Lecture 2
Derivation of the finite difference equations

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

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

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

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

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

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

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

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

Forward Difference Formulas

First Order Accuracy

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

Second Order Accuracy

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

Backward Difference Formulas

First Order Accuracy

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

Second Order Accuracy

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

Central Difference Formulas

Second Order Accuracy

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

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

Fourth Order Accuracy

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

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

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

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

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

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

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

(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.