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

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

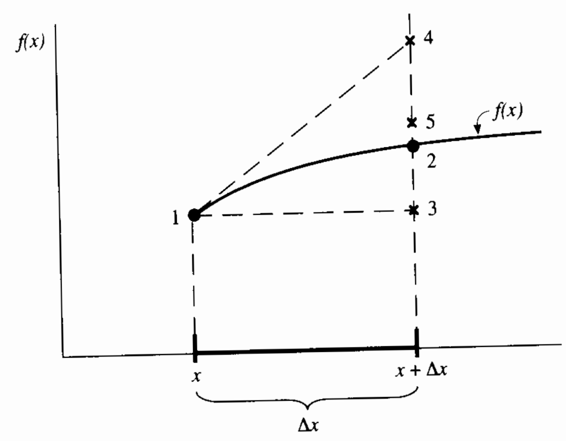

FIG. E4.1
Illustration of behavior of the first three terms in a Taylor series (for Example 4.1).

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

$$f(x) = \sin 2\pi x \tag{E.2}$$

$$\text{At } x = 0.2: \qquad f(x) = 0.9511$$

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),

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

$$f(0.22) \approx f(0.2) + 2\pi \cos[2\pi(0.2)](0.02)$$

$$\approx 0.9511 + 0.388 = 0.9899$$

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