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Computational Fluid Dynamics

Finite Difference Method

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FDM: Basics

- **The finite difference method is based on the properties of the Taylor series and on the straight forward application of the definition of derivatives.**
- **The earliest work in this filed is due to Euler in 1768.**
- **For a function $u(x)$, the derivative at point x is defined as**

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

- **This means that**

(Actual derivative)=(approximate derivative)+(truncation error)

- **The power Δx with which the error goes to zero for $\Delta x \to 0$ is called the order of the difference equation.**
- **Expanding $u(x+\Delta x)$ around $u(x)$, we get**

$$u(x+\Delta x) = u(x) + \Delta x \,.\, u_x + \frac{(\Delta x)^2}{2!} u_{xx} + \ldots \quad \rightarrow$$

$$\frac{u(x+\Delta x) - u(x)}{\Delta x} = u_x + \frac{(\Delta x)}{2!} u_{xx} + \ldots = u_x + O(\Delta x)$$

Various Differences

- **There are three difference forms:**

$$\left(u_x\right)_i = \frac{u_{i+1} - u_i}{\Delta x} + O(\Delta x) \qquad \textit{forward}$$

$$\left(u_x\right)_i = \frac{u_i - u_{i-1}}{\Delta x} + O(\Delta x) \qquad \textit{backward}$$

$$\left\{\begin{array}{l} \left(u_x\right)_i = \dfrac{u_{i+1} - u_{i-1}}{2\Delta x} + O(\Delta x^2) \\ \left(u_x\right)_{i+1/2} = \dfrac{u_{i+1} - u_i}{\Delta x} + O(\Delta x^2) \\ \left(u_x\right)_{i-1/2} = \dfrac{u_i - u_{i-1}}{\Delta x} + O(\Delta x^2) \end{array}\right. \qquad \textit{central}$$

Using Arbitrary Number of Points

- **We can involve as many points as we want to obtain a required accuracy. For example, we can write:**

$$(u_x)_i = \frac{au_i + bu_{i-1} + cu_{i-2}}{\Delta x} + O(\Delta x^2)$$

- **The coefficients** a, b **and** c **are obtained as**

$$u_{i-2} = u_i - 2\,\Delta x\,(u_x)_i + 2\,(\Delta x)^2\,(u_{xx})_i - \frac{(2\Delta x)^3}{6}(u_{xxx})_i + \ldots$$

$$u_{i-1} = u_i - \Delta x\,(u_x)_i + \frac{(\Delta x)^2}{2}(u_{xx})_i - \frac{(\Delta x)^3}{6}(u_{xxx})_i + \ldots$$

- **Then,**

$$au_i + bu_{i-1} + cu_{i-2} = (a+b+c)u_i - \Delta x(2c+b)(u_x)_i + \frac{(\Delta x)^3}{2}(4c+b)(u_{xx})_i + O(\Delta x^3)$$

- **This requires**

$$\begin{cases} a+b+c=0 \\ 2c+b=-1 \\ 4c+b=0 \end{cases} \rightarrow \begin{cases} a=3/2 \\ b=-2 \\ c=1/2 \end{cases} \rightarrow (u_x)_i = \frac{3u_i - 4u_{i-1} + u_{i-2}}{2\Delta x}$$

Using Arbitrary…

- **A similar relation can be written using $i, i+1$ and $i+2$**

$$(u_x)_i = \frac{-3u_i + 4u_{i+1} - u_{i+2}}{\Delta x} + O(\Delta x^2)$$

- **For the second order derivatives, we can write:**

$$(u_{xx})_i = \frac{(u_x)_{i+1} - (u_x)_i}{\Delta x} = \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2} + O(\Delta x^2)$$

- **Another form which is first order can be written as**

$$(u_{xx})_i = \frac{u_i - 2u_{i-1} + u_{i-2}}{(\Delta x)^2} + O(\Delta x)$$

General Method for Deriving Formulas

- **We use the following operator**

$$E u_i = u_{i+1} \qquad (displacement\ operator)$$
$$E^{-1} u_i = u_{i-1}$$
$$E^n u_i = u_{i+n} \qquad (in\ general)$$

- **Also use**

δ^+	:	*forward difference operator*	$\delta^+ u_i = u_{i+1} - u_i$
δ^-	:	*backward difference operator*	$\delta^- u_i = u_i - u_{i-1}$
δ	:	*central difference operator*	$\delta u_i = u_{i+1/2} - u_{i-1/2}$
$\bar{\delta}$	:	*central difference operator*	$\bar{\delta} u_i = (u_{i+1} - u_{i-1})/2$
μ	:	*averaging operator*	$\mu u_i = (u_{i+1/2} + u_{i-1/2})/2$
D	:	*differential operator*	$D u_i = \dfrac{\partial u}{\partial x} = u_x$

- **We note that**

$$\delta^+ = E - 1 \qquad \qquad \delta^- = 1 - 1/E$$

General Method...

- **This results in the following relations:**

$$\delta^- = E^{-1}\delta^+$$
$$\delta^+\delta^- = \delta^-\delta^+ = \delta^+ - \delta^- = \delta^2$$
$$\delta = E^{1/2} - E^{-1/2} = (E - E^{-1})/2$$
$$\mu = (E^{1/2} + E^{-1/2})/2$$

- **For n repeated actions of the operator δ, we have**

$$\left(\delta^+\right)^2 = \delta^+\delta^+ = E^2 - 2E + 1$$
$$\left(\delta^+\right)^3 = (E-1)^3 = E^3 - 3E^2 + 3E - 1$$

Difference Formulas for First Derivatives

- **Using the Taylor expansion, we get**

$$u(x+\Delta x) = u(x) + \Delta x \, . u_x + \frac{(\Delta x)^2}{2!} u_{xx} + \frac{(\Delta x)^3}{3!} u_{xxx} + ...$$

- **Or**

$$E\,u(x) = \left(1 + \Delta x \, . D + \frac{(\Delta x\, D)^2}{2!} + \frac{(\Delta x\, D)^3}{3!} + \ldots \right) u(x) \qquad \rightarrow$$

$$E\,u(x) = e^{\Delta x\, D}\, u(x) \quad \rightarrow \quad E = \exp(\Delta x\, D) \quad \rightarrow \quad \Delta x\, D = \ln(E)$$

- **Forward Difference: from the above relations, we can write**

$$\Delta x\, D = \ln(E) = \ln(1+\delta^+) = \delta^+ - \frac{(\delta^+)^2}{2} + \frac{(\delta^+)^3}{3} - \frac{(\delta^+)^4}{4} + \ldots$$

- **Keeping the first three terms, we get**

$$(u_x)_i = D\,u_i = \frac{-3u_i + 4u_{i+1} - u_{i+2}}{2\,\Delta x} + \frac{(\Delta x)^2}{3} u_{xxx}$$

Difference formulas…

- **Backward difference:**

$$\Delta x\, D = \ln(E) = -\ln(1-\delta^-) = \delta^- + \frac{(\delta^-)^2}{2} + \frac{(\delta^-)^3}{3} + \frac{(\delta^-)^4}{4} + \ldots$$

or

$$(u_x)_i = D u_i = \frac{3u_i - 4u_{i-1} + u_{i-2}}{2\,\Delta x} + \frac{(\Delta x)^2}{3} u_{xxx}$$

- **Central Difference:**

$$\delta u_i = u_{i+1/2} - u_{i-1/2} = (E^{1/2} - E^{-1/2})u_i \quad \rightarrow$$

$$\delta = \exp(\Delta x\, D/2) - \exp(-\Delta x\, D/2) = 2\sinh(\Delta x\, D/2) \quad \rightarrow$$

$$\Delta x\, D = 2\sinh^{-1}(\delta/2) = 2\left[\frac{\delta}{2} - \frac{1}{2\times 3}\left(\frac{\delta}{2}\right)^3 + \frac{1\times 3}{2\times 4\times 5}\left(\frac{\delta}{2}\right)^5 - \frac{1\times 3\times 5}{2\times 4\times 6\times 7}\left(\frac{\delta}{2}\right)^7 + \ldots\right]$$

$$= \delta - \frac{\delta^3}{24} + \frac{3\delta^5}{640} - \frac{5\delta^7}{7168} + \ldots$$

- **Keeping the <u>first term</u>, we obtain**

$$(u_x)_i = \frac{u_{i+1/2} - u_{i-1/2}}{\Delta x} - \frac{(\Delta x)^2}{24} u_{xxx}$$

Difference formulas…

- **Keeping the <u>first two terms</u>, we obtain:**

$$(u_x)_i = \frac{-u_{i+3/2} + 27u_{i+1/2} - 27u_{i-1/2} + u_{i-3/2}}{24\,\Delta x} + \frac{3}{640}(\Delta x)^4 \frac{\partial^5 u}{\partial x^5}$$

- **We could use $\bar{\delta}$ to get**

$$\bar{\delta} = \frac{1}{2}\left(E - E^{-1}\right) = \frac{1}{2}(e^{\Delta x\, D} - e^{-\Delta x\, D}) = \sinh(\Delta x\, D) \quad \rightarrow$$

$$\Delta x\, D = \sinh^{-1}(\bar{\delta}) = \bar{\delta} - \frac{(\bar{\delta})^3}{6} + \frac{3}{2\times 4\times 5}(\bar{\delta})^5 - \ldots$$

- **Nothing that** $\mu^2 = 1 + \delta^2/4$ **or**

$$1 = \mu(1+\delta^2/4)^{-1/2} = \mu\left(1 - \frac{\delta^2}{8} + \frac{3\delta^4}{128} - \frac{5\delta^6}{1024} + \ldots\right)$$

- **We obtain**

$$\Delta x\, D = \mu\left(\delta - \frac{1}{3!}\delta^3 + \frac{1^2\times 2^2}{5!}\delta^5 - \ldots\right) = \bar{\delta}\left(1 - \frac{1}{3!}\delta^2 + \frac{2^2}{5!}\delta^4 - \frac{2^2\times 3^2}{7!}\delta^6 + \ldots\right)$$

Difference formulas…

- Then, keeping one term, we get

$$(u_x)_i = \frac{u_{i+1} - u_{i-1}}{2\,\Delta x} - \frac{(\Delta x)^2}{6} u_{xxx}$$

- And keeping two terms, we get

$$(u_x)_i = \frac{-u_{i+2} + 8u_{i+1} - 8u_{i-1} + u_{i-2}}{12\,\Delta x} + \frac{(\Delta x)^4}{30} u_{xxxxx}$$

Higher Order Derivatives

- For higher-order derivatives, we can use a <u>one-sided</u> forward difference as

$$\left(\frac{\partial^n u}{\partial x^n}\right)_i = D^n u_i = \frac{1}{\Delta x^n}\left[\ln(1+\delta^+)\right]^n u_i$$
$$= \frac{1}{\Delta x^n}\left[\left(\delta^+\right)^n - \frac{n}{2}\left(\delta^+\right)^{n+1} + \frac{n(3n+5)}{24}\left(\delta^+\right)^{n+2} - \frac{n(n+2)(n+3)}{48}\left(\delta^+\right)^{n+3} + \dots\right]u_i$$

- This can be written in terms of the backward and central differences as

$$\left(\frac{\partial^n u}{\partial x^n}\right)_i = \frac{-1}{\Delta x^n}\left[\ln(1-\delta^-)\right]^n u_i \qquad \left(\frac{\partial^n u}{\partial x^n}\right)_i = \left[\frac{2}{\Delta x}\sinh^{-1}\left(\frac{\delta}{2}\right)\right]^n u_i$$

- For <u>even</u> values of n, the central difference form generates formulas using the <u>integer mesh points</u>. For <u>odd</u> values of n, the formulas involve points at <u>half-integer mesh points</u>.
- For the following equation, the inverse is true:

$$D^n u_i = \frac{\mu\delta^n}{\Delta x^n}\left(1 - \frac{n+3}{24}\delta^2 + \frac{5n^2+52n+135}{5760}\delta^4 + \dots\right)u_i$$

Higher Order Derivatives

- **For example, we obtain the followings:**

$$(u_{xx})_i = \frac{1}{\Delta x^2}\left[(\delta^+)^2 - (\delta^+)^3 + \frac{11}{12}(\delta^+)^4 - \frac{5}{6}(\delta^+)^5 + \ldots\right]u_i$$

$$(u_{xx})_i = \frac{1}{\Delta x^2}\left[(\delta^-)^2 + (\delta^-)^3 + \frac{11}{12}(\delta^-)^4 + \frac{5}{6}(\delta^-)^5 + \ldots\right]u_i$$

$$(u_{xx})_i = \frac{1}{\Delta x^2}\left[(\delta)^2 - \frac{1}{12}(\delta)^4 + \frac{1}{90}(\delta)^6 - \frac{1}{560}(\delta)^8 + O(\Delta x^8)\right]u_i$$

- **By keeping only the <u>first term</u>, these formulas give:**

$$(u_{xx})_i = \frac{1}{\Delta x^2}(u_{i+2} - 2u_{i+1} + u_i) - \Delta x . u_{xxx} \quad (1st\ order\ \ forward)$$

$$(u_{xx})_i = \frac{1}{\Delta x^2}(u_i - 2u_{i-1} + u_{i-2}) + \Delta x . u_{xxx} \quad (1st\ order\ backward)$$

$$(u_{xx})_i = \frac{1}{\Delta x^2}(u_{i+1} - 2u_i + u_{i-1}) - \frac{\Delta x^2}{12} . u_{xxxx} \quad (2nd\ order\ central)$$

$$(u_{xx})_i = \frac{1}{2\Delta x^2}(u_{i+3/2} - u_{i+1/2} - u_{i-1/2} + u_{i-3/2}) - \frac{5\Delta x^2}{24} . u_{xxxx} \quad (2nd\ order\ central)$$

Higher Order Derivatives…

- The one-sided difference formulas are only first-order accurate, while the central difference always leads to a higher-order of accuracy.
- By keeping the first two terms of the above formulas, we obtain higher-order formulas:

$$(u_{xx})_i = \frac{1}{\Delta x^2}(2u_i - 5u_{i+1} + 4u_{i+2} - u_{i+3}) + \frac{11\Delta x^2}{12}.u_{xxxx} \quad (2nd\ order\ forward)$$

$$(u_{xx})_i = \frac{1}{\Delta x^2}(2u_i - 5u_{i-1} + 4u_{i-2} - u_{i-3}) - \frac{11\Delta x^2}{12}.u_{xxxx} \quad (2nd\ order\ backward)$$

$$(u_{xx})_i = \frac{1}{12\Delta x^2}(-u_{i+2} + 16u_{i+1} - 30u_i + 16u_{i-1} - u_{i-2}) + \frac{\Delta x^4}{90}.u_{xxxxxx} \quad (4th\ order\ central)$$

$$(u_{xx})_i = \frac{1}{48\Delta x^2}(-5u_{i+5/2} + 39u_{i+3/2} - 34u_{i+1/2} - 34u_{i-1/2} + 39u_{i-3/2} - 5u_{i-5/2}) + \frac{259\Delta x^4}{5760}.u_{xxxxxx} \quad (4th\ order\ central)$$

- For a term like $\frac{\partial}{\partial x}\left(k(x)\frac{\partial u}{\partial x}\right)$, we can use: (2^{nd} order central)

$$\frac{\partial}{\partial x}\left[k(x)\frac{\partial}{\partial x}\right]u_i = \frac{1}{(\Delta x)^2}\delta^+\left(k_{i-1/2}\delta^-\right)u_i + O(\Delta x^2)$$

$$= \frac{k_{i+1/2}(u_{i+1} - u_i)}{(\Delta x)^2} - \frac{k_{i-1/2}(u_i - u_{i-1})}{(\Delta x)^2} + O(\Delta x^2)$$

3rd Order Derivatives

- **As an special case, we can easily show that**

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

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

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

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

$$\left(\frac{\partial^3 u}{\partial x^3}\right)_i = \frac{1}{(\Delta x)^3}\left(u_{i+3/2} - 3u_{i+1/2} + 3u_{i-1/2} - u_{i-3/2}\right) - \frac{(\Delta x)^2}{8}\frac{\partial^5 u}{\partial x^5} \qquad 2nd\ order\ central$$

$$\left(\frac{\partial^3 u}{\partial x^3}\right)_i = \frac{1}{8(\Delta x)^3}\left(-u_{i+5/2} + 13u_{i+3/2} - 34u_{i+1/2} + 34u_{i-1/2} - 13u_{i-3/2} + u_{i-5/2}\right) - \frac{37(\Delta x)^4}{1920}\frac{\partial^7 u}{\partial x^7} \qquad 4th\ order\ central$$

- **Also, using integer points, we get:**

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

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

4th Order Derivatives

- **Similarly, for the 4th order formulas, we get**

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

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

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

Implicit FD Formulas

- **Implicit formulas are defined as expressions where derivatives at different mesh points appear simultaneously.**
- **We can generate implicit formulas from previous explicit formulas.**
- **For example starting with**

$$\Delta x\, D = \mu\delta\left(1+\delta^2/6\right)^{-1} + O(\Delta x^5) \;\rightarrow$$

$$\left(1+\delta^2/6\right)D = \frac{\mu\delta}{\Delta x} + O(\Delta x^4) \;\rightarrow$$

$$\frac{1}{6}\left[(u_x)_{i+1} + 4(u_x)_i + (u_x)_{i-1}\right] = \frac{u_{i+1}-u_{i-1}}{2\Delta x} + O(\Delta x^4)$$

- **The last equation is called rational fraction or Pade's differencing.**

Implicit FD Formulas…

- The use of this formulas results in the following tri-diagonal system:

$$\begin{bmatrix} \ddots & & & & 0 \\ 1 & 4 & 1 & & \\ & 1 & 4 & 1 & \\ & & 1 & 4 & 1 \\ 0 & & & & \ddots \end{bmatrix} \begin{bmatrix} 0 \\ \vdots \\ (u_x)_{i-1} \\ (u_x)_i \\ (u_x)_{i+1} \\ \vdots \\ 0 \end{bmatrix} = \frac{3}{\Delta x} \begin{bmatrix} 0 \\ \vdots \\ u_i - u_{i-2} \\ u_{i+1} - u_{i-1} \\ u_{i+2} - u_i \\ \vdots \\ 0 \end{bmatrix}$$

- The reason why the formulas are higher order is that each u_x depends on all values of $u's$.

Derivation of Implicit Formulas

- **If we use a three point expression, we can write a general form as**

$$
\begin{aligned}
&a^{+}u_{i+1} + a^{0}u_{i} + a^{-}u_{i-1} + \\
&b^{+}\left(u_{x}\right)_{i+1} + b^{0}\left(u_{x}\right)_{i} + b^{-}\left(u_{x}\right)_{i-1} + \\
&c^{+}\left(u_{xx}\right)_{i+1} + c^{0}\left(u_{xx}\right)_{i} + c^{-}\left(u_{xx}\right)_{i-1} = 0
\end{aligned}
$$

- **Developing all the variables in a Taylor series about point i, We get**
- **In order to get a 2nd order accuracy for the second derivative, we request the coefficients up to the third order derivatives of the truncation error to vanish, i.e.:**

$$
\begin{aligned}
u_{i\pm1} = u_i \pm \Delta x\left(u_x\right)_i + \frac{(\Delta x)^2}{2}\left(u_{xx}\right)_i \pm \frac{(\Delta x)^3}{6}\left(u_{xxx}\right)_i + \frac{(\Delta x)^4}{24}\left(u_{xxxx}\right)_i \\
\pm \frac{(\Delta x)^5}{5!}\left(u_{xxxxx}\right)_i + \frac{(\Delta x)^6}{6!}\left(u_{xxxxxx}\right)_i \pm \ldots..
\end{aligned}
$$

Derivation of Implicit Formulas…

- **For the first derivative, we get**

$$(u_x)_{i\pm1} = (u_x)_i \pm \Delta x\,(u_{xx})_i + \frac{(\Delta x)^2}{2}(u_{xxx})_i \pm \frac{(\Delta x)^3}{6}(u_{xxxx})_i + \frac{(\Delta x)^4}{24}(u_{xxxxx})_i \pm \frac{(\Delta x)^5}{5!}(u_{xxxxxx})_i + \frac{(\Delta x)^6}{6!}(u_{xxxxxxx})_i \pm .....$$

- **And for the second derivative, we get**

$$(u_{xx})_{i\pm1} = (u_{xx})_i \pm \Delta x\,(u_{xxx})_i + \frac{(\Delta x)^2}{2}(u_{xxxx})_i \pm \frac{(\Delta x)^3}{6}(u_{xxxxx})_i + \frac{(\Delta x)^4}{24}(u_{xxxxxx})_i \pm \frac{(\Delta x)^5}{5!}(u_{xxxxxxx})_i + \frac{(\Delta x)^6}{6!}(u_{xxxxxxxx})_i \pm .....$$

Derivation of Implicit Formulas…

- **In order to get a 2nd order accuracy for the 2nd derivative, we request that the coefficients up to the 3rd order derivatives of the truncation error to vanish:**

$$\begin{cases} a^+ + a^0 - a^- = 0 \\ \Delta x\left(a^+ - a^-\right) + b^+ + b^0 + b^- = 0 \\ \dfrac{\Delta x^2}{2}\left(a^+ + a^-\right) + \Delta x\left(b^+ - b^-\right) + c^+ + c^0 + c^- = 0 \\ \dfrac{\Delta x^3}{6}\left(a^+ - a^-\right) + \dfrac{\Delta x^2}{2}\left(b^+ - b^-\right) + \Delta x\left(c^+ - c^-\right) = 0 \end{cases} \rightarrow$$

$$\begin{cases} a^+ = \dfrac{1}{2\Delta x}\left[-5b^+ - b^- + \dfrac{2}{\Delta x}(2c^- - 4c^+ - c^0)\right] \\ a^0 = \dfrac{2}{\Delta x}\left[b^+ - b^- + \dfrac{1}{\Delta x}(c^+ + c^0 - c^-)\right] \\ a^- = \dfrac{1}{2\Delta x}\left[b^+ + 5b^- + \dfrac{2}{\Delta x}(2c^+ - 4c^- - c^0)\right] \\ b^0 = 2\left(b^+ + b^-\right) + \dfrac{6}{\Delta x}\left(c^+ - c^-\right) \end{cases}$$

Derivation of Implicit Formulas…

- And the truncation error R reduces to

$$R = \frac{\Delta x^3}{24}\left[2(b^+ - b^-) + \frac{10}{\Delta x}(c^+ - c^-) - \frac{2}{\Delta x}c^0\right]\frac{\partial^4 u}{\partial x^4} +$$
$$\frac{\Delta x^4}{120}\left[2(b^+ - b^-) + \frac{14}{\Delta x}(c^+ - c^-)\right]\frac{\partial^5 u}{\partial x^5} +$$
$$\frac{\Delta x^5}{6!}\left[4(b^+ - b^-) + \frac{28}{\Delta x}(c^+ + c^-) - \frac{2}{\Delta x}c^0\right]\frac{\partial^6 u}{\partial x^6} +$$
$$\frac{\Delta x^6}{7!}\left[4(b^+ + b^-) + \frac{36}{\Delta x}(c^+ - c^-)\right]\frac{\partial^7 u}{\partial x^7} +$$
$$\frac{\Delta x^7}{8!}\left[6(b^+ - b^-) + \frac{54}{\Delta x}(c^+ + c^-) - \frac{2}{\Delta x}c^0\right]\frac{\partial^8 u}{\partial x^8}$$

- This gives a four parameter family of implicit relations.
- One parameter may be set arbitrarily to one since our original form is homogeneous.

Derivation of Implicit Formulas…

- **If we choose to make the first three terms in R equal to zero, we obtain:**

$$b^{+} = \frac{1}{\Delta x}\left(8c^{+} + c^{-}\right)$$
$$b^{-} = \frac{1}{\Delta x}\left(c^{+} + 8c^{-}\right)$$
$$c^{0} = -4\left(c^{+} + c^{-}\right)$$

- **Then, we get:**

$$\frac{3}{2\Delta x^2}(13+3\alpha)u_{i+1} - \frac{24}{\Delta x^2}(1+\alpha)u_i + \frac{3}{2\Delta x^2}(3+13\alpha)u_{i-1} - \frac{1}{\Delta x}(8+\alpha)(u_x)_{i+1} - \frac{8}{\Delta x}(1-\alpha)(u_x)_i + \frac{1}{\Delta x}(1+8\alpha)(u_x)_{i-1} + (u_{xx})_{i+1} - 4(1+\alpha)(u_{xx})_i + \alpha(u_{xx})_{i-1} = 0$$

- **Where $\alpha = c^{-}/c^{+}$ and**

$$R = \frac{8\Delta x^5}{7!}(1-\alpha)\frac{\partial^7 u}{\partial x^7} + \frac{\Delta x^6}{8!}(1+\alpha)\frac{\partial^8 u}{\partial x^8}$$

Derivation of Implicit Formulas…

- **The unique, implicit relation of order six is obtained from $\alpha = 1$:**

$$\frac{24}{\Delta x^2}\left(u_{i+1} - 2u_i + u_{i-1}\right) - \frac{9}{\Delta x}\left[\left(u_x\right)_{i+1} - \left(u_x\right)_{i-1}\right] + \left(u_{xx}\right)_{i+1} - 8\left(u_{xx}\right)_i + \left(u_{xx}\right)_{i-1} = 0$$

with

$$R = \frac{2}{8!}\Delta x^6 \frac{\partial^8 u}{\partial x^8}$$

- **The unique 4th order relation is obtained from $c^+ = c^0 = c^- = 0$ and $\beta = b^- / b^+$:**

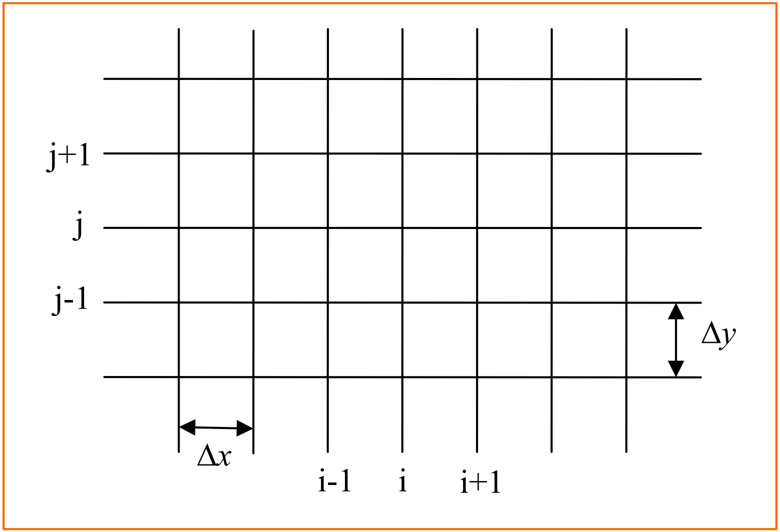
$$\frac{1}{2\Delta x}(-5-\beta)u_{i+1} + \frac{2}{\Delta x}(1-\beta)u_i + \frac{1}{2\Delta x}(1+5\beta)u_{i-1} + \left(u_x\right)_{i+1} + 2(1+\beta)\left(u_x\right)_i + \beta\left(u_x\right)_{i-1} = 0$$

with

$$R = \frac{\Delta x^3}{12}(1-\beta)\frac{\partial^4 u}{\partial x^4} + \frac{\Delta x^4}{60}(1+\beta)\frac{\partial^5 u}{\partial x^5}$$

Note: SPECIAL CASE $\beta = 1$

Multi-dimensional FDM Formulas



- **In a 2D space a rectangular mesh can be obtained by**

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

Multi-dimensional FDM Formulas

- If we denote $u(x_i, y_j)$ by u_{ij}, we can apply the previous formulas on either variables x and y.
- For example: (1st order formulas)

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

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

- And a second order formula can be written as

$$\left(u_{xx}\right)_{ij} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} - \frac{\Delta x^2}{12} u_{xxxx}$$

Multi-dimensional FDM Formulas

- **Laplace Equation:**

$$\left(u_{xx} + u_{yy}\right)_{ij} = \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{\Delta x^2} + \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{\Delta y^2} + O(\Delta x^2, \Delta y^2)$$

- **For** $\Delta x = \Delta y$ **, we get**

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

- **A more general term** $\nabla.\left(k\,\nabla\right)$ **can be written as**

$$\nabla.\left(k\,\nabla\right) = \frac{1}{\Delta x^2}\left(\delta_x^+ \, k_{i+1/2,j} \, \delta_x^-\right)u_{ij} + \frac{1}{\Delta y^2}\left(\delta_y^+ \, k_{i,j+1/2} \, \delta_y^-\right)u_{ij} + O(\Delta x^2, \Delta y^2)$$

- **We could use another form as**

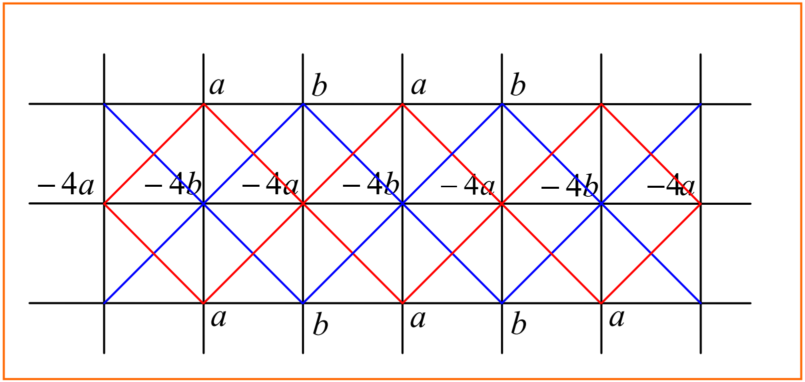
$$\nabla^2 = \frac{1}{\Delta x^2}\left(\mu_y \delta_x\right)^2 + \frac{1}{\Delta y^2}\left(\mu_x \delta_y\right)^2$$

Multi-dimensional FDM Formulas

- Which gives the following formula for $\Delta x = \Delta y$:

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

- This formula is not suitable as it decouples the odd-numbered points from the even-number points. This means that for a situation where the solution oscillates between values a and b, the results satisfy the Laplace equation while it is not right.



Multi-dimensional FDM Formulas

- **We can combine the last two methods to obtain a family of nine-point schemes as** $(\Delta x = \Delta y)$

$$\nabla^2 u_{ij} = \frac{1}{\Delta x^2}\left[\left(\delta_x^2 + \delta_y^2\right) + \frac{b}{2}\delta_x^2\delta_y^2\right] = \Delta u_{ij} + \frac{\Delta x^2}{12}\left(u_{xxxx} + u_{yyyy} + 6b\,u_{xxyy}\right)$$

- **For** $b = 2/3$ **, this is equivalent to a Galerkin finite element discretization of the Laplace operator using bilinear quadrilateral elements on the same mesh.**

Mixed Derivatives

- The simplest 2nd order central formula is

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

- A first order formula in both x and y is

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

- We should note that the above formula is 2nd order at $(i+1/2, j+1/2)$.

- The following formula is the most general 2nd order mixed derivative formula: ($a+b=1$)

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

NON-UNIFORM GRIDS

- **In a general mesh, Δx may vary. So, we should be careful of the order of the approximations:**

$$(u_x)_i = \frac{u_{i+1} - u_i}{\Delta x_{i+1}} - \frac{\Delta x_{i+1}}{2} u_{xx} \qquad (first\ order)$$

$$(u_x)_i = \frac{u_i - u_{i-1}}{\Delta x_i} + \frac{\Delta x_i}{2} u_{xx} \qquad (first\ order)$$

- **Combining these formulas, one gets:**

$$(u_x)_i = \frac{1}{\Delta x_i + \Delta x_{i+1}} \left[\frac{\Delta x_i}{\Delta x_{i+1}} (u_{i+1} - u_i) + \frac{\Delta x_{i+1}}{\Delta x_i} (u_i - u_{i-1}) \right] - \frac{\Delta x_i \Delta x_{i+1}}{6} u_{xxx} \qquad (2nd\ \ order)$$

- **A 2nd order formula for the 2nd derivative is**

$$(u_{xx})_i = \left(\frac{u_{i+1} - u_i}{\Delta x_{i+1}} - \frac{u_i - u_{i-1}}{\Delta x_i} \right) \frac{2}{\Delta x_{i+1} + \Delta x_i} + \frac{1}{3} (\Delta x_{i+1} - \Delta x_i)\, u_{xxx} - \frac{\Delta x_{i+1}^3 + \Delta x_i^3}{12(\Delta x_{i+1} + \Delta x_i)} u_{xxxx}$$

NON-UNIFORM GRIDS

- **Note that if the mesh size varies abruptly, for example if $\Delta x_{i+1} \approx 2\Delta x_i$, then the formula will be only 1st order accurate.**
- **It is a general property of finite difference method on non-uniform meshes that if the mesh size does not vary smoothly, a loss of accuracy is unavoidable.**