Lecture 13
APPROXIMATION OF SECOMD ORDER DERIVATIVES

13.1 APPROXIMATION OF SECOND ORDER DERIVATIVES

Second order derivatives appear in diffusive terms of transport/conservation equations. To obtain a finite difference approximation of the second derivative at a point, we can either use the approximation of the first derivatives or extend any of the techniques described in the previous lecture for the first order derivatives. We discuss application of each of these approaches in the sequel.

13.2 USE OF APPROXIMATIONS OF FIRST ORDER DERIVATIVE

To obtain the second order derivative at a point, one may use approximation of first order derivatives. For example, an approximation of the second order derivative can be obtained using the forward difference formula

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_i \approx \frac{\left(\frac{\partial f}{\partial x}\right)_{i+1} - \left(\frac{\partial f}{\partial x}\right)_i}{x_{i+1} - x_i} \tag{13.1}$$

We can use a different formula (say, BDS) for the approximation of the first order derivatives in the preceding equation which results in

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_i \approx \frac{\frac{f_{i+1} - f_i}{x_{i+1} - x_i} - \frac{f_i - f_{i-1}}{x_i - x_{i-1}}}{x_{i+1} - x_i} = \frac{f_{i+1}\left(x_i - x_{i-1}\right) + f_{i-1}\left(x_{i+1} - x_i\right) - f_i\left(x_{i+1} - x_i\right)}{\left(x_{i+1} - x_i\right)^2\left(x_i - x_{i-1}\right)} \tag{13.2}$$

On a uniform grid, Eq. (13.2) reduces to

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_i \approx \frac{f_{i+1} + f_{i-1} - 2 f_i}{\left(\Delta x\right)^2} \tag{13.3}$$

Approximation (13.1) is first order accurate. A better approximation for the second order derivative can be obtained using CDS at points halfway between nodes, i.e.

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_i \approx \frac{\left(\frac{\partial f}{\partial x}\right)_{i+\frac{1}{2}} - \left(\frac{\partial f}{\partial x}\right)_{i-\frac{1}{2}}}{\left(x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}\right)} \tag{13.4}$$

CDS is also used for approximation of the first order derivatives in Eq. (13.4), i.e.

$$\left(\frac{\partial f}{\partial x}\right)_{i+\frac{1}{2}} \approx \frac{f_{i+1} - f_i}{x_{i+1} - x_i} \quad \text{and} \quad \left(\frac{\partial f}{\partial x}\right)_{i-\frac{1}{2}} \approx \frac{f_i - f_{i-1}}{x_i - x_{i-1}} \tag{13.5}$$

Substitution of Eq. (13.5) into Eq. (13.4) yields the following formula for the second order derivative

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_i \approx \frac{f_{i+1}\left(x_i - x_{i-1}\right) + f_{i-1}\left(x_{i+1} - x_i\right) - f_i\left(x_{i+1} - x_{i-1}\right)}{\frac{1}{2}\left(x_{i+1} - x_{i-1}\right)\left(x_{i+1} - x_i\right)\left(x_i - x_{i-1}\right)} \tag{13.6}$$

On a uniform grid, Eq. (13.6) reduces to Eq. (13.3).

13.3 TAYLOR SERIES EXPANSION

Using Taylor series expansion about $x = x_i$, function values at grid points x_{i+1} and x_{i-1} can be expressed as

$$f_{i+1} = f_i + \left(x_{i+1} - x_i\right)\left(\frac{\partial f}{\partial x}\right)_i + \frac{\left(x_{i+1} - x_i\right)^2}{2!}\left(\frac{\partial^2 f}{\partial x^2}\right)_i + \frac{\left(x_{i+1} - x_i\right)^3}{3!}\left(\frac{\partial^3 f}{\partial x^3}\right)_i + H \tag{13.7}$$

$$f_{i-1} = f_i - \left(x_i - x_{i-1}\right)\left(\frac{\partial f}{\partial x}\right)_i + \frac{\left(x_i - x_{i-1}\right)^2}{2!}\left(\frac{\partial^2 f}{\partial x^2}\right)_i - \frac{\left(x_i - x_{i-1}\right)^3}{3!}\left(\frac{\partial^3 f}{\partial x^3}\right)_i + H \tag{13.8}$$

Multiply Eq. (13.8) by $\left(x_{i+1} - x_i\right)$ and add it to $\left(x_i - x_{i-1}\right)\times$ Eq. (13.7) to eliminate the first order derivative. Rearrangement of the resulting equation leads to the following relation for the second order derivative:

$$\begin{aligned}\left(\frac{\partial^2 f}{\partial x^2}\right)_i = {}& \frac{f_{i+1}\left(x_i - x_{i-1}\right) + f_{i-1}\left(x_{i+1} - x_i\right) - f_i\left(x_{i+1} - x_{i-1}\right)}{\frac{1}{2}\left(x_{i+1} - x_{i-1}\right)\left(x_{i+1} - x_i\right)\left(x_i - x_{i-1}\right)} \\ & - \frac{1}{3}\left[\left(x_{i+1} - x_i\right) - \left(x_i - x_{i-1}\right)\right]\left(\frac{\partial^3 f}{\partial x^3}\right)_i + H\end{aligned} \tag{13.9}$$

which is identical to Eq. (13.6) obtained using CDS. The leading term in the truncation error of preceding approximation is formally of first order on a non-uniform grid, and of second order on uniform grids. However, even for a non-uniform grid, the truncation error is reduced as in a second order scheme with the grid refinement (Ferziger and Peric, 2003).

A general procedure on uniform grids

On uniform grids, we can define the difference approximation for the second order derivative as (Chung, 2010)

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_i \approx \frac{af_i + bf_{i-1} + cf_{i+1} + df_{i-2} + ef_{i+2} + \ldots}{\Delta x^2} \tag{13.10}$$

Coefficients a, b, c, d, e, …. can be determined from Taylor series expansion for the function values involved at the RHS around point x_i. Using this approach, the three point central difference formula (13.3) can be derived starting with the relation

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_i \approx \frac{af_i + bf_{i-1} + cf_{i+1}}{\Delta x^2} \tag{13.11}$$

Taylor series expansion for f_{i-1} and f_{i+1} lead to the following relation:

$$\begin{aligned}\frac{af_i + bf_{i-1} + cf_{i+1}}{\Delta x^2} &= \frac{(a+b+c)}{\Delta x^2} f_i + \frac{(c-b)}{\Delta x}\left(\frac{\partial f}{\partial x}\right)_i + \frac{(b+c)}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i \\ &+ (c-b)\frac{\Delta x}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i + (b+c)\frac{\Delta x^2}{24}\left(\frac{\partial^4 f}{\partial x^4}\right)_i + \ldots.\end{aligned} \tag{13.12}$$

From the preceding equation, it is clear that Eq. (13.11) will represent an approximation for the second order derivative if and only if $a+b+c=0, b-c=0$ and $b+c=2.$ Clearly, $b=c=1$ and $a=-2.$ Thus, we obtain the following central difference approximation

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_i = \frac{f_{i+1} + f_{i-1} - 2f_i}{(\Delta x)^2} - \frac{\Delta x^2}{12}\left(\frac{\partial^4 f}{\partial x^4}\right)_i \tag{13.13}$$

which is second order accurate. Similarly, we can derive the following one-sided formula

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_i = \frac{f_i - 2f_{i-1} + f_{i-2}}{(\Delta x)^2} + \Delta x\left(\frac{\partial^3 f}{\partial x^3}\right)_i \tag{13.14}$$

which is only first order accurate (Chung, 2010). Further, using this approach, we can easily derive a higher order central difference approximation using function values at five points (for details, see Example 13.1 below) given by

$$\left(\frac{\partial f}{\partial x}\right)_i = \frac{-30f_i + 16(f_{i-1} + f_{i+1}) - (f_{i-2} + f_{i+2})}{12\Delta x^2} + O\left(\Delta x^4\right) \tag{13.15}$$

Example 13.1

Derive a five point central difference formula for the second order derivative on uniform grid using Taylor series expansion and Eq. (13.10).

Solution

Five point central difference formula for the second order derivative can expressed as

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_i \approx \frac{af_i + bf_{i-1} + cf_{i+1} + df_{i-2} + ef_{i+2}}{\Delta x^2} \tag{i}$$

Taylor series expansions for $f_{i-2}, f_{i-1}, f_{i+1}$ and f_{i+2}, we get

$$\begin{aligned}\frac{af_i + bf_{i-1} + cf_{i+1} + df_{i-2} + ef_{i+2}}{\Delta x^2} &= \frac{(a+b+c+d+e)}{\Delta x^2} f_i + \frac{(-b+c-2d+2e)}{\Delta x}\left(\frac{\partial f}{\partial x}\right)_i \\ &+ \frac{1}{2}(b+c+4d+4e)\left(\frac{\partial^2 f}{\partial x^2}\right)_i + \frac{\Delta x}{6}(-b+c-8d+8e)\left(\frac{\partial^3 f}{\partial x^3}\right)_i \\ &+ \frac{\Delta x^2}{24}(b+c+16d+16e)\left(\frac{\partial^4 f}{\partial x^4}\right)_i + \frac{\Delta x^3}{120}(-b+c-32d+32e)\left(\frac{\partial^5 f}{\partial x^5}\right)_i \\ &+ \frac{\Delta x^4}{720}(b+c+64d+64e)\left(\frac{\partial^6 f}{\partial x^6}\right)_i + H\end{aligned} \tag{ii}$$

Equations (i) and (iv) indicate that the coefficients in Eq. (i) must satisfy the following conditions:

$$a+b+c+d+e=0 \quad \text{(iii)}$$
$$-b+c-2d+2e=0 \quad \text{(iv)}$$
$$b+c+4d+4e=2 \quad \text{(v)}$$
$$-b+c-8d+8e=0 \quad \text{(vi)}$$
$$b+c+16d+16e \quad \text{(vii)}$$

Solving Eqs. (v)-(vii), we get

$$a=-5/2, \quad b=c=4/3, \quad d=e=-1/12 \quad \text{(viii)}$$

The truncation error (TE) is given by

$$\varepsilon_\tau = -\frac{\Delta x^4}{720}(b+c+64d+64e)\left(\frac{\partial^6 f}{\partial x^6}\right)_i = \frac{\Delta x^4}{90}\left(\frac{\partial^6 f}{\partial x^6}\right)_i \quad \text{(ix)}$$

Therefore, the desired five-point central difference formula is

$$\boxed{\left(\frac{\partial f}{\partial x}\right)_i \approx \frac{-30 f_i + 16(f_{i-1}+f_{i+1}) - (f_{i-2}+f_{i+2})}{12\Delta x^2}, \qquad \text{TE}\sim O\left(\Delta x^4\right)} \quad \text{(x)}$$

13.4 POLYNOMIAL FITTING

For any function, an interpolating polynomial of degree n can be fit using function values at $(n+1)$ data points and approximation to all derivatives up to order n can be obtained by differentiation.

- Use of quadratic interpolation loads to three point CDS formula (13.3) or (13.13) for the second order derivative.
- In general, truncation error of the approximation to second order derivative obtained by fitting a polynomial of degree n is of order $(n-1)$.
- One order is gained (i.e., truncation error is of order n) if grid spacing is uniform and an even-order polynomials is used. For example, polynomial of degree 4 on uniform grid leads to the fourth order accurate formula given by Eq. (13.15).

Example 13.2
Derive Eq. (13.15) by fitting a polynomial of degree 4 on uniform grid. Also obtain the corresponding approximations for the first, third and fourth order derivatives.

Solution
To obtain a central difference approximation, we can fit the following 4th degree polynomial through five points $x_{i-2}, x_{i-1}, x_i, x_{i+1}$ and x_{i+2} :

$$f(x) \approx a_0 + a_1(x-x_i)x + a_2(x-x_i)^2 + a_3(x-x_i)^3 + a_4(x-x_i)^4 \quad \text{(i)}$$

Formal differentiation of the preceding equation leads to the following relations:

$$\left(\frac{\partial f}{\partial x}\right)_i = a_1, \quad \left(\frac{\partial^2 f}{\partial x^2}\right)_i = 2a_2, \quad \left(\frac{\partial^3 f}{\partial x^3}\right)_i = 6a_3, \quad \left(\frac{\partial^4 f}{\partial x^4}\right)_i = 24a_4 \quad \text{(ii)}$$

To obtain the values of coefficients a_i, we fit the interpolation curve (i) to the function values at points $x_{i-2}, x_{i-1}, x_i, x_{i+1}$ and x_{i+2}, which results in the following set of linear equations:

$$f_i = a_0 \tag{iii}$$
$$f_{i-2} = f_i + a_1(-2\Delta x) + a_2(-2\Delta x)^2 + a_3(-2\Delta x)^3 + a_2(-2\Delta x)^4 \tag{iv}$$
$$f_{i-1} = f_i + a_1(-\Delta x) + a_2(-\Delta x)^2 + a_3(-\Delta x)^3 + a_2(-\Delta x)^4 \tag{v}$$
$$f_{i+1} = f_i + a_1(\Delta x) + a_2(\Delta x)^2 + a_3(\Delta x)^3 + a_2(\Delta x)^4 \tag{vi}$$
$$f_{i+2} = f_i + a_1(2\Delta x) + a_2(2\Delta x)^2 + a_3(2\Delta x)^3 + a_2(2\Delta x)^4 \tag{vii}$$

Solution of simultaneous Eqs. (iv)-(vii) yields the following values for coefficients a_i:

$$\begin{aligned} a_1 &= \frac{f_{i-2} - 8f_{i-1} + 8f_{i+1} - f_{i+2}}{12\Delta x}, \qquad & a_2 &= \frac{-f_{i-2} + 16f_{i-1} - 30f_i + 16f_{i+1} - f_{i+2}}{24\Delta x^2} \\ a_3 &= \frac{-f_{i-2} + 2f_{i-1} - 2f_{i+1} + f_{i+2}}{12\Delta x^3}, \qquad & a_4 &= \frac{f_{i-2} - 4f_{i-1} + 6f_i - 4f_{i+1} + f_{i+2}}{24\Delta x^4} \end{aligned} \tag{viii}$$

Thus, approximations for the derivatives obtained from two-sided 4th degree polynomial fitting on a uniform grid are

$$\left(\frac{\partial f}{\partial x}\right)_i \equiv a_1 = \frac{f_{i-2} - 8f_{i-1} + 8f_{i+1} - f_{i+2}}{12\Delta x} \tag{ix}$$
$$\left(\frac{\partial^2 f}{\partial x^2}\right)_i = 2a_2 = \frac{-f_{i-2} + 16f_{i-1} - 30f_i + 16f_{i+1} - f_{i+2}}{12\Delta x^2} \tag{x}$$
$$\left(\frac{\partial^3 f}{\partial x^3}\right)_i = 6a_3 = \frac{-f_{i-2} + 2f_{i-1} - 2f_{i+1} + f_{i+2}}{2\Delta x^3} \tag{xi}$$
$$\left(\frac{\partial^4 f}{\partial x^4}\right)_i = 24a_4 = \frac{f_{i-2} - 4f_{i-1} + 6f_i - 4f_{i+1} + f_{i+2}}{\Delta x^4} \tag{xii}$$

Equation (x) is the same as Eq. (13.15) derived earlier using Taylor series expansion.

13.5 APPROXIMATION OF SECOND ORDER DERIVATIVE IN GENERIC TRANSPORT EQUATION

The diffusion term in the generic conservation equation involves a second order derivative of the form $\partial(\Gamma\partial\phi/\partial x)/\partial x$. If Γ is constant, this term becomes $\Gamma(\partial^2\phi/\partial x^2)$ and finite difference approximations in the preceding section can be used. Otherwise, we have to employ suitable finite difference approximations for the first order derivatives for inner and outer derivatives. The most popular approach is to employ the central difference approximation for both the inner and outer derivatives. Let us use the values of the inner first order derivative at points mid-way between the nodes and central difference formula to obtain the approximation for the outer derivative given by

$$\left[\frac{\partial}{\partial x}\left(\Gamma\frac{\partial\phi}{\partial x}\right)\right]_i \approx \frac{\left(\Gamma\frac{\partial\phi}{\partial x}\right)_{i+\frac{1}{2}} - \left(\Gamma\frac{\partial\phi}{\partial x}\right)_{i-\frac{1}{2}}}{\left(x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}\right)} \tag{13.16}$$

Central difference approximation of the first order derivatives on RHS of the preceding equation are

$$\left(\frac{\partial \phi}{\partial x}\right)_{i+\frac{1}{2}} = \frac{\left(\phi_{i+1} - \phi_i\right)}{x_{i+1} - x_i} \quad \text{and} \quad \left(\frac{\partial \phi}{\partial x}\right)_{i-\frac{1}{2}} = \frac{\left(\phi_i - \phi_{i-1}\right)}{x_i - x_{i-1}} \tag{13.17}$$

Combining Eq. (13.16) and Eq. (13.17), we get

$$\left[\frac{\partial}{\partial x}\left(\Gamma \frac{\partial \phi}{\partial x}\right)\right]_i \approx \frac{\Gamma_{i+\frac{1}{2}} \dfrac{\left(\phi_{i+1} - \phi_i\right)}{x_{i+1} - x_i} - \Gamma_{i-\frac{1}{2}} \dfrac{\left(\phi_i - \phi_{i-1}\right)}{x_i - x_{i-1}}}{\dfrac{1}{2}\left(x_{i+1} - x_{i-1}\right)} \tag{13.18}$$

On a uniform grid, the preceding equation simplifies to

$$\left[\frac{\partial}{\partial x}\left(\Gamma \frac{\partial \phi}{\partial x}\right)\right]_i \approx \frac{\Gamma_{i+\frac{1}{2}}\left(\phi_{i+1} - \phi_i\right) - \Gamma_{i-\frac{1}{2}}\left(\phi_i - \phi_{i-1}\right)}{(\Delta x)^2} \tag{13.19}$$

Note that if Γ is a function of ϕ, values at a point midway between the nodes can be evaluated using simple average of function values at the neighbouring nodes, i.e.

$$\Gamma_{i+\frac{1}{2}} \approx \Gamma\left(\frac{1}{2}\left(\phi_{i+1} + \phi_i\right), \frac{1}{2}(x_{i+1} + x_i)\right) \tag{13.20}$$

Other approximations can be easily obtained using different finite difference approximations for the inner and outer derivatives.

REFERENCES

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