Derivation of Finite Difference Equations

The basic idea of finite difference methods is simple: derivatives in differential equations are written in terms of discrete quantities of dependent and independent variables, resulting in simultaneous algebraic equations with all unknowns prescribed at discrete mesh points for the entire domain.

In fluid dynamics applications, appropriate types of differencing schemes and suitable methods of solution are chosen, depending on the particular physics of the flows, which may include inviscid, viscous, incompressible, compressible, irrotational, rotational, laminar, turbulent, subsonic, transonic, supersonic, or hypersonic flows. Different forms of the finite difference equations are written to conform to these different physical phenomena encountered in fluid dynamics.

In this chapter, we present various methods for deriving finite difference equations of low and high orders of accuracy. Truncation errors, as related to the orders of accuracy involved in the approximations, will also be discussed.

3.1 SIMPLE METHODS

Consider a function $u(x)$ and its derivative at point x,

$$\frac{\partial u(x)}{\partial x} = \lim_{\Delta x \to 0} \frac{u(x + \Delta x) - u(x)}{\Delta x} \tag{3.1.1}$$

If $u(x + \Delta x)$ is expanded in Taylor series about $u(x)$, we obtain

$$u(x + \Delta x) = u(x) + \Delta x \frac{\partial u(x)}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 u(x)}{\partial x^2} + \frac{(\Delta x)^3}{3!} \frac{\partial^3 u(x)}{\partial x^3} + \cdots \tag{3.1.2}$$

Substituting (3.1.2) into (3.1.1) yields

$$\frac{\partial u(x)}{\partial x} = \lim_{\Delta x \to 0} \left(\frac{\partial u(x)}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 u(x)}{\partial x^2} + \cdots \right) \tag{3.1.3}$$

Or it is seen from (3.1.2) that

$$\frac{u(x + \Delta x) - u(x)}{\Delta x} = \frac{\partial u(x)}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 u(x)}{\partial x^2} + \cdots = \frac{\partial u(x)}{\partial x} + \mathrm{O}(\Delta x) \tag{3.1.4}$$

The derivative $\frac{\partial u(x)}{\partial x}$ in (3.1.4) is of first order in Δx, indicating that the truncation error $\mathrm{O}(\Delta x)$ goes to zero like the first power in Δx. The finite difference form given by (3.1.1), (3.1.3), and (3.1.4) is said to be of the first order accuracy.

Referring to Figure 1.2.1, we may write u in Taylor series at $i+1$ and $i-1$,

$$u_{i+1} = u_i + \Delta x\left(\frac{\partial u}{\partial x}\right)_i + \frac{\Delta x^2}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i + \frac{\Delta x^3}{3!}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \frac{\Delta x^4}{4!}\left(\frac{\partial^4 u}{\partial x^4}\right)_i + \cdots \tag{3.1.5}$$

$$u_{i-1} = u_i - \Delta x\left(\frac{\partial u}{\partial x}\right)_i + \frac{\Delta x^2}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i - \frac{\Delta x^3}{3!}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \frac{\Delta x^4}{4!}\left(\frac{\partial^4 u}{\partial x^4}\right)_i + \cdots \tag{3.1.6}$$

Rearranging (3.1.5), we arrive at the forward difference:

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1} - u_i}{\Delta x} + \mathrm{O}(\Delta x) \tag{3.1.7}$$

Likewise, from (3.1.6), we have the backward difference:

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_i - u_{i-1}}{\Delta x} + \mathrm{O}(\Delta x) \tag{3.1.8}$$

A central difference is obtained by subtracting (3.1.6) from (3.1.5):

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + \mathrm{O}(\Delta x^2) \tag{3.1.9}$$

It is seen that the truncation errors for the forward and backward differences are first order, whereas the central difference yields a second order truncation error.

Finally, by adding (3.1.5) and (3.1.6), we have

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} = \left(\frac{\partial^2 u}{\partial x^2}\right)_i + \frac{(\Delta x)^2}{12}\left(\frac{\partial^4 u}{\partial x^4}\right)_i + \cdots \tag{3.1.10}$$

This leads to the finite difference formula for the second derivative with second order accuracy,

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + \mathrm{O}(\Delta x^2) \tag{3.1.11}$$

Note that these results were intuitively obtained in Section 1.2 by approximations of slopes of a curve, without the notion of truncation errors.

3.2 GENERAL METHODS

In general, finite difference equations may be generated for any order derivative with any number of points involved (any order accuracy). For example, let us consider a first derivative associated with three points such that

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{au_i + bu_{i-1} + cu_{i-2}}{\Delta x} \tag{3.2.1}$$

The coefficients a, b, c may be determined from a Taylor series expansion of upstream nodes u_{i-1} and u_{i-2} about u_i (one-sided upstream or backward difference)

$$u_{i-1} = u_i + (-\Delta x)\left(\frac{\partial u}{\partial x}\right)_i + \frac{(-\Delta x)^2}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i + \frac{(-\Delta x)^3}{3!}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \cdots \tag{3.2.2a}$$

$$u_{i-2} = u_i + (-2\Delta x)\left(\frac{\partial u}{\partial x}\right)_i + \frac{(-2\Delta x)^2}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i + \frac{(-2\Delta x)^3}{3!}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \cdots \tag{3.2.2b}$$

from which we obtain

$$\begin{aligned} au_i + bu_{i-1} + cu_{i-2} &= (a+b+c)u_i - \Delta x(b+2c)\left(\frac{\partial u}{\partial x}\right)_i \\ &\quad + \frac{\Delta x^2}{2}(b+4c)\left(\frac{\partial^2 u}{\partial x^2}\right)_i + \mathrm{O}(\Delta x^3) \end{aligned} \tag{3.2.3}$$

It follows from (3.2.1) and (3.2.3) that the following three conditions must be satisfied:

$$a + b + c = 0 \tag{3.2.4a}$$

$$b + 2c = -1 \tag{3.2.4b}$$

$$b + 4c = 0 \tag{3.2.4c}$$

The solution of (3.2.4) yields $a = 3/2$, $b = -2$, and $c = 1/2$. Thus, from (3.2.1) we obtain

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{3u_i - 4u_{i-1} + u_{i-2}}{2\Delta x} + \mathrm{O}(\Delta x^2) \tag{3.2.5}$$

If the downstream nodes u_{i+1} and u_{i+2} are used (one-sided downstream or forward difference), then we have

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{-3u_i + 4u_{i+1} - u_{i+2}}{2\Delta x} + \mathrm{O}(\Delta x^2) \tag{3.2.6}$$

A similar approach may be used to determine the finite difference formula for a second derivative. In view of (3.2.3) and setting

$$a + b + c = 0 \tag{3.2.7a}$$

$$b + 2c = 0 \tag{3.2.7b}$$

$$b + 4c = 2 \tag{3.2.7c}$$

we obtain

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{u_i - 2u_{i-1} + u_{i-2}}{\Delta x^2} + \Delta x \frac{\partial^3 u}{\partial x^3} + \cdots \tag{3.2.8}$$

This implies that the one-sided formula provides only the first order accuracy in contrast to the two-sided formula, which gives the second order accuracy as seen in (3.1.11).

The foregoing procedure may be transformed into a systematic form in terms of "displacement" and "difference" operators so that difference formulas may be obtained with a preselected order of accuracy [Hildebrand, 1956; Kopal, 1961; Collatz, 1966], among others. These results are summarized next.

Forward Difference Formulas

The Taylor series expansion (3.1.2) may be written in terms of the displacement operator E and the derivative operator D,

$$Eu(x) = [1 + \Delta x D + (\Delta x D)^2/2! + (\Delta x D)^3/3! + \cdots]\, u(x) \tag{3.2.9}$$

with $Du = \frac{\partial u}{\partial x}$, $E = e^{\Delta x D}$, and $D = \frac{1}{\Delta x} \ln E$. These definitions lead to the first derivative of u at i in the form

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{1}{\Delta x} \ln(1 + \delta^+) u_i = \frac{1}{\Delta x}\left(\delta^+ - \frac{\delta^{+2}}{2} + \frac{\delta^{+3}}{3} - \frac{\delta^{+4}}{4} + \cdots\right) u_i \tag{3.2.10}$$

where δ^+ is the forward difference operator,

$$\delta^+ = E - 1, \qquad \delta^+ u_i = u_{i+1} - u_i \tag{3.2.11}$$

with E being defined such that

$$Eu_i = u_{i+1}, \qquad E^n u_i = u_{i+n} \tag{3.2.12}$$

It is now obvious that the order of accuracy increases with the number of terms kept on the right-hand side of (3.2.10) given by

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{1}{\Delta x}\left((E - 1) - \frac{(E-1)^2}{2} + \frac{(E-1)^3}{3} - \frac{(E-1)^4}{4} + \cdots\right) u_i \tag{3.2.13}$$

which leads to

First Order Accuracy

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1} - u_i}{\Delta x} - \frac{\Delta x}{2} \frac{\partial^2 u}{\partial x^2} \tag{3.2.14}$$

Second Order Accuracy

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{-3u_i + 4u_{i+1} - u_{i+2}}{2\Delta x} + \frac{\Delta x^2}{3} \frac{\partial^3 u}{\partial x^3} \tag{3.2.15}$$

Backward Difference Formulas

A backward difference formula can be derived similarly in the form

$$\begin{aligned}\left(\frac{\partial u}{\partial x}\right)_i &= \frac{-1}{\Delta x} \ln(1 - \delta^-) u_i = \frac{1}{\Delta x}\left(\delta^- + \frac{\delta^{-2}}{2} + \frac{\delta^{-3}}{3} + \frac{\delta^{-4}}{4} + \cdots\right) u_i \\ &= \frac{1}{\Delta x}\left[(1 - E^{-1}) + \frac{(1 - E^{-1})^2}{2} + \frac{(1 - E^{-1})^3}{3} + \frac{(1 - E^{-1})^4}{4} + \cdots\right] u_i\end{aligned} \tag{3.2.16}$$

where δ^- is the backward difference operator,

$$\delta^- = 1 - E^{-1}, \qquad \delta^- u_i = u_i - u_{i-1} \tag{3.2.17}$$

with

$$E^{-1} u_i = u_{i-1} \tag{3.2.18}$$

These definitions lead to the following schemes:

First Order Accuracy

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_i - u_{i-1}}{\Delta x} + \frac{\Delta x}{2}\frac{\partial^2 u}{\partial x^2} \tag{3.2.19}$$

Second Order Accuracy

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{3u_i - 4u_{i-1} + u_{i-2}}{2\Delta x} + \frac{\Delta x^2}{3}\frac{\partial^3 u}{\partial x^3} \tag{3.2.20}$$

Central Difference Formulas

The central difference formulas are derived using the following definitions:

$$\delta u_i = u_{i+1/2} - u_{i-1/2} = \left(E^{1/2} - E^{-1/2}\right)u_i \tag{3.2.21}$$

with

$$\delta = e^{\Delta x D/2} - e^{-\Delta x D/2} = 2\sinh(\Delta x D/2) \tag{3.2.22}$$

which leads to the first derivative of u at i in the form

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{1}{\Delta x}\left(2\sinh^{-1}\frac{\delta}{2}\right)u_i = \frac{1}{\Delta x}\left(\delta - \frac{\delta^3}{24} + \frac{3\delta^5}{640} - \frac{5\delta^7}{7168} + \cdots\right)u_i \tag{3.2.23}$$

With these definitions, we obtain

Second Order Accuracy (with the first term)

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+\frac{1}{2}} - u_{i-\frac{1}{2}}}{\Delta x} - \frac{\Delta x^2}{24}\frac{\partial^3 u}{\partial x^3} \tag{3.2.24}$$

Fourth Order Accuracy (with the first two terms)

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{1}{24\Delta x}\left(-u_{i+\frac{3}{2}} + 27u_{i+\frac{1}{2}} - 27u_{i-\frac{1}{2}} + u_{i-\frac{3}{2}}\right) + \frac{3}{640}\Delta x^4\frac{\partial^5 u}{\partial x^5} \tag{3.2.25}$$

The half-integer mesh points may be avoided by choosing

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{1}{\Delta x}\left(\bar{\delta} - \frac{\bar{\delta}^3}{3!} + \frac{3^2}{5!}\bar{\delta}^5 + \cdots\right)u_i \tag{3.2.26}$$

where $\bar{\delta}$ is the alternative central difference operator such that

$$\bar{\delta}u_i = \frac{1}{2}(E - E^{-1})\,u_i = \frac{1}{2}(u_{i+1} - u_{i-1}) \tag{3.2.27}$$

These definitions provide

Second Order Accuracy

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} - \frac{(\Delta x)^2}{6}\frac{\partial^3 u}{\partial x^3} \tag{3.2.28}$$

Fourth Order Accuracy

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{-u_{i+2} + 8u_{i+1} - 8u_{i-1} + u_{i-2}}{12\Delta x} + \frac{\Delta x^4}{30}\frac{\partial^5 u}{\partial x^5} \tag{3.2.29}$$

3.3 HIGHER ORDER DERIVATIVES

Finite difference formulas for higher-order derivatives may be derived using the operator technique similarly to the one employed for the first order derivative. Let us consider the forward difference relation given by (3.2.10) and extend it to higher order derivatives as

$$\begin{aligned}\left(\frac{\partial^n u}{\partial x^n}\right)_i &= \frac{1}{\Delta x^n}[\ln(1+\delta^+)]^n u_i \\ &= \frac{1}{\Delta x^n}\left[\delta^{+n} - \frac{n}{2}\delta^{+(n+1)} + \frac{n(3n+5)}{24}\delta^{+(n+2)}\right. \\ &\quad \left. - \frac{n(n+2)(n+3)}{48}\delta^{+(n+3)} + \cdots\right]u_i \end{aligned} \tag{3.3.1}$$

Similarly for the backward difference, we write

$$\begin{aligned}\left(\frac{\partial^n u}{\partial x^n}\right)_i &= \frac{-1}{\Delta x^n}[\ln(1-\delta^-)]^n u_i \\ &= \frac{1}{\Delta x^n}\left(\delta^- + \frac{\delta^{-2}}{2} + \frac{\delta^{-3}}{3} + \cdots\right)^n u_i \\ &= \frac{1}{\Delta x^n}\left[\delta^{-n} + \frac{n}{2}\delta^{-(n+1)} + \frac{n(3n+5)}{24}\delta^{-(n+2)}\right. \\ &\quad \left. + \frac{n(n+2)(n+3)}{48}\delta^{-(n+3)} + \cdots\right]u_i \end{aligned} \tag{3.3.2}$$

The central difference formulas are in the form

$$\begin{aligned}\left(\frac{\partial^n u}{\partial x^n}\right)_i &= \left(\frac{2}{\Delta x}\sinh^{-1}\frac{\delta}{2}\right)^n u_i \\ &= \frac{1}{\Delta x^n}\left[\delta - \frac{\delta^3}{24} + \frac{3\delta^5}{640} - \frac{5\delta^7}{7168} + \cdots\right]^n u_i \\ &= \frac{1}{\Delta x^n}\delta^n\left[1 - \frac{n}{24}\delta^2 + \frac{n}{64}\left(\frac{22+5n}{90}\right)\delta^4\right. \\ &\quad \left. - \frac{n}{4^5}\left(\frac{5}{7} + \frac{n-1}{5} + \frac{(n-1)(n-2)}{3^5}\right)\delta^6 + \cdots\right]u_i \end{aligned} \tag{3.3.3}$$

If n is even, the difference formulas are obtained at the integer mesh points. If n is uneven, however, the difference formulas involve half-integer mesh points. In order to maintain the integer mesh points, we may use

$$\begin{aligned}\left(\frac{\partial^n u}{\partial x^n}\right)_i &= \frac{\mu}{\left(1+\frac{\delta^2}{4}\right)^{\frac{1}{2}}}\left(\frac{2}{\Delta x}\sinh^{-1}\frac{\delta}{2}\right)^n u_i \\ &= \mu\frac{\delta^n}{\Delta x^n}\left[1 - \frac{n+3}{24}\delta^2 + \frac{5n^2+52n+135}{5760}\delta^4 + \cdots\right]u_i \end{aligned} \tag{3.3.4}$$

where

$$\mu = \left(1 + \frac{\delta^2}{4}\right)^{\frac{1}{2}}$$

Based on these formulas, we summarize the second, third, and fourth order derivatives below.

Second Order Derivative ($n = 2$)

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{1}{\Delta x^2}\left(\delta^{+2} - \delta^{+3} + \frac{11}{12}\delta^{+4} - \frac{5}{6}\delta^{+5} + \cdots\right)u_i, \qquad \text{from (3.3.1)} \qquad (3.3.5a)$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{1}{\Delta x^2}\left(\delta^{-2} + \delta^{-3} + \frac{11}{12}\delta^{-4} + \frac{5}{6}\delta^{-5} + \cdots\right)u_i, \qquad \text{from (3.3.2)} \qquad (3.3.5b)$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{1}{\Delta x^2}\left(\delta^2 - \frac{\delta^4}{12} + \frac{\delta^6}{90} - \frac{\delta^8}{560} + \cdots\right)u_i, \qquad \text{from (3.3.3)} \qquad (3.3.5c)$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{\mu}{\Delta x^2}\left(\delta^2 - \frac{5\delta^4}{24} + \frac{259}{5760}\delta^6 + O(\Delta x^8)\right)u_i, \qquad \text{from (3.3.4)} \qquad (3.3.5d)$$

Forward Difference

First Order Accuracy

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{1}{\Delta x^2}(u_{i+2} - 2u_{i+1} + u_i) - \Delta x\frac{\partial^3 u}{\partial x^3} \qquad (3.3.6)$$

Second Order Accuracy

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{1}{\Delta x^2}(2u_i - 5u_{i+1} + 4u_{i+2} - u_{i+3}) + \frac{11}{12}\Delta x^2\frac{\partial^4 u}{\partial x^4} \qquad (3.3.7)$$

Backward Difference

First Order Accuracy

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{1}{\Delta x^2}(u_i - 2u_{i-1} + u_{i-2}) + \Delta x\frac{\partial^3 u}{\partial x^3} \qquad (3.3.8)$$

Second Order Accuracy

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{1}{\Delta x^2}(2u_i - 5u_{i-1} + 4u_{i-2} - u_{i-3}) - \frac{11}{12}\Delta x^2\frac{\partial^4 u}{\partial x^4} \qquad (3.3.9)$$

Central Difference

Second Order Accuracy

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{1}{\Delta x^2}(u_{i+1} - 2u_i + u_{i-1}) - \frac{\Delta x^2}{12}\frac{\partial^4 u}{\partial x^4} \qquad (3.3.10)$$

Fourth Order Accuracy

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{1}{12\Delta x^2}(-u_{i+2} + 16u_{i+1} - 30u_i + 16u_{i-1} - u_{i-2}) + \frac{\Delta x^4}{90}\frac{\partial^6 u}{\partial x^6} \qquad (3.3.11)$$

Central Difference – Half Integer Points

Second Order Accuracy

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{1}{2\Delta x^2}\left(u_{i+\frac{3}{2}} - u_{i+\frac{1}{2}} - u_{i-\frac{1}{2}} + u_{i-\frac{3}{2}}\right) - \frac{5}{24}\Delta x^2 \frac{\partial^4 u}{\partial x^4} \tag{3.3.12}$$

Fourth Order Accuracy

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{1}{48\Delta x^2}\left(-5u_{i+\frac{5}{2}} + 39u_{i+\frac{3}{2}} - 34u_{i+\frac{1}{2}} - 34u_{i-\frac{1}{2}} + 39u_{i-\frac{3}{2}} - 5u_{i-\frac{5}{2}}\right) + \frac{259}{5760}\Delta x^4 \frac{\partial^6 u}{\partial x^6} \tag{3.3.13}$$

Note that the last scheme requires six mesh points to achieve the fourth order accuracy, whereas for the same accuracy, the scheme given by (3.3.11) requires only five mesh points.

Third Order Derivative ($n = 3$)

Forward Difference

First Order Accuracy

$$\left(\frac{\partial^3 u}{\partial x^3}\right)_i = \frac{1}{\Delta x^3}(u_{i+3} - 3u_{i+2} + 3u_{i+1} - u_i) - \frac{\Delta x}{2}\frac{\partial^4 u}{\partial x^4} \tag{3.3.14}$$

Second Order Accuracy

$$\left(\frac{\partial^3 u}{\partial x^3}\right)_i = \frac{1}{2\Delta x^3}(-3u_{i+4} + 14u_{i+3} - 24u_{i+2} + 18u_{i+1} - 5u_i) + \frac{21}{12}\Delta x^2 \frac{\partial^5 u}{\partial x^5} \tag{3.3.15}$$

Backward Difference

First Order Accuracy

$$\left(\frac{\partial^3 u}{\partial x^3}\right)_i = \frac{1}{\Delta x^3}(u_i - 3u_{i-1} + 3u_{i-2} - u_{i-3}) + \frac{\Delta x}{2}\frac{\partial^4 u}{\partial x^4} \tag{3.3.16}$$

Second Order Accuracy

$$\left(\frac{\partial^3 u}{\partial x^3}\right)_i = \frac{1}{2\Delta x^3}(5u_i - 18u_{i-1} + 24u_{i-2} - 14u_{i-3} + 3u_{i-4}) - \frac{21}{12}\Delta x^2 \frac{\partial^5 u}{\partial x^5} \tag{3.3.17}$$

Central Difference

Second Order Accuracy

$$\left(\frac{\partial^3 u}{\partial x^3}\right)_i = \frac{1}{2\Delta x^3}(u_{i+2} - 2u_{i+1} + 2u_{i-1} - u_{i-2}) - \frac{1}{4}\Delta x^2 \frac{\partial^5 u}{\partial x^5} \tag{3.3.18}$$

Fourth Order Accuracy

$$\left(\frac{\partial^3 u}{\partial x^3}\right)_i = \frac{1}{8\Delta x^3}(-u_{i+3} + 8u_{i+2} - 13u_{i+1} - 13u_{i-1} - 8u_{i-2} + u_{i-3}) + \frac{7}{120}\Delta x^4 \frac{\partial^7 u}{\partial x^7} \tag{3.3.19}$$

Central Difference – Half Integer Points

Second Order Accuracy

$$\left(\frac{\partial^3 u}{\partial x^3}\right)_i = \frac{1}{\Delta x^3}\left(u_{i+\frac{3}{2}} - 3u_{i+\frac{1}{2}} + 3u_{i-\frac{1}{2}} - u_{i-\frac{3}{2}}\right) - \frac{\Delta x^2}{8}\frac{\partial^5 u}{\partial x^5} \tag{3.3.20a}$$

Fourth Order Accuracy

$$\left(\frac{\partial^3 u}{\partial x^3}\right)_i = \frac{1}{8\Delta x^3}\left(-u_{i+\frac{5}{2}} + 13u_{i+\frac{3}{2}} - 34u_{i+\frac{1}{2}} + 34u_{i-\frac{1}{2}} - 13u_{i-\frac{3}{2}} + u_{i-\frac{5}{2}}\right) + \frac{37}{1920}\Delta x^4\frac{\partial^7 u}{\partial x^7} \tag{3.3.20b}$$

Fourth Order Derivative

Forward Difference (first order accuracy)

$$\left(\frac{\partial^4 u}{\partial x^4}\right)_i = \frac{1}{\Delta x^4}(u_{i+4} - 4u_{i+3} + 6u_{i+2} - 4u_{i+1} + u_i) - 2\Delta x\frac{\partial^5 u}{\partial x^5} \tag{3.2.21}$$

Backward Difference (first order accuracy)

$$\left(\frac{\partial^4 u}{\partial x^4}\right)_i = \frac{1}{\Delta x^4}(u_i - 4u_{i-1} + 6u_{i-2} - 4u_{i-3} + u_{i-4}) + 2\Delta x\frac{\partial^5 u}{\partial x^5} \tag{3.2.22}$$

Central Difference (second order accuracy)

$$\left(\frac{\partial^4 u}{\partial x^4}\right)_i = \frac{1}{\Delta x^4}(u_{i+2} - 4u_{i+1} + 6u_i - 4u_{i-1} + u_{i-2}) - \frac{\Delta x^2}{6}\frac{\partial^6 u}{\partial x^6} \tag{3.2.23}$$

Various order finite difference formulas up to fourth order derivatives are summarized in Table 3.3.1.

3.4 MULTIDIMENSIONAL FINITE DIFFERENCE FORMULAS

Multidimensional finite difference formulas can be derived using the results of one-dimensional formulas. For two-dimensions, we consider

$$x_i = x_0 + i\Delta x$$
$$y_j = y_0 + j\Delta y$$

as defined in Figure 3.4.1. The forward and backward operators are now given by $\delta_x^{\pm}$ and $\delta_y^{\pm}$ for x- and y-directions, respectively. The first partial derivatives in the x- and y-directions are

$$\left(\frac{\partial u}{\partial x}\right)_{ij} = \frac{1}{\Delta x}\delta_x^+ u_{ij} + O(\Delta x) = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + O(\Delta x) \tag{3.4.1}$$

$$\left(\frac{\partial u}{\partial y}\right)_{ij} = \frac{1}{\Delta y}\delta_y^+ u_{ij} + O(\Delta x) = \frac{u_{i,j+1} - u_{i,j}}{\Delta y} + O(\Delta y) \tag{3.4.2}$$

Table 3.3.1 Various Order Finite Difference Formulas

(a) Forward Difference, O(Δx)

	u_i	u_{i+1}	u_{i+2}	u_{i+3}	u_{i+4}
$\Delta x \frac{\partial u}{\partial x}$	–1	1			
$\Delta x^2 \frac{\partial^2 u}{\partial x^2}$	1	–2	1		
$\Delta x^3 \frac{\partial^3 u}{\partial x^3}$	–1	3	–3	1	
$\Delta x^4 \frac{\partial^4 u}{\partial x^4}$	1	–4	6	–4	1

(b) Backward Difference, O(Δx)

	u_{i-4}	u_{i-3}	u_{i-2}	u_{i-1}	u_i
$\Delta x \frac{\partial u}{\partial x}$				–1	1
$\Delta x^2 \frac{\partial^2 u}{\partial x^2}$			1	–2	1
$\Delta x^3 \frac{\partial^3 u}{\partial x^3}$		–1	3	–3	1
$\Delta x^4 \frac{\partial^4 u}{\partial x^4}$	1	–4	6	–4	1

(c) Central Difference, O(Δx^2)

	u_{i-2}	u_{i-1}	u_i	u_{i+1}	u_{i+2}
$2\Delta x \frac{\partial u}{\partial x}$		–1	0	1	
$\Delta x^2 \frac{\partial^2 u}{\partial x^2}$		1	–2	1	
$2\Delta x^3 \frac{\partial^3 u}{\partial x^3}$	–1	2	0	2	1
$\Delta x^4 \frac{\partial^4 u}{\partial x^4}$	1	–4	6	–4	1

(d) Forward Difference, O(Δx^2)

	u_i	u_{i+1}	u_{i+2}	u_{i+3}	u_{i+4}	u_{i+5}
$2\Delta x \frac{\partial u}{\partial x}$	–3	4	–1			
$\Delta x^2 \frac{\partial^2 u}{\partial x^2}$	2	–5	4	–1		
$2\Delta x^3 \frac{\partial^3 u}{\partial x^3}$	–5	18	–24	14	–3	
$\Delta x^4 \frac{\partial^4 u}{\partial x^4}$	3	–14	26	–24	11	–2

(e) Backward Difference, O(Δx^2)

	u_{i-5}	u_{i-4}	u_{i-3}	u_{i-2}	u_{i-1}	u_i
$2\Delta x \frac{\partial u}{\partial x}$				1	–4	3
$\Delta x^2 \frac{\partial^2 u}{\partial x^2}$			–1	4	–5	2
$2\Delta x^3 \frac{\partial^3 u}{\partial x^3}$		3	–14	24	–18	5
$\Delta x^4 \frac{\partial^4 u}{\partial x^4}$	–2	11	–24	26	–14	3

(f) Central Difference, O(Δx^4)

	u_{i-3}	u_{i-2}	u_{i-1}	u_i	u_{i+1}	u_{i+2}	u_{i+3}
$12\Delta x \frac{\partial u}{\partial x}$		1	–8	0	8	–1	
$12\Delta x^2 \frac{\partial^2 u}{\partial x^2}$		–1	16	–30	16	–1	
$8\Delta x^3 \frac{\partial^3 u}{\partial x^3}$	1	–8	13	0	–13	8	–1
$6\Delta x^4 \frac{\partial^4 u}{\partial x^4}$	–1	12	–39	56	–39	12	–1

Similarly, the second order central difference formulas for the second order derivatives are of the form

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{ij} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} - \frac{\Delta x^2}{12}\frac{\partial^4 u}{\partial x^4} \tag{3.4.3}$$

$$\left(\frac{\partial^2 u}{\partial y^2}\right)_{ij} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} - \frac{\Delta y^2}{12}\frac{\partial^4 u}{\partial x^4} \tag{3.4.4}$$

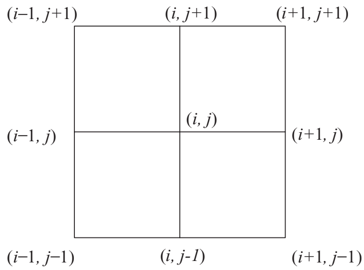


Figure 3.4.1 Two-dimensional mesh.

Let us now consider the Laplace equation

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

whose finite difference formula is obtained as the sum of (3.4.3) and (3.4.4), resulting in a five-point scheme

$$\Delta u_{ij} = \left(\frac{\delta_x^2}{\Delta x^2} + \frac{\delta_y^2}{\Delta y^2}\right)u_{ij} = \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{\Delta x^2} + \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{\Delta y^2} + O(\Delta x^2, \Delta y^2) \tag{3.4.5a}$$

For $\Delta x = \Delta y$

$$\Delta^{(1)} u_{ij} = \frac{u_{i+1,j} + u_{i-1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}}{\Delta x^2} - \frac{\Delta x^2}{12}\left(\frac{\partial^4 u}{\partial x^4} + \frac{\partial^4 u}{\partial y^4}\right) \tag{3.4.5b}$$

as graphically shown in Figure 3.4.2a.

An alternative representation of (3.4.5a) is given by

$$\begin{aligned}\Delta^{(2)} u_{ij} &= \left[\left(\frac{1}{\Delta x}\mu_y\delta_x\right)^2 + \left(\frac{1}{\Delta y}\mu_x\delta_y\right)^2\right]u_{ij} \\ &= \left[\frac{1}{4\Delta x^2}\left(E_y + 2 + E_y^{-1}\right)\left(E_x - 2 + E_x^{-1}\right)\right. \\ &\quad \left. + \frac{1}{4\Delta y^2}\left(E_x + 2 + E_x^{-1}\right)\left(E_y - 2 + E_y^{-1}\right)\right] u_{ij}\end{aligned} \tag{3.4.6}$$

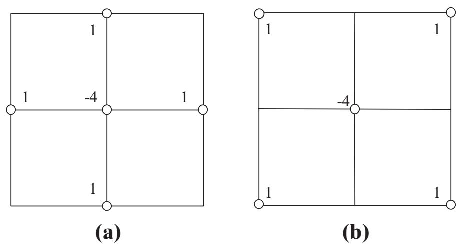


Figure 3.4.2 Five-point finite difference mesh. **(a)** Regular operator. **(b)** Shift operator.

where E_x and E_y are the shift operators resulting from

$$\delta_x^2 = \left(E_x^{\frac{1}{2}} - E_x^{-\frac{1}{2}}\right)^2 = E_x - 2 + E_x^{-1}$$

$$\mu_y^2 = \left[\frac{1}{2}\left(E_y^{\frac{1}{2}} + E_y^{-\frac{1}{2}}\right)\right]^2 = \frac{1}{4}\left(E_y + 2 + E_y^{-1}\right)$$

etc.
For $\Delta x = \Delta y$, (3.4.6) is simplified as (Figure 3.4.2b)

$$\Delta^{(2)} u_{ij} = \frac{1}{4\Delta x^2}(u_{i+1,j+1} + u_{i+1,j-1} + u_{i-1,j-1} + u_{i-1,j+1} - 4u_{i,j}) \tag{3.4.7}$$

For higher order terms, we may write

$$\begin{aligned}\Delta^{(2)} u_{ij} &= \left(1 + \frac{\Delta y^2}{4}\frac{\partial^2}{\partial y^2}\right)\left(\frac{\partial^2 u}{\partial x^2} + \frac{\Delta x^2}{12}\frac{\partial^4 u}{\partial x^4}\right)_{ij} + \left(1 + \frac{\Delta x^2}{4}\frac{\partial^2}{\partial x^2}\right)\left(\frac{\partial^2 u}{\partial y^2} + \frac{\Delta y^2}{12}\frac{\partial^4 u}{\partial y^4}\right)_{ij} \\ &= \Delta u_{ij} + \frac{1}{12}\Delta x^2 \frac{\partial^4 u}{\partial x^4} + \frac{1}{12}\Delta y^2 \frac{\partial^4 u}{\partial y^4} + \left(\frac{\Delta x^2 + \Delta y^2}{4}\right)\frac{\partial^4 u}{\partial x^4 \partial y^4} + \cdots \end{aligned} \tag{3.4.8}$$

with the truncation error being $O(\Delta x^2, \Delta y^2)$. Note that this scheme involves the odd-numbered nodes detached from the even-numbered nodes (Figure 3.4.3). Note that point (i, j) is coupled to the points marked by a square, while there is no connection to the even-numbered points marked by a circle. Thus, the solution oscillates between the two values a and b when passing from an even to odd-numbered point, satisfying the difference equation $\Delta^{(2)} u_{ij} = 0$. However, it will not satisfy the difference equation (3.4.5).

The well-known nine-point formula can be derived by combining (3.4.8) with $\Delta^{(1)} u_{ij}$.

$$\begin{aligned}\Delta^{(3)} u_{ij} &= \left(a\Delta^{(1)} + b\Delta^{(2)}\right) u_{ij} \\ &= \frac{1}{\Delta x^2}\left[(\delta x^2 + \delta y^2) + \frac{b}{2}\delta x^2 \delta y^2\right] u_{ij} = \Delta^{(1)} u_{ij} + \frac{b}{2}\delta x^2 \delta y^2 u_{ij} \\ &= \Delta u_{ij} + \frac{\Delta x^2}{12}\left[\frac{\partial^4 u}{\partial x^4} + \frac{\partial^4 u}{\partial y^4} + 6b\frac{\partial^4 u}{\partial x^4 \partial y^4}\right]\end{aligned} \tag{3.4.9}$$

where $a + b = 1$. For $b = 2/3$, we arrive at the scheme depicted in Figure 3.4.4a, which can also be obtained from finite elements. For $b = 1/3$, the Dahlquist and Bjorck scheme

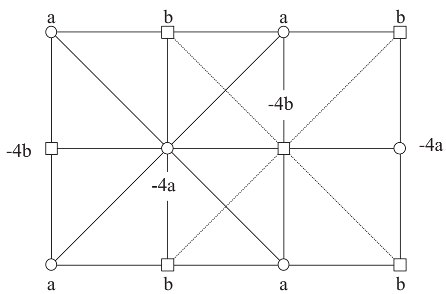


Figure 3.4.3 Odd-even oscillations of the five-point scheme.

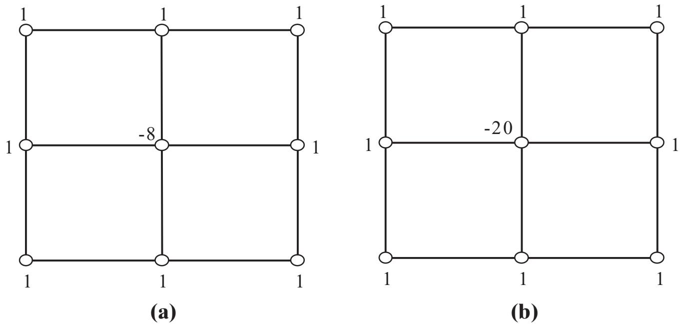


Figure 3.4.4 Nine-point molecule. (**a**) Nine-point formula with $b = 2/3$. (**b**) Nine-point formula with $b = 1/3$.

[1974] arises as shown in Figure 3.4.4b, providing the truncation error

$$-\frac{\Delta x^2}{12}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)^2 u = -\frac{\Delta x^2}{12}\Delta^2 u$$

For $\Delta u = \lambda u$, the nine-point operator with $\Delta^{(3)} = \frac{2}{3}\Delta^{(1)} + \frac{1}{3}\Delta^{(2)}$ gives a truncation error

$$-\lambda^2\frac{\Delta x^2}{12}u$$

Therefore, the corrected difference scheme

$$\Delta^{(3)}u_{i,j} = \left(\lambda + \lambda^2\frac{\Delta x^2}{12}\right)u$$

has a fourth order truncation error.

An extension to three-dimensional geometries is straightforward. Some applications to 3-D problems will be discussed in Chapter 7.

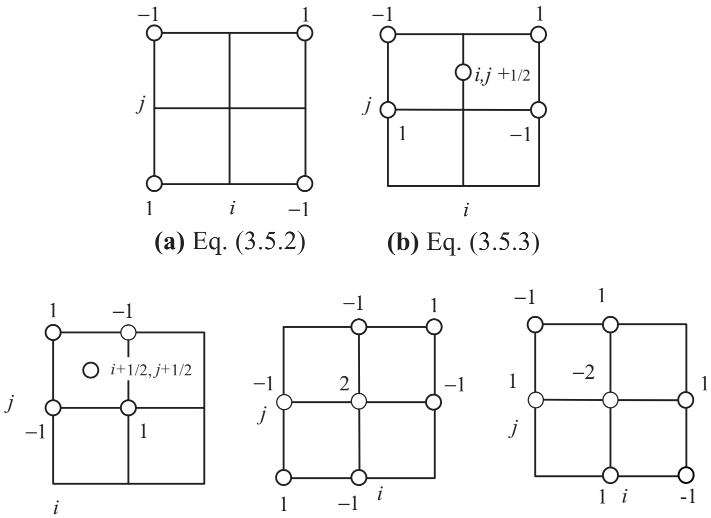
3.5 MIXED DERIVATIVES

The simplest, second order central formula for the mixed derivative is obtained from the application of (3.2.3) in both directions x and y.

$$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{ij} = \frac{1}{\Delta x \Delta y}\mu_x\delta_x\left[\left(1-\frac{\delta x^2}{6}+O(\Delta x^4)\right)\right]\mu_y\delta_y\left[\left(1-\frac{\delta y^2}{6}+O(\Delta y^4)\right)\right]u_{i,j} \tag{3.5.1}$$

This leads to a second order accuracy (Figure 3.5.1a),

$$\begin{aligned}\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{ij} &= \frac{1}{\Delta x \Delta y}(\mu_x\delta_x\mu_y\delta_y)\,u_{i,j} + O(\Delta x^2, \Delta y^2)\\ &= \frac{u_{i+1,j+1}-u_{i+1,j-1}-u_{i-1,j+1}+u_{i-1,j-1}}{4\Delta x\Delta y} + O(\Delta x^2, \Delta y^2)\end{aligned} \tag{3.5.2}$$



(a) Eq. (3.5.2) **(b)** Eq. (3.5.3)

(c) Eq. (3.5.5) **(d)** Eq. (3.5.7) **(e)** Eq. (3.5.8)

Figure 3.5.1 Mixed derivatives.

An alternative approach as shown in Figure 3.5.1b is given by

$$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{ij} = \frac{1}{\Delta x \Delta y}(\mu_x \delta_x \delta_y^+)\, u_{ij} + O(\Delta x^2, \Delta y)$$
$$= \frac{1}{2\Delta x \Delta y}(u_{i+1,j+1} - u_{i-1,j+1} - u_{i+1,j} + u_{i-1,j}) + O(\Delta x^2, \Delta y) \qquad (3.5.3)$$

A similar form can be obtained for the truncation error of $O(\Delta x, \Delta y^2)$. A first order in both x and y is derived in the form

$$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_i = \frac{1}{\Delta x \Delta y}\delta_x^+ \delta_y^+ u_{ij} + O(\Delta x, \Delta y)$$
$$= \frac{1}{\Delta x \Delta y}(u_{i+1,j+1} - u_{i+1,j} - u_{i,j+1} + u_{i,j}) + O(\Delta x, \Delta y) \qquad (3.5.4)$$

This scheme can be altered to give a second order accuracy at $i + \frac{1}{2}$, $j + \frac{1}{2}$,

$$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i+\frac{1}{2}, j+\frac{1}{2}} = \frac{1}{\Delta x \Delta y}\delta_x \delta_y u_{i+\frac{1}{2}, j+\frac{1}{2}} + O(\Delta x^2, \Delta y^2)$$
$$= \frac{1}{\Delta x \Delta y}(u_{i+1,j+1} - u_{i+1,j} - u_{i,j+1} + u_{i,j}) + O(\Delta x^2, \Delta y^2) \qquad (3.5.5)$$

as shown in Figure (3.5.1c).

Applying backward differences in both directions, we obtain

$$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_i = \frac{1}{\Delta x \Delta y}\delta_x^- \delta_y^- u_{ij} + O(\Delta x, \Delta y)$$
$$= \frac{1}{\Delta x \Delta y}(u_{i-1,j-1} - u_{i-1,j} - u_{i,j-1} + u_{i,j}) + O(\Delta x, \Delta y)$$
$$= \frac{1}{\Delta x \Delta y}\delta_x \delta_y u_{i-\frac{1}{2}, j-\frac{1}{2}} + O(\Delta x, \Delta y) \qquad (3.5.6)$$

Summing (3.5.4) and (3.5.6), we obtain a second order formula,

$$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_i = \frac{1}{2\Delta x \Delta y}[\delta_x^+\delta_y^+ + \delta_x^-\delta_y^-]u_{ij} + O(\Delta x^2, \Delta y^2)$$
$$= \frac{1}{2\Delta x \Delta y}[u_{i+1,j+1} - u_{i+1,j} - u_{i,j+1} + u_{i-1,j-1} - u_{i-1,j} - u_{i,j-1} + 2u_{ij}]$$
$$+ O(\Delta x^2, \Delta y^2) \tag{3.5.7}$$

This is shown in Figure 3.5.1d. Another form can be obtained by combining forward and backward differences as (Figure 3.5.1e)

$$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_i = \frac{1}{2\Delta x \Delta y}[\delta_x^+\delta_y^- + \delta_x^-\delta_y^+]u_{ij} + O(\Delta x^2, \Delta y^2)$$
$$= \frac{1}{2\Delta x \Delta y}[u_{i+1,j} - u_{i+1,j-1} + u_{i,j+1} + u_{i,j-1} - u_{i-1,j+1} + u_{i-1,j} - 2u_{ij}]$$
$$= \frac{1}{2\Delta x \Delta y}\left(\delta_x\delta_y u_{i+\frac{1}{2},j-\frac{1}{2}} + \delta_x\delta_y u_{i-\frac{1}{2},j+\frac{1}{2}}\right) + O(\Delta x^2 \Delta y^2) \tag{3.5.8}$$

Combining (3.5.7) and (3.5.8), we recover the fully central second order approximation (3.5.2). Therefore, the most general second order mixed derivative approximation can be obtained by an arbitrary linear combination of (3.5.7) and (3.5.8) [Mitchell and Griffiths, 1980].

$$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_i = \frac{1}{2\Delta x \Delta y}\delta_x\delta_y\left(au_{i+\frac{1}{2},j+\frac{1}{2}} + au_{i-\frac{1}{2},j-\frac{1}{2}} + bu_{i+\frac{1}{2},j-\frac{1}{2}} + bu_{i-\frac{1}{2},j+\frac{1}{2}}\right)$$
$$+ O(\Delta x^2, \Delta y^2) \tag{3.5.9}$$

with $a + b = 1$.

3.6 NONUNIFORM MESH

The standard Taylor series expansion may be applied to nonuniform meshes. The first derivative one-sided first order formula takes the form

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1} - u_i}{\Delta x_{i+1}} - \frac{\Delta x_{i+1}}{2}\frac{\partial^2 u}{\partial x^2} \tag{3.6.1a}$$

The backward formula becomes

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_i - u_{i-1}}{\Delta x_i} + \frac{\Delta x_i}{2}\frac{\partial^2 u}{\partial x^2} \tag{3.6.1b}$$

where $\Delta x_i = x_i - x_{i-1}$, etc.

The central difference is obtained by combining (3.6.1a) and (3.6.1b), which will lead to the second order formula

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{1}{\Delta x_i + \Delta x_{i+1}}\left[\frac{\Delta x_i}{\Delta x_{i+1}}(u_{i+1} - u_i) + \frac{\Delta x_{i+1}}{\Delta x_i}(u_i - u_{i-1})\right] - \frac{\Delta x_i \Delta x_{i+1}}{6}\frac{\partial^3 u}{\partial x^3} \tag{3.6.2}$$

It can also be shown that Taylor expansion leads to a forward or backward scheme. For example, for a forward scheme, we obtain

$$\left(\frac{\partial u}{\partial x}\right)_i = \left(\frac{\Delta x_{i+1} + \Delta x_{i+2}}{\Delta x_{i+2}} \frac{u_{i+1} - u_i}{\Delta x_{i+1}} - \frac{\Delta x_{i+1}}{\Delta x_{i+2}} \frac{u_{i+2} - u_i}{\Delta x_{i+1} + \Delta x_{i+2}}\right) + \frac{\Delta x_{i+1}(\Delta x_{i+1} + \Delta x_{i+2})}{6} \frac{\partial^3 u}{\partial x^3} \tag{3.6.3}$$

The three-point central difference formula for the second derivative is of the form

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \left(\frac{u_{i+1} - u_i}{\Delta x_{i+1}} - \frac{u_i - u_{i-1}}{\Delta x_i}\right) \frac{2}{\Delta x_{i+1} + \Delta x_i} + \frac{1}{3}(\Delta x_{i+1} - \Delta x_i) \frac{\partial^3 u}{\partial x^3} - \frac{\Delta x_{i+1}^3 + \Delta x_i^3}{12(\Delta x_{i+1} + \Delta x_i)} \frac{\partial^4 u}{\partial x^4} \tag{3.6.4}$$

Note that a loss of accuracy in nonuniform meshes is expected to occur and abrupt changes in mesh size in (3.6.4) result in the first order accuracy. For example, the third order accuracy of (3.6.4) is reduced to the second order for $\Delta x_{i+1} = \Delta x_i$.

3.7 HIGHER ORDER ACCURACY SCHEMES

For many applications in fluid dynamics with discontinuities and/or high gradients such as in shock waves and turbulence, it is necessary that higher order accuracy be provided in constructing difference equations for the first order, second order, and higher order derivatives. Lele [1992] presents various finite difference schemes which are generalization of the Padé scheme [Hildebrand, 1956; Kopal, 1961; Collatz, 1966]. These generalizations for the first order derivatives are given by

$$\beta u'_{i-2} + \alpha u'_{i-1} + u'_i + \alpha u'_{i+1} + \beta u'_{i+2} = a\frac{u_{i+1} - u_{i-1}}{2\Delta x} + b\frac{u_{i+2} - u_{i-2}}{4\Delta x} + c\frac{u_{i+3} - u_{i-3}}{6\Delta x} \tag{3.7.1}$$

with $u' = du/dx$. The relations between the coefficients a, b, c and α and β are derived by matching the Taylor series coefficients of various orders. Similarly, the generalizations for the second order derivatives are given by

$$\beta u''_{i-2} + \alpha u''_{i-1} + u''_i + \alpha u''_{i+1} + \beta u''_{i+2} = a\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + b\frac{u_{i+2} - 2u_i + u_{i-2}}{4\Delta x^2} + c\frac{u_{i+3} - 2u_i + u_{i-3}}{9\Delta x^2} \tag{3.7.2}$$

with $u'' = d^2u/dx^2$. Again, the relations between the coefficients a, b, c and α and β are derived by matching the Taylor series coeffcients of various orders.

Higher Order Accuracy for the First Order Derivatives

Fourth Order Accuracy. Note that, for $\alpha = \beta = 0$ and $a = 4/3, b = -1/3$, and $c = 0$ inserted in (3.7.1), the first order derivative in (3.7.1) leads to the well-known fourth order central difference scheme.

$$u'_i = \frac{du_i}{dx} = \frac{1}{12\Delta x}(u_{i-2} - 8u_{i-1} + 8u_{i+1} - u_{i+2}) \tag{3.7.3}$$

Other higher order accuracy schemes for the first order derivative are obtained from (3.7.1) as follows:

Sixth Order Accuracy

$$\alpha = 1/3, \quad \beta = 0, \quad a = 14/9, \quad b = 1/9, \quad c = 0$$

Eighth Order Accuracy

$$\alpha = 4/9, \quad \beta = 1/36, \quad a = 40/27, \quad b = 25/54, \quad c = 0$$

Higher Order Accuracy for the Second Order Derivatives

Fourth Order Accuracy. The fourth order accuracy for the second order derivative arises from (3.7.2) by inserting the same constants as in the first order derivative.

$$u_i'' = d^2u_i/dx^2 = \frac{1}{12\Delta x^2}(-u_{i-2} + 16u_{i-1} - 30u_i + 16u_{i+1} - u_{i+2}) \tag{3.7.4}$$

Higher order accuracy schemes for the second order derivative are obtained by inserting the following constants in (3.7.2):

Sixth Order Accuracy

$$\alpha = 2/11, \quad \beta = 0, \quad a = 12/11, \quad b = 3/11, \quad c = 0$$

Eighth Order Accuracy

$$\alpha = 344/1179, \qquad \beta = \frac{38\alpha - 9}{214},$$

$$a = \frac{696 - 1191\alpha}{428}, \qquad b = \frac{2454\alpha - 294}{535}, \qquad c = \frac{1179\alpha - 344}{2140}$$

These higher order accuracy derivatives have been used extensively in the analysis of shock waves and turbulence, as will be discussed in Part Five, Applications.

3.8 ACCURACY OF FINITE DIFFERENCE SOLUTIONS

The finite difference formulas and their subsequent use in boundary value problems must assure accuracy in portraying the physical aspect of the problem that has been modeled. The accuracy depends on consistency, stability, and convergence as defined below:

(a) *Consistency* A finite difference equation is consistent if it becomes the corresponding partial differential equation as the grid size and time step approach zero, or truncation errors are zero. This is usually the case if finite difference formulas are derived from the Taylor series.

(b) *Stability* A numerical scheme used for the solution of finite difference equations is stable if the error remains bounded. Certain criteria must be satisfied in order to achieve stability. This subject will be elaborated upon in Sections 4.2 and 4.3.

(c) *Convergence* A finite difference scheme is convergent if its solution approaches that of the partial differential equation as the grid size approaches zero. Both consistency and stability are prerequisite to convergence.

The ultimate goal of any numerical scheme is a convergence to the exact solution as the mesh size is reduced. Discrete time step sizes are chosen adequately as related to the mesh sizes so that the solution process is stable. The finite difference formulas studied in this chapter will be used for developing such numerical schemes. Here, the stability and convergence are important factors for the success in CFD projects and will be addressed continuously for the rest of this book.

3.9 SUMMARY

In this chapter, we have demonstrated that finite difference equations can be derived in many different ways. Simple methods and more rigorous general methods by means of finite difference operator, derivative operator, forward difference operator, and backward difference operator are introduced. Applications to various order derivatives in multidimensions are presented.

We have also shown how to obtain finite difference equations for higher order accuracy. They are particularly useful for complex physical phenomena such as in shock waves and turbulence, as will be shown in Part Five, Applications.

Our ultimate goal is the accuracy of the solution of differential equations. In order to achieve this accuracy, it is necessary that difference equations satisfy three criteria: consistency, stability, and convergence. Among these, the properties of consistency and stability reside in the realm of the development of finite difference equations. Convergence prevails if the requirements of consistency and stability are satisfied. The consequence of satisfaction of these criteria leads to the assurance of accuracy in CFD.

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