Boussineq Equations: Derivation and Numerical Approximation

(The derivation is based on the notes provided in https://classes.soe.ucsc.edu/ams227/Fall13/lecturenotes/Chapter3.pdf)

1 Setup and Derivation

We consider a channel flow (with an arbitary angle w.r.t. gravity) subjected to a temperature gradient between the two walls. Viscosity is assumed to be a function of temperature.

$$\mu = f(T). \tag{1}$$

The Cartesian coordinate system is fixed with respect to the channel which is assumed to be infinitely long in the stream-wise $(x_1 = x)$ and span-wise $(x_3 = z)$ directions. The wall (with the wall normal coordinate $x_2 = y$) is assumed to be of height H.

In the absence of any flow, the steady state density, pressure and temperature (hydrostatic) are:

$$\overline{\rho}(\mathbf{x}) = \rho_{ref} + \rho_0(\mathbf{x}), \tag{2a}$$

$$\overline{p}(\mathbf{x}) = p_{ref} + p_0(\mathbf{x}),\tag{2b}$$

$$\overline{T}(\mathbf{x}) = T_{ref} + T_0(\mathbf{x}). \tag{2c}$$

The reference values for each of the three variables are the mean values and the terms with subscript 0 are relatively small deviations about the mean i.e.

$$\rho_0(\mathbf{x}) << \rho_{ref},\tag{3a}$$

$$p_0(\mathbf{x}) << p_{ref},\tag{3b}$$

$$T_0(\mathbf{x}) << T_{ref}. \tag{3c}$$

In the presence of an unsteady flow with velocity $\mathbf{u}(\mathbf{x},t)$ the perturbations in these three variables are:

$$\rho(\mathbf{x},t) = \overline{\rho}(\mathbf{x}) + \hat{\rho}(\mathbf{x},t), \tag{4a}$$

$$p(\mathbf{x},t) = \overline{p}(\mathbf{x}) + \hat{p}(\mathbf{x},t), \tag{4b}$$

$$T(\mathbf{x},t) = \overline{T}(\mathbf{x}) + \hat{T}(\mathbf{x},t).$$
 (4c)

The governing equations for mass, momentum and energy conservation are:

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u} = 0, \tag{5a}$$

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p - \rho \mathbf{g} + \nabla \cdot \left(\mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right), \tag{5b}$$

$$\rho c_v \frac{DT}{Dt} = -p\nabla \cdot \mathbf{u} + \nabla \cdot (k\nabla T). \tag{5c}$$

We have assumed absence of a heat flux and removed the (often) negligible viscous dissipation of heat from the energy equation. The hydrostatic balance is:

$$\nabla \overline{p} = -\overline{\rho} \mathbf{g},\tag{6a}$$

$$\nabla \cdot (k\nabla \overline{T}) = 0. \tag{6b}$$

Defining the characteristic density and temperature difference to be that between the top and the bottom wall in the hydrostatic case:

$$\Delta \rho_0 = |\overline{\rho}(H) - \overline{\rho}(0)|, \tag{7a}$$

$$\Delta T_0 = |\overline{T}(H) - \overline{T}(0)|,\tag{7b}$$

and dimensionalising the governing equations with the following:

$$\tilde{\mathbf{x}} = \frac{\mathbf{x}}{H}, \quad \tilde{\mathbf{u}} = \frac{\mathbf{u}}{U}, \quad \tilde{t} = t\frac{U}{H}, \quad \tilde{T} = \frac{T}{\Delta T_0}, \quad \tilde{p} = \frac{p}{\rho_{ref}U^2}, \quad \tilde{\rho} = \frac{\rho}{\Delta \rho_0}, \quad \tilde{\mu} = \frac{\mu}{\mu_{ref}}.$$
 (8)

The mass conservation equation is:

$$\frac{U\Delta\rho_0}{H}\frac{\partial\tilde{\rho}_0 + \tilde{\hat{\rho}}}{\partial\tilde{t}} + \frac{U}{H}(\rho_{ref} + \Delta\rho_0(\tilde{\rho}_0 + \tilde{\hat{\rho}}))\tilde{\nabla} \cdot \tilde{u} + \frac{U\Delta\rho_0}{H}\tilde{u} \cdot \tilde{\nabla}(\tilde{\rho}_0 + \tilde{\hat{\rho}}) = 0, \tag{9}$$

or

$$\frac{\partial(\tilde{\rho_0} + \hat{\tilde{\rho}})}{\partial \tilde{t}} + \left(\frac{\rho_{ref}}{\Delta \rho_0} + (\tilde{\rho_0} + \tilde{\hat{\rho}})\right) \tilde{\nabla} \cdot \tilde{u} + \tilde{u} \cdot \tilde{\nabla}(\tilde{\rho_0} + \tilde{\hat{\rho}}) = 0, \tag{10}$$

where $\tilde{\rho} = \tilde{\rho_0} + \tilde{\hat{\rho}}$. As $\rho_{ref} >> \Delta \rho_0$

$$\tilde{\nabla} \cdot \tilde{u} = 0. \tag{11}$$

The momentum equation is non-dimensionalised as following:

$$\frac{U^{2}}{H}(\rho_{ref} + \Delta \rho_{0}(\tilde{\rho_{0}} + \tilde{\hat{\rho}}))\frac{D\tilde{u}}{D\tilde{t}} = -\frac{\rho_{ref}U^{2}}{H}\tilde{\nabla}\tilde{p} - (\rho_{ref} + \Delta \rho_{0}(\tilde{\rho_{0}} + \tilde{\hat{\rho}}))\mathbf{g} + \frac{\mu_{ref}U}{H^{2}}\tilde{\nabla}\cdot\left(\tilde{\mu}\left(\tilde{\nabla}\tilde{\mathbf{u}} + (\tilde{\nabla}\tilde{\mathbf{u}})^{T}\right)\right),\tag{12}$$

or using the hydrostatic relationship

$$\frac{D\tilde{u}}{D\tilde{t}} = -\tilde{\nabla}\tilde{\hat{p}} - \frac{H\Delta\rho_0}{U^2\rho_{ref}}\tilde{\hat{\rho}}\mathbf{g} + \frac{\mu_{ref}}{\rho_{ref}HU}\tilde{\nabla}\cdot\left(\tilde{\mu}\left(\tilde{\nabla}\tilde{\mathbf{u}} + (\tilde{\nabla}\tilde{\mathbf{u}})^T\right)\right). \tag{13}$$

The energy equation can be non-dimensionalised as following:

$$(\rho_{ref} + \Delta \rho_0(\tilde{\rho_0} + \tilde{\hat{\rho}})) \frac{\Delta T_0 U}{H} c_v \frac{D\tilde{T}}{D\tilde{t}} = -\frac{\rho_{ref} U^3}{H} \tilde{p} \tilde{\nabla} \cdot \tilde{\mathbf{u}} + \frac{\Delta T_0}{H^2} \tilde{\nabla} \cdot (k \tilde{\nabla} \tilde{T}), \tag{14}$$

or

$$\frac{D\tilde{T}}{D\tilde{t}} = -\frac{U^2}{c_v \Delta T_0} \tilde{p} \tilde{\nabla} \cdot \tilde{\mathbf{u}} + \frac{1}{c_v \rho_{ref} H U} \tilde{\nabla} \cdot (k \tilde{\nabla} \tilde{T}), \tag{15}$$

Decomposing the pressure and temperature into hydrostatic part and perturbation about it and using the hydrostatic relation

$$\frac{D\tilde{T}}{D\tilde{t}} + \tilde{\mathbf{u}} \cdot \tilde{\nabla}\tilde{T}_0 = -\frac{U^2\tilde{p}_{ref}}{c_v\Delta T_0}\tilde{\nabla} \cdot \tilde{\mathbf{u}} + \frac{1}{c_v\rho_{ref}HU}\tilde{\nabla} \cdot (k\tilde{\nabla}\tilde{T}), \tag{16}$$

1.1 Liquids

$$\frac{\hat{\rho}}{\rho_{ref}} = \frac{1}{\rho_{ref}} \left(\frac{\partial \rho}{\partial T}\right)_{\bar{\rho},\bar{T}} \hat{T} = -\alpha \hat{T},\tag{17}$$

where α is the coefficient of thermal expansion. In the non-dimensional form this is

$$\frac{\Delta \rho_0 \tilde{\hat{\rho}}}{\rho_{ref}} = -\alpha \Delta T_0 \tilde{\hat{T}}.$$
 (18)

Therefore, the momentum equation can be re-written as

$$\frac{D\tilde{u}}{D\tilde{t}} = -\tilde{\nabla}\tilde{\hat{p}} + \frac{H\alpha\Delta T_0}{U^2}\tilde{\hat{T}}\mathbf{g} + \frac{\mu_{ref}}{\rho_{ref}HU}\tilde{\nabla}\cdot\left(\tilde{\mu}\left(\tilde{\nabla}\tilde{\mathbf{u}} + (\tilde{\nabla}\tilde{\mathbf{u}})^T\right)\right). \tag{19}$$

For liquids (as they are incompressible) the energy/ temperature scalar transport equation is:

$$\frac{D\tilde{T}}{D\tilde{t}} + \tilde{\mathbf{u}} \cdot \tilde{\nabla} \tilde{T}_0 = \frac{1}{\rho_{ref} H U} \tilde{\nabla} \cdot (k \tilde{\nabla} \tilde{T}), \tag{20}$$

Defining the non-dimensional groups

$$Ri_b = \frac{\alpha \Delta T_0 gH}{U^2}, Re = \frac{\rho_{ref} UH}{\mu_{ref}}, Pr = \frac{\mu_{ref}}{\rho_{ref}(k/c_v)}, \tag{21}$$

dropping and noting $\hat{T} = T$, $\hat{p} = p$ we can re-write the equations as following:

$$\nabla \cdot \mathbf{u} = 0, \tag{22a}$$

$$\frac{D\mathbf{u}}{Dt} = -\nabla p + Ri_b T \mathbf{n} + \frac{1}{Re} \nabla \cdot \left(\mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right), \tag{22b}$$

$$\frac{DT}{Dt} + \mathbf{u} \cdot \nabla T_0 = \frac{1}{PrRe} \nabla^2 T. \tag{22c}$$

We emphasise that T and p are the deviation from hydrostatic temperature and pressure distributions and T_0 is the hydrostatic temperature deviation from its mean.

Pressure poisson can be derived by taking the gradient of equation (22b) and using incompressibility.

$$\frac{\partial}{\partial x_i} \left(\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right) = \frac{\partial}{\partial x_i} \left(-\frac{\partial p}{\partial x_i} + Ri_b T n_i + \frac{1}{Re} \left[\frac{\partial}{\partial x_j} \left(\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right) \right] \right)$$
(23a)

$$\frac{\partial u_j}{\partial x_i} \frac{\partial u_i}{\partial x_j} = -\frac{\partial^2 p}{\partial x_i^2} + Ri_b \frac{\partial T}{\partial x_i} n_i + \frac{1}{Re} \frac{\partial}{\partial x_i} \left[\frac{\partial \mu}{\partial x_j} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \mu \frac{\partial^2 u_i}{\partial x_j^2} \right]$$
(23b)

$$\frac{\partial u_j}{\partial x_i} \frac{\partial u_i}{\partial x_j} = -\frac{\partial^2 p}{\partial x_i^2} + Ri_b \frac{\partial T}{\partial x_i} n_i + \frac{1}{Re} \left[\frac{\partial^2 \mu}{\partial x_j \partial x_i} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \frac{\partial \mu}{\partial x_j} \frac{\partial^2 u_j}{\partial x_i^2} + \frac{\partial \mu}{\partial x_i} \frac{\partial^2 u_i}{\partial x_j^2} \right]$$
(23c)

$$\frac{\partial^2 p}{\partial x_i^2} = -\frac{\partial u_j}{\partial x_i} \frac{\partial u_i}{\partial x_j} + Ri_b \frac{\partial T}{\partial x_i} n_i + \frac{1}{Re} \left[\frac{\partial^2 \mu}{\partial x_j \partial x_i} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + 2 \frac{\partial \mu}{\partial x_j} \frac{\partial^2 u_j}{\partial x_i^2} \right]$$
(23d)

We need this to set the initial condition for pressure.

1.2 Gases

We will consider gases later.

2 Numerical Discretisation

This section is based on Tom Bewley's algorithm provided in the book Numerical Renaissance: http://numerical-renaissance.com/NR.pdf

2.1 Spatial Discretisation

We will assume x and z to be periodic and calculate the derivatives in these directions using spectral differentiation. The grid is uniform in these directions and in the wall normal direction y, the grid will be modified to cluster near the walls with the following equation:

$$y_j = \tanh\left(C\left(\frac{2(j-1)}{NY} - 1\right)\right) \tag{24}$$

for the base grid $j \in [0, ..., NY + 2]$. The fractional grid is defined to lie exactly between the two base grid points:

$$y_{j+1/2} = \frac{1}{2}(y_j + y_{j+1}). (25)$$

The spatial derivatives in the x and z are calculated spectrally using fast Fourier transform algorithm and the spatial derivatives in the wall normal y direction are evaluated using central finite difference schemes. Variables are stored in the following manner:

- Base grid (j): v
- Fractional grid (j + 1/2): u, w, p and T

We may need v at the fractional grid and the fractional grid variables at the base grid. To interpolate we use the following:

$$\bar{v}_{j+1/2} = \frac{1}{2} (v_{j+1} + v_j)$$
 (26a)

$$\check{u}_j = \frac{1}{2\Delta y_j} \left(\Delta y_{j+1/2} u_{j+1/2} + \Delta y_{j-1/2} u_{j-1/2} \right)$$
(26b)

$$\check{u}_j = \frac{1}{2\Delta y_j} \left(\Delta y_{j-1/2} u_{j+1/2} + \Delta y_{j+1/2} u_{j-1/2} \right)$$
(26c)

2.1.1 x-momentum equation

$$\frac{\partial u}{\partial t} = -\left[\frac{\partial u^2}{\partial x} + \frac{\partial uv}{\partial y} + \frac{\partial uw}{\partial z}\right] - \frac{\partial p}{\partial x} + Ri_b T n_1
+ \frac{1}{Re} \left[\frac{\partial}{\partial x} \left(2\mu \frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y} \left(\mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)\right) + \frac{\partial}{\partial z} \left(\mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)\right)\right]$$
(27)

$$\frac{\partial u}{\partial t}\bigg|_{i,j+1/2,k} = -\left[\frac{\delta_{s}u^{2}}{\delta x}\bigg|_{j+1/2} + \frac{(\bar{u}v)_{j+1} - (\bar{u}v)_{j}}{\Delta y_{j+1/2}} + \frac{\delta_{s}uw}{\delta z}\bigg|_{j+1/2}\right] - \frac{\delta_{s}p}{\delta x}\bigg|_{j+1/2} \\
+ Ri_{b}n_{1}T|_{j+1/2} + \frac{1}{Re}\left[\frac{\delta_{s}}{\delta x}\left(2\mu\frac{\delta_{s}u}{\delta x}\right)\bigg|_{j+1/2} + \frac{\delta_{s}}{\delta z}\left(\mu\left(\frac{\delta_{s}u}{\delta z} + \frac{\delta_{s}w}{\delta x}\right)\right)\bigg|_{j+1/2} \\
+ \frac{1}{\Delta y_{j+1/2}}\left(\check{\mu}_{j+1}\left(\frac{u_{j+3/2} - u_{j+1/2}}{\Delta y_{j+1}} + \frac{\delta_{s}v}{\delta x}\bigg|_{j+1}\right) - \check{\mu}_{j}\left(\frac{u_{j+1/2} - u_{j-1/2}}{\Delta y_{j}} + \frac{\delta_{s}v}{\delta x}\bigg|_{j}\right)\right] \tag{28}$$

2.1.2 y-momentum equation

$$\frac{\partial v}{\partial t} = -\left[\frac{\partial uv}{\partial x} + \frac{\partial v^2}{\partial y} + \frac{\partial vw}{\partial z}\right] - \frac{\partial p}{\partial y} + Ri_b T n_2
+ \frac{1}{Re} \left[\frac{\partial}{\partial x} \left(\mu \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right)\right) + \frac{\partial}{\partial y} \left(2\mu \frac{\partial v}{\partial y}\right) + \frac{\partial}{\partial z} \left(\mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right)\right)\right]$$
(29)

$$\frac{\partial v}{\partial t}\bigg|_{i,j,k} = -\left[\frac{\delta_{s}\check{u}v}{\delta x}\bigg|_{j} + \frac{(\bar{v}^{2})_{j+1/2} - (\bar{v}^{2})_{j-1/2}}{\Delta y_{j}} + \frac{\delta_{s}v\check{w}}{\delta z}\bigg|_{j}\right] - \frac{p_{j+1/2} - p_{j-1/2}}{\Delta y_{j}} + Ri_{b}n_{2}\check{T}|_{j}
+ \frac{1}{Re}\left[\frac{\delta_{s}}{\delta x}\Big(\check{\mu}_{j}\Big(\frac{\delta_{s}v}{\delta x}\bigg|_{j} + \frac{u_{j+1/2} - u_{j-1/2}}{\Delta y_{j}}\Big)\Big) + \frac{2}{\Delta y_{j}}\Big(\mu_{j+1/2}\frac{v_{j+1} - v_{j}}{\Delta y_{j+1/2}} - \mu_{j-1/2}\frac{v_{j} - v_{j-1}}{\Delta y_{j-1/2}}\Big) \right]
+ \frac{\delta_{s}}{\delta z}\Big(\check{\mu}_{j}\Big(\frac{\delta_{s}v}{\delta z}\bigg|_{j} + \frac{w_{j+1/2} - w_{j-1/2}}{\Delta y_{j}}\Big)\right]$$
(30)

2.1.3 z-momentum equation

$$\frac{\partial w}{\partial t} = -\left[\frac{\partial uw}{\partial x} + \frac{\partial vw}{\partial y} + \frac{\partial w^2}{\partial z}\right] - \frac{\partial p}{\partial z} + Ri_b T n_3
+ \frac{1}{Re} \left[\frac{\partial}{\partial x} \left(\mu \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z}\right)\right) + \frac{\partial}{\partial y} \left(\mu \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z}\right)\right) + \frac{\partial}{\partial z} \left(2\mu \frac{\partial w}{\partial z}\right)\right]$$
(31)

$$\frac{\partial w}{\partial t}\bigg|_{i,j+1/2,k} = -\left[\frac{\delta_s u w}{\delta x}\bigg|_{j+1/2} + \frac{(v\bar{w})_{j+1} - (v\bar{w})_j}{\Delta y_{j+1/2}} + \frac{\delta_s w^2}{\delta z}\bigg|_{j+1/2}\right] - \frac{\delta_s p}{\delta z}\bigg|_{j+1/2} \\
+ Ri_b n_3 T|_{j+1/2} + \frac{1}{Re}\left[\frac{\delta_s}{\delta x}\bigg(\mu\bigg(\frac{\delta_s w}{\delta x} + \frac{\delta_s u}{\delta z}\bigg)\bigg)\bigg|_{j+1/2} + \frac{\delta_s}{\delta z}\bigg(2\mu\frac{\delta_s w}{\delta z}\bigg)\bigg|_{j+1/2} \\
+ \frac{1}{\Delta y_{j+1/2}}\bigg(\check{\check{\mu}}_{j+1}\bigg(\frac{w_{j+3/2} - w_{j+1/2}}{\Delta y_{j+1}} + \frac{\delta_s v}{\delta z}\bigg|_{j+1}\bigg) - \check{\check{\mu}}_j\bigg(\frac{w_{j+1/2} - w_{j-1/2}}{\Delta y_j} + \frac{\delta_s v}{\delta z}\bigg|_{j}\bigg)\bigg] \tag{32}$$

2.1.4 Scalar equation

$$\frac{\partial T}{\partial t} = -\left[\frac{\partial(uT)}{\partial x} + \frac{\partial(vT)}{\partial y} + \frac{\partial(wT)}{\partial z} + \frac{\partial(uT_0)}{\partial z} + \frac{\partial(vT_0)}{\partial x} + \frac{\partial(wT_0)}{\partial z}\right] + \frac{1}{PrRe}\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right)$$
(33)

$$\frac{\partial T}{\partial t}\Big|_{i,j+1/2,k} = -\left[\frac{\delta_s(u(T+T_0))}{\delta x}\Big|_{j+1/2} + \frac{(v(\mathring{T}+\mathring{T}_0))_{j+1} - (v(\mathring{T}+\mathring{T}_0))_{j}}{\Delta y_{j+1/2}} + \frac{\delta_s(w(T+T_0))}{\delta z}\Big|_{j+1/2}\right] + \frac{1}{PrRe}\left(\frac{\delta_s^2 T}{\delta x^2}\Big|_{j+1/2} + \frac{1}{\Delta y_{j+1/2}}\left(\frac{T_{j+3/2} - T_{j+1/2}}{\Delta y_{j+1}} - \frac{T_{j+1/2} - T_{j-1/2}}{\Delta y_{j}}\right) + \frac{\delta_s^2 T}{\delta z^2}\Big|_{j+1/2}\right)$$
(34)

2.1.5 Incompressibility

$$\nabla \cdot \mathbf{u} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = \frac{\delta_s u_{j+1/2}}{\delta x} + \frac{v_{j+1} - v_j}{\Delta y_{j+1/2}} + \frac{\delta_s w_{j+1/2}}{\delta z}$$
(35)

2.1.6 Pressure Poisson Operator

$$\nabla^{2} p = \frac{\partial^{2} p}{\partial x^{2}} + \frac{\partial^{2} p}{\partial y^{2}} + \frac{\partial^{2} p}{\partial z^{2}} = \frac{\delta_{s}^{2} p_{j+1/2}}{\delta x^{2}} + \frac{1}{\Delta y_{j+1/2}} \left(\frac{p_{j+3/2} - p_{j+1/2}}{\Delta y_{j+1}} - \frac{p_{j+1/2} - p_{j-1/2}}{\Delta y_{j}} \right) + \frac{\delta_{s}^{2} p_{j+1/2}}{\delta z^{2}}$$
(36)

2.2 Temporal Discretisation

The low storage third order Runge-Kutta Wray scheme that treats part of the terms implicitly using Crank Nicholson and part explicitly using Runge- Kutte scheme is used for time advancement. For a pde

$$\frac{\partial \phi}{\partial t} = N(\phi) + A(\phi) \tag{37}$$

the terms condensed into $N(\phi)$ are treated explicitly and in $A(\phi)$ implicitly. Therefore, $A(\phi)$ must be either linear or linearised appropriately. The three substeps required for a Δt from $t^n \to t^{n+1} = t^n + \Delta t$ advancement in time are:

$$\phi' = \phi^n + \gamma_1 \Delta t N(\phi^n) + \zeta_1 \Delta t N(\phi^{-n}) + \alpha_1 \Delta t \frac{A(\phi') + A(\phi^n)}{2}, \tag{38a}$$

$$\phi'' = \phi' + \gamma_2 \Delta t N(\phi') + \zeta_2 \Delta t N(\phi^n) + \alpha_2 \Delta t \frac{A(\phi'') + A(\phi')}{2}, \tag{38b}$$

$$\phi^{n+1} = \phi'' + \gamma_3 \Delta t N(\phi'') + \zeta_3 \Delta t N(\phi') + \alpha_3 \Delta t \frac{A(\phi^{n+1}) + A(\phi'')}{2}.$$
 (38c)

The coefficient are given by:

$$\gamma_1 = \frac{8}{15}, \gamma_2 = \frac{5}{12}, \gamma_3 = \frac{3}{4}, \zeta_1 = 0, \zeta_2 = -\frac{17}{60}, \zeta_3 = -\frac{5}{12}, \alpha_1 = \frac{8}{15}, \alpha_2 = \frac{2}{15}, \alpha_3 = \frac{1}{3}$$
 (39)

Writing each of these step as rk = 1, 2 and 3, the equations (38) can be compactly written as:

$$\phi^{rk} = \phi^{rk-1} + \gamma_{rk} \Delta t N(\phi^{rk-1}) + \zeta_{rk} \Delta t N(\phi^{rk-2}) + \alpha_{rk} \Delta t \frac{A(\phi^{rk}) + A(\phi^{rk-1})}{2}$$
(40)

We will consider the terms involving spatial derivatives in the wall parallel (x and z) directions explicitly as they are calculated spectrally. It is not theoretically impossible to treat them as one could write the spectral derivatives as a product with spectral derivative matrix. However, such a matrix will be dense and hence inverting it would not be efficient. Due to the stretched grid used, the grid size is largely reduced near the wall. This would require a very small step size Δt if treated explicitly. Hence, in the terms involving the wall normal derivatives are treated implicitly. Some of these need to be linearised and are explained below.

2.2.1 Scalar Equation

Considering first the scalar equation with ϕ in (38) as T. The explicit terms are:

$$N(\phi) = -\left[\frac{\delta_s(u(T+T_0))}{\delta x}\Big|_{j+1/2} + -\frac{(v(\check{T}+\check{T}_0))_{j+1} - (v(\check{T}+\check{T}_0))_j}{\Delta y_{j+1/2}} + \frac{\delta_s(w(T+T_0))}{\delta z}\Big|_{j+1/2}\right] + \frac{1}{PrRe}\left(\frac{\delta_s^2 T}{\delta x^2}\Big|_{j+1/2} + \frac{\delta_s^2 T}{\delta z^2}\Big|_{j+1/2}\right)$$
(41)

The implicit terms are:

$$A(\phi) = \frac{1}{PrRe} \left(\frac{1}{\Delta y_{j+1/2}} \left(\frac{T_{j+3/2} - T_{j+1/2}}{\Delta y_{j+1}} - \frac{T_{j+1/2} - T_{j-1/2}}{\Delta y_j} \right) \right)$$
(42)

Hence, solving the temperature equation at the time step rk will provide:

$$T^{rk} \to \mu^{rk} \tag{43}$$

2.2.2 Momentum Equations

The momentum equations can be re-written as:

$$\mathbf{u}^{rk} = \mathbf{u}^{rk-1} + \gamma_{rk} \Delta t N(\mathbf{u}^{rk-1}) + \zeta_{rk} \Delta t N(\mathbf{u}^{rk-2}) + \alpha_{rk} \Delta t \frac{A(\mathbf{u}^{rk}) + A(\mathbf{u}^{rk-1})}{2} - \alpha_{rk} \Delta t \frac{\delta p^{rk-1}}{\delta x_i} - \alpha_{rk} \Delta t \frac{\delta q}{\delta x_i}$$

$$(44)$$

where

$$q := p^{rk} - p^{rk-1} \tag{45}$$

The fractional step strategy is to break the momentum equation into two distinct steps:

$$\mathbf{v}^{rk} = \mathbf{u}^{rk-1} + \gamma_{rk} \Delta t N(\mathbf{u}^{rk-1}) + \zeta_{rk} \Delta t N(\mathbf{u}^{rk-2}) + \alpha_{rk} \Delta t \frac{A(\mathbf{v}^{rk}) + A(\mathbf{u}^{rk-1})}{2} - \alpha_{rk} \Delta t \frac{\delta p^{rk-1}}{\delta x_i}$$
(46)

with

$$\mathbf{u}^{rk} = \mathbf{v}^{rk} - \alpha_{rk} \Delta t \nabla q, \tag{47}$$

$$\nabla \cdot (\mathbf{u}^{rk}) = 0 = \nabla \cdot (\mathbf{v}^{rk}) - \alpha_{rk} \Delta t \nabla^2 q. \tag{48}$$

Therefore,

$$\nabla^2 q = \frac{1}{\alpha_{rk} \Delta t} \nabla \cdot (\mathbf{v}^{rk}), \tag{49}$$

and update the pressure as

$$p^{rk} = p^{rk-1} + q. (50)$$

y momentum equation: First consider the y momentum equation (to avoid confusion we will use v_2 as y component of intermediate velocity \mathbf{v} and u_2 as that for the actual velocity \mathbf{u}):

$$A(u_2^{rk}) = -\frac{\delta(u_2^{rk})^2}{\delta y} + Ri_b n_2 \check{\tilde{T}}^{rk} + \frac{2}{Re} \frac{\delta}{\delta y} \left(\mu^{rk} \frac{\delta u_2^{rk}}{\delta y} \right)$$
 (51)

(although there are cross derivative terms involving the y- derivative, but they must be treated explicitly due to the use of spectral derivatives)

$$\tilde{A}(v_2^{rk}) = -\frac{\delta(v_2^{rk})^2}{\delta y} + Ri_b n_2 \tilde{T}^{rk} + \frac{2}{Re} \frac{\delta}{\delta y} \left(\mu^{rk} \frac{\delta v_2^{rk}}{\delta y} \right), \tag{52}$$

$$\mathcal{O}((\Delta t)^2) = (v_2^{rk} - u_2^{rk-1})^2 = (v_2^{rk})^2 - 2v_2^{rk}u_2^{rk-1} + (u_2^{rk-1})^2 = 0 \rightarrow (v_2^{rk})^2 = 2v_2^{rk}u_2^{rk-1} - (u_2^{rk-1})^2. \tag{53}$$

The fully explicit terms thus generated from this approximation exactly cancels the first term in the $A(u_2^{rk})$ in equation (51). Therefore,

$$A(u_2^{rk}) = Ri_b n_2 \check{T}^{rk} + \frac{2}{Re} \frac{\delta}{\delta u} \left(\mu^{rk} \frac{\delta u_2^{rk}}{\delta u} \right), \tag{54}$$

and,

$$A(v_2^{rk}) = -2\frac{\delta(v_2^{rk}u_2^{rk-1})}{\delta y} + Ri_b n_2 \check{T}^{rk} + \frac{2}{Re} \frac{\delta}{\delta y} \left(\mu^{rk} \frac{\delta v_2^{rk}}{\delta y}\right). \tag{55}$$

As we already know the T at the current step from solving the scalar equation first, the Crank-Nicholson terms are modified to:

$$A(u_2^{rk}) = Ri_b n_2(\check{\check{T}}^{rk} + \check{\check{T}}^{rk+1}) + \frac{2}{Re} \frac{\delta}{\delta y} \left(\mu^{rk} \frac{\delta u_2^{rk}}{\delta y} \right), \tag{56}$$

and,

$$A(v_2^{rk}) = -2\frac{\delta(v_2^{rk}u_2^{rk-1})}{\delta y} + \frac{2}{Re}\frac{\delta}{\delta y}\left(\mu^{rk}\frac{\delta v_2^{rk}}{\delta y}\right). \tag{57}$$

Also,

$$N(v^{rk}) = -\frac{\delta(uv)^{rk}}{\delta x} - \frac{\delta(vw)^{rk}}{\delta z} + \frac{1}{Re} \left[\frac{\delta}{\delta x} \left(\mu^{rk} \left(\frac{\delta v^{rk}}{\delta x} + \frac{\delta u^{rk}}{\delta y} \right) \right) + \frac{\delta}{\delta z} \left(\mu^{rk} \left(\frac{\delta v^{rk}}{\delta z} + \frac{\delta w^{rk}}{\delta y} \right) \right) \right]$$
(58)

Now we can solve for v_2 . We have all the ingredients to solve for v_1 and v_3 .

x momentum equation:

$$A(u_1^{rk}) = -\frac{\delta(u_1^{rk}u_2^{rk})}{\delta y} + Ri_b n_1 T^{rk} + \frac{1}{Re} \left[\frac{\delta}{\delta y} \left(\mu^{rk} \frac{\delta u_1^{rk}}{\delta y} \right) + \frac{\delta}{\delta y} \left(\mu^{rk} \frac{\delta u_2^{rk}}{\delta x} \right) \right], \tag{59}$$

$$A(v_1^{rk}) = -\frac{\delta(v_1^{rk}v_2^{rk})}{\delta y} + Ri_b n_1 T^{rk} + \frac{1}{Re} \left[\frac{\delta}{\delta y} \left(\mu^{rk} \frac{\delta v_1^{rk}}{\delta y} \right) + \frac{\delta}{\delta y} \left(\mu^{rk} \frac{\delta v_2^{rk}}{\delta x} \right) \right]. \tag{60}$$

As we already know the T and v_2 at the current step from solving the scalar v_2 equation first, the Crank-Nicholson terms are modified to:

$$A(u_1^{rk}) = -\frac{\delta(u_1^{rk}u_2^{rk})}{\delta y} + Ri_b n_1(T^{rk} + T^{rk+1}) + \frac{1}{Re} \left[\frac{\delta}{\delta y} \left(\mu^{rk} \frac{\delta u_1^{rk}}{\delta y} \right) + \frac{\delta}{\delta y} \left(\mu^{rk} \frac{\delta u_2^{rk}}{\delta x} \right) + \frac{\delta}{\delta y} \left(\mu^{rk+1} \frac{\delta v_2^{rk+1}}{\delta x} \right) \right], \tag{61}$$

$$A(v_1^{rk}) = -\frac{\delta(v_1^{rk}v_2^{rk})}{\delta y} + \frac{1}{Re}\frac{\delta}{\delta y} \left(\mu^{rk}\frac{\delta v_1^{rk}}{\delta y}\right). \tag{62}$$

The explicit term is:

$$N(u^{rk}) = -\frac{\delta(u^2)^{rk}}{\delta x} - \frac{\delta(uw)^{rk}}{\delta z} + \frac{1}{Re} \left[\frac{\delta}{\delta x} \left(2\mu^{rk} \frac{\delta u^{rk}}{\delta x} \right) + \frac{\delta}{\delta z} \left(\mu^{rk} \left(\frac{\delta u^{rk}}{\delta z} + \frac{\delta w^{rk}}{\delta x} \right) \right]. \tag{63}$$

z momentum equation:

$$A(u_3^{rk}) = -\frac{\delta(u_2^{rk}u_3^{rk})}{\delta y} + Ri_b n_3 T^{rk} + \frac{1}{Re} \left[\frac{\delta}{\delta y} \left(\mu^{rk} \frac{\delta u_3^{rk}}{\delta y} \right) + \frac{\delta}{\delta y} \left(\mu^{rk} \frac{\delta u_2^{rk}}{\delta z} \right) \right], \tag{64}$$

$$A(v_3^{rk}) = -\frac{\delta(v_2^{rk}v_3^{rk})}{\delta y} + Ri_b n_3 T^{rk} + \frac{1}{Re} \left[\frac{\delta}{\delta y} \left(\mu^{rk} \frac{\delta v_3^{rk}}{\delta y} \right) + \frac{\delta}{\delta y} \left(\mu^{rk} \frac{\delta v_2^{rk}}{\delta z} \right) \right]. \tag{65}$$

As we already know the T and v_2 at the current step from solving the scalar v_2 equation first, the Crank-Nicholson terms are modified to:

$$A(u_3^{rk}) = -\frac{\delta(u_2^{rk}u_3^{rk})}{\delta y} + Ri_b n_3 (T^{rk} + T^{rk+1}) + \frac{1}{Re} \left[\frac{\delta}{\delta y} \left(\mu^{rk} \frac{\delta u_3^{rk}}{\delta y} \right) + \frac{\delta}{\delta y} \left(\mu^{rk} \frac{\delta u_2^{rk}}{\delta z} \right) + \frac{\delta}{\delta y} \left(\mu^{rk+1} \frac{\delta v_2^{rk+1}}{\delta z} \right) \right], \tag{66}$$

$$A(v_3^{rk}) = -\frac{\delta(v_2^{rk}v_3^{rk})}{\delta y} + \frac{1}{Re}\frac{\delta}{\delta y} \left(\mu^{rk}\frac{\delta v_3^{rk}}{\delta y}\right). \tag{67}$$

The explicit term is:

$$N(w^{rk}) = -\frac{\delta(uw)^{rk}}{\delta x} - \frac{\delta(w^2)^{rk}}{\delta z} + \frac{1}{Re} \left[\frac{\delta}{\delta z} \left(2\mu^{rk} \frac{\delta w^{rk}}{\delta z} \right) + \frac{\delta}{\delta x} \left(\mu^{rk} \left(\frac{\delta u^{rk}}{\delta z} + \frac{\delta w^{rk}}{\delta x} \right) \right] \right]. \tag{68}$$