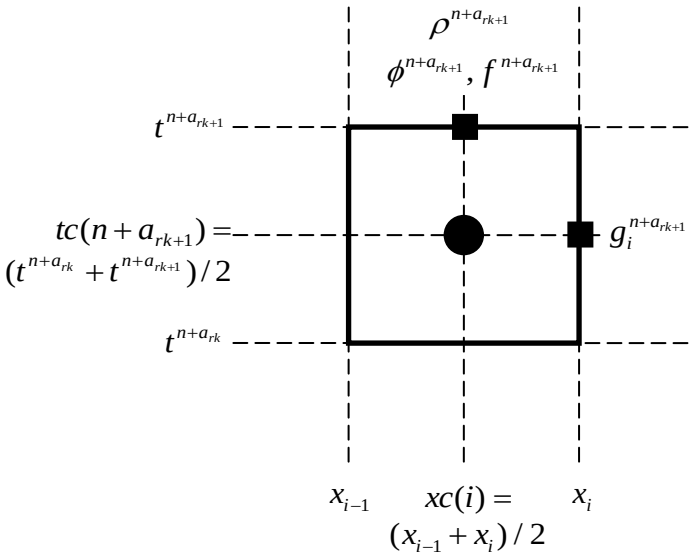

Figure 1. Scalar staggered cell. NB: The RHS of the scalar equation is evaluated at the center of the spatio-tempral cell, identified by a black dot.

- Calculate: $(g_j^{n+a_{rk+1}})^{iter-1} = ((\overline{\overline{\rho}^{x_j}}^{t})^{n+a_{rk+1}})^{iter-1} \times (u_j^{n+a_{rk+1}})^{iter-1}$, $((\overline{\phi}^{t})^{n+a_{rk+1}})^{iter-1}$, $((\overline{\rho D_\phi}^{t})^{n+a_{rk+1}})^{iter-1}$

- Initialize scalar fields: $f^{n+a_{rk}} = \rho^{n+a_{rk}} \times \phi^{n+a_{rk}}$

- Solve scalar equations: $\partial_t(f)+\partial_{x_j}(g_j\overline{\overline{\phi}^{x_j}}^t)=\partial_{x_j}(\overline{\overline{\rho D_\phi}^{x_j}}^t\partial_{x_j}(\overline{\phi}^t))$, where $f=(\rho\phi)$ and $g_j=(\overline{\overline{\rho}^{x_j}}^t u_j)$, and provide $(f^{n+a_{rk+1}})^{iter}$, $(RHS_\phi^{rk})^{iter}$

- Calculate intermediate value $(\phi^{n+a_{rk+1}})^{iter*}=(f^{n+a_{rk+1}})^{iter}/(\rho^{n+a_{rk+1}})^{iter-1}$

- Impose boundary conditions

STEP 3: EQUATION OF STATE

Next the thermodynamic equation of state is called to update the density field through the gas molecular weight and provisional results from the scalar advancement as follows,

- Calculate $(\rho^{n+a_{rk+1}})^{iter}=(M^{n+a_{rk+1}}/T^{n+a_{rk+1}})^{iter*}$

STEP 4: UPDATE SCALAR FIELDS

Scalar fields are now updated based on the new density field found on STEP 3.

- Calculate $(\phi^{n+a_{rk+1}})^{iter}=(f^{n+a_{rk+1}})^{iter}/(\rho^{n+a_{rk+1}})^{iter}$

- Impose boundary conditions

STEP 5: MOMENTUM EQUATIONS

The equations are now advanced by first calculating time averaged momentum (g_i) and velocity fields u_i from the current and previous iteration. Each spatial component of the calculated values is now used in the discretization following the spatio-temporal staggered cell convention shown by figure 2 to obtain the momentum field. The intermediate velocity is now calculated and boundary conditions are applied leading to an update of the intermediate momentum field.

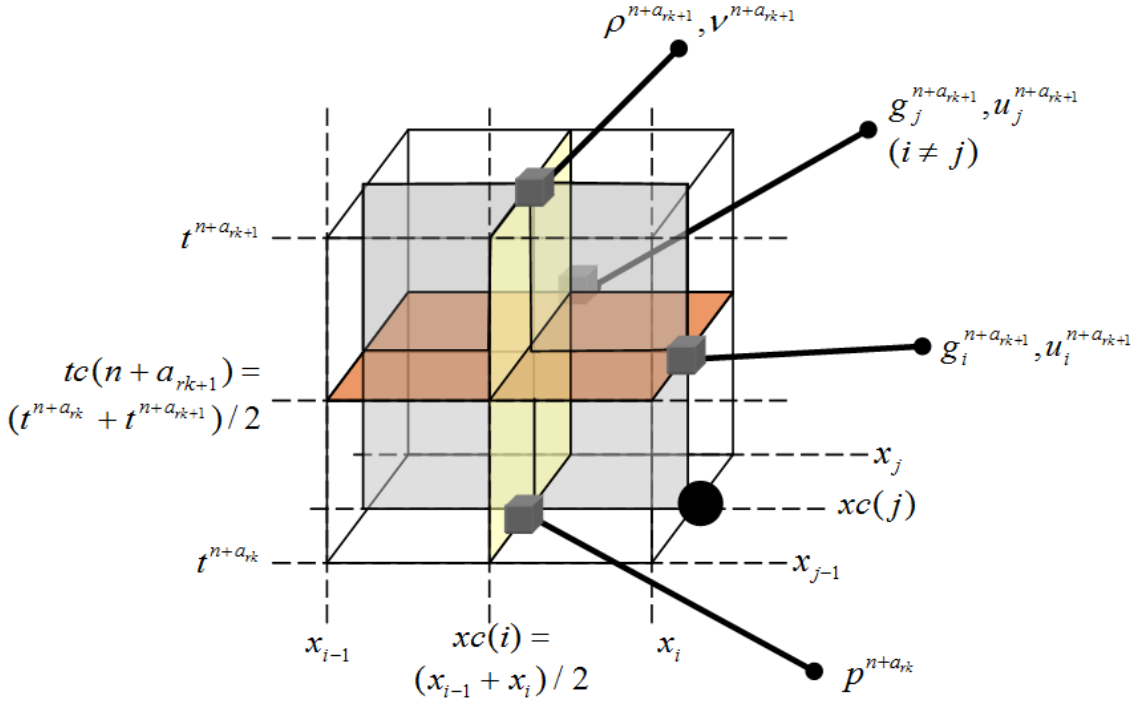

Figure 2. Momentum staggered cell. NB: The RHS of this equation is evaluated at the bottom right of the spatio-tempral cell, identified by a black dot.

- Calculate: $(g_j^{n+a_{rk+1}})^{iter**} = ((\overline{\rho}^{x_j})^t)^{n+a_{rk+1}})^{iter} \times (u_j^{n+a_{rk+1}})^{iter-1}$, $((\overline{g_j}^t)^{n+a_{rk+1}})^{iter**}, ((\overline{u_j}^t)^{n+a_{rk+1}})^{iter-1}$

- Initialize momentum field: $g_j^{n+a_{rk}}$

- Solve momentum equations: $\partial_t(g_i) + \partial_{x_j}(\overline{\overline{g_j}^{x_i}}^t \overline{u_i}^{x_j t}) = -\partial_{x_i} p + \partial_{x_j}(\tau_{ij})$, where $\tau_{ij} = 2\rho\nu[\partial_{x_i}(\overline{u_i}^t) - \partial_{x_k}(\overline{u_k}^t)/3]$, if $i = j$, and $\tau_{ij} = \overline{\overline{\rho\nu}^{x_i}}^{x_j}[\partial_{x_j}(\overline{u_i}^t) + \partial_{x_i}(\overline{u_j}^t)]$, if $i \neq j$, and provide $(g_j^{n+a_{rk+1}})^{iter}$, $(RHS_{u_j}^{rk})^{iter}$

- Calculate intermediate velocity $(\widetilde{u_j^{n+a_{rk+1}}})^{iter} = (g_j^{n+a_{rk+1}})^{iter} / ((\overline{\rho}^{x_j})^t)^{n+a_{rk+1}})^{iter}$

- Impose boundary conditions

- Calculate intermediate momentum field $(\widetilde{g_j^{n+a_{rk+1}}})^{iter} = ((\overline{\rho}^{x_j})^t)^{n+a_{rk+1}})^{iter} \times (\widetilde{u_j^{n+a_{rk+1}}})^{iter}$

STEP 6: PRESSURE EQUATION

This step requires the solution of the Poisson equation to determine the pressure field correction used in the enforcement of the continuity equation. Application of fractional step method including the density fields lead to the following Poisson expresison:

- Solve pressure equation: $\partial_{x_k}(\partial_{x_k}\delta p) = \frac{1}{(t^{n+a_{rk+1}} - t^{n+a_{rk}})}[\partial_{x_j} g_j + \frac{\partial \rho}{\partial t}]]$ or

$$\partial_{x_k}(\partial_{x_k}\delta p) = \frac{1}{2bk(rk)\Delta t}[\partial_{x_j}(\overbrace{g_j^{n+a_{rk+1}}})^{iter} + \frac{(\rho^{n+a_{rk+1}})^{iter} - \rho^{n+a_{rk}}}{2bk(rk)\Delta t}], \text{ and provide}$$

$$(\delta p^{n+a_{rk+1}})^{iter} = (p^{n+a_{rk+1}})^{iter} - p^{n+a_{rk}}$$

Enforcement of the Neumann condition for the Poisson equation is applied by assuming the mass flux correction to be zero on the boundaries. This is a required compatibility condition.

STEP 7: UPDATE VELOCITY AND PRESSURE (end of iterative loop)

- Calculate:

$$(g_j^{n+a_{rk+1}})^{iter} = (\overbrace{g_j^{n+a_{rk+1}}})^{iter} - 2bk(rk)\Delta t \times \partial_{x_j}((\delta p^{n+a_{rk+1}})^{iter}) \quad ,$$

$$(u_j^{n+a_{rk+1}})^{iter} = (g_j^{n+a_{rk+1}})^{iter} / ((\overline{\overline{\rho}^{x_j}}^{t})^{n+a_{rk+1}})^{iter}$$

$$(p^{n+a_{rk+1}})^{iter} = p^{n+a_{rk}} + (\delta p^{n+a_{rk+1}})^{iter}$$

- Impose boundary conditions

- Prepare for next Runge-Kutta stage and update values of $\rho^{n+a_{rk}}$ and $\rho^{n+a_{rk-1}}$

Updating the velocity and pressure fields ensures that density based continuity equation is satisfied. Steps 2 through 7 of the present iterative scheme define a single density iteration. Successful convergence of this loop is based on a criteria consisting of reaching below density change ($\Delta\rho_{max}$) threshold levels calculated from the previous and current density values.

6. Summary

The basic modeling aspects of boundary layer turbulent flows have been derived and introduced. The subgrid scale models used in the LES3D-MP variable density transport equations are also clearly presented. The time advancement method, including a semi-implicit Crank-Nicholson treatment for the wall-normal diffusion components are described since this is typical of CFD codes in the community where wall normal diffusion plays a big role in the numerical solution. Boundary layer calculations are typical cases where the viscous core introduces numerical stiffness slowing down the calculation. Introducing implicit treatment for the viscous wall-normal term reduces the amount of numerical stiffness and provides more efficient calculations.

The numerical method, developed by Charles Pierce has been presented where a new convention for staggering fields has been introduced [3]. Classical staggering is applied to all the fields in space for conservation and stability properties [2]. Additionally, time staggering is included due to the introduction of two density field levels corresponding to the previous and current sub-step of the variable density transport field equations. Application of the developments presented will be shown in the verification and validation chapters of this proposal.

References

[1] Germano, M., Piomelli, U., Cabot, W.H., “A dynamic subgrid-scale eddy viscosity model”, 1991, Physics of Fluids, A 3, pp 1760-1765.

[2] Keating, A., “Large-eddy simulation of heat transfer in turbulent channel flow and in the turbulent flow downstream of a backward facing step”, 2004, PhD Thesis, Department of Mechanical Engineering. The University of Queensland, Brisbane, Australia.

[3] Pierce, C., “Progress variable approach for Large-eddy simulation of turbulent combustion”, 2001, PhD Thesis, Department of Mechanical Engineering, Stanford University, USA.

[4] Pope, S., “Turbulent Flows”, 2000, Cambridge University Press.

[5] Lilly, D.K., “A proposed modification of the Germano subgrid-scale closure method”, 1992, Physics of Fluids, A 4, pp 635-645.

[6] Yoshiwaza, A., “Statistical theory for compressible turbulent shear flows, with applications to subgrid modeling”, 1986, Physics of Fluids, A 29, pp 2152-2164.

[7] Erlebacher, G., Hussaini, M.Y., Speziale, C.G., and Zang, T.A., “Toward the large-eddy simulation of compressible turbulent flows”, 1992, J. Fluid Mechanics, 238, pp 155-185.

[8] Moin, P., Squires, K.D., Cabot, W.H., and Lee, S., “A dynamic subgrid-scale model for compressible turbulence and scalar transport”, 1991. *Phys. Fluids A*, **3**, 2746–2757.

[9] Martin, P., Piomelli, U., Candler, G., “Subgrid-Scale Models for Compressible Large-Eddy Simulations”, 2000 Theoret. Comput. Fluid Dynamics, 13, pp 361-376.

[10] Ma, T., “Large-eddy simulation of variable density flows”, 2006, PhD Thesis, Department of Mechanical Engineering. The University of Maryland, College Park, USA.