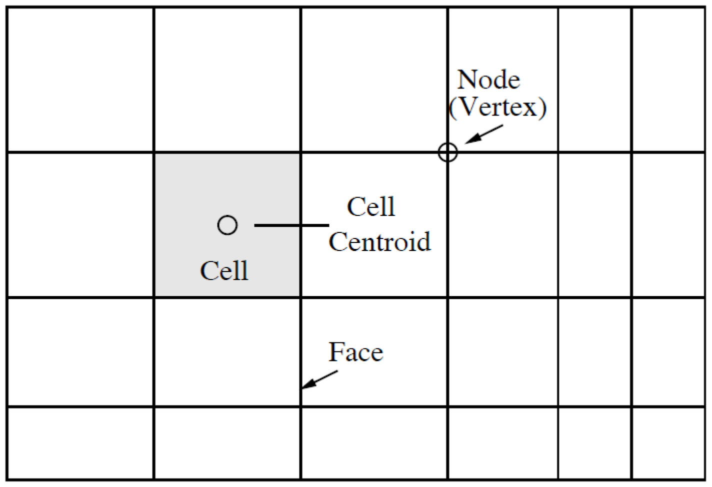
Introduction to Computational Fluid Dynamics

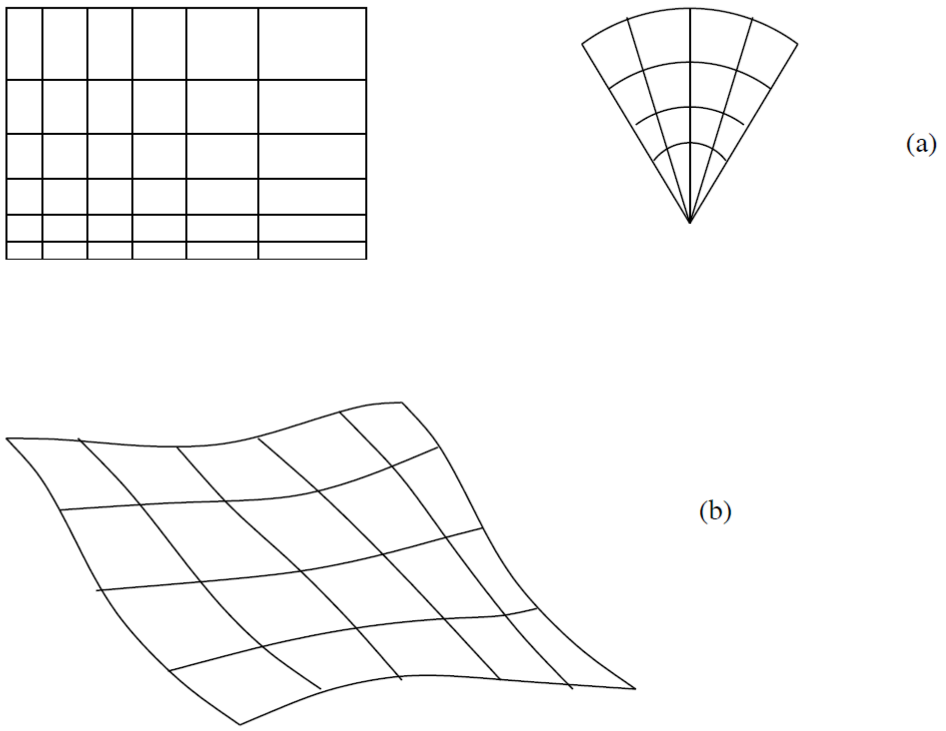
FINITE VOLUME METHOD

(Jayathi Y. Murthy, Numerical Methods in Heat, Mass, and Momentum Transfer, Purdue University, Spring 2002)

Mesh terminology and types

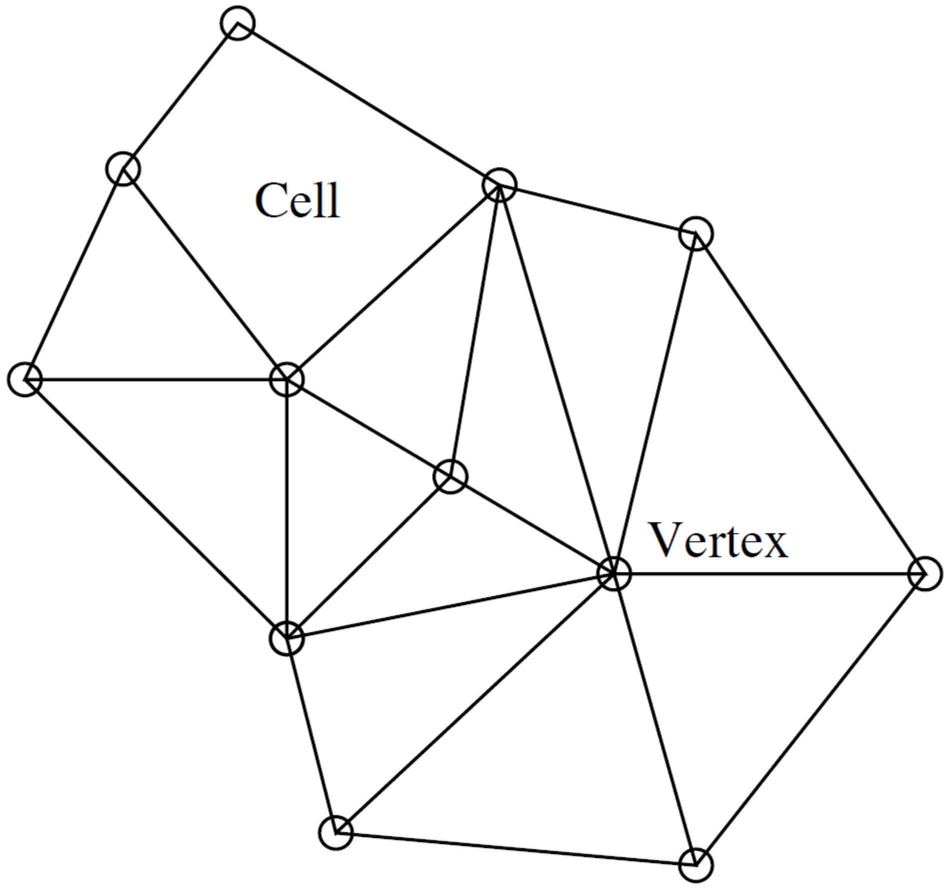


Mesh Terminology

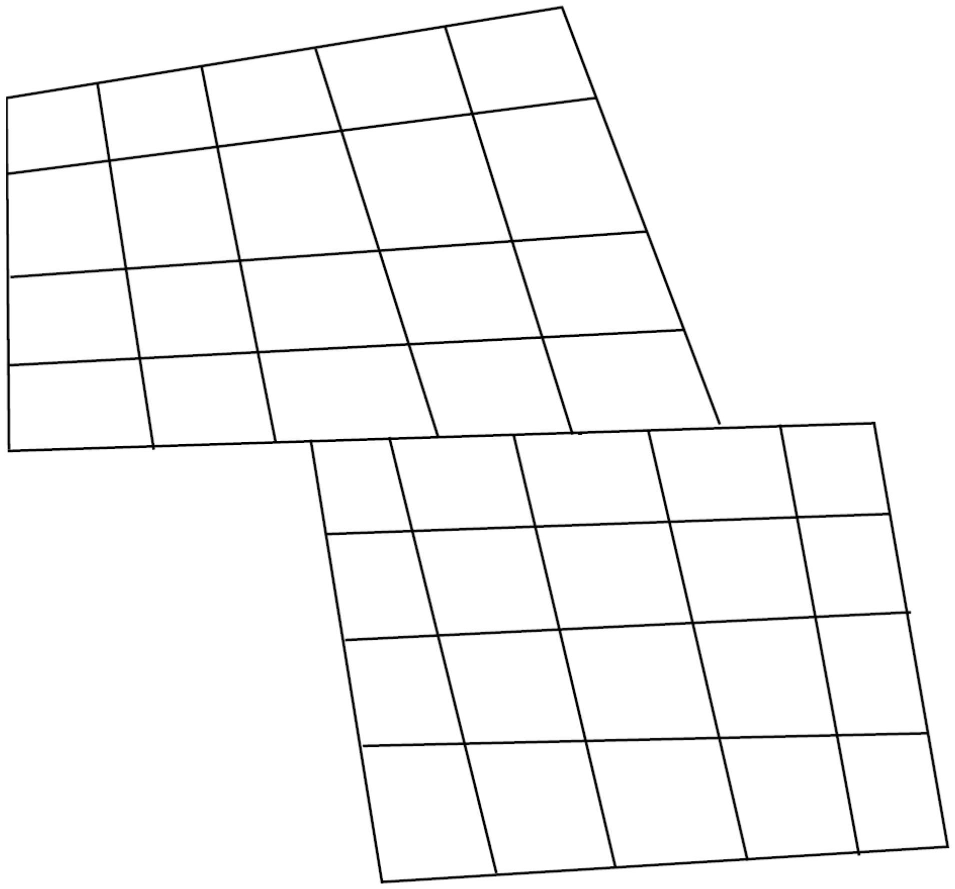


Regular and Body-Fitted Meshes

(structured mesh - every interior vertex in the domain is connected to the same number of neighbour vertices)

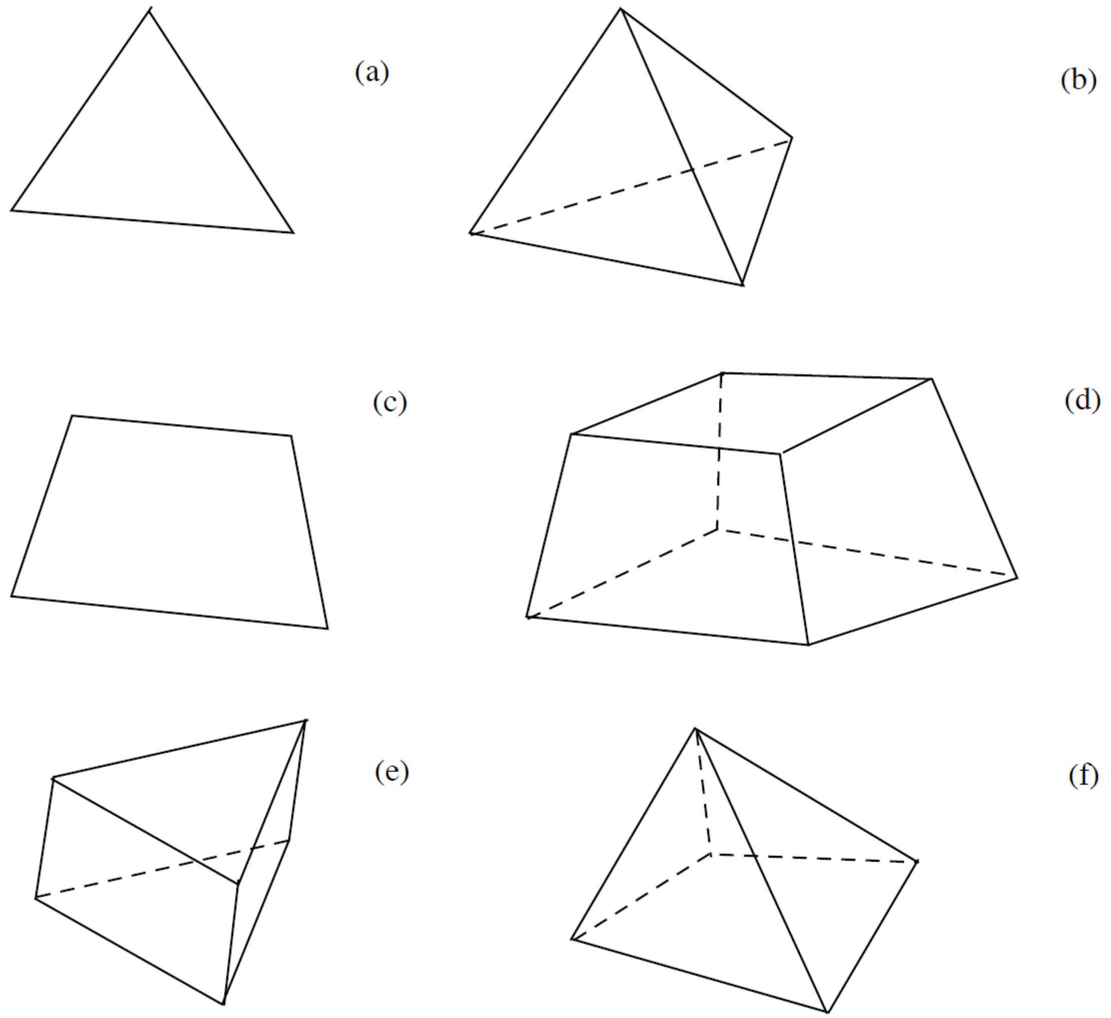


Unstructured Mesh



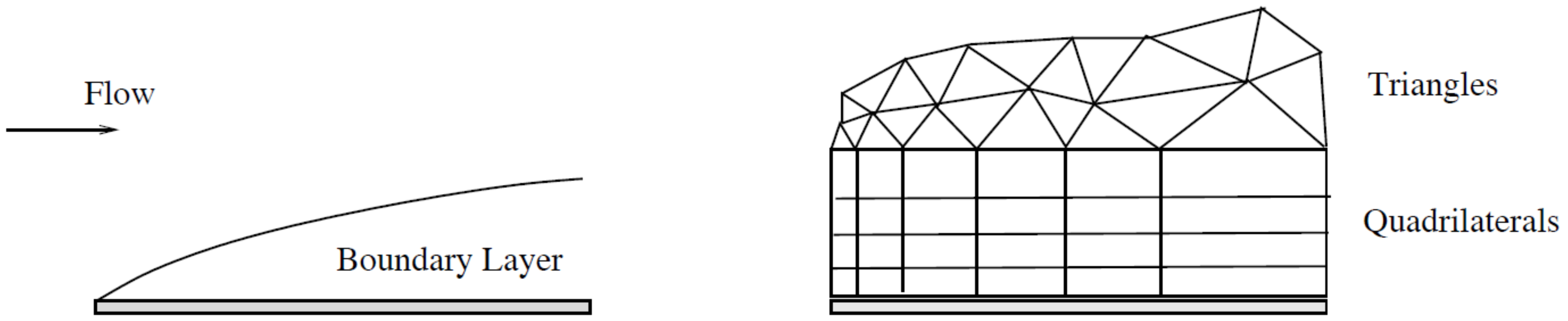
Non-Conformal Mesh

(non-conformal mesh - the vertices of a cell or element may fall on the faces of neighboring cells or elements)



Cell Shapes: (a) Triangle, (b) Tetrahedron, (c) Quadrilateral, (d) Hexahedron, (e) Prism, and (f) Pyramid

•



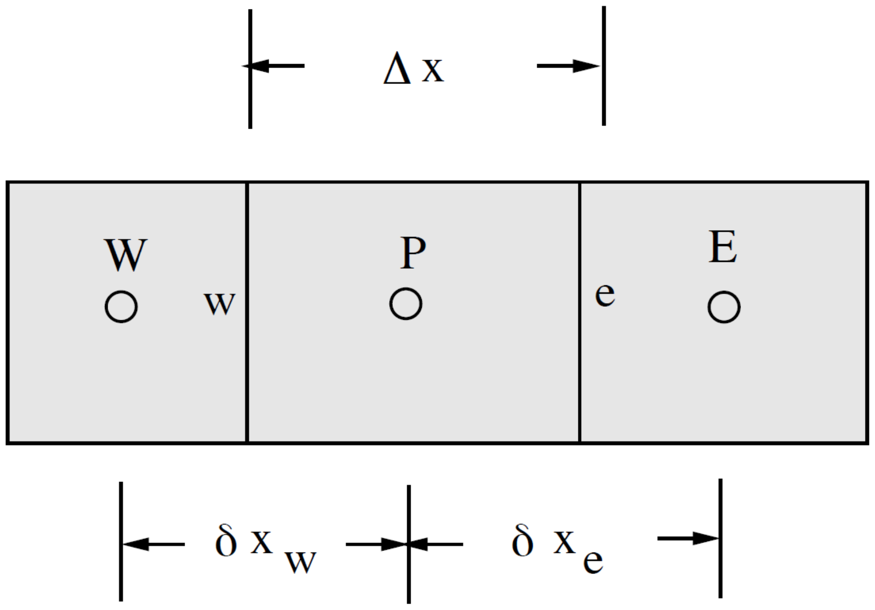
Hybrid Mesh in Boundary Layer

Finite Volume Discretization

Consider the 1D diffusion equation

$$\frac{d}{dx}\left(\Gamma\frac{d\phi}{dx}\right)+S=0$$

on the following control volume:



: Arrangement of Control Volumes

We focus on the cell associated with P. We start by integrating over the cell P. This yields

$$\int_w^e \frac{d}{dx}\left(\Gamma\frac{d\phi}{dx}\right)dx + \int_w^e S dx = 0$$

One obtain

$$\left(\Gamma\frac{d\phi}{dx}\right)_e - \left(\Gamma\frac{d\phi}{dx}\right)_w + \int_w^e S dx = 0$$

We now make a profile assumption, i.e., we make an assumption about how ϕ varies between cell centroids. If we assume that ϕ varies linearly between cell centroids, we may write

$$\frac{\Gamma_e\left(\phi_E - \phi_P\right)}{\left(\delta x_e\right)} - \frac{\Gamma_w\left(\phi_P - \phi_W\right)}{\left(\delta x_w\right)} + \overline{S}\Delta x = 0 \tag{2.15}$$

Here $\overline{S}$ is the average value of S in the control volume. We note that the above equation is no longer exact because of the approximation in assuming that ϕ varies in a piece-wise linear fashion between grid points.

Introduction to Computational Fluid Dynamics

Collecting terms, we obtain

$$a_P\phi_P = a_E\phi_E + a_W\phi_W + b$$

where

$$\begin{aligned} a_E &= \Gamma_e/(\delta x_e) \\ a_W &= \Gamma_w/(\delta x_w) \\ a_P &= a_E + a_W \\ b &= \overline{S}\Delta x \end{aligned}$$

Similar equation may be derived for all cells in the domain, yielding a set of algebraic equations, as before; these may be solved using a variety of direct or iterative methods.

We note the following about the discretization process.

1. The process starts with the statement of conservation over the cell. We then find cell values of ϕ which satisfy this conservation statement. Thus conservation is guaranteed for each cell, regardless of mesh size.

2. Conservation does not guarantee accuracy, however. The solution for ϕ may be inaccurate, but conservative.

3. The quantity $-(\Gamma d\phi/dx)_e$ is diffusion flux on the e face. The cell balance is written in terms of *face* fluxes. The gradient of ϕ must therefore be evaluated at the *faces* of the cell.

4. The profile assumptions for ϕ and S need not be the same.

Two-Dimensional Diffusion in Rectangular Domain

Let us consider the steady two-dimensional diffusion of a scalar ϕ in a rectangular domain. From Equation 1.10, the governing scalar transport equation may be written as

$$\nabla \cdot \mathbf{J} = S \tag{3.1}$$

where $\mathbf{J} = J_x\mathbf{i} + J_y\mathbf{j}$ is the diffusion flux vector and is given by

$$\mathbf{J} = -\Gamma\nabla\phi \tag{3.2}$$

In Cartesian geometries, the gradient operator is given by

$$\nabla = \frac{\partial}{\partial x}\mathbf{i} + \frac{\partial}{\partial y}\mathbf{j} \tag{3.3}$$

We note that Equation 3.1 is written in conservative or divergence form. When Γ is constant and S is zero, the equation defaults to the familiar Laplace equation. When Γ is constant and S is non-zero, the Poisson equation is obtained.

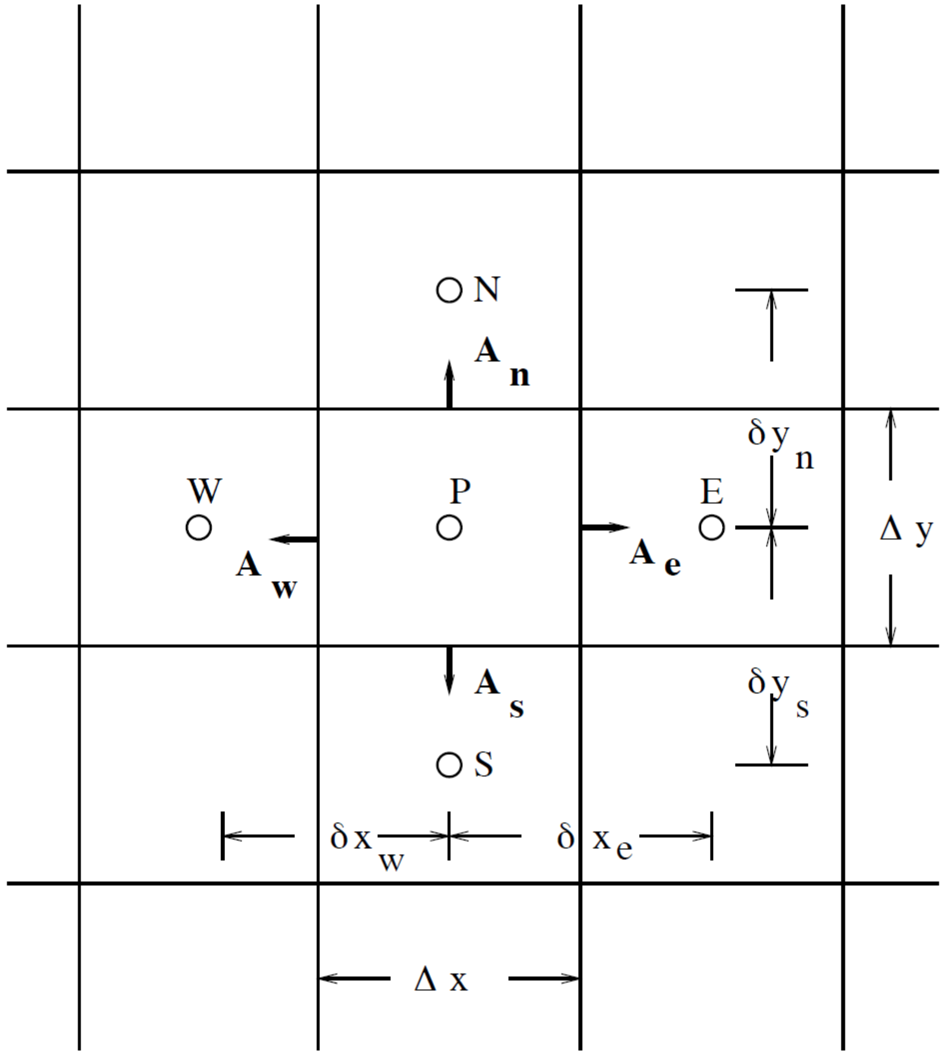


Figure 3.1: Two-Dimensional Control Volume

We begin the process of discretization by integrating Equation 3.1 over the cell P:

$$\int_{\Delta\mathcal{V}} \nabla \cdot \mathbf{J} \, d\mathcal{V} = \int_{\Delta\mathcal{V}} S \, d\mathcal{V} \tag{3.4}$$

Next, we apply the divergence theorem to yield

$$\int_A \mathbf{J} \cdot d\mathbf{A} = \int_{\Delta\mathcal{V}} S \, d\mathcal{V} \tag{3.5}$$

The first integral represents the integral over the control surface A of the cell. We have made no approximations thus far.

We now make a profile assumption about the flux vector **J**. We assume that **J** varies linearly over each face of the cell P, so that it may be represented by its value at the face centroid. We also assume that the mean value of the source term S over the control volume is $\overline{S}$. Thus,

$$(\mathbf{J} \cdot \mathbf{A})_e + (\mathbf{J} \cdot \mathbf{A})_w + (\mathbf{J} \cdot \mathbf{A})_n + (\mathbf{J} \cdot \mathbf{A})_s = \overline{S}\Delta\mathcal{V} \tag{3.6}$$

or, more compactly

$$\sum_{\mathrm{f=e,w,n,s}} \mathbf{J}_f \cdot \mathbf{A}_f = \overline{S}\Delta\mathcal{V} \tag{3.7}$$

The face areas $\mathbf{A}_e$ and $\mathbf{A}_w$ are given by

$$\begin{aligned} \mathbf{A}_e &= \Delta y\,\mathbf{i} \\ \mathbf{A}_w &= -\Delta y\,\mathbf{i} \end{aligned} \tag{3.8}$$

The other area vectors may be written analogously. Further

$$\begin{aligned} \mathbf{J}_e \cdot \mathbf{A}_e &= -\Gamma_e \Delta y \left(\frac{\partial \phi}{\partial x}\right)_e \\ \mathbf{J}_w \cdot \mathbf{A}_w &= \Gamma_w \Delta y \left(\frac{\partial \phi}{\partial x}\right)_w \end{aligned} \tag{3.9}$$

The transport in the other directions may be written analogously.

In order to complete the discretization process, we make one more round of profile assumptions. We assume that ϕ varies linearly between cell centroids. Thus, Equation 3.9 may be written as

$$\begin{aligned} \mathbf{J}_e \cdot \mathbf{A}_e &= -\Gamma_e \Delta y \frac{\phi_E - \phi_P}{(\delta x)_e} \\ \mathbf{J}_w \cdot \mathbf{A}_w &= \Gamma_w \Delta y \frac{\phi_P - \phi_W}{(\delta x)_w} \end{aligned} \tag{3.10}$$

Let us assume that the source term S has the form

$$S = S_C + S_P \phi \tag{3.11}$$

with $S_P \leq 0$. We say that S has been *linearized*. We will see later how general forms of S can be written in this way. We write the volume-averaged source term $\overline{S}$ in the cell P as

$$\overline{S} = S_C + S_P \phi_P \tag{3.12}$$

Substituting Equations 3.10, 3.8 and 3.12 into Equation 3.6 yields a discrete equation for ϕ_P:

$$a_P \phi_P = a_E \phi_E + a_W \phi_W + a_N \phi_N + a_S \phi_S + b \tag{3.13}$$

where

$$\begin{aligned} & & a_N &= \frac{\Gamma_n \Delta x}{(\delta y)_n} \\ a_E &= \frac{\Gamma_e \Delta y}{(\delta x)_e} & a_S &= \frac{\Gamma_s \Delta x}{(\delta y)_s} \\ a_W &= \frac{\Gamma_w \Delta y}{(\delta x)_w} & a_P &= a_E + a_W + a_N + a_S - S_P \Delta x \Delta y \\ & & b &= S_C \Delta x \Delta y \end{aligned} \tag{3.14}$$

Equation 3.13 may be written in a more compact form as

$$a_P \phi_P = \sum_{\text{nb}} a_{\text{nb}} \phi_{\text{nb}} + b \tag{3.15}$$

Here, the subscript *nb* denotes the cell neighbors E, W, N, and S.

We make the following important points about the discretization we have done so far:

1. The discrete equation expresses a balance of discrete flux (the $\mathbf{J}$'s) and the source term. Thus conservation over individual control volumes is guaranteed. However, overall conservation in the calculation domain is not guaranteed unless the diffusion transfer from one cell enters the next cell. For example, in writing the balance for cell E, we must ensure that the flux used on the face e is $\mathbf{J}_e$, and that it is discretized *exactly* as in Equation 3.10.

2. The coefficients a_P and a_{nb} are all of the same sign. In our case they are all positive. This has physical meaning. If the temperature at E is increased, we would expect the temperature at P to increase, not decrease. (The solution to our elliptic partial differential equation also has this property). Many higher order schemes do not have this property. This does not mean these schemes are wrong – it means they do not have a property we would like to have if at all possible.

3. We require that S_P in Equation 3.11 be negative. This also has physical meaning. If for example S is a temperature source, we do not want a situation where as T increases, S increases indefinitely. We control this behavior in the numerical scheme by insisting that S_P be kept negative.

4. When $S_P = 0$, we have

$$a_P = \sum_{\text{nb}} a_{\text{nb}} \tag{3.16}$$

Equation 3.13 may then be written as

$$\phi_P = \sum_{\text{nb}} \left(\frac{a_{\text{nb}}}{a_P} \phi_{\text{nb}} \right) \tag{3.17}$$

where $\sum_{\text{nb}}(a_{\text{nb}}/a_P) = 1$. Since ϕ_P is the weighted sum of its neighbor values, it is always bounded by them. By extension, ϕ_P is always bounded by the boundary values of ϕ. We notice that this property is also shared by our canonical elliptic equation.

When $S \neq 0$, ϕ_P need not be bounded in this manner, and can overshoot or undershoot its boundary values, but this is perfectly physical. The amount of overshoot is determined by the magnitude of S_C and S_P with respect to the a_{nb}'s.

5. If $S_P = 0$ and $a_P = \sum_{\text{nb}} a_{\text{nb}}$, we notice that ϕ and $\phi + C$ are solutions to Equation 3.13. This is also true of the original differential equation, Equation 3.1. The solution can be made unique by specifying boundary conditions on ϕ which fix the value of ϕ at some point on the boundary.

Boundary Conditions

A typical boundary control volume is shown in Figure 3.2. A boundary control volume is one which has one or more faces on the boundary. Discrete values of ϕ are stored at cell centroids, as before. In addition, we store discrete values of ϕ at the centroids of boundary faces.

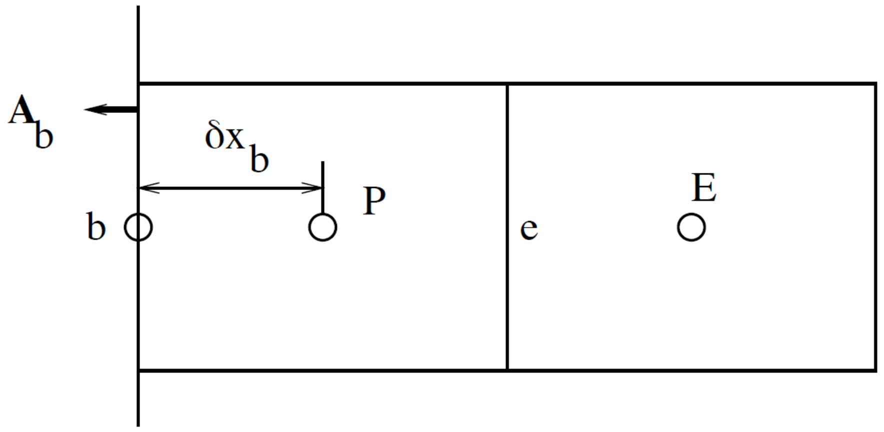


Figure 3.2: Boundary Control Volume

Let us consider the discretization process for a near-boundary control volume centered about the cell centroid P with a face on the boundary. The boundary face centroid is denoted by b. The face area vector of the boundary face is $\mathbf{A}_b$, and points outward from the cell P as shown.

Integrating the governing transport equation over the cell P as before yields

$$(\mathbf{J}\cdot\mathbf{A})_b + (\mathbf{J}\cdot\mathbf{A})_e + (\mathbf{J}\cdot\mathbf{A})_n + (\mathbf{J}\cdot\mathbf{A})_s = \overline{S}\Delta\mathcal{V} \tag{3.18}$$

The fluxes on the interior faces are discretized as before. The boundary area vector $\mathbf{A}_b$ is given by

$$\mathbf{A}_b = -\Delta y\,\mathbf{i} \tag{3.19}$$

Let us assume that the boundary flux $\mathbf{J}_b$ is given by the boundary face centroid value. Thus

$$\mathbf{J}_b = -\Gamma_b \nabla\phi_b \tag{3.20}$$

$$\mathbf{J}_b\cdot\mathbf{A}_b = \Delta y \Gamma_b \nabla\phi_b \tag{3.21}$$

Assuming that ϕ varies linearly between b and P, we write

$$\mathbf{J}_b\cdot\mathbf{A}_b = \Delta y \Gamma_b \frac{(\phi_P - \phi_b)}{(\delta x)_b} \tag{3.22}$$

3.2.1 Dirichlet Boundary Condition

The boundary condition is given by

$$\phi_b = \phi_{b,\text{given}} \tag{3.23}$$

Using $\phi_{b,\text{given}}$ in Equation 3.22, and including $\mathbf{J_b} \cdot \mathbf{A}_b$ in Equation 3.18 yields the following discrete equation for boundary cell P:

$$a_P\phi_P = a_E\phi_E + a_N\phi_N + a_S\phi_S + b \tag{3.24}$$

where

$$\begin{aligned} a_E &= \frac{\Gamma_e \Delta y}{(\delta x)_e} & & \\ a_N &= \frac{\Gamma_n \Delta x}{(\delta y)_n} & a_b &= \frac{\Gamma_b \Delta y}{(\delta x)_b} \\ & & a_P &= a_E + a_N + a_S + a_b - S_P \Delta x \Delta y \\ a_S &= \frac{\Gamma_s \Delta x}{(\delta y)_s} & b &= a_b \phi_b + S_C \Delta x \Delta y \end{aligned} \tag{3.25}$$

Neumann Boundary Condition

Here, we are given the normal gradient of ϕ at the boundary:

$$-(\Gamma\nabla\phi)_b \cdot \mathbf{i} = q_{b,\text{given}} \tag{3.26}$$

We are in effect given the flux $\mathbf{J}_b$ at Neumann boundaries:

$$\mathbf{J}_b \cdot \mathbf{A}_b = -q_{b,\text{given}}\Delta y \tag{3.27}$$

We may thus include $(-q_{b,\text{given}}\Delta y)$ directly in Equation 3.18 to yield the following discrete equation for the boundary cell P:

$$a_P\phi_P = a_E\phi_E + a_N\phi_N + a_S\phi_S + b \tag{3.28}$$

where

$$\begin{aligned} a_E &= \frac{\Gamma_e\Delta y}{(\delta x)_e} & a_S &= \frac{\Gamma_s\Delta x}{(\delta y)_s} \\ a_N &= \frac{\Gamma_n\Delta x}{(\delta y)_n} & a_P &= a_E + a_N + a_S - S_P\Delta x\Delta y \\ & & b &= q_{b,\text{given}}\Delta y + S_C\Delta x\Delta y \end{aligned} \tag{3.29}$$

Once ϕ_P is computed, the boundary value, ϕ_b may be computed using Equation 3.22:

$$\phi_b = \frac{q_{b,\text{given}} + (\Gamma_b/\delta x_b)\phi_P}{(\Gamma_b/\delta x_b)} \tag{3.30}$$

Mixed Boundary Condition

The mixed boundary condition is given by

$$-(\Gamma\nabla\phi)_b \cdot \mathbf{i} = h_b(\phi_\infty - \phi) \tag{3.31}$$

Since $\mathbf{A}_b = \Delta y\mathbf{i}$, we are given that

$$\mathbf{J}_b \cdot \mathbf{A}_b = -h_b(\phi_\infty - \phi)\Delta y \tag{3.32}$$

Using Equation 3.22 we may write

$$\Gamma_b \frac{(\phi_P - \phi_b)}{\delta x_b} = -h_b(\phi_\infty - \phi_b) \tag{3.33}$$

We may thus write ϕ_b as

$$\phi_b = \frac{h_b \phi_\infty + (\Gamma_b/\delta x_b)\phi_P}{h_b + (\Gamma_b/\delta x_b)} \tag{3.34}$$

Using Equation 3.34 to eliminate ϕ_b from Equation 3.33 we may write

$$\mathbf{J}_b \cdot \mathbf{A}_b = -R_{eq}(\phi_\infty - \phi_P)\Delta y \tag{3.35}$$

where

$$R_{eq} = \frac{h_b(\Gamma_b/\delta x_b)}{h_b + (\Gamma_b/\delta x_b)} \tag{3.36}$$

We are now ready to write the discretization equation for the boundary control volume P. Substituting the boundary flux from Equation 3.35 into Equation 3.18 given the following discrete equation for ϕ_P:

$$a_P \phi_P = a_E \phi_E + a_N \phi_N + a_S \phi_S + b \tag{3.37}$$

where

$$\begin{aligned} a_E &= \frac{\Gamma_e \Delta y}{(\delta x)_e} \\ a_N &= \frac{\Gamma_n \Delta x}{(\delta y)_n} & a_b &= R_{eq}\Delta y \\ a_S &= \frac{\Gamma_s \Delta x}{(\delta y)_s} & a_P &= a_E + a_N + a_S + a_b - S_P \Delta x \Delta y \\ && b &= R_{eq}\Delta y \phi_\infty + S_C \Delta x \Delta y \end{aligned} \tag{3.38}$$

The boundary value, ϕ_b, may be computed from Equation 3.34 once a solution has been obtained. It is bounded by ϕ_P and ϕ_∞, as shown by Equation 3.34.

Unsteady Conduction

Let us now consider the unsteady counterpart of Equation 3.1:

$$\frac{\partial}{\partial t}(\rho\phi) + \nabla \cdot \mathbf{J} = S \tag{3.39}$$

We are given initial conditions $\phi(x,y,0)$. As we saw in a previous chapter, time is a “marching” coordinate. By knowing the initial condition, and taking discrete time steps Δt, we wish to obtain the solution for ϕ at a each discrete time instant.

In order to discretize Equation 3.39, we integrate it over the control volume as usual. We also integrate it over the time step Δt, i.e., from t to $t + \Delta t$.

$$\int_{\Delta t}\int_{\Delta \mathscr{V}} \frac{\partial}{\partial t}(\rho\phi)\, d\mathscr{V}\, dt + \int_{\Delta t}\int_{\Delta \mathscr{V}} \nabla \cdot \mathbf{J} d\mathscr{V}\, dt = \int_{\Delta t}\int_{\Delta \mathscr{V}} S d\mathscr{V}\, dt \tag{3.40}$$

Applying the divergence theorem as before, we obtain

$$\int_{\Delta \mathscr{V}} \left((\rho\phi)^1 - (\rho\phi)^0\right) d\mathscr{V} + \int_{\Delta t}\int_{A} \mathbf{J} \cdot d\mathbf{A} dt = \int_{\Delta t}\int_{\Delta \mathscr{V}} S d\mathscr{V}\, dt \tag{3.41}$$

The superscripts 1 and 0 in the first integral denote the values at the times $t+\Delta t$ and t respectively. Let us consider each term in turn. If we assume that

$$\int_{\Delta \mathscr{V}} \rho\phi \, d\mathscr{V} = (\rho\phi)_P \Delta \mathscr{V} \tag{3.42}$$

we may write the unsteady term as

$$\Delta \mathscr{V} \left((\rho\phi)_P^1 - (\rho\phi)_P^0 \right) \tag{3.43}$$

We now turn to the flux term. If we assume as before that the flux on a face is represented by its centroid value, we may write the term as

$$\int_{\Delta t} \sum_{\mathrm{f=e,w,n,s}} \mathbf{J}_f \cdot \mathbf{A}_f dt \tag{3.44}$$

We are now required to make a profile assumption about how the flux $\mathbf{J}$ varies with time. Let us assume that it can be interpolated between time instants $t+\Delta t$ and t using a factor f between zero and one:

$$\int_{\Delta t} \mathbf{J} \cdot \mathbf{A} dt = \left(f\mathbf{J}^1 \cdot \mathbf{A} + (1-f)\,\mathbf{J}^0 \cdot \mathbf{A} \right) \Delta t \tag{3.45}$$

Proceeding as before, making linear profile assumptions for ϕ between grid points, we may write

$$\begin{aligned} \mathbf{J}_e^1 \cdot \mathbf{A}_e &= -\Gamma_e \Delta y \frac{\phi_E^1 - \phi_P^1}{(\delta x)_e} \\ \mathbf{J}_w^1 \cdot \mathbf{A}_w &= \Gamma_w \Delta y \frac{\phi_P^1 - \phi_W^1}{(\delta x)_w} \end{aligned} \tag{3.46}$$

$$\begin{aligned} \mathbf{J}_e^0 \cdot \mathbf{A}_e &= -\Gamma_e \Delta y \frac{\phi_E^0 - \phi_P^0}{(\delta x)_e} \\ \mathbf{J}_w^0 \cdot \mathbf{A}_w &= \Gamma_w \Delta y \frac{\phi_P^0 - \phi_W^0}{(\delta x)_w} \end{aligned} \tag{3.47}$$

Let us now examine the source term. Linearizing S as $S_C + S_P\phi$ and further assuming that

$$\int_{\Delta \mathcal{V}} (S_C + S_P\phi)\, d\mathcal{V} = (S_C + S_P\phi_P)\, \Delta\mathcal{V} \tag{3.48}$$

we have

$$\int_{\Delta t}\int_{\Delta \mathcal{V}} S d\mathcal{V}\, dt = \int_{\Delta t} (S_C + S_P\phi_P)\, \Delta\mathcal{V}\, dt \tag{3.49}$$

Again, interpolating S between $t+\Delta t$ and t using a weighting factor f between zero and one:

$$\int_{\Delta t} \left(S_C + S_P\phi_P\right) \Delta \mathcal{V}\, dt = f\left(S_C + S_P\phi_P\right)^1 \Delta \mathcal{V} \Delta t + (1-f)\left(S_C + S_P\phi_P\right)^0 \Delta \mathcal{V} \Delta t \quad (3.50)$$

For simplicity, let us drop the superscript 1 and let the un-superscripted value represent the value at time $t+\Delta t$. The values at time t are represented as before with the superscript 0. Collecting terms and dividing through by Δt, we obtain the following discrete equation for ϕ:

$$a_P\phi_P = \sum_{\text{nb}} a_{\text{nb}}\left(f\phi_{\text{nb}} + (1-f)\phi_{\text{nb}}^0\right) + b + \left(a_P^0 - (1-f)\sum_{\text{nb}} a_{\text{nb}}\right)\phi_P^0 \quad (3.51)$$

where nb denotes E, W, N and S. Further

$$\begin{aligned} a_E &= \frac{\Gamma_e \Delta y}{(\delta x)_e} & a_S &= \frac{\Gamma_s \Delta x}{(\delta y)_s} \\ a_W &= \frac{\Gamma_w \Delta y}{(\delta x)_w} & a_P^0 &= \frac{\rho \Delta \mathcal{V}}{\Delta t} \\ a_N &= \frac{\Gamma_n \Delta x}{(\delta y)_n} & a_P &= f\sum_{\text{nb}} a_{\text{nb}} - fS_P\Delta\mathcal{V} + a_P^0 \\ & & b &= \left(fS_C + (1-f)S_C^0 + (1-f)S_P^0\phi_P^0\right)\Delta\mathcal{V} \end{aligned} \quad (3.52)$$

The Explicit Scheme

If we set $f = 0$, we obtain the explicit scheme. This means that the flux and source terms are evaluated using values exclusively from the previous time step. In this limit, we obtain the following discrete equations:

$$a_P\phi_P = \sum_{\text{nb}} a_{\text{nb}}\phi^0_{\text{nb}} + b + \left(a^0_P - \sum_{\text{nb}} a_{\text{nb}}\right)\phi^0_P \tag{3.53}$$

$$\begin{aligned}
a_E &= \frac{\Gamma_e \Delta y}{(\delta x)_e} & a_S &= \frac{\Gamma_s \Delta x}{(\delta y)_s} \\
a_W &= \frac{\Gamma_w \Delta y}{(\delta x)_w} & a^0_P &= \frac{\rho \Delta \mathcal{V}}{\Delta t} \\
& & a_P &= a^0_P \\
a_N &= \frac{\Gamma_n \Delta x}{(\delta y)_n} & b &= \left(S^0_C + S^0_P \phi^0_P\right)\Delta \mathcal{V}
\end{aligned} \tag{3.54}$$

3.3.2 The Fully-Implicit Scheme

The fully-implicit scheme is obtained by setting $f = 1$ in Equation 3.51. In this limit, we obtain the following discrete equation for ϕ_P.

$$a_P \phi_P = \sum_{\text{nb}} a_{\text{nb}} \phi_{\text{nb}} + b + a_P^0 \phi_P^0 \tag{3.59}$$

$$\begin{aligned} a_E &= \frac{\Gamma_e \Delta y}{(\delta x)_e} \\ a_W &= \frac{\Gamma_w \Delta y}{(\delta x)_w} & a_P^0 &= \frac{\rho \Delta \mathcal{V}}{\Delta t} \\ a_N &= \frac{\Gamma_n \Delta x}{(\delta y)_n} & a_P &= \sum_{\text{nb}} a_{\text{nb}} - S_P \Delta \mathcal{V} + a_P^0 \\ a_S &= \frac{\Gamma_s \Delta x}{(\delta y)_s} & b &= S_C \Delta \mathcal{V} \end{aligned} \tag{3.60}$$

The Crank-Nicholson Scheme

The Crank-Nicholson Scheme is obtained by setting $f = 0.5$. With this value of f, our discrete equation becomes

$$a_P \phi_P = \sum_{\text{nb}} a_{\text{nb}} \left(0.5\phi_{\text{nb}} + 0.5\phi^0_{\text{nb}}\right) + b + \left(a^0_P - 0.5 \sum_{\text{nb}} a_{\text{nb}}\right) \phi^0_P \qquad (3.61)$$

$$\begin{aligned} a_E &= \frac{\Gamma_e \Delta y}{(\delta x)_e} \\ a_W &= \frac{\Gamma_w \Delta y}{(\delta x)_w} & a^0_P &= \frac{\rho \Delta \mathcal{V}}{\Delta t} \\ a_N &= \frac{\Gamma_n \Delta x}{(\delta y)_n} & a_P &= 0.5 \sum_{\text{nb}} a_{\text{nb}} - 0.5 S_P \Delta \mathcal{V} + a^0_P \\ a_S &= \frac{\Gamma_s \Delta x}{(\delta y)_s} & b &= 0.5 \left(\left(S_C + S^0_C\right) + S^0_P \phi^0_P\right) \Delta \mathcal{V} \end{aligned} \qquad (3.62)$$

3.6.1 Interpolation of Γ

We notice in our discretization that the diffusion flux is evaluated at the *face* of the control volume. As a result, we must specify the face value of the diffusion coefficient Γ. Since we store Γ at cell centroids, we must find a way to interpolate Γ to the face.

Referring to the notation in Figure 3.5, it is possible to simple interpolate Γ linearly as:

$$\Gamma_e = f_e \Gamma_P + (1 - f_e)\Gamma_E \tag{3.79}$$

where

$$f_e = \frac{0.5\Delta x_E}{(\delta x)_e} \tag{3.80}$$

As long as Γ_e is smoothly varying, this is a perfectly adequate interpolation. When ϕ is used to represent energy or temperature, step jumps in Γ may be encountered at conjugate boundaries. It is useful to devise an interpolation procedure which accounts for these jumps.

Our desire is to represent the interface flux correctly. Let J_e be the magnitude of the flux vector $\mathbf{J}_e$. Let us assume locally one-dimensional diffusion. In this limit, we may write

$$J_e = -\frac{(\phi_E - \phi_P)}{(0.5\Delta x_P)/\Gamma_P + (0.5\Delta x_E)/\Gamma_E} \tag{3.81}$$

Thus, an equivalent interface diffusion coefficient may be defined as

$$\frac{\delta x_e}{\Gamma_e} = \frac{0.5\Delta x_P}{\Gamma_P} + \frac{0.5\Delta x_E}{\Gamma_E} \tag{3.82}$$

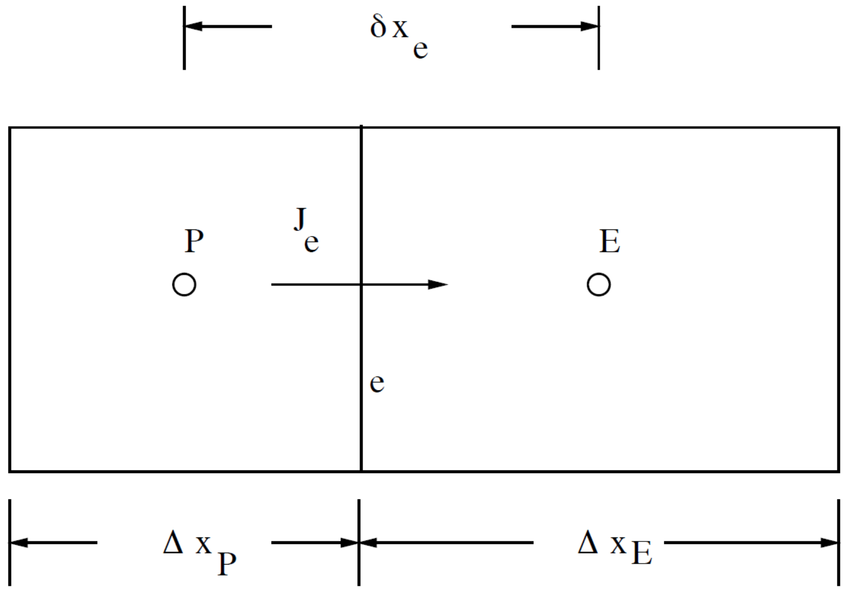


Figure 3.5: Diffusion Transport at Conjugate Boundaries

Introduction to Computational Fluid Dynamics

The term $\delta x_e/\Gamma_e$ may be seen as a *resistance* to the diffusion transfer between P and E. We may write Γ_e as

$$\Gamma_e = \left(\frac{1 - f_e}{\Gamma_P} + \frac{f_e}{\Gamma_E} \right)^{-1} \qquad (3.83)$$

Equation 3.83 represents a *harmonic mean* interpolation for Γ. The properties of this interpolation may be better understood if we consider the case $f_e = 0.5$, i.e., the face e lies midway between P and E. In this case,

$$\Gamma_e = \frac{2\Gamma_P\Gamma_E}{\Gamma_P + \Gamma_E} \qquad (3.84)$$

Source Linearization and Treatment of Non-Linearity

Our goal is to reduce our differential equation to a set of algebraic equations in the discrete values of ϕ. When the scalar transport is non-linear, the resulting algebraic set is also non-linear. Non-linearity can arise from a number of different sources. For example, in diffusion problems, the diffusion coefficient may be a function of ϕ, such as in the case of temperature-dependent thermal conductivity. The source term S may also be a function of ϕ. In radiative heat transfer in participating media, for example, the source term in the energy equation contains fourth powers of the temperature. There are many ways to treat non-linearities. Here, we will treat non-linearities through *Picard* iteration. In this method, the coefficients a_P, a_{nb}, S_C and S_P are evaluated using prevailing values of ϕ. They are updated as ϕ is updated by iteration.

We said previously that the source term S could be written in the form

$$S = S_C + S_P \phi \tag{3.85}$$

We now examine how this can be done when S is a non-linear function of ϕ.

Let the prevailing value of ϕ be called ϕ^*. This is the value that exists at the current iteration. We write a Taylor series expansion for S about its prevailing value $S^* = S(\phi^*)$:

$$S = S^* + \left(\frac{\partial S}{\partial \phi}\right)^* (\phi - \phi^*) \tag{3.86}$$

so that

$$\begin{aligned} S_C &= S^* - \left(\frac{\partial S}{\partial \phi}\right)^* \phi^* \\ S_P &= \left(\frac{\partial S}{\partial \phi}\right)^* \end{aligned} \tag{3.87}$$

Here, $(\partial S/\partial \phi)^*$ is the gradient evaluated at the prevailing value ϕ^*. For most problems of interest to us, $\partial S/\partial \phi$ is negative, resulting in a negative S_P. This ensures that the source tends to decrease as ϕ increases, providing a stabilizing effect. However, this type of dependence is not always guaranteed.

Under-Relaxation

When using iterative methods for obtaining solutions or when iterating to resolve non-linearities, it is frequently necessary to control the rate at which variables are changing during iterations. When we have a strong non-linearity in a temperature source term, for example, and our initial guess is far from the solution, we may get large oscillations in the temperature computed during the first few iterations, making it difficult for the iteration to proceed. In such cases, we often employ *under-relaxation*.

Let the current iterate of ϕ be ϕ_P^*. We know that ϕ_P satisfies

$$a_P\phi_P = \sum_{\mathrm{nb}} a_{\mathrm{nb}}\phi_{\mathrm{nb}} + b \qquad (3.88)$$

so that after the system has been solved for the current iteration, we expect to compute a value of ϕ_P of

$$\phi_P = \frac{\sum_{\mathrm{nb}} a_{\mathrm{nb}}\phi_{\mathrm{nb}} + b}{a_P} \qquad (3.89)$$

We do not, however, want ϕ_P to change as much as Equation 3.89 implies. The change in ϕ_P from one iteration to the next is given by

$$\frac{\sum_{\mathrm{nb}} a_{\mathrm{nb}} \phi_{\mathrm{nb}} + b}{a_P} - \phi_P^* \tag{3.90}$$

We wish to make ϕ_P change only by a fraction α of this change. Thus

$$\phi_P = \phi_P^* + \alpha \left(\frac{\sum_{\mathrm{nb}} a_{\mathrm{nb}} \phi_{\mathrm{nb}} + b}{a_P} - \phi_P^* \right) \tag{3.91}$$

Collecting terms, we may write

$$\frac{a_P}{\alpha} \phi_P = \sum_{\mathrm{nb}} a_{\mathrm{nb}} \phi_{\mathrm{nb}} + b + \frac{1-\alpha}{\alpha} a_P \phi_P^* \tag{3.92}$$

Introduction to Computational Fluid Dynamics

When the iterations converge to a solution, i.e., when $\phi_P = \phi_P^*$, the original discrete equation is recovered. So we are assured that under-relaxation is only a change in the path to solution, and not in the discretization itself. Thus, both under-relaxed and un-underrelaxed equations yield the same final solution.

Though over-relaxation ($\alpha > 1$) is a possibility, we will for the most part be using $\alpha \leq 1$. With $\alpha \leq 1$, we are assured that $a_P/\alpha > \sum_{\text{nb}} a_{\text{nb}}$. This allows us to satisfy the Scarborough criterion.

(the matrix is diagonally dominant)

We note the similarity of under-relaxation to time-stepping. The initial guess acts as the initial condition. The terms a_P/α and $((1-\alpha)/\alpha)a_p\phi_P^*$ represent the effect of the unsteady terms.