Chapter 3

An Introduction to

Finite Difference Calculus

Third Session Contents:

1) **Difference operators theory**
2) **Difference approximation**
3) **Implicit finite difference equations**
4) **Fourier analysis error and numerical accuracy**

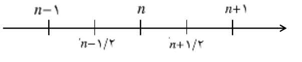
Difference Operators Theory

$y = f(x)$

$h = x_{n+1} - x_n$

$y_n = f(x_n)$

$$\begin{cases} \Delta y_n = y_{n+1} - y_n & \text{Forward difference operator} \\ \nabla y_n = y_n - y_{n-1} & \text{Backward difference operator} \\ \delta y_n = y_{n+1/2} - y_{n-1/2} & \text{Central difference operator} \\ \mu y_n = \frac{1}{2}(y_{n+1/2} + y_{n-1/2}) & \text{Averaging difference operator} \\ E y_n = y_{n+1} & \text{Transport operator} \\ D y_n = \left.\frac{dy}{dx}\right|_n & \text{Derivative operator} \end{cases}$$



Difference Operators Theory

Other relations between operators

$\Delta = E - 1$ $\quad \nabla = 1 - E^{-1}$ $\quad E^k f_n = f_{n+k}$ $\quad E^{-1} f_n = f_{n-1}$

$\delta = E^{1/2} - E^{-1/2}$ $\quad \mu = \frac{1}{2}\left(E^{1/2} + E^{-1/2}\right)$ $\quad E^{1/2} f_n = f_{n+1/2}$ $\quad E^{-1/2} f_n = f_{n-1/2}$

Finding a relation for D operator

Taylor series → $f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \dots$

$$E f(x) = \left[1 + hD + \frac{h^2 D^2}{2!} + \dots\right] f(x) = e^{hD} f(x)$$

→ $E = e^{hD}$

Difference Operators Theory

$\Delta = E - 1$ $\quad \nabla = 1 - E^{-1}$ $\quad E^k f_n = f_{n+k}$ $\quad E^{-1} f_n = f_{n-1}$

$\delta = E^{1/2} - E^{-1/2}$ $\quad \mu = \frac{1}{2}\left(E^{1/2} + E^{-1/2}\right)$ $\quad E^{1/2} f_n = f_{n+1/2}$ $\quad E^{-1/2} f_n = f_{n-1/2}$

$$\begin{cases} \Delta = e^{hD} - 1 \\ \nabla = 1 - e^{-hD} \\ \delta = e^{hD/2} - e^{-hD/2} = 2\sinh(\frac{hD}{2}) \\ \mu = \frac{1}{2}\left(e^{hD/2} + e^{-hD/2}\right) = \cosh(\frac{hD}{2}) \end{cases} \Rightarrow \begin{cases} D = \frac{1}{h}\ln(1 + \Delta) \\ D = -\frac{1}{h}\ln(1 - \nabla) \\ D = \frac{2}{h}\sinh^{-1}(\frac{\delta}{2}) \\ D = \frac{2}{h}\cosh^{-1}(\mu) \end{cases}$$

Difference Approximation

$$D = \frac{1}{h}\ln(1+\Delta) = \frac{1}{h}\left(\Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 + \dots\right)$$

Keeping the first term of right side $\longrightarrow$ $Df_n \simeq \frac{1}{h}\Delta f_n = \frac{f_{n+1} - f_n}{h}$

Keeping the first two terms at right side $\longrightarrow$

$$Df_n \simeq \frac{1}{h}\left(\Delta f_n - \frac{1}{2}\Delta^2 f_n\right)$$
$$= \frac{1}{h}\left\{f_{n+1} - f_n - \frac{1}{2}(f_{n+2} - 2f_{n+1} + f_n)\right\}$$
$$\simeq \frac{1}{h}\left(-\frac{1}{2}f_{n+2} + 2f_{n+1} - \frac{3}{2}f_n\right)$$

$$\hookrightarrow Df_n \simeq \frac{1}{2h}(-f_{n+2} + 4f_{n+1} - 3f_n)$$

$$\left.\begin{aligned} &\Delta = e^{hD} - 1 = hD + \frac{h^2}{2!}D^2 + \dots \\ &\Delta = O(h) \end{aligned}\right\} Df_n = \frac{1}{2h}(-f_{n+2} + 4f_{n+1} - 3f_n) + O(h^2)$$

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Difference Approximation

For finding the truncation error

$$Df_n = \frac{1}{h}\Delta f_n + \text{T.E.}$$

$$\text{T.E.} = \frac{1}{h}\left(-\frac{1}{2}\Delta^2 f_n + \frac{1}{3}\Delta^3 f_n + \dots\right) \xrightarrow{\Delta = O(h)} \text{T.E.} \simeq O(h)$$

One can also use the following equations for finding a new definition for D

$$D = \frac{2}{h}\sinh^{-1}\left(\frac{\delta}{2}\right)$$

$$\left.\begin{aligned} \sinh^{-1} x &= x - \frac{1}{2}\frac{x^3}{3} + \frac{1\times 3}{2\times 4}\frac{x^5}{5} - \frac{1\times 3\times 5}{2\times 4\times 6}\frac{x^7}{7} + \dots \\ &= \sum_{n=0}^{\infty}\frac{(-1)^n}{2^{2n}}\frac{(2n)!}{(n!)^2}\frac{x^{2n+1}}{2n+1} \end{aligned}\right\} D = \frac{2}{h}\left\{\frac{\delta}{2} - \frac{\delta^3}{48} + \dots\right\} \simeq \frac{\delta}{h} - \frac{\delta^3}{24h}$$

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Difference Approximation

Considering the first term of the right-hand side

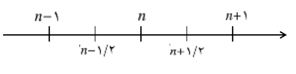
$$Df_n \simeq \frac{E^{1/2}f_n - E^{-1/2}f_n}{h} = \frac{f_{n+1/2} - f_{n-1/2}}{h}$$ **Central difference approximation**

$$\mu\delta = 2\sinh\left(\frac{hD}{2}\right)\cosh\left(\frac{hD}{2}\right) = \sinh(hD)$$

$$D = \frac{1}{h}\sinh^{-1}(\mu\delta) = \frac{1}{h}\left\{\mu\delta - \frac{1}{6}(\mu\delta)^3 + \dots\right\}$$

Considering the first term of right-hand side and neglecting the higher order term:

$$Df_n = \frac{\mu\delta}{h}f_n = \frac{\mu}{h}(\delta f_n) = \frac{\mu}{h}(f_{n+1/2} - f_{n-1/2})$$
$$Df_n = \frac{1}{2h}\{(f_{n+1} + f_n) - (f_n + f_{n-1})\}$$
$$Df_n = \frac{1}{2h}(f_{n+1} - f_{n-1})$$



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Difference Approximation

New central difference operator:

$$\bar{\delta} = \mu\delta$$
$$\bar{\delta} = \mu\delta = \mu\left(E^{1/2} - E^{-1/2}\right) = \frac{1}{2}\left(E^1 + E^0 - E^0 - E^{-1}\right)$$
$$\bar{\delta} = \frac{1}{2}\left(E^1 - E^{-1}\right)$$

$$D = \frac{1}{h}\sinh^{-1}(\mu\delta) = \frac{1}{h}\left\{\mu\delta - \frac{1}{6}(\mu\delta)^3 + \dots\right\} \Rightarrow D = \frac{1}{h}\left\{\bar{\delta} - \frac{\bar{\delta}^3}{6} + \frac{3}{2\times 4\times 5}\bar{\delta}^5 + \dots\right\}$$

$$\mu^2 = 1 + \frac{\delta^2}{4}$$

Multiplying both side by μ^{-2}

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

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Difference Approximation

$$D = \frac{2}{h}\left\{\frac{\delta}{2} - \frac{\delta^3}{48} + \frac{3}{1280}\delta^5 + \dots\right\} \longrightarrow hD = \mu\left\{\delta - \frac{1}{3!}\delta^3 + \frac{1^2 3^2}{5!}\delta^5 + \dots\right\}$$
$$= \bar{\delta}\left\{1 - \frac{\delta^2}{3!} + \frac{2^2}{5!}\delta^4 - \frac{2^2 3^2}{7!}\delta^6 + \dots\right\}$$

Considering the first term of right-hand side

$$(f_x)_n = \frac{f_{n+1} - f_{n-1}}{2\Delta x} - \frac{(\Delta x)^2}{6} f_{xxx}$$

Considering the first and second terms one can obtain:

$$(f_x)_n = \frac{-f_{n+2} + 8f_{n+1} - 8f_{n-1} + f_{n-2}}{12\Delta x} + \frac{(\Delta x)^4}{30}\frac{\partial^5 f}{\partial x^5}$$

Which is the standard form we have obtained before.

Compact Implicit Finite Difference

From the previous section:

$$hD = \bar{\delta}\left\{1 - \frac{\delta^2}{3!} + \frac{2^2}{5!}\delta^4 - \frac{2^2 \cdot 3^2}{7!}\delta^6 + \dots\right\}$$

Considering the first and second terms of the above equation:

$$hD = \mu\delta\left(1 - \frac{\delta^2}{6}\right) + O(h^5) \quad \text{(I)}$$

Using Newton's expansion $\longrightarrow$ $hD = \dfrac{\mu\delta}{1 + \dfrac{\delta^2}{6}} + O(h^5)$ (II) **Rational fraction or Pade difference scheme**

Using (I) equation for f_n $\quad (Df_n)_i = \dfrac{-f_{n+2} + 8f_{n+1} - 8f_{n-1} + f_{n-2}}{12h} + \dfrac{h^4}{30}\dfrac{\partial^5 f_n}{\partial x^5}$

Using (II) equation for f_n $\quad h\left(1 + \dfrac{\delta^2}{6}\right)Df_n = (\mu\delta)\, f_n + O(h^5)$

Compact Implicit Finite Difference

Using $\bar{\delta} = \mu\delta$ and, δ^2

$$h\left[1 + \frac{1}{6}\left(E^{1/2} - E^{-1/2}\right)^2\right]Df_n = \frac{f_{n+1} - f_{n-1}}{2} + O(h^5)$$
$$h\left[1 + \frac{1}{6}\left(E + E^{-1} - 2\right)\right]Df_n = \frac{f_{n+1} - f_{n-1}}{2} + O(h^5)$$

Utilizing transform operator

$$\frac{h}{6}\left[Df_{n+1} + 4Df_n + Df_{n-1}\right] = \frac{f_{n+1} - f_{n-1}}{2} + O(h^5)$$
$$Df_{n+1} + 4Df_n + Df_{n-1} = \frac{3}{h}(f_{n+1} - f_{n-1}) + O(h^4)$$
$$f'_{n+1} + 4f'_n + f'_{n-1} = \frac{3}{h}(f_{n+1} - f_{n-1}) + O(h^4)$$

$\Rightarrow$ **Hermitian Scheme or Compact implicit method**

Fourier Analysis Error and Numerical Accuracy

Joseph Fourier

Born: March 21, 1768, Auxerre, France

Died: May 16, 1830, Paris, France

Education: École Normale Supérieure

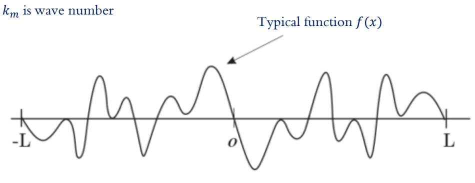
Jean-Baptiste Joseph Fourier was a French mathematician and physicist born in Auxerre and best known for initiating the investigation of Fourier series and their applications to problems of heat transfer and vibrations.

Fourier Analysis Error and Numerical Accuracy

Fourier series:

$$f(x) = \sum_m A_m e^{ik_m x}$$

k_m is wave number



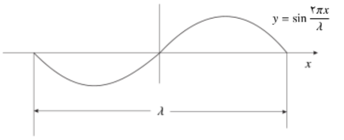
Schematic diagram of a typical function variation versus x

Fourier analysis Error and Numerical Accuracy

$$e^{ik_m x} = \cos k_m x + i \sin k_m x$$

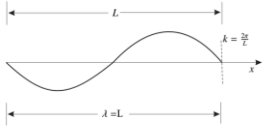
k_m is wave number

λ is wave length

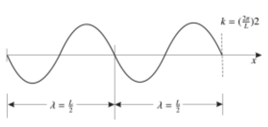


$$y = \sin \frac{٢\pi x}{\lambda} \quad \& \quad y = \sin k_m x \longrightarrow k_m = \frac{٢\pi}{\lambda}$$

Fourier Analysis Error and Numerical Accuracy

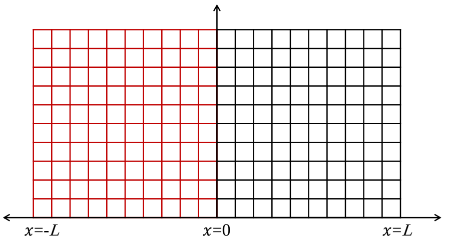


$$\longrightarrow \quad k_١ = \frac{٢\pi}{L}$$



$$\longrightarrow \quad k_٢ = \frac{٢\pi}{L/٢} = \left(\frac{٢\pi}{L}\right) \times ٢$$

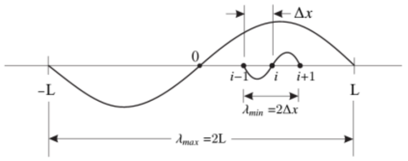
Fourier Analysis Error and Numerical Accuracy



$$k_m = \left(\frac{٢\pi}{٢L}\right)m, \qquad m = ٠, ١, ٢, ٣, \ldots, M, \qquad \lambda_{\max} = ٢L \longrightarrow$$

M* is the number of waves in the specific domain like 2*L

Fourier Analysis Error and Numerical Accuracy



The smallest and the largest waves for the typical function

For a computational domain with N grids in the specific domain of L:

$\Delta x = L/N \longrightarrow \lambda_{\min} = 2L/N$

$k_m = \frac{2\pi}{2L/N} = \frac{2\pi}{L}\frac{N}{2}$

Fourier Analysis Error and Numerical Accuracy

For a domain with N+1 grid points:

$f(x) = \sum_{m=-N}^{N} A_m e^{ik_m x}$

If A_m is a function of time: $f(x,t) = \sum_{m=-N}^{N} A_m(t) e^{ik_m x}$

Which could be defined as an exponential as following:

$$f(x,t) = \sum_{m=-N}^{N} e^{at} e^{ik_m x}$$

Fourier Analysis of the First Derivative

A discretized periodic function with periodicity of λ_m

$f(x_j) = \sum_{m=-N}^{N} \tilde{f}(k_m) e^{ik_m x_j}$ $\quad k_m = \frac{2\pi}{L} m$

The largest wave length $\quad \lambda_{max} = N\Delta x$

The smallest wave length $\quad \lambda_{min} = 2\Delta x$

Fourier series for N[th] derivative: $(\widetilde{\mathcal{D}^n f_j})_m = (ik_m)^n \tilde{f}(k_m) \rightarrow \frac{\partial^n \widetilde{f(x)}}{\partial x^n} = (ik_m)^n \tilde{f}(k)$

Finite difference relation:

$$\begin{cases} \mathcal{D}f = \dfrac{f_{j+1} - f_{j-1}}{2\Delta x} \\ (\widetilde{\mathcal{D}f_j}) = \dfrac{[e^{ik_m(\Delta x)} - e^{ik_m(-\Delta x)}]}{2\Delta x} \tilde{f}(k_m) \end{cases}$$

Fourier Analysis of the First Derivative

$$ik_m \tilde{f}(k_m) = \frac{[e^{ik_m(\Delta x)} - e^{ik_m(-\Delta x)}]}{2\Delta x} \tilde{f}(k_m)$$

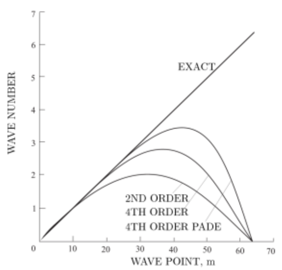
Defining the Modified wave number: $k'_{2m} = \frac{\sin\theta_m}{\Delta x}$ which $\theta_m = \Delta x k_m$

Pade scheme:

$$\begin{cases} \mathcal{D}f = \dfrac{f_{j-2} - 8f_{j-1} + 8f_{j+1} - f_{j+2}}{12\Delta x} \\ k'_{4m} = \dfrac{8\sin\theta_m - \sin 2\theta_m}{6\Delta x} \end{cases} \qquad \begin{cases} k'_{4pm} = \dfrac{3\sin\theta_m}{\Delta x(2 + \cos\theta_m)} \\ \left[1 + \dfrac{\delta^2}{6}\right]\mathcal{D}f = \dfrac{f_{j+1} - f_{j-1}}{2\Delta x} \end{cases}$$

where $\quad \delta^2 f = f_{j+1} - 2f_j + f_{j-1}$

Fourier Analysis of the First Derivative



Comparing the analytical and numerical wave number for N=64 and $\lambda_{max} = 20\pi$ (first derivative)

Results:

- Higher order methods are more accurate
- Different methods with the same order of T.E. have different errors
- By increasing the wave number, the error related to finite difference method will increase too.
- Higher order methods needs less points for achieving the same errors
- For the small wave numbers, the error approaches zero with different rates depending on order of T.E.

Fourier Analysis of the Second Derivative

Diffusion terms in momentum equations:

$\mu_{\text{eff}}\left(\frac{\partial^2 f}{\partial x^2}\right)$ which μ_{eff} Effective viscosity coefficient

Second order, central finite difference

$$\mathcal{D}^2 f = \frac{f_{j+1} - 2f_j + f_{j-1}}{\Delta x^2} \qquad k''_{2m} = -\frac{2(\cos\theta_m - 1)}{\Delta x^2}$$

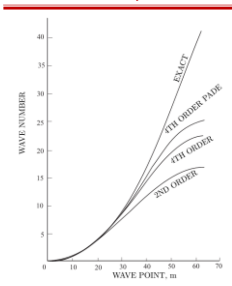
"prime" is used to show the derivative order

Pade method

$$\begin{cases} \mathcal{D}^2 f = \dfrac{-f_{j-2} + 16 f_{j-1} - 30 f_j + 16 f_{j+1} - f_{j+2}}{12\Delta x^2} \\ k''_{4m} = \dfrac{15 - 16\cos\theta_m + \cos 2\theta_m}{6\Delta x^2} \end{cases}$$

$$\begin{cases} \left[1 + \dfrac{\delta^2}{12}\right]\mathcal{D}^2 f = \dfrac{\delta^2 f}{\Delta x^2} \\ k''_{4pm} = \dfrac{12(1 - \cos\theta_m)}{(5 + \cos\theta_m)\Delta x^2} \end{cases}$$

Fourier Analysis of the Second Derivative



Comparing the analytical and numerical wave number for N=64 and $\lambda_{max} = 20\pi$ (second derivative)

Results:

- Higher order methods are more accurate
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- For the small wave numbers, the error approaches zero with different rates depending on order of T.E.