Analytical solutions of partial differential equations involve closed-form expressions which give the variation of the dependent variables *continuously* throughout the domain. In contrast, numerical solutions can give answers at only *discrete points* in the domain, called *grid points*. For example, consider Fig. 4.1, which shows a section of a discrete grid in the xy plane. For convenience, let us assume that the spacing of the grid points in the x direction is uniform and given by Δx and that the spacing of the points in the y direction is also uniform and given by Δy, as shown in Fig. 4.1. In general, Δx and Δy are different. Indeed, it is not absolutely necessary that Δx or Δy be uniform; we could deal with totally unequal spacing in both directions, where Δx is a different value between each successive pairs of grid points, and similarly for Δy. However, the majority of CFD applications involve numerical solutions on a grid which contains uniform spacing in each direction, because this greatly simplifies the programming of the solution, saves storage space, and usually results in greater accuracy. This uniform spacing does not have to occur in the physical xy space; as is frequently done in CFD, the numerical calculations are carried out in a transformed computational space which has uniform spacing in the transformed independent variables but which corresponds to nonuniform spacing in the physical plane. These matters will be discussed in detail in Chap. 5. In any event, in this chapter we will assume uniform spacing in each coordinate direction but not necessarily equal spacing for both directions; i.e., we will assume Δx and Δy to be constants, but Δx does not have to equal Δy. (We should note that recent research in CFD has focused on *unstructured* grids, where the grid points are placed in the flow field in a very irregular fashion; this is in contrast to a *structured* grid which reflects some type of consistent geometrical regularity. Figure 4.1 is an example of a structured grid. Some aspects of unstructured grids will be discussed in Chap. 5.)

Returning to Fig. 4.1, the grid points are identified by an index i which runs in the x direction and an index j which runs in the y direction. Hence, if (i, j) is the index for point P in Fig. 4.1, then the point immediately to the right of P is labeled as $(i + 1, j)$, the point immediately to the left is $(i - 1, j)$, the point directly above is $(i, j + 1)$, and the point directly below is $(i, j - 1)$.

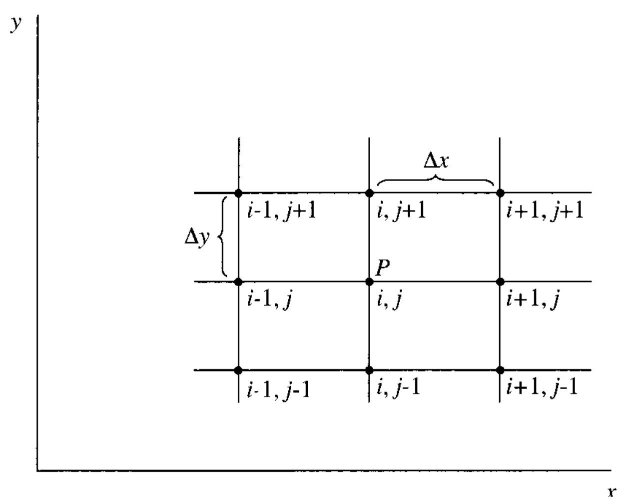


FIG. 4.1
Discrete grid points.

We are now in a position to elaborate on the word "discretization." Imagine that we have a two-dimensional flow field which is governed by the Navier-Stokes equations, or as the case may be, the Euler equations, as derived in Chap. 2. These are partial differential equations. An analytical solution of these equations would provide, in principle, closed-form expressions for u, v, p, ρ, etc., as functions of x and y, which could be used to give values of the flow-field variables at *any* point we wish to choose in the flow, i.e., at any of the infinite number of (x, y) points in the domain. On the other hand, if the partial derivatives in the governing equations are replaced by approximate algebraic difference quotients (to be derived in the next section), where the algebraic difference quotients are expressed strictly in terms of the flow-field variables at two or more of the discrete grid points shown in Fig. 4.1, then the partial differential equations are totally replaced by a system of *algebraic* equations which can be solved for the values of the flow-field variables at the discrete grid points *only*. In this sense, the original partial differential equations have been discretized. Moreover, this method of discretization is called the *method of finite differences*. Finite-difference solutions are widely employed in CFD, and hence much of this chapter will be devoted to matters concerning finite differences.

So this is what discretization means. All methods in CFD utilize some form of discretization. The purpose of this chapter is to derive and discuss the more common forms of discretization in use today for finite-difference applications. This constitutes one of the three main headings in Fig. 4.2, which is the road map for this

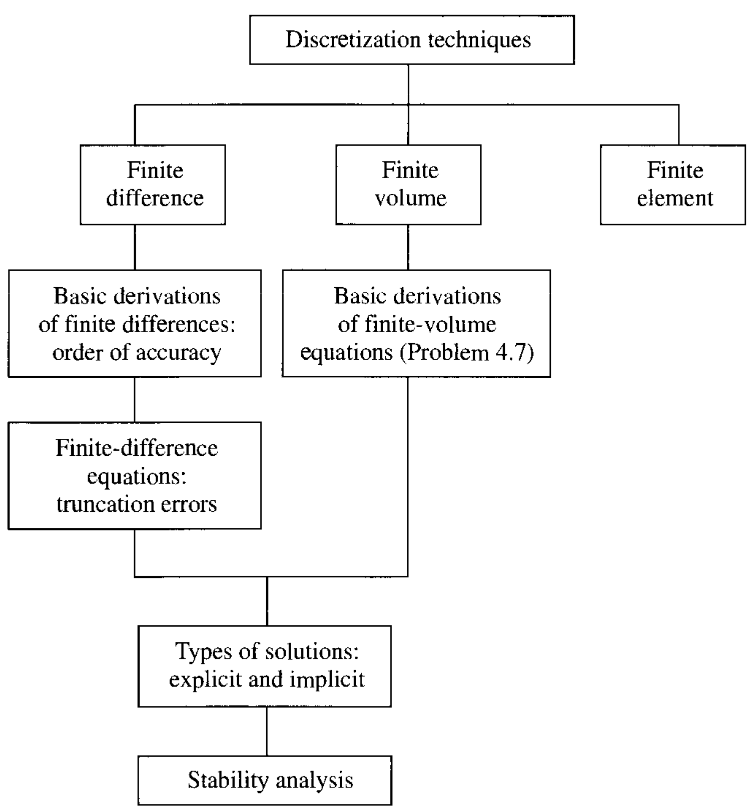


FIG. 4.2
Road map for Chap. 4.

chapter. The second and third main headings are labeled finite volume and finite element, respectively. Both finite-volume and finite-element methods have been in widespread use in computational mechanics for years. However, we will not discuss finite-volume or finite-element methods in this book, mainly because of length constraints. The essential aspects of finite volume discretization are dealt with via Problem 4.7 at the end of this chapter. It is important to note that CFD can be approached using any of the three main types of discretization: finite difference, finite volume, or finite element, as displayed in Fig. 4.2.

Examining the road map in Fig. 4.2 further, the purpose of the present chapter is to construct the basic discretization formulas for finite differences, while at the same time addressing the order of accuracy of these formulas. The road map in Fig. 4.2 gives us our marching orders—let's go to it!

4.2 INTRODUCTION TO FINITE DIFFERENCES

Here, we are interested in replacing a partial derivative with a suitable algebraic difference quotient, i.e., a *finite difference*. Most common finite-difference representations of derivatives are based on Taylor's series expansions. For example, referring to Fig. 4.1, if $u_{i,j}$ denotes the x component of velocity at point (i, j), then the velocity $u_{i+1,j}$ at point $(i + 1, j)$ can be expressed in terms of a Taylor series expanded about point (i, j) as follows:

$$u_{i+1,j} = u_{i,j} + \left(\frac{\partial u}{\partial x}\right)_{i,j} \Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \frac{(\Delta x)^2}{2} + \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} \frac{(\Delta x)^3}{6} + \cdots \tag{4.1}$$

Equation (4.1) is mathematically an exact expression for $u_{i+1,j}$ if (1) the number of terms is infinite and the series converges and/or (2) $\Delta x \to 0$.

Example 4.1. Since some readers may not be totally comfortable with the concept of a Taylor series, we will review some aspects in this example.

First, consider a continuous function of x, namely, $f(x)$, with all derivatives defined at x. Then, the value of f at a location $x + \Delta x$ can be estimated from a Taylor series expanded about point x, that is,

$$f(x + \Delta x) = f(x) + \frac{\partial f}{\partial x} \Delta x + \frac{\partial^2 f}{\partial x^2} \frac{(\Delta x)^2}{2} + \cdots \frac{\partial^n f}{\partial x^n} \frac{(\Delta x)^n}{n!} + \cdots \tag{E.1}$$

[Note in Eq. (E.1) that we continue to use the partial derivative nomenclature to be consistent with Eq. (4.1), although for a function of one variable, the derivatives in Eq. (E.1) are really ordinary derivatives.] The significance of Eq. (E.1) is diagramed in Fig. E4.1. Assume that we know the value of f at x (point 1 in Fig. E4.1); we want to calculate the value of f at $x + \Delta x$ (point 2 in Fig. E4.1) using Eq. (E.1). Examining the right-hand side of Eq. (E4.1), we see that the first term, $f(x)$, is not a good guess for $f(x + \Delta x)$, unless, of course, the function $f(x)$ is a horizontal line between points 1 and 2. An improved guess is made by approximately accounting for the slope of the curve at point 1, which is the role of the second term, $\partial f/\partial x\, \Delta x$, in Eq. (E.1). To obtain an even better estimate of f at $x + \Delta x$, the third term, $\partial^2 f/\partial x^2\, (\Delta x)^2/2$, is added, which approximately accounts for the curvature between points 1 and 2. In general, to obtain

$$\boxed{\underbrace{f(x+\Delta x)=f(x)}_{\substack{\text{First guess}\\ \text{(not very good)}}} + \underbrace{\frac{\partial f}{\partial x}\Delta x}_{\substack{\text{Add to capture}\\ \text{slope}}} + \underbrace{\frac{\partial^2 f}{\partial x^2}\frac{(\Delta x)^2}{2}}_{\substack{\text{Add to account}\\ \text{for curvature}}} + \cdots}$$

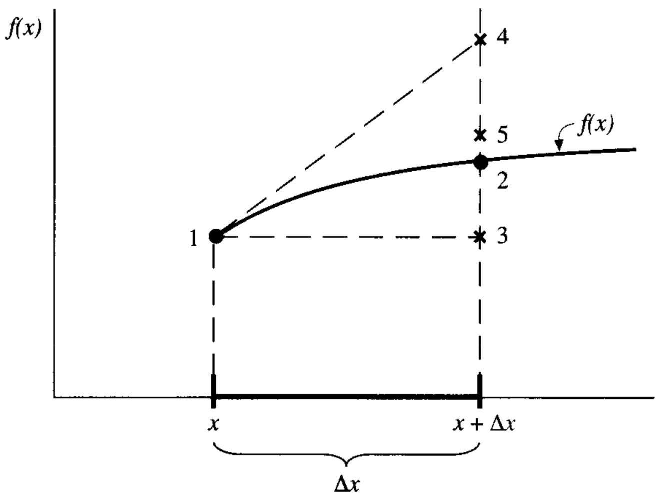


FIG. E4.1
Illustration of behavior of the first three terms in a Taylor series (for Example 4.1).

more accuracy, additional higher-order terms must be included. Indeed, Eq. (E.1) becomes an *exact* representation of $f(x + \Delta x)$ only when an infinite number of terms is carried on the right-hand side. To examine some numbers, let

$$\begin{aligned} f(x) &= \sin 2\pi x \\ \text{At } x = 0.2: \qquad f(x) &= 0.9511 \end{aligned} \tag{E.2}$$

This *exact* value of $f(0.2)$ corresponds to point 1 in Fig. E4.1. Now, let $\Delta x = 0.02$. We wish to evaluate $f(x + \Delta x) = f(0.22)$. From Eq. (E.2), we have the *exact* value:

$$\text{At } x = 0.22: \qquad f(x) = 0.9823$$

This corresponds to point 2 in Fig. E4.1. Now, let us *estimate* $f(0.22)$ using Eq. (E.1). Using just the first term on the right-hand side of Eq. (E.1), we have

$$f(0.22) \approx f(0.2) = 0.9511$$

This corresponds to point 3 in Fig. E4.1. The percentage error in this estimate is $[(0.9823 - 0.9511)/0.9823] \times 100 = 3.176$ percent. Using two terms in Eq. (E.1),

$$\begin{aligned} f(x+\Delta x) &\approx f(x) + \frac{\partial f}{\partial x}\Delta x \\ f(0.22) &\approx f(0.2) + 2\pi \cos\,[2\pi(0.2)](0.02) \\ &\approx 0.9511 + 0.388 = 0.9899 \end{aligned}$$

This corresponds to point 4 in Fig. E4.1. The percentage error in this estimate is $[0.9899 - 0.9823)/0.9823] \times 100 = 0.775$ percent. This is much closer than the previous estimate. Finally, to obtain yet an even better estimate, let us use three terms in Eq. (E.1).

$$f(x+\Delta x) \approx f(x) + \frac{\partial f}{\partial x}\Delta x + \frac{\partial^2 f}{\partial x^2}\frac{(\Delta x)^2}{2}$$

$$\begin{aligned} f(0.22) &\approx f(0.2) + 2\pi \cos\,[2\pi(0.2)](0.02) - 4\pi^2 \sin\,[2\pi(0.2)]\frac{(0.02)^2}{2} \\ &\approx 0.9511 + 0.0388 - 0.0075 \\ &\approx 0.9824 \end{aligned}$$

This corresponds to point 5 in Fig. E4.1. The percentage error in this estimate is $[(0.9824 - 0.9823)/0.9823] \times 100 = 0.01$ percent. *This is a very close estimate of $f(0.22)$ using just three terms in the Taylor series given by Eq. (E.1).*

Let us now return to Eq. (4.1) and pursue our discussion of finite-difference representations of derivatives. Solving Eq. (4.1) for $(\partial u/\partial x)_{i,j}$, we obtain

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \underbrace{\frac{u_{i+1,j} - u_{i,j}}{\Delta x}}_{\substack{\text{Finite-}\\ \text{difference}\\ \text{representation}}} \underbrace{- \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}\frac{\Delta x}{2} - \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j}\frac{(\Delta x)^2}{6} + \cdots}_{\text{Truncation error}} \tag{4.2}$$

In Eq. (4.2), the actual partial derivative evaluated at point (i, j) is given on the left side. The first term on the right side, namely, $(u_{i+1,j} - u_{i,j})/\Delta x$, is a finite-difference representation of the partial derivative. The remaining terms on the right side constitute the *truncation error*. That is, if we wish to *approximate* the partial derivative with the above algebraic finite-difference quotient,

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} \approx \frac{u_{i+1,j} - u_{i,j}}{\Delta x} \tag{4.3}$$

then the truncation error in Eq. (4.2) tells us what is being neglected in this approximation. In Eq. (4.2), the lowest-order term in the truncation error involves Δx to the first power; hence, the finite-difference expression in Eq. (4.3) is called *first-order-accurate*. We can more formally write Eq. (4.2) as

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + O(\Delta x) \tag{4.4}$$

In Eq. (4.4), the symbol $O(\Delta x)$ is a formal mathematical notation which represents "terms of order Δx." Equation (4.4) is a more precise notation than Eq. (4.3), which involves the "approximately equal" notation; in Eq. (4.4) the order of magnitude of the truncation error is shown explicitly by the notation. Also referring to Fig. 4.1, note that the finite-difference expression in Eq. (4.4) uses information to the *right* of grid point (i, j); that is, it uses $u_{i+1,j}$ as well as $u_{i,j}$. No information to the left of (i, j) is used. As a result, the finite difference in Eq. (4.4) is called a *forward difference*. For this reason, we now identify the first-order-accurate difference representation for the derivative $(\partial u/\partial x)_{i,j}$ expressed by Eq. (4.4) as a *first-order forward difference*, repeated below.

$$\boxed{\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + O(\Delta x)} \tag{4.4}$$

Let us now write a Taylor series expansion for $u_{i-1,j}$, expanded about $u_{i,j}$.

$$u_{i-1,j} = u_{i,j} + \left(\frac{\partial u}{\partial x}\right)_{i,j}(-\Delta x) + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}\frac{(-\Delta x)^2}{2} + \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j}\frac{(-\Delta x)^3}{6} + \cdots$$

or

$$u_{i-1,j} = u_{i,j} - \left(\frac{\partial u}{\partial x}\right)_{i,j}\Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}\frac{(\Delta x)^2}{2} - \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j}\frac{(\Delta x)^3}{6} + \cdots \tag{4.5}$$

Solving for $(\partial u/\partial x)_{i,j}$, we obtain

$$\boxed{\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i,j} - u_{i-1,j}}{\Delta x} + O(\Delta x)} \tag{4.6}$$

The information used in forming the finite-difference quotient in Eq. (4.6) comes from the *left* of grid point (i, j); that is, it uses $u_{i-1,j}$ as well as $u_{i,j}$. No information to the right of (i, j) is used. As a result, the finite difference in Eq. (4.6) is called a *rearward* (or *backward*) *difference*. Moreover, the lowest-order term in the truncation error involves Δx to the first power. As a result, the finite difference in Eq. (4.6) is called a *first-order rearward difference.*

In most applications in CFD, first-order accuracy is not sufficient. To construct a finite-difference quotient of second-order accuracy, simply subtract Eq. (4.5) from Eq. (4.1):

$$u_{i+1,j} - u_{i-1,j} = 2\left(\frac{\partial u}{\partial x}\right)_{i,j}\Delta x + 2\left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j}\frac{(\Delta x)^3}{6} + \cdots \tag{4.7}$$

Equation (4.7) can be written as

$$\boxed{\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} + O(\Delta x)^2} \tag{4.8}$$

The information used in forming the finite-difference quotient in Eq. (4.8) comes from *both* sides of the grid point located at (i, j); that is, it uses $u_{i+1,j}$ as well as $u_{i-1,j}$. Grid point (i, j) falls between the two adjacent grid points. Moreover, in the truncation error in Eq. (4.7), the lowest-order terms involves $(\Delta x)^2$, which is second-order accuracy. Hence, the finite-difference quotient in Eq. (4.8) is called a *second-order central difference.*

Difference expressions for the y derivatives are obtained in exactly the same fashion. (See Prob. 4.1 and 4.2.) The results are directly analogous to the previous equations for the x derivatives. They are:

$$\left(\frac{\partial u}{\partial y}\right)_{i,j} = \begin{cases} \dfrac{u_{i,j+1} - u_{i,j}}{\Delta y} + O(\Delta y) & \textit{Forward difference} \quad (4.9) \\[2ex] \dfrac{u_{i,j} - u_{i,j-1}}{\Delta y} + O(\Delta y) & \textit{Rearward difference} \quad (4.10) \\[2ex] \dfrac{u_{i,j+1} - u_{i,j-1}}{2\Delta y} + O(\Delta y)^2 & \textit{Central difference} \quad (4.11) \end{cases}$$

Equations (4.4), (4.6), and (4.8) to (4.11) are examples of finite-difference quotients for *first* partial derivatives. Is this all that we need for CFD? Let us return to Chap. 2 for a moment and take a look at the governing equations of motion. If we are dealing with inviscid flows only, the governing equations are the Euler equations, summarized in Sec. 2.8.2 and expressed by Eqs. (2.82) to (2.86). Note that the highest-order derivatives which appear in the Euler equations are first partial derivatives. Hence, finite differences for the first derivatives, such as those expressed by Eqs. (4.4), (4.6), and (4.8), are all that we need for the numerical solution of inviscid flows. On the other hand, if we are dealing with viscous flows, the governing equations are the Navier-Stokes equations, summarized in Sec. 2.8.1 and expressed by Eqs. (2.29), (2.50), (2.56), and (2.66). Note that the highest-order derivatives which appear in the Navier-Stokes equations are *second* partial derivatives, as reflected in the viscous terms such as $\partial\tau_{xy}/\partial x = \partial/\partial x\ [\mu(\partial v/\partial x + \partial u/\partial y)]$ which appears in Eq. (2.50*b*), and $\partial/\partial x\ (k\ \partial T/\partial x)$ which appears in Eq. (2.66). When expanded, these terms involve such second partial derivatives as $\partial^2 u/\partial x\,\partial y$ and $\partial^2 T/\partial x^2$, just for example. Consequently, there is a need for discretizing second-order derivatives for CFD. We can obtain such finite-difference expressions by continuing with a Taylor series analysis, as follows.

Summing the Taylor series expansions given by Eqs. (4.1) and (4.5), we have

$$u_{i+1,j} + u_{i-1,j} = 2u_{i,j} + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}(\Delta x)^2 + \left(\frac{\partial^4 u}{\partial x^4}\right)_{i,j}\frac{(\Delta x)^4}{12} + \cdots$$

Solving for $(\partial^2 u/\partial x)_{i,j}$,

$$\boxed{\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2} + O(\Delta x)^2} \qquad (4.12)$$

In Eq. (4.12), the first term on the right-hand side is a central finite difference for the second derivative with respect to x evaluated at grid point (i, j); from the remaining order-of-magnitude term, we see that this central difference is of second-order accuracy. An analogous expression can easily be obtained for the second derivative with respect to y, with the result that

$$\left(\frac{\partial^2 u}{\partial y^2}\right)_{i,j} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\Delta y)^2} + O(\Delta y)^2 \tag{4.13}$$

Equations (4.12) and (4.13) are examples of *second-order central second differences.*

For the case of mixed derivatives, such as $\partial^2 u/\partial x\, \partial y$, appropriate finite-difference quotients can be found as follows. Differentiating Eq. (4.1) with respect to y, we have

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j} = \left(\frac{\partial u}{\partial y}\right)_{i,j} + \left(\frac{\partial^2 u}{\partial x\, \partial y}\right)_{i,j} \Delta x + \left(\frac{\partial^3 u}{\partial x^2\, \partial y}\right)_{i,j} \frac{(\Delta x)^2}{2} + \left(\frac{\partial^4 u}{\partial x^3\, \partial y}\right)_{i,j} \frac{(\Delta x)^3}{6} + \cdots \tag{4.14}$$

Differentiating Eq. (4.5) with respect to y, we have

$$\left(\frac{\partial u}{\partial y}\right)_{i-1,j} = \left(\frac{\partial u}{\partial y}\right)_{i,j} - \left(\frac{\partial^2 u}{\partial x\, \partial y}\right)_{i,j} \Delta x + \left(\frac{\partial^3 u}{\partial x^2\, \partial y}\right)_{i,j} \frac{(\Delta x)^2}{2} + \left(\frac{\partial^4 u}{\partial x^3\, \partial y}\right)_{i,j} \frac{(\Delta x)^3}{6} + \cdots \tag{4.15}$$

Subtracting Eq. (4.15) from Eq. (4.14) yields

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j} - \left(\frac{\partial u}{\partial y}\right)_{i-1,j} = 2\left(\frac{\partial^2 u}{\partial x\, \partial y}\right)_{i,j} \Delta x + \left(\frac{\partial^4 u}{\partial x^3\, \partial y}\right)_{i,j} \frac{(\Delta x)^3}{6} + \cdots$$

Solving for $(\partial^2 u/\partial x\, \partial y)_{i,j}$, which is the mixed derivative for which we are seeking a finite-difference expression, the above equation yields

$$\left(\frac{\partial^2 u}{\partial x\, \partial y}\right)_{i,j} = \frac{(\partial u/\partial y)_{i+1,j} - (\partial u/\partial y)_{i-1,j}}{2\Delta x} - \left(\frac{\partial^4 u}{\partial x^3\, \partial y}\right)_{i,j} \frac{(\Delta x)^2}{12} + \cdots \tag{4.16}$$

In Eq. (4.16), the first term on the right-hand-side involves $\partial u/\partial y$, first evaluated at grid point $(i + 1, j)$ and then at grid point $(i - 1, j)$. Returning to the grid sketched in Fig. 4.1, we can see that $\partial u/\partial y$ at each of these two grid points can be replaced with a second-order central difference patterned after that given by Eq. (4.11) but using appropriate grid points first centered on $(i + 1, j)$ and then on $(i - 1, j)$. To be more specific, in Eq. (4.16) first replace $(\partial u/\partial y)_{i+1,j}$ with

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j} = \frac{u_{i+1,j+1} - u_{i+1,j-1}}{2\Delta y} + O(\Delta y)^2$$

and then replace $(\partial u/\partial y)_{i-1,j}$ with the analogous difference,

$$\left(\frac{\partial u}{\partial y}\right)_{i-1,j} = \frac{u_{i-1,j+1} - u_{i-1,j-1}}{2\Delta y} + O(\Delta y)^2$$

In this fashion, Eq. (4.16) becomes

$$\boxed{\left(\frac{\partial^2 u}{\partial x\, \partial y}\right)_{i,j} = \frac{u_{i+1,j+1} - u_{i+1,j-1} - u_{i-1,j+1} + u_{i-1,j-1}}{4\Delta x\, \Delta y} + O[(\Delta x)^2, (\Delta y)^2]} \tag{4.17}$$

The truncation error in Eq. (4.17) comes from Eq. (4.16), where the lowest-order neglected term is of $O(\Delta x)^2$, and from the fact that the central difference in Eq. (4.11) is of $O(\Delta y)^2$, Hence, the truncation error in Eq. (4.17) must be $O[(\Delta x)^2, (\Delta y)^2]$. Equation (4.17) gives a *second-order central difference for the mixed derivative*, $(\partial^2 u/\partial x\, \partial y)_{i,j}$.

It is important to note that when the governing flow equations are used in the form of Eq. (2.93), only first derivatives are needed, even for viscous flows. The dependent variables being differentiated are U, F, G, and H in Eq. (2.93), and only as first derivatives. Hence, these derivatives can be replaced with the appropriate finite-difference expressions for first derivatives, such as Eqs. (4.4), (4.6), and (4.8) to (4.11). In turn, some elements of F, G, and H involve viscous stresses, such as τ_{xx}, τ_{xy}, and thermal conduction terms. These terms depend on velocity or temperature gradients, which are also first derivatives. Hence, the finite-difference forms for first derivatives can also be used for the viscous terms *inside* F, G, and H. In this fashion, the need to use a finite-difference expression for second derivatives, such as Eqs. (4.12), (4.13), and (4.17), is circumvented.

To this stage, we have derived a number of different forms of finite-difference expressions for various partial derivatives. To help reinforce these finite differences in your mind, the graphical concept of *finite-difference modules* is useful. All the above difference expressions can be nicely displayed in the context of the finite-difference modules shown in Fig. 4.3. This figure is a concise review of the finite-difference forms we have discussed, as well as illustrating on a grid the specific grid points that participate in the formation of each finite difference. These participating grid points are shown by large filled circles connected by bold lines; such a schematic is called a finite-difference module. The plus and minus signs adjacent to the participating grid points remind us of whether the information at each of these points is added or subtracted to form the appropriate finite differences; similarly, a (-2) beside a grid point connotes that twice the variable at that grid point is subtracted in the formation of the finite-difference quotient. Compare the (+), $(-)$, and (-2) in the finite-difference modules with the corresponding formula for the finite difference which appears to the left of each module in Fig. 4.3.

The finite-difference expressions derived in this section and displayed in Fig. 4.3 represent just the "tip of the iceberg." Many other difference approximations can be obtained for the same derivatives we treated above. In particular, more

First-order forward difference with respect to x $\quad \left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x}$

First-order rearward difference with respect to x $\quad \left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i,j} - u_{i-1,j}}{\Delta x}$

Second-order central difference with respect to x $\quad \left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x}$

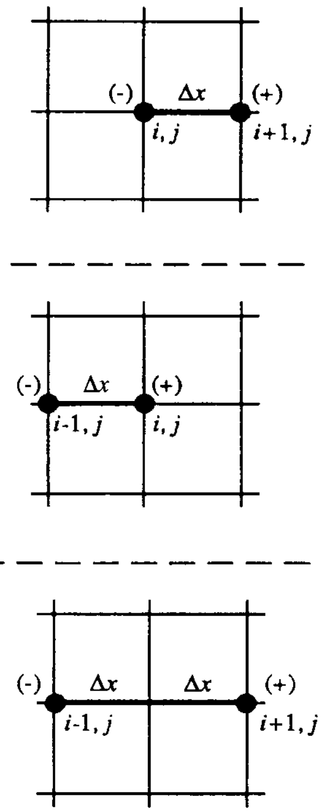


FIG. 4.3
Finite-difference expressions with their appropriate finite-difference modules.

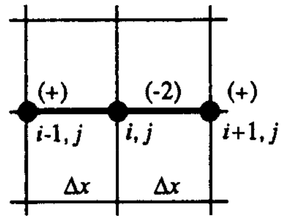
accurate finite-difference quotients can be derived, exhibiting third-order accuracy, fourth-order accuracy, and more. Such higher-order-accurate difference quotients generally involve information at more grid points than those we have derived. For example, a fourth-order-accurate central finite-difference for $\partial^2 u/\partial x^2$ is

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} = \frac{-u_{i+2,j} + 16u_{i+1,j} - 30u_{i,j} + 16u_{i-1,j} - u_{i-2,j}}{12(\Delta x)^2} + \mathrm{O}(\Delta x)^4 \qquad (4.18)$$

Note that information at five grid points is required to form this fourth-order finite difference; compare this with Eq. (4.12), where $(\partial^2 u/\partial x^2)_{i,j}$ is represented in terms of information at only three grid points, albeit with only second-order accuracy. Equation (4.18) can be derived by repeated application of Taylor's series expanded about grid points $(i + 1, j)$, (i, j), and $(i - 1, j)$; the details are considered in Prob. 4.5. We are simply emphasizing that an almost unlimited number of finite-difference expressions can be derived with ever-increasing accuracy. In the past, second-order accuracy has been considered sufficient for most CFD applications, so the types of difference quotients we have derived in this section have been, by far, the most

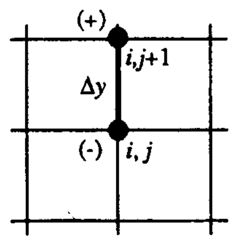
Second-order central second difference with respect to x

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2}$$



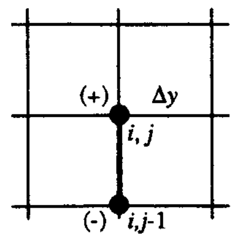
First-order forward difference with respect to y

$$\left(\frac{\partial u}{\partial y}\right)_{i,j} = \frac{u_{i,j+1} - u_{i,j}}{\Delta y}$$



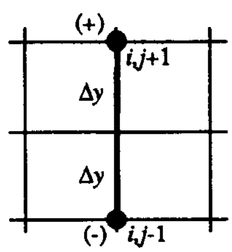
First-order rearward difference with respect to y

$$\left(\frac{\partial u}{\partial y}\right)_{i,j} = \frac{u_{i,j} - u_{i,j-1}}{\Delta y}$$



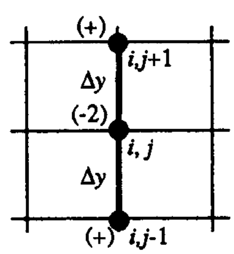
Second-order central difference with respect to y

$$\left(\frac{\partial u}{\partial y}\right)_{i,j} = \frac{u_{i,j+1} - u_{i,j-1}}{2\Delta y}$$



Second-order central second difference with respect to y

$$\left(\frac{\partial^2 u}{\partial y^2}\right)_{i,j} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\Delta y)^2}$$



Second-order central mixed difference with respect to x and y

$$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j} = \frac{u_{i+1,j+1} + u_{i-1,j-1} - u_{i-1,j+1} - u_{i+1,j-1}}{4\Delta x\, \Delta y}$$

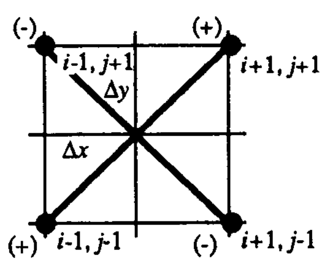


FIG. 4.3 *(continued)*

commonly used forms. The pros and cons of higher-order accuracy are as follows:

1. Higher-order-accurate difference quotients, such as displayed in Eq. (4.18), by requiring more grid points, result in more computer time required for each time wise or spatial step—a con.
2. On the other hand, a higher-order difference scheme may require a smaller number of total grid points in a flow solution to obtain comparable overall accuracy—a pro.
3. Higher-order difference schemes may result in a "higher- quality" solution, such as captured shock waves that are sharper and more distinct—also a pro. In fact, this aspect is a matter of current research in CFD.

For these reasons, the matter of what degree of accuracy is desirable for various CFD solutions is not clear-cut. Because second-order accuracy has been previously accepted in the vast majority of CFD applications, and because the purpose of this book is to present a basic introduction to the elements of CFD without undue complication, we will consider that second-order accuracy will be sufficient for our purposes in this and subsequent chapters. For a detailed tabulation of many forms of difference quotients, see pp. 44 and 45 of Ref. 13.

We have one more item of business before finishing this section on finite-difference quotients. We pose the following question: What happens at a boundary? What type of differencing is possible when we have only one direction to go, namely, the direction away from the boundary? For example, consider Fig. 4.4, which illustrates a portion of a boundary to a flow field, with the y axis perpendicular to the boundary. Let grid point 1 be on the boundary, with points 2 and 3 a distance Δy and $2\Delta y$ above the boundary, respectively. We wish to construct a finite-difference approximation for $\partial u/\partial y$ at the boundary. It is easy to construct a forward difference as

$$\left(\frac{\partial u}{\partial y}\right)_1 = \frac{u_2 - u_1}{\Delta y} + O(\Delta y) \tag{4.19}$$

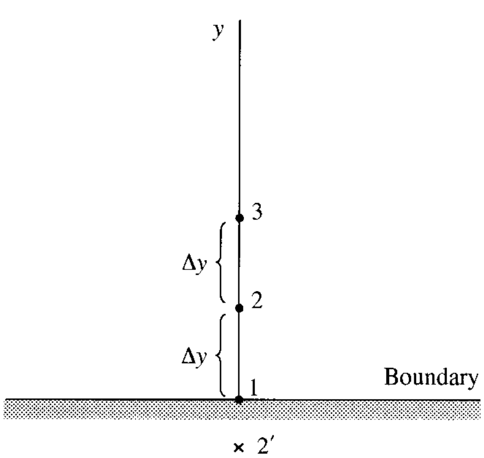


FIG. 4.4
Grid points at a boundary

which is of first-order accuracy. However, how do we obtain a result which is of second-order accuracy? Our central difference in Eq. (4.11) fails us because it requires another point beneath the boundary, such as illustrated as point $2'$ in Fig. 4.4. Point $2'$ is outside the domain of computation, and we generally have no information about u at this point. In the early days of CFD, many solutions attempted to sidestep this problem by assuming that $u_{2'} = u_2$. This is called the *reflection boundary condition*. In most cases it does not make physical sense and is just as inaccurate, if not more so, than the forward difference given by Eq. (4.19).

So we ask the question again, how do we find a second-order-accurate finite-difference at the boundary? The answer is straightforward, as we will describe here. Moreover, we will seize this occasion to illustrate an alternative approach to the construction of finite-difference quotients—alternative to the Taylor's series analyses presented earlier. We will use a *polynomial approach*, as follows. Assume at the boundary shown in Fig. 4.4 that u can be expressed by the polynomial

$$u = a + by + cy^2 \tag{4.20}$$

Applied successively to the grid points in Fig. 4.4, Eq. (4.20) yields at grid point 1 where $y = 0$,

$$u_1 = a \tag{4.21}$$

and at grid point 2 where $y = \Delta y$,

$$u_2 = a + b\,\Delta y + c(\Delta y)^2 \tag{4.22}$$

and at grid point 3 where $y = 2\Delta y$,

$$u_3 = a + b(2\Delta y) + c(2\Delta y)^2 \tag{4.23}$$

Solving Eqs. (4.21) to (4.23) for b, we obtain

$$b = \frac{-3u_1 + 4u_2 - u_3}{2\Delta y} \tag{4.24}$$

Returning to Eq. (4.20), and differentiating with respect to y,

$$\frac{\partial u}{\partial y} = b + 2cy \tag{4.25}$$

Equation (4.25), evaluated at the boundary where $y = 0$, yields

$$\left(\frac{\partial u}{\partial y}\right)_1 = b \tag{4.26}$$

Combining Eqs. (4.24) and (4.26), we obtain

$$\left(\frac{\partial u}{\partial y}\right)_1 = \frac{-3u_1 + 4u_2 - u_3}{2\Delta y} \tag{4.27}$$

Equation (4.27) is a one-sided finite-difference expression for the derivative at the boundary—called *one-sided* because it uses information only on one side of the grid point at the boundary, namely, information only *above* grid point 1 in Fig. 4.4. Also, Eq. (4.27) was derived using a polynomial expression, namely, Eq. (4.20), rather than a Taylor series representation. This illustrates an alternative approach to the formulation of finite-difference quotients; indeed, all our previous results as summarized in Fig. 4.3 could have been obtained using this polynomial approach. It remains to show the order of accuracy of Eq. (4.27). Here, we have to appeal to a Taylor series again. Consider a Taylor series expansion about the point 1.

$$u(y) = u_1 + \left(\frac{\partial u}{\partial y}\right)_1 y + \left(\frac{\partial^2 u}{\partial y^2}\right)_1 \frac{y^2}{2} + \left(\frac{\partial^3 u}{\partial y^3}\right)_1 \frac{y^3}{6} + \cdots \tag{4.28}$$

Compare Eqs. (4.28) and (4.20). Our assumed polynomial expression in Eq. (4.20) is the same as using the first three terms in the Taylor series. Hence, Eq. (4.20) is of $O(\Delta y)^3$. Now examine the numerator of Eq. (4.27); here u_1, u_2, and u_3 can all be expressed in terms of the polynomial given by Eq. (4.20). Since Eq. (4.20) is of $O(\Delta y)^3$, then the numerator of Eq. (4.27) is also of $O(\Delta y)^3$. However, in forming the derivative in Eq. (4.27), we divided by Δy, which then makes Eq. (4.27) of $O(\Delta y)^2$. Thus, we can write from Eq. (4.27)

$$\left(\frac{\partial u}{\partial y}\right)_1 = \frac{-3u_1 + 4u_2 - u_3}{2\Delta y} + O(\Delta y)^2 \tag{4.29}$$

This is our desired second-order-accurate difference quotient at the boundary.

Both Eqs. (4.19) and (4.29) are called *one-sided differences*, because they express a derivative at a point in terms of dependent variables on *only one side* of that point. Moreover, these equations are general; i.e., they are not in any way limited to application just at a boundary; they can be applied at internal grid points as well. It just so happens that we have taken advantage of our discussion of finite-difference quotients at a boundary to derive such one-sided differences. Of course, as we have seen here, one-sided differences are essentially mandatory for a representation of a derivative at a boundary, but such one-sided differences simply offer another option when applied *internally* within the domain of the overall calculations. Furthermore, Eq. (4.29) displays a one-sided finite difference of second-order accuracy; many other one-sided difference formulas for a derivative at a point can be derived with higher orders of accuracy using additional grid points to one side of that point. In some CFD applications, it is not unusual to see four- and five-point one-sided differences applied at a boundary. This is especially true for viscous flow calculations. In such calculations, the shear stress and heat transfer at the wall, due to a flow over that wall, are of particular importance. The shear stress at the wall is given by (see, for example, chap. 12 of Ref. 8)

$$\tau_w = \mu\left(\frac{\partial u}{\partial y}\right)_w \tag{4.30}$$