Chapter 3

Finite-Volume Space Discretization of PDEs

Learning Objectives. Students will be able to:

- Transform a partial differential equation from differential form into control volume form.
- Compute fluxes on a uniform mesh for any problem whose differential form contains no higher than second derivatives.
- Compute the flux integral for a control volume, given the fluxes at the boundaries of the CV.

Suppose we write our PDE with as many terms as possible in divergence form (the left-hand side (LHS) of Eq. 3.1) with the remaining terms written as a source term (the right-hand side (RHS)):

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} = S \tag{3.1}$$

This form is much more general than it looks. In particular, it is a simple matter to write the Navier-Stokes equations in this form, with no source term; turbulence and chemistry models (among other effects) add source terms.

Unless specified otherwise, we will assume throughout the course that the exact solution to the PDE is sufficiently *smooth*. That is, that we can take as many derivatives as we need of the exact solution, and that all of those derivatives are finite.

Before we can compute the solution of this problem, we must rewrite the PDE into a system of algebraic equations relating the solution at one time level to the solution at the next time level. The first step in this process is space discretization, which will convert the PDE into a system of coupled ODEs describing the variation of solution unknowns with time. Next, these ODEs are discretized in time to produce a set of algebraic equations.

3.1 Transformation of a PDE into Control Volume Form

If we integrate Equation 3.1 over a three-dimensional control volume, we get

$$\begin{aligned}
\int_{CV} \frac{\partial U}{\partial t} dV + \int_{CV} \frac{\partial F}{\partial x} dV + \int_{CV} \frac{\partial G}{\partial y} dV + \int_{CV} \frac{\partial H}{\partial z} dV &= \int_{CV} S\, dV \\
\int_{CV} \frac{\partial U}{\partial t} dV + \int_{CV} \left(\frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} \right) dV &= \int_{CV} S\, dV \\
\int_{CV} \frac{\partial U}{\partial t} dV + \int_{CV} \nabla \cdot \vec{F}\, dV &= \int_{CV} S\, dV
\end{aligned}$$

where the last equation arises by defining $\vec{F} = F\hat{\imath} + G\hat{\jmath} + H\hat{k}$. Using Gauss's theorem, we get

$$\int_{CV} \frac{\partial U}{\partial t} dV + \oint_{\partial(CV)} \vec{F} \cdot \vec{n}\, dA = \int_{CV} S\, dV$$

If we assume that the size and shape of the control volume is fixed (computationally, assume that the mesh is not moving), we can simplify a bit further.

$$\frac{d}{dt} \int_{CV} U\, dV + \oint_{\partial(CV)} \vec{F} \cdot \vec{n}\, dA = \int_{CV} S\, dV \tag{3.2}$$

It's worth pointing out that often the derivation of physical PDEs in differential form involves a balance over some small region (our control volume), with the PDE arising in the limit of infinitesimal control volumes.

In the finite-volume method, we abandon hope of knowing anything about the details of the solution within a control volume and instead content ourselves with computing $\bar{U} \equiv \frac{1}{V} \int_{CV} U\, dV$, just as we do in conventional pencil-and-paper control volume analysis. This average value is *not necessarily the value of the solution at any fixed point within the control volume*, including its centroid; forgetting this fact can lead to unfortunate misunderstandings when developing finite-volume algorithms.[1]

If we also define a mean source term contribution $\bar{S} \equiv \frac{1}{V} \int_{CV} S\, dV$, we can write Equation 3.2 as follows.

$$\frac{d\bar{U}}{dt} = -\frac{1}{V} \oint_{\partial(CV)} \vec{F} \cdot \vec{n}\, dA + \bar{S} \tag{3.3}$$

[1] Nevertheless, it isn't hard to show (by expanding in a Taylor series and integrating over the control volume) that $\bar{U}$ is within $O(\Delta x^2)$ of U at the centroid of the control volume for problems with smooth solutions. Likewise, $\bar{S}$ can be evaluated to within $O\left(\Delta x^2\right)$ by taking its value as $\bar{S} \approx S(\bar{U})$.

This equation states that the average value $\bar{U}$ of the solution in the control volume changes at a rate determined by the volume average of the net flux of stuff across the boundaries of the control volume $\frac{1}{V}\oint \vec{F}\cdot\vec{n}\,dA$ and the average rate of production of stuff inside the control volume $\bar{S}$.

Also, Equation 3.3 suggests that for a general time-varying problem, the process of advancing the solution from one time level $t = n\Delta t$ to the next ($(n+1)\Delta t$) requires four operations:

1. Evaluation of the flux $\vec{F}$ at the surface of the control volume.
2. Integration of the normal flux $\vec{F}\cdot\vec{n}$ around the boundary of the control volume.
3. Evaluation and integration of the source term S over the control volume.
4. Updating the control volume average value $\bar{U}$.

3.2 Second-order Accurate Flux for the Poisson Equation

Poisson's equation in two dimensions is:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = S.$$

Integrating over control volumes, we have

$$\begin{aligned}
\int_{CV}\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) dA &= \int_{CV} S\,dA && (3.4)\\
\int_{CV}\nabla\cdot\begin{pmatrix}\frac{\partial T}{\partial x}\\ \frac{\partial T}{\partial y}\end{pmatrix} dA &= \bar{S}A && (3.5)\\
\oint_{\partial CV}(\nabla T)\cdot\vec{n}\,ds &= \bar{S}A && (3.6)
\end{aligned}$$

The last transformation uses Gauss's theorem. So the flux in Poisson's equation is $\begin{pmatrix}\frac{\partial T}{\partial x} & \frac{\partial T}{\partial y}\end{pmatrix}^T$. The normal component of this flux is $\frac{\partial T}{\partial x}$ on faces perpendicular to the x-axis and $\frac{\partial T}{\partial y}$ on faces perpendicular to the y-axis.

Recall that the derivative can be defined as

$$\left.\frac{dT}{dx}\right|_{x_0} = \lim_{\varepsilon\to 0}\frac{T(x_0+\varepsilon) - T(x_0-\varepsilon)}{2\varepsilon}, \tag{3.7}$$

assuming that the limit exists. This is the well-known centered difference formula. Note that the difference between the total and partial derivative here is simply that the partial derivative carries along a non-varying second independent variable:

$$\left.\frac{\partial T}{\partial x}\right|_{x_0} = \lim_{\varepsilon \to 0} \frac{T(x_0+\varepsilon, y) - T(x_0-\varepsilon, y)}{2\varepsilon}, \tag{3.8}$$

Our problem with applying this directly is that we don't have values of the solution like $T(x_0+\varepsilon)$ available to us; all we have are control volume averages. Can we use control volume averages in Eqs. 3.7 and 3.8 and still approximate the derivative accurately enough? That is, what is the error in approximating

$$\left.\frac{dT}{dx}\right|_{i+\frac{1}{2}} \approx \frac{\overline{T}_{i+1} - \overline{T}_i}{\Delta x}$$

That is, if we take some arbitrary smooth function $T(x)$ and compute its control volume averages $\overline{T}_i$ and $\overline{T}_{i+1}$ for control volumes i and $i+1$, respectively, how accurately can we approximate the derivative $T'(x)$ at $i+\frac{1}{2}$ using only those two control volume averages?

To determine this, we need to use Taylor series[2] and integration to express the control volume averages in control volumes i and $i+1$ in terms of the solution and its derivatives at the interface between these control volumes, where $x = x_{i+\frac{1}{2}}$. We must use that location to evaluate derivatives because we are planning to compare our results to the derivative First, for control volume $i+1$, we have:

$$\begin{aligned}
\overline{T}_{i+1} &= \frac{1}{\Delta x}\int_{x_{i+\frac{1}{2}}}^{x_{i+\frac{3}{2}}} \left(T_{i+\frac{1}{2}} + \left(x - x_{i+\frac{1}{2}}\right) \left.\frac{dT}{dx}\right|_{i+\frac{1}{2}} + \frac{\left(x - x_{i+\frac{1}{2}}\right)^2}{2} \left.\frac{d^2T}{dx^2}\right|_{i+\frac{1}{2}} + \frac{\left(x - x_{i+\frac{1}{2}}\right)^3}{6} \left.\frac{d^3T}{dx^3}\right|_{i+\frac{1}{2}} + \cdots \right) dx \\
&= \frac{1}{\Delta x}\int_0^{\Delta x} \left(T_{i+\frac{1}{2}} + \xi \left.\frac{dT}{dx}\right|_{i+\frac{1}{2}} + \frac{\xi^2}{2} \left.\frac{d^2T}{dx^2}\right|_{i+\frac{1}{2}} + \frac{\xi^3}{6} \left.\frac{d^3T}{dx^3}\right|_{i+\frac{1}{2}} + \cdots \right) d\xi \\
&= \frac{1}{\Delta x} \left(\xi T_{i+\frac{1}{2}} + \frac{\xi^2}{2} \left.\frac{dT}{dx}\right|_{i+\frac{1}{2}} + \frac{\xi^3}{6} \left.\frac{d^2T}{dx^2}\right|_{i+\frac{1}{2}} + \frac{\xi^4}{24} \left.\frac{d^3T}{dx^3}\right|_{i+\frac{1}{2}} + \cdots \right)_0^{\Delta x} \\
&= T_{i+\frac{1}{2}} + \frac{\Delta x}{2} \left.\frac{dT}{dx}\right|_{i+\frac{1}{2}} + \frac{\Delta x^2}{6} \left.\frac{d^2T}{dx^2}\right|_{i+\frac{1}{2}} + \frac{\Delta x^3}{24} \left.\frac{d^3T}{dx^3}\right|_{i+\frac{1}{2}} + \cdots
\end{aligned} \tag{3.9}$$

[2]A good reference if you'd like to refresh your memory on Taylor series is the Khan Academy videos on the topic, which are filed under AP Calculus at khanacademy.org.

Note carefully that this is not the pointwise value of $T(x_i)$; all terms after the second are different for the control volume average than for the Taylor expansion of the function at that point. Should we need more terms for our accuracy analysis, we can always compute them simply integrating more terms in the series. Similarly, we can write:

$$\overline{T}_i = T_{i+\frac{1}{2}} - \frac{\Delta x}{2}\left.\frac{dT}{dx}\right|_{i+\frac{1}{2}} + \frac{\Delta x^2}{6}\left.\frac{d^2T}{dx^2}\right|_{i+\frac{1}{2}} - \frac{\Delta x^3}{24}\left.\frac{d^3T}{dx^3}\right|_{i+\frac{1}{2}} + \cdots$$

In practice, this amounts to using different limits in the already-evaluated indefinite integral, Eq. 3.9. Combining these,

$$\frac{\overline{T}_{i+1} - \overline{T}_i}{\Delta x} = \left.\frac{dT}{dx}\right|_{i+\frac{1}{2}} + \frac{\Delta x^2}{12}\left.\frac{d^3T}{dx^3}\right|_{i+\frac{1}{2}} + O\left(\varepsilon^4\right) \tag{3.10}$$

Another way to write this is to use *Taylor tables*. Basically, this approach is just a convenient way to avoid writing out all of every term each time you expand something in a Taylor series. Each column of the Taylor table represents one term in the Taylor series expansion, and each row represents an expression that is being expanded. The entries in the table are coefficients. Here's the previous example done using a Taylor table.

	$T(x_0)$	$\left.\frac{\partial T}{\partial x}\right\|_{x_0}$	$\left.\frac{\partial^2 T}{\partial x^2}\right\|_{x_0}$	$\left.\frac{\partial^3 T}{\partial x^3}\right\|_{x_0}$
$\frac{\overline{T}_{i+1}}{\Delta x}$	$\frac{1}{\Delta x}$	$\frac{1}{2}$	$\frac{\Delta x}{6}$	$\frac{\Delta x^2}{24}$
$-\frac{\overline{T}_i}{\Delta x}$	$-\frac{1}{\Delta x}$	$\frac{1}{2}$	$-\frac{\Delta x}{6}$	$\frac{\Delta x^2}{24}$
$\frac{\overline{T}_{i+1}-\overline{T}_i}{\Delta x}$	0	1	0	$\frac{\Delta x^2}{12}$

The *truncation error* in a difference approximation D of a differential operator $\mathbf{D}$ is defined to be $D - \mathbf{D}$.[3] An approximation is said to be k^{th}*-order accurate* if and only if the leading-order term in the truncation error is $O\left(\varepsilon^k\right)$.

For our example, the truncation error is $\frac{\Delta x^2}{12}\left.\frac{\partial^3 T}{\partial x^3}\right|_{x_0} + O\left(\Delta x^4\right)$. This approximation is therefore second-order accurate, and the error in the approximation will fall by a factor of four each time Δx is reduced by a factor of two.

[3] You may also see this definition with the sign reversed; the difference is largely philosophical.

Returning to our example of Poisson's equation, Equation 3.10 implies that we can write

$$\left.\frac{\partial T}{\partial x}\right|_{i+\frac{1}{2},j} = \frac{\bar{T}_{i+1,j} - \bar{T}_{i,j}}{\Delta x} + O\left(\Delta x^2\right)$$

and

$$\left.\frac{\partial T}{\partial y}\right|_{i,j+\frac{1}{2}} = \frac{\bar{T}_{i,j+1} - \bar{T}_{i,j}}{\Delta y} + O\left(\Delta y^2\right)$$

Now we're going

3.3 Flux Integrals

Equation 3.3 requires us to evaluate the integral of the normal flux around each control volume. That is, we need to compute $\oint_{\partial CV} \vec{F} \cdot \vec{n}\, dl$. For the control volume of Figure 3.1,

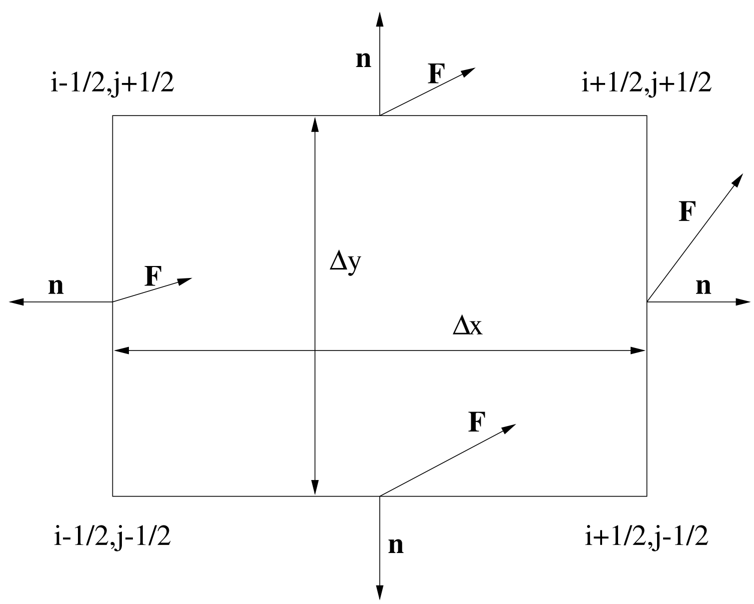

Figure 3.1: Flux integration around a finite volume.

we can write this as

$$
\begin{aligned}
\oint_{\partial CV} \vec{F}\cdot\vec{n}\,dl &= \vec{F}_{i+\frac{1}{2},j}\cdot\vec{n}_{i+\frac{1}{2},j}\Delta y+\vec{F}_{i,j+\frac{1}{2}}\cdot\vec{n}_{i,j+\frac{1}{2}}\Delta x \\
&\quad +\vec{F}_{i-\frac{1}{2},j}\cdot\vec{n}_{i-\frac{1}{2},j}\Delta y+\vec{F}_{i,j-\frac{1}{2}}\cdot\vec{n}_{i,j-\frac{1}{2}}\Delta x \\
&= \left(F_{x;i+\frac{1}{2},j}-F_{x;i-\frac{1}{2},j}\right)\Delta y+\left(F_{y;i,j+\frac{1}{2}}-F_{y;i,j-\frac{1}{2}}\right)\Delta x
\end{aligned}
$$

Returning once again to our Poisson example, we have to second-order accuracy

$$
\begin{aligned}
F_{x;i+\frac{1}{2},j} &= \frac{\bar{T}_{i+1,j}-\bar{T}_{i,j}}{\Delta x} \\
F_{x;i-\frac{1}{2},j} &= \frac{\bar{T}_{i,j}-\bar{T}_{i-1,j}}{\Delta x} \\
F_{x;i,j+\frac{1}{2}} &= \frac{\bar{T}_{i,j+1}-\bar{T}_{i,j}}{\Delta y} \\
F_{x;i,j-\frac{1}{2}} &= \frac{\bar{T}_{i,j}-\bar{T}_{i,j-1}}{\Delta y} \\
\oint_{\partial CV} \vec{F}\cdot\vec{n}\,dl &= \left(\bar{T}_{i+1,j}-2\bar{T}_{i,j}+\bar{T}_{i-1,j}\right)\frac{\Delta y}{\Delta x}+\left(\bar{T}_{i,j+1}-2\bar{T}_{i,j}+\bar{T}_{i,j-1}\right)\frac{\Delta x}{\Delta y}
\end{aligned}
$$

Substituting this into Equation 3.6 and dividing by $A=\Delta x\Delta y$, we get the canonical finite-volume discretization of Poisson's equation.

$$
\frac{\bar{T}_{i+1,j}-2\bar{T}_{i,j}+\bar{T}_{i-1,j}}{\Delta x^2}+\frac{\bar{T}_{i,j+1}-2\bar{T}_{i,j}+\bar{T}_{i,j-1}}{\Delta y^2}=\bar{S} \tag{3.11}
$$

It is easy to show by Taylor analysis that the left-hand side of Equation 3.11 is a second-order accurate approximation to the Laplacian of $\bar{T}$ at i,j. In this Taylor analysis, because we're looking to match $\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}$ evaluated at the center of control volume i,j, we would need to expand $T\,(x,y)$ in a two-dimensional Taylor series about that center.

3.4 Problems

1. Show that, for a smooth function, the difference between $T_i$and $\bar{T}_i$ is $O\left(\Delta x^2\right)$. (Hint: expand T in a Taylor series about $x=x_i$.

2. Show that

$$\overline{\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right)}_{i,j}=\frac{\bar{T}_{i+1,j}-2\bar{T}_{i,j}+\bar{T}_{i-1,j}}{\Delta x^2}+\frac{\bar{T}_{i,j+1}-2\bar{T}_{i,j}+\bar{T}_{i,j-1}}{\Delta y^2}+O\left(\Delta x^2,\Delta y^2\right)$$

3. **High-order accurate flux evaluation for Poisson's equation.** Suppose that we wanted a more accurate approximation for the flux for Poisson's equation than we got in Section 3.2. We could choose to use four control volume averages to compute the flux: $\overline{T}_{i+2}$, $\overline{T}_{i+1}$, $\overline{T}_i$, and $\overline{T}_{i-1}$. Find the most accurate possible approximation to the $\frac{\partial T}{\partial x}_{i+\frac{1}{2}}$ and determine the leading-order truncation error term. Combine this flux with its analog at $i-\frac{1}{2}$ to get a high-order approximation to the Laplacian in 1D, and find the truncation error for this Laplacian approximation.

4. Show that the flux for the control volume boundary at $i+\frac{1}{2}$ for the wave equation really is $T_{i+\frac{1}{2}}$.

5. **First-order upwind flux for the wave equation.** The flux $T_{i+\frac{1}{2}}$ can be approximated most simply by using data from the control volume upwind of the interface; for a positive wave speed, this is control volume i. Show that this approximation is only first-order accurate.

6. **Centered flux for the wave equation.** Suppose we were to use two control volume averages ($\bar{T}_i$ and $\bar{T}_{i+1}$) to evaluate the flux at $i+\frac{1}{2}$. Find an expression for the flux, determine the accuracy of the flux (including the leading-order term in the truncation error), and find the flux integral for the 1D case.

7. **Upwind extrapolated flux for the wave equation**. Suppose that we wanted a more accurate approximation for the flux for the wave equation while still using upwind data. We could choose to use two control volume averages to compute the flux at $i+\frac{1}{2}$: $\overline{T}_i$ and $\overline{T}_{i-1}$. Find the most accurate possible approximation to the flux and determine the leading-order truncation error term.

Chapter 8

The Incompressible Energy Equation

The incompressible energy equation is useful both in its own right for predicting energy transfer and to provide experience combining convective and diffusive terms in the same governing equation before moving on to the Navier-Stokes equations, which are mathematically similar in many ways but have the added complication of being a coupled system of equations.

Also, the same equation can be used to model other physical processes. For example, if T is interpreted as a chemical species concentration and the viscous dissipation term on the right-hand side of the energy equation (see below) is replaced by an appropriate source term, then the energy equation correctly models species concentration in chemically reacting flow.

The differential form of the incompressible energy equation can be written as:

$$\begin{aligned}\frac{\partial T}{\partial t}+\frac{\partial uT}{\partial x}+\frac{\partial vT}{\partial y} &= \frac{1}{\mathrm{Re}\cdot\mathrm{Pr}}\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right)\\ &\quad +\frac{\mathrm{Ec}}{\mathrm{Re}}\left(2\left(\frac{\partial u}{\partial x}\right)^2+2\left(\frac{\partial v}{\partial y}\right)^2+\left(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}\right)^2\right)\end{aligned}$$

Applying Gauss's Theorem over an arbitrary fixed control volume, we can arrive at the integral form of the energy equation:

$$\begin{aligned}\frac{\partial \bar{T}}{\partial t}A+\oint_{\partial CV}\vec{v}T\cdot\vec{n}\,ds &= \frac{1}{\mathrm{Re}\cdot\mathrm{Pr}}\oint_{\partial CV}\nabla T\cdot\vec{n}\,ds\\ &\quad +\frac{\mathrm{Ec}}{\mathrm{Re}}\int_{CV}\left(2\left(\frac{\partial u}{\partial x}\right)^2+2\left(\frac{\partial v}{\partial y}\right)^2+\left(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}\right)^2\right)dA\end{aligned}$$

For a finite volume in a 2D uniform mesh:

$$\begin{aligned}
\frac{d\bar{T}_{i,j}}{dt}\Delta x\Delta y & & \frac{1}{\mathrm{Re}\cdot\mathrm{Pr}}\left(\frac{\partial T}{\partial x}\Big|_{i-\frac{1}{2},j}^{i+\frac{1}{2},j}\Delta y+\frac{\partial T}{\partial y}\Big|_{i,j-\frac{1}{2}}^{i,j+\frac{1}{2}}\Delta x\right)\\
+(uT)_{i-\frac{1}{2},j}^{i+\frac{1}{2},j}\Delta y &=& +\frac{\mathrm{Ec}}{\mathrm{Re}}\left(2\left(\frac{u_{i+1,j}-u_{i-1,j}}{2\Delta x}\right)^2+2\left(\frac{v_{i,j+1}-v_{i,j-1}}{2\Delta y}\right)^2\right)\Delta x\Delta y\\
+(vT)_{i,j-\frac{1}{2}}^{i,j+\frac{1}{2}}\Delta x & & +\frac{\mathrm{Ec}}{\mathrm{Re}}\left(\frac{v_{i+1,j}-v_{i-1,j}}{2\Delta x}+\frac{u_{i,j+1}-u_{i,j-1}}{2\Delta y}\right)^2\Delta x\Delta y
\end{aligned}$$

Abbreviating the (constant) viscous dissipation terms as $S_{i,j}$ and combining the convective and diffusive fluxes, we arrive at last at a fairly compact form of the equation.

$$\frac{d\bar{T}_{i,j}}{dt}+\frac{1}{\Delta x}\left(uT-\frac{1}{\mathrm{Re}\cdot\mathrm{Pr}}\frac{\partial T}{\partial x}\right)_{i-\frac{1}{2},j}^{i+\frac{1}{2},j}+\frac{1}{\Delta y}\left(vT-\frac{1}{\mathrm{Re}\cdot\mathrm{Pr}}\frac{\partial T}{\partial y}\right)_{i,j-\frac{1}{2}}^{i,j+\frac{1}{2}}=S_{i,j} \tag{8.1}$$

8.1 Simple Discretization of the Incompressible Energy Equation

We can write a simple sum of the fluxes in the x-direction from Equation 8.1 by using centered approximations for both the convective and diffusive fluxes. Both of these approximations are second-order accurate. (See Sections 3.6 and 3.2 for more information.)

$$\begin{aligned}
\frac{1}{\Delta x}\left(uT-\frac{1}{\mathrm{Re}\cdot\mathrm{Pr}}\frac{\partial T}{\partial x}\right)_{i-\frac{1}{2},j}^{i+\frac{1}{2},j} &=& \frac{1}{\Delta x}\left(\frac{u_{i+1,j}\bar{T}_{i+1,j}-u_{i-1,j}\bar{T}_{i-1,j}}{2}\right.\\
&-& \left.\frac{1}{\mathrm{Re}\cdot\mathrm{Pr}}\left(\frac{\bar{T}_{i+1,j}-\bar{T}_{i,j}}{\Delta x}-\frac{\bar{T}_{i,j}-\bar{T}_{i-1,j}}{\Delta x}\right)\right)\\
&=& \frac{1}{\Delta x}\left(\frac{u_{i+1,j}\bar{T}_{i+1,j}-u_{i-1,j}\bar{T}_{i-1,j}}{2}\right.\\
&-& \left.\frac{1}{\mathrm{Re}\cdot\mathrm{Pr}}\left(\frac{\bar{T}_{i+1,j}-2\bar{T}_{i,j}+\bar{T}_{i-1,j}}{\Delta x}\right)\right)
\end{aligned}$$

where the integral limit-like notation on the LHS indicates that this is the net flux across those two faces. Combining this flux summation with the analogous sum in the y-direction, we arrive at the following semi-discrete form of the energy equation.

$$
\begin{aligned}
\frac{d\bar{T}_{i,j}}{dt} \quad = \quad & -\frac{1}{\Delta x}\left(\frac{u_{i+1,j}\bar{T}_{i+1,j}-u_{i-1,j}\bar{T}_{i-1,j}}{2}\right. \\
& \left. -\frac{1}{\text{Re}\cdot\text{Pr}}\left(\frac{\bar{T}_{i+1,j}-2\bar{T}_{i,j}+\bar{T}_{i-1,j}}{\Delta x}\right)\right) \\
& -\frac{1}{\Delta y}\left(\frac{v_{i,j+1}\bar{T}_{i,j+1}-v_{i,j-1}\bar{T}_{i,j-1}}{2}\right. \\
& \left. -\frac{1}{\text{Re}\cdot\text{Pr}}\left(\frac{\bar{T}_{i,j+1}-2\bar{T}_{i,j}+\bar{T}_{i,j-1}}{\Delta y}\right)\right) \\
& +S_{i,j}
\end{aligned}
$$

This scheme is second-order accurate in space. Now let's examine the eigenvalues for this problem, reduced to one dimension:

$$
\begin{aligned}
\frac{d\bar{T}_{i}}{dt} \quad = \quad & -\frac{1}{\Delta x}\left(\frac{u_{i+1}\bar{T}_{i+1}-u_{i-1}\bar{T}_{i-1}}{2}\right. \\
& \left. -\frac{1}{\text{Re}\cdot\text{Pr}}\left(\frac{\bar{T}_{i+1}-2\bar{T}_{i}+\bar{T}_{i-1}}{\Delta x}\right)\right) \\
& +S_{i}
\end{aligned}
$$

For a periodic domain, the discretization of this problem is

$$
\frac{d\bar{T}_i}{dt} = B_p\left(\frac{u_{i-1}}{2\Delta x}+\frac{1}{\text{Re}\cdot\text{Pr}\cdot\Delta x^2}, -\frac{2}{\text{Re}\cdot\text{Pr}\cdot\Delta x^2}, -\frac{u_{i+1}}{2\Delta x}+\frac{1}{\text{Re}\cdot\text{Pr}\cdot\Delta x^2}\right)\bar{T}_i
$$

So we can use our usual procedure for finding the eigenvalues, which gives us, for constant velocity u,

$$
\lambda = \frac{-u}{\Delta x} I \sin\phi - \frac{2}{\text{Re}\cdot\text{Pr}\cdot\Delta x^2}\left(1-\cos\phi\right)
$$

8.2 Time Discretization of the Energy Equation

8.2.1 Implicit Euler time advance applied to the energy equation

If we write the energy equation in fully-discrete form using the implicit Euler time advance scheme, we arrive at the following equation:

$$
\begin{aligned}
\frac{\bar{T}^{n+1}_{i,j}-\bar{T}^{n}_{i,j}}{\Delta t} \quad = \quad & -\frac{1}{\Delta x}\left(\frac{u_{i+1,j}\bar{T}^{n+1}_{i+1,j}-u_{i-1,j}\bar{T}^{n+1}_{i-1,j}}{2}\right. \\
& \left.-\frac{1}{\mathrm{Re}\cdot\mathrm{Pr}}\left(\frac{\bar{T}^{n+1}_{i+1,j}-2\bar{T}^{n+1}_{i,j}+\bar{T}^{n+1}_{i-1,j}}{\Delta x}\right)\right) \\
& -\frac{1}{\Delta y}\left(\frac{v_{i,j+1}\bar{T}^{n+1}_{i,j+1}-v_{i,j-1}\bar{T}^{n+1}_{i,j-1}}{2}\right. \\
& \left.-\frac{1}{\mathrm{Re}\cdot\mathrm{Pr}}\left(\frac{\bar{T}^{n+1}_{i,j+1}-2\bar{T}^{n+1}_{i,j}+\bar{T}^{n+1}_{i,j-1}}{\Delta y}\right)\right) \\
& +S_{i,j}
\end{aligned}
$$

In practice, we will typically want to write this in what is called δ-form by replacing $T^{n+1}_{i,j} \equiv T^{n}_{i,j}+\delta T^{n+1}_{i,j}$ and simplifying. δ-form is much more convenient near steady state, where round off errors in the calculation of T can easily exceed δT, the change in T from one time level to the next. Also, as we'll see later in the course, δ-form is more convenient for non-linear problems.

$$
\begin{aligned}
\frac{\overline{\delta T}_{i,j}}{\Delta t} \quad &+ \quad \frac{1}{\Delta x}\left(\frac{u_{i+1,j}\overline{\delta T}_{i+1,j} - u_{i-1,j}\overline{\delta T}_{i-1,j}}{2}\right. \\
&\qquad \left. - \frac{1}{\text{Re}\cdot\text{Pr}}\left(\frac{\overline{\delta T}_{i+1,j} - 2\overline{\delta T}_{i,j} + \overline{\delta T}_{i-1,j}}{\Delta x}\right)\right) \\
&+ \quad \frac{1}{\Delta y}\left(\frac{v_{i,j+1}\overline{\delta T}_{i,j+1} - v_{i,j-1}\overline{\delta T}_{i,j-1}}{2}\right. \\
&\qquad \left. - \frac{1}{\text{Re}\cdot\text{Pr}}\left(\frac{\overline{\delta T}_{i,j+1} - 2\overline{\delta T}_{i,j} + \overline{\delta T}_{i,j-1}}{\Delta y}\right)\right) \\
&= \quad -\frac{1}{\Delta x}\left(\frac{u_{i+1,j}\bar{T}^n_{i+1,j} - u_{i-1,j}\bar{T}^n_{i-1,j}}{2}\right. \\
&\qquad \left. - \frac{1}{\text{Re}\cdot\text{Pr}}\left(\frac{\bar{T}^n_{i+1,j} - 2\bar{T}^n_{i,j} + \bar{T}^n_{i-1,j}}{\Delta x}\right)\right) \\
&- \quad \frac{1}{\Delta y}\left(\frac{v_{i,j+1}\bar{T}^n_{i,j+1} - v_{i,j-1}\bar{T}^n_{i,j-1}}{2}\right. \\
&\qquad \left. - \frac{1}{\text{Re}\cdot\text{Pr}}\left(\frac{\bar{T}^n_{i,j+1} - 2\bar{T}^n_{i,j} + \bar{T}^n_{i,j-1}}{\Delta y}\right)\right) \\
&+ \quad S_{i,j}
\end{aligned}
\tag{8.2}
$$

The right-hand side is the flux integral evaluated at time level n.

8.2.2 Trapezoidal time advance applied to the energy equation

If we write the energy equation in fully-discrete δ-form using the trapezoidal time advance scheme (see Problem 6.4), we arrive at the following equation:

$$\begin{aligned}
\frac{\overline{\delta T}_{i,j}}{\Delta t} &+ \frac{1}{2\Delta x}\left(\frac{u_{i+1,j}\overline{\delta T}_{i+1,j} - u_{i-1,j}\overline{\delta T}_{i-1,j}}{2}\right. \\
&\qquad \left. -\frac{1}{\mathrm{Re{\cdot}Pr}}\left(\frac{\overline{\delta T}_{i+1,j} - 2\overline{\delta T}_{i,j} + \overline{\delta T}_{i-1,j}}{\Delta x}\right)\right) \\
&+ \frac{1}{2\Delta y}\left(\frac{v_{i,j+1}\overline{\delta T}_{i,j+1} - v_{i,j-1}\overline{\delta T}_{i,j-1}}{2}\right. \\
&\qquad \left. -\frac{1}{\mathrm{Re{\cdot}Pr}}\left(\frac{\overline{\delta T}_{i,j+1} - 2\overline{\delta T}_{i,j} + \overline{\delta T}_{i,j-1}}{\Delta y}\right)\right) \\
&= -\frac{1}{\Delta x}\left(\frac{u_{i+1,j}\bar{T}^n_{i+1,j} - u_{i-1,j}\bar{T}^n_{i-1,j}}{2}\right. \\
&\qquad \left. -\frac{1}{\mathrm{Re{\cdot}Pr}}\left(\frac{\bar{T}^n_{i+1,j} - 2\bar{T}^n_{i,j} + \bar{T}^n_{i-1,j}}{\Delta x}\right)\right) \\
&- \frac{1}{\Delta y}\left(\frac{v_{i,j+1}\bar{T}^n_{i,j+1} - v_{i,j-1}\bar{T}^n_{i,j-1}}{2}\right. \\
&\qquad \left. -\frac{1}{\mathrm{Re{\cdot}Pr}}\left(\frac{\bar{T}^n_{i,j+1} - 2\bar{T}^n_{i,j} + \bar{T}^n_{i,j-1}}{\Delta y}\right)\right) \\
&+ S_{i,j}
\end{aligned} \tag{8.3}$$

The difference between this equation and the fully-implicit version is a factor of two on the left-hand side. This small difference in the equation makes the big difference between first- and second-order accuracy in time. This is because this scheme blends explicit Euler and implicit Euler time advance together in precisely the proper proportions to cancel their first-order errors.

8.3 Boundary Conditions

Boundary conditions for the energy equation fall into two categories: those that are analogous to Poisson equation boundary conditions and those that aren't. Generally speaking, we can use the same approach for temperature boundary conditions at walls as for the Poisson equation (see Section 4.2). For inflow and outflow boundaries, there are differences.

8.3.1 Inflow boundaries

At inflow boundaries, the temperature is usually specified in terms of known upstream values. Because the temperature at the boundary is known, the flux across the boundary can easily be calculated. Generally this is most easily done by setting a ghost cell value in the same way as for Dirichlet boundary conditions for the Poisson equation(see Section 4.2.2).

8.3.2 Outflow boundaries

At outflow boundaries, there are two fairly common choices for boundary conditions. First, the temperature at the outflow may be determined strictly by the upstream temperature in the computational domain as fluid convects out; in this case, the temperature for the ghost cell would typically be extrapolated from interior data:

$$T_{i_{\max}+1,j} = 2T_{i_{\max},j} - T_{i_{\max}-1,j}$$

The other common choice is to assume that the temperature gradient is zero normal to the boundary; this is completely equivalent to a Neumann boundary condition applied to the Poisson equation (see Section 4.2.1).

8.4 Approximate Factorization

Both implicit discretizations for the energy equation require the solution of a matrix that does not have a simple, tightly-banded structure. However, it is possible to factor this matrix approximately into two scalar tri-diagonal matrices using a technique called *approximate factorization.*

Learning Objectives. Students will be able to:

- Describe the approximate factorization scheme as applied to the implicit Euler and trapezoidal time advance schemes. Prove that approximate factorization does not affect the order of time accuracy.
- Outline how to advance the energy equation in time using an implicit time advance scheme and approximate factorization.

Regardless of how we choose to do the space discretization for the two-dimensional energy equation, we will end up with a semi-discrete equation of the form:

$$\frac{d}{dt}\begin{pmatrix} \bar{T}_{1,1} \\ \bar{T}_{2,1} \\ \bar{T}_{3,1} \\ \vdots \\ \bar{T}_{i-1,j} \\ \bar{T}_{i,j} \\ \bar{T}_{i+1,j} \\ \vdots \\ \bar{T}_{i_{\max},j_{\max}} \end{pmatrix} + [D_x]\begin{pmatrix} \bar{T}_{1,1} \\ \bar{T}_{2,1} \\ \bar{T}_{3,1} \\ \vdots \\ \bar{T}_{i-1,j} \\ \bar{T}_{i,j} \\ \bar{T}_{i+1,j} \\ \vdots \\ \bar{T}_{i_{\max},j_{\max}} \end{pmatrix} + [D_y]\begin{pmatrix} \bar{T}_{1,1} \\ \bar{T}_{2,1} \\ \bar{T}_{3,1} \\ \vdots \\ \bar{T}_{i-1,j} \\ \bar{T}_{i,j} \\ \bar{T}_{i+1,j} \\ \vdots \\ \bar{T}_{i_{\max},j_{\max}} \end{pmatrix} = \begin{pmatrix} \bar{S}_{1,1} \\ \bar{S}_{2,1} \\ \bar{S}_{3,1} \\ \vdots \\ \bar{S}_{i-1,j} \\ \bar{S}_{i,j} \\ \bar{S}_{i+1,j} \\ \vdots \\ \bar{S}_{i_{\max},j_{\max}} \end{pmatrix}$$

or, more compactly,

$$\frac{d\vec{T}}{dt} + [D_x]\,\vec{T} + [D_y]\,\vec{T} = \vec{S}$$

where $[D_x]$ and $[D_y]$ are matrix representation of the space discretization in the x- and y-directions, respectively.

8.4.0.1 Implicit Euler Time Advance

If we use the implicit Euler time advance scheme, we get the following fully-discrete form for the problem:

$$\begin{aligned} \frac{\vec{T}^{n+1} - \vec{T}^{n}}{\Delta t} + [D_x]\,\vec{T}^{n+1} + [D_y]\,\vec{T}^{n+1} &= \vec{S} \\ \left([I] + \Delta t\,[D_x] + \Delta t\,[D_y]\right)\overrightarrow{\delta T} &= -\Delta t\left([D_x]\,\vec{T}^{n} + [D_y]\,\vec{T}^{n}\right) + \Delta t\,\vec{S} \end{aligned} \tag{8.4}$$

The right-hand side of Equation 8.4 is the flux integral at time level n. The left-hand side is a matrix with structure similar or identical to the system of equations we would have had to solve for the Laplace equation. That is, the matrix looks roughly like this for a 4-by-4 mesh:

$$\left[\begin{array}{cccccccccccccccc}
D & x & & & y & & & & & & & & & & & \\
X & D & x & & & y & & & & & & & & & & \\
& X & D & x & & & y & & & & & & & & & \\
& & X & D & & & & y & & & & & & & & \\
Y & & & & D & x & & & y & & & & & & & \\
& Y & & & X & D & x & & & y & & & & & & \\
& & Y & & & X & D & x & & & y & & & & & \\
& & & Y & & & X & D & & & & y & & & & \\
& & & & Y & & & & D & x & & & y & & & \\
& & & & & Y & & & X & D & x & & & y & & \\
& & & & & & Y & & & X & D & x & & & y & \\
& & & & & & & Y & & & X & D & & & & y \\
& & & & & & & & Y & & & & D & x & & \\
& & & & & & & & & Y & & & X & D & x & \\
& & & & & & & & & & Y & & & X & D & x \\
& & & & & & & & & & & Y & & & X & D
\end{array}\right] \tag{8.5}$$

This system of equations is impractical to solve directly for the same reasons that we discussed for the Laplace equation. In this case, however, we have an option that was not available to us in that case: approximate factorization. We can re-write the left-hand side of Equation 8.4 as

$$\left([I]+\Delta t\,[D_x]+\Delta t\,[D_y]\right)\overrightarrow{\delta T} \quad\approx\quad \left([I]+\Delta t\,[D_x]\right)\left([I]+\Delta t\,[D_y]\right)\overrightarrow{\delta T} \tag{8.6}$$

This is a win, because each of $[D_x]$ and $[D_y]$ are tri-diagonal.[1] The question is, does this factorization produce an unacceptable error? To find out, expand the approximately factored form:

$$\left([I]+\Delta t\,[D_x]\right)\left([I]+\Delta t\,[D_y]\right)\overrightarrow{\delta T} = \left([I]+\Delta t\,[D_x]+\Delta t\,[D_y]+\Delta t^2\,[D_x]\,[D_y]\right)\overrightarrow{\delta T} \tag{8.7}$$

Comparing Equations 8.6 and 8.7, we see that the approximate factorization introduces an error of $O\left(\Delta t^2\overrightarrow{\delta T}\right) = O\left(\Delta t^3\right)$ (where the equality reflects the fact that $\overrightarrow{\delta T} \sim \Delta t$). But we know that the implicit Euler scheme is only first-order accurate in time, so there is *already* an error of $O\left(\Delta t^2\right)$ *before* we do the approximate factorization. Therefore, the factorization itself does not hurt time accuracy.

[1] $[D_y]$ is only tri-diagonal in the sense of having two diagonals adjacent to the main diagonal if we reorder the unknowns in $\vec{T}$ so that the j index varies more rapidly than the i index.

8.4.0.2 Trapezoidal Time Advance

If instead we use the trapezoidal (centered implicit) time advance scheme, we get the following fully-discrete form for the problem:

$$\begin{aligned}
\frac{\vec{T}^{n+1}-\vec{T}^{n}}{\Delta t}+[D_x]\frac{\vec{T}^{n+1}+\vec{T}^{n}}{2}+[D_y]\frac{\vec{T}^{n+1}+\vec{T}^{n}}{2} &= \vec{S} \\
\left([I]+\frac{\Delta t}{2}[D_x]+\frac{\Delta t}{2}[D_y]\right)\overrightarrow{\delta T} &= -\Delta t\left([D_x]\vec{T}^n+[D_y]\vec{T}^n\right)+\Delta t\,\vec{S} \qquad (8.8)
\end{aligned}$$

The right-hand side of Equation 8.8 is again the flux integral at time level n. The left-hand side is nearly identical to the matrix in Equation 8.4, except for the factors of 2. If we apply approximate factorization, we can re-write the left-hand side of Equation 8.8 as

$$\left([I]+\frac{\Delta t}{2}[D_x]+\frac{\Delta t}{2}[D_y]\right)\overrightarrow{\delta T}\approx\left([I]+\frac{\Delta t}{2}[D_x]\right)\left([I]+\frac{\Delta t}{2}[D_y]\right)\overrightarrow{\delta T}$$

When we re-expand the approximately factored form, we get:

$$\left([I]+\frac{\Delta t}{2}[D_x]\right)\left([I]+\frac{\Delta t}{2}[D_y]\right)\overrightarrow{\delta T}=\left([I]+\frac{\Delta t}{2}[D_x]+\frac{\Delta t}{2}[D_y]+\frac{\Delta t^2}{4}[D_x][D_y]\right)\overrightarrow{\delta T}$$

As for the implicit Euler scheme, approximate factorization introduces an error of $O\left(\Delta t^3\right)$. The trapezoidal time advance scheme is second-order accurate in time, so there is *already* an error of $O\left(\Delta t^3\right)$ *before* we do the approximate factorization. Therefore, the factorization itself does not hurt the order of accuracy. Approximately factor the LHS of this equation and show that second-order accuracy is still achieved.

8.4.1 Application of Approximate Factorization

To apply approximate factorization in practice, we combine (for example) Equations 8.4 and 8.6:

$$([I]+\Delta t\,[D_x])([I]+\Delta t\,[D_y])\overrightarrow{\delta T}=-\Delta t\left([D_x]\vec{T}^n+[D_y]\vec{T}^n\right)+\Delta t\,\vec{S}$$

We can solve this system of equations in two steps:

$$\begin{aligned}
([I]+\Delta t\,[D_x])\overrightarrow{\delta \tilde{T}} &= -\Delta t\left([D_x]\vec{T}^n+[D_y]\vec{T}^n\right)+\Delta t\,\vec{S} \\
([I]+\Delta t\,[D_y])\overrightarrow{\delta T} &= \overrightarrow{\delta \tilde{T}}
\end{aligned}$$

That is, instead of solving one large matrix problem, we can now solve a series of small matrix problems along lines in the mesh. First, for every line of constant j (lines parallel to the x-axis) we solve for an intermediate variable along that line $\overrightarrow{\delta\tilde{T}}_j$:

$$([I] + \Delta t\,[D_x])_j\,\overrightarrow{\delta\tilde{T}_j} = -\Delta t\left([D_x]\,\vec{T}^n + [D_y]\,\vec{T}^n\right)_j + \Delta t\,\vec{S} \tag{8.9}$$

Then, for every line of constant i (lines parallel to the y-axis) we solve for the update to the solution along that line $\overrightarrow{\delta T}_i$:

$$([I] + \Delta t\,[D_y])_i\,\overrightarrow{\delta T_i} = \overrightarrow{\delta\tilde{T}_i} \tag{8.10}$$

That all sounds very nice, but it *is* a little abstract. To make it more concrete, consider the case of the two-dimensional heat equation. For this case, we can write Equation 8.4 for the interior control volume $(4,2)$ as:

$$\begin{aligned}
\left(1+\frac{2\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta x^2}+\frac{2\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta y^2}\right)\delta T_{4,2} &\qquad -\left(\frac{2\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta x^2}+\frac{2\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta y^2}\right)T^n_{4,2}\\
+\left(\frac{u\Delta t}{2\Delta x}-\frac{\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta x^2}\right)\delta T_{5,2} &\qquad -\left(\frac{u\Delta t}{2\Delta x}-\frac{\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta x^2}\right)T^n_{5,2}\\
+\left(-\frac{u\Delta t}{2\Delta x}-\frac{\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta x^2}\right)\delta T_{3,2} &= -\left(-\frac{u\Delta t}{2\Delta x}-\frac{\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta x^2}\right)T^n_{3,2}\\
+\left(\frac{v\Delta t}{2\Delta y}-\frac{\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta y^2}\right)\delta T_{4,3} &\qquad -\left(\frac{v\Delta t}{2\Delta y}-\frac{\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta y^2}\right)T^n_{4,3}\\
+\left(-\frac{v\Delta t}{2\Delta y}-\frac{\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta y^2}\right)\delta T_{4,1} &\qquad -\left(-\frac{v\Delta t}{2\Delta y}-\frac{\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta y^2}\right)T^n_{4,1}
\end{aligned}$$

Applying approximate factorization, we have two equations, one for $\delta\tilde{T}_{4,2}$ (solved for simultaneously with $\delta\tilde{T}_{5,2}$ and $\delta\tilde{T}_{3,2}$, etc.) and the other for $\delta T_{4,2}$ (solved for simultaneously with $\delta T_{4,3}$ and $\delta T_{4,1}$, etc).

$$\begin{aligned}
&\qquad -\left(\frac{2\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta x^2}+\frac{2\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta y^2}\right)T^n_{4,2}\\
+\left(\frac{u\Delta t}{2\Delta x}-\frac{\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta x^2}\right)\delta\tilde{T}_{5,2} &\qquad -\left(\frac{u\Delta t}{2\Delta x}-\frac{\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta x^2}\right)T^n_{5,2}\\
\left(1+\frac{2\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta x^2}\right)\delta\tilde{T}_{4,2} &= -\left(-\frac{u\Delta t}{2\Delta x}-\frac{\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta x^2}\right)T^n_{3,2}\\
+\left(-\frac{u\Delta t}{2\Delta x}-\frac{\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta x^2}\right)\delta\tilde{T}_{3,2} &\qquad -\left(\frac{v\Delta t}{2\Delta y}-\frac{\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta y^2}\right)T^n_{4,3}\\
&\qquad -\left(-\frac{v\Delta t}{2\Delta y}-\frac{\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta y^2}\right)T^n_{4,1}
\end{aligned}$$

$$
\begin{aligned}
&+\left(\frac{v\Delta t}{2\Delta y}-\frac{\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta y^2}\right)\delta T_{4,3}\\
&\left(1+\frac{2\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta y^2}\right)\delta T_{4,2} \quad = \quad \delta\tilde{T}_{4,2}\\
&+\left(-\frac{v\Delta t}{2\Delta y}-\frac{\Delta t}{\mathrm{Re}\cdot\mathrm{Pr}\cdot\Delta y^2}\right)\delta T_{4,1}
\end{aligned}
$$

These last two equations are specific instances of Equations 8.9 and 8.10.

Let us return now to the full form of these equations. If we completely ignore boundary conditions, then the compact matrix forms of the difference operators are given by:

$$
[D_x]=\frac{1}{Re\cdot Pr\cdot\Delta x^2}\begin{bmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & -1 & 2 & -1 & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 2 \end{bmatrix}+\frac{u}{2\Delta x}\begin{bmatrix} 0 & 1 & & & & \\ -1 & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & -1 & 0 & 1 & \\ & & & -1 & 0 & 1 \\ & & & & -1 & 0 \end{bmatrix}
$$

and

$$
[D_y]=\frac{1}{Re\cdot Pr\cdot\Delta y^2}\begin{bmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & -1 & 2 & -1 & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 2 \end{bmatrix}+\frac{v}{2\Delta y}\begin{bmatrix} 0 & 1 & & & & \\ -1 & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & -1 & 0 & 1 & \\ & & & -1 & 0 & 1 \\ & & & & -1 & 0 \end{bmatrix}
$$

So if we define $\alpha\equiv\frac{1}{Re\cdot Pr}$, Equation 8.9 becomes

$$
\begin{bmatrix}
1+\frac{2\alpha\Delta t}{\Delta x^2} & -\frac{\alpha\Delta t}{\Delta x^2}+\frac{u}{2\Delta x} & & & & \\
-\frac{\alpha\Delta t}{\Delta x^2}-\frac{u}{2\Delta x} & 1+\frac{2\alpha\Delta t}{\Delta x^2} & -\frac{\alpha\Delta t}{\Delta x^2}+\frac{u}{2\Delta x} & & & \\
& -\frac{\alpha\Delta t}{\Delta x^2}-\frac{u}{2\Delta x} & 1+\frac{2\alpha\Delta t}{\Delta x^2} & -\frac{\alpha\Delta t}{\Delta x^2}+\frac{u}{2\Delta x} & & \\
& & -\frac{\alpha\Delta t}{\Delta x^2}-\frac{u}{2\Delta x} & 1+\frac{2\alpha\Delta t}{\Delta x^2} & -\frac{\alpha\Delta t}{\Delta x^2}+\frac{u}{2\Delta x} & \\
& & & -\frac{\alpha\Delta t}{\Delta x^2}-\frac{u}{2\Delta x} & 1+\frac{2\alpha\Delta t}{\Delta x^2} & -\frac{\alpha\Delta t}{\Delta x^2}+\frac{u}{2\Delta x} \\
& & & & -\frac{\alpha\Delta t}{\Delta x^2}-\frac{u}{2\Delta x} & 1+\frac{2\alpha\Delta t}{\Delta x^2}
\end{bmatrix}
\begin{pmatrix} \delta\tilde{T}_{1,j} \\ \delta\tilde{T}_{2,j} \\ \delta\tilde{T}_{3,j} \\ \delta\tilde{T}_{4,j} \\ \delta\tilde{T}_{5,j} \\ \delta\tilde{T}_{6,j} \end{pmatrix} = \mathrm{RHS} \tag{8.11}
$$

We would solve 6 of these equations (using the Thomas algorithm, described in Appendix C), one for each value of j. Next we apply Equation 8.10, which for this case becomes

$$
\begin{bmatrix}
1+\frac{2\alpha\Delta t}{\Delta y^2} & -\frac{\alpha\Delta t}{\Delta y^2}+\frac{v}{2\Delta y} & & & & \\
-\frac{\alpha\Delta t}{\Delta y^2}-\frac{v}{2\Delta y} & 1+\frac{2\alpha\Delta t}{\Delta y^2} & -\frac{\alpha\Delta t}{\Delta y^2}+\frac{v}{2\Delta y} & & & \\
& -\frac{\alpha\Delta t}{\Delta y^2}-\frac{v}{2\Delta y} & 1+\frac{2\alpha\Delta t}{\Delta y^2} & -\frac{\alpha\Delta t}{\Delta y^2}+\frac{v}{2\Delta y} & & \\
& & -\frac{\alpha\Delta t}{\Delta y^2}-\frac{v}{2\Delta y} & 1+\frac{2\alpha\Delta t}{\Delta y^2} & -\frac{\alpha\Delta t}{\Delta y^2}+\frac{v}{2\Delta y} & \\
& & & -\frac{\alpha\Delta t}{\Delta y^2}-\frac{v}{2\Delta y} & 1+\frac{2\alpha\Delta t}{\Delta y^2} & -\frac{\alpha\Delta t}{\Delta y^2}+\frac{v}{2\Delta y} \\
& & & & -\frac{\alpha\Delta t}{\Delta y^2}-\frac{v}{2\Delta y} & 1+\frac{2\alpha\Delta t}{\Delta y^2}
\end{bmatrix}
\begin{pmatrix} \delta T_{i,1} \\ \delta T_{i,2} \\ \delta T_{i,3} \\ \delta T_{i,4} \\ \delta T_{i,5} \\ \delta T_{i,6} \end{pmatrix} = \begin{pmatrix} \delta\tilde{T}_{i,1} \\ \delta\tilde{T}_{i,2} \\ \delta\tilde{T}_{i,3} \\ \delta\tilde{T}_{i,4} \\ \delta\tilde{T}_{i,5} \\ \delta\tilde{T}_{i,6} \end{pmatrix}
$$

We solve this equation 6 times as well, once for each i. This gives us $\delta T_{i,j}$ for all i and j in the mesh. We can update the solution (including possible ghost cells) and continue to the next time step.

8.4.2 Implicit Implementation of Boundary Conditions

With implicit time advance, we need to be able to apply boundary conditions implicitly as well. That is, the changes in solution must be computed so that the boundary conditions are still satisfied at the new time level $n+1$. We will examine both Dirichlet and Neumann boundary conditions in this context. In both cases, we will assume that the boundary condition is satisfied at time level n.

8.4.2.1 Implicit Dirichlet boundary conditions

Dirichlet boundary conditions are typically enforced using a ghost cell, with the requirement that

$$\frac{\overline{T}_{i,1} + \overline{T}_{i,0}}{2} = T_w$$

We know that this is true at time level n and wish to update the solution so that it will also be true at time level $n+1$. That is,

$$\begin{aligned} \frac{\overline{T}^n_{i,1} + \overline{T}^n_{i,0}}{2} &= T_w \\ \frac{\overline{T}^{n+1}_{i,1} + \overline{T}^{n+1}_{i,0}}{2} &= T_w \end{aligned}$$

If we subtract these two equations, we get

$$\begin{aligned} \frac{\delta\overline{T}_{i,1} + \delta\overline{T}_{i,0}}{2} &= 0 \\ \delta\overline{T}_{i,0} &= -\delta\overline{T}_{i,1} \end{aligned}$$

8.4.2.2 Implicit Neumann boundary conditions

Neumann boundary conditions are also typically enforced using a ghost cell, with the requirement that

$$\frac{\overline{T}_{i,1} - \overline{T}_{i,0}}{\Delta y} = \left.\frac{\partial T}{\partial y}\right._w$$

We know that this is true at time level n and wish to update the solution so that it will also be true at time level $n+1$. That is,

$$\begin{aligned}
\frac{\overline{T}_{i,1}^{n+1} - \overline{T}_{i,0}^{n+1}}{\Delta y} &= \frac{\partial T}{\partial y}_w \\
\frac{\overline{T}_{i,1}^{n} - \overline{T}_{i,0}^{n}}{\Delta y} &= \frac{\partial T}{\partial y}_w
\end{aligned}$$

If we subtract these two equations, we get

$$\begin{aligned}
\frac{\delta\overline{T}_{i,1} - \delta\overline{T}_{i,0}}{\Delta y} &= 0 \\
\delta\overline{T}_{i,0} &= \delta\overline{T}_{i,1}
\end{aligned}$$

8.4.2.3 Enforcement in conjunction with tri-diagonal solution

These boundary conditions are added to the tri-diagonal system. In fact, boundary conditions of some sort are required to close these systems, which require the ghost cell control volumes for flux computation but may not yet contain boundary conditions (as written in Equation 8.11, for example). The full and correct version of that equation, with a Dirichlet condition at $i = \frac{1}{2}$ and Neumann at $i = 6\frac{1}{2}$ is in fact:

$$\begin{bmatrix}
1 & 1 & & & & & & \\
-\frac{\alpha\Delta t}{\Delta x^2} - \frac{u}{2\Delta x} & 1 + \frac{2\alpha\Delta t}{\Delta x^2} & -\frac{\alpha\Delta t}{\Delta x^2} + \frac{u}{2\Delta x} & & & & & \\
 & -\frac{\alpha\Delta t}{\Delta x^2} - \frac{u}{2\Delta x} & 1 + \frac{2\alpha\Delta t}{\Delta x^2} & \ddots & & & & \\
 & & \ddots & \ddots & \ddots & & & \\
 & & & \ddots & \ddots & \ddots & & \\
 & & & & \ddots & 1 + \frac{2\alpha\Delta t}{\Delta x^2} & -\frac{\alpha\Delta t}{\Delta x^2} + \frac{u}{2\Delta x} & \\
 & & & & & -\frac{\alpha\Delta t}{\Delta x^2} - \frac{u}{2\Delta x} & 1 + \frac{2\alpha\Delta t}{\Delta x^2} & -\frac{\alpha\Delta t}{\Delta x^2} + \frac{u}{2\Delta x} \\
 & & & & & & 1 & -1
\end{bmatrix}
\begin{pmatrix}
\delta\tilde{T}_{0,j} \\ \delta\tilde{T}_{1,j} \\ \delta\tilde{T}_{2,j} \\ \delta\tilde{T}_{3,j} \\ \delta\tilde{T}_{4,j} \\ \delta\tilde{T}_{5,j} \\ \delta\tilde{T}_{6,j} \\ \delta\tilde{T}_{7,j}
\end{pmatrix}
=
\begin{pmatrix}
0 \\ \mathrm{RHS}_1 \\ \mathrm{RHS}_2 \\ \mathrm{RHS}_3 \\ \mathrm{RHS}_4 \\ \mathrm{RHS}_5 \\ \mathrm{RHS}_6 \\ 0
\end{pmatrix} \tag{8.12}$$

This enlarged system is solved in the usual way.