Finite Difference Method

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Reactor Physics, KTH

Overview

- Deterministic vs. Stochastic
- FD Method
  - Discretization
  - Derivative Approximation
  - Accuracy
- Local Truncation Error
- First and Second Derivatives
- Matrix Representation

Diffusion Equation

$$-\phi_{xx}(x,y)-\phi_{yy}(x,y)+B^2\phi(x,y)=S(x,y) \qquad a\le x,y\le b$$

$$\frac{1}{v}\frac{\partial\phi(\mathbf{r},t)}{\partial t}=S(\mathbf{r},t)+\nu\Sigma_f(\mathbf{r})\phi(\mathbf{r},t)-\Sigma_a(\mathbf{r})\phi+\nabla\left[D(\mathbf{r})\nabla\phi(\mathbf{r},t)\right]$$

$$-\nabla\left[D(\mathbf{r})\nabla\phi(\mathbf{r})\right]+\Sigma_a(\mathbf{r})\phi=\frac{\nu\Sigma_f(\mathbf{r})}{k}\phi(\mathbf{r})$$

General Approaches

NDE/NTE

Deterministic (FD Method)	Stochastic (Simulations)
• Attila (com) • Dragon (open) • Dif3D (ANL) • …	• MCNP (LANL) • KENO (ORNL) • Serpent (open) • …

FD Method

1. **Discretization**

$$x \longrightarrow \left[x_0, x_1, \ldots, x_{N+1}\right]^T \equiv \mathbf{x}$$

$$y(x) \longrightarrow \left[y_0, y_1, \ldots, y_{N+1}\right]^T \equiv \mathbf{y}$$

2. **Approximation**

$$\frac{dy(x_i)}{dx} \longrightarrow \frac{y_{i+1} - y_i}{x_{i+1} - x_i}$$

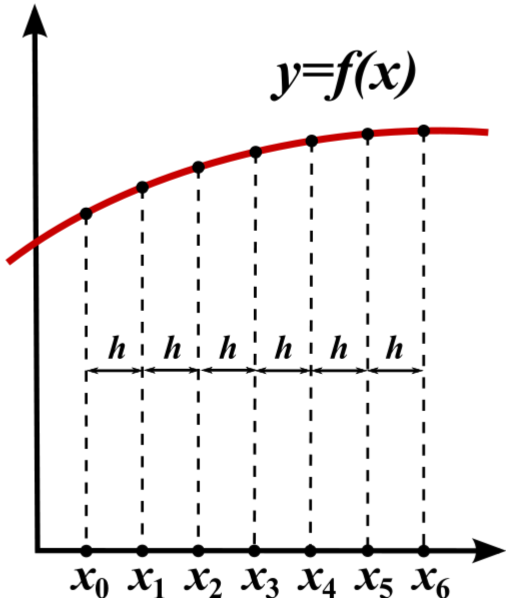
3. **Solving FD equations**

$$\mathbf{Ay} = \mathbf{s}$$

4. **Answering the question**

$$\left|y(x_i) - y_i\right| \le Ch^m \qquad h = \max_i \left(x_{i+1} - x_i\right)$$

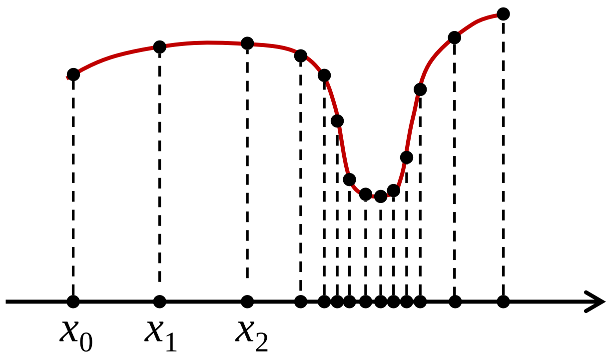
Discretization



$$\mathbf{D}y(x) = S(x)$$

$$x \in [a,b] \longrightarrow [x_0, x_1, \ldots, x_{N+1}] \equiv \mathbf{x}$$

$$y = y(x) \longrightarrow [y_0, y_1, \ldots, y_{N+1}] \equiv \mathbf{y}$$

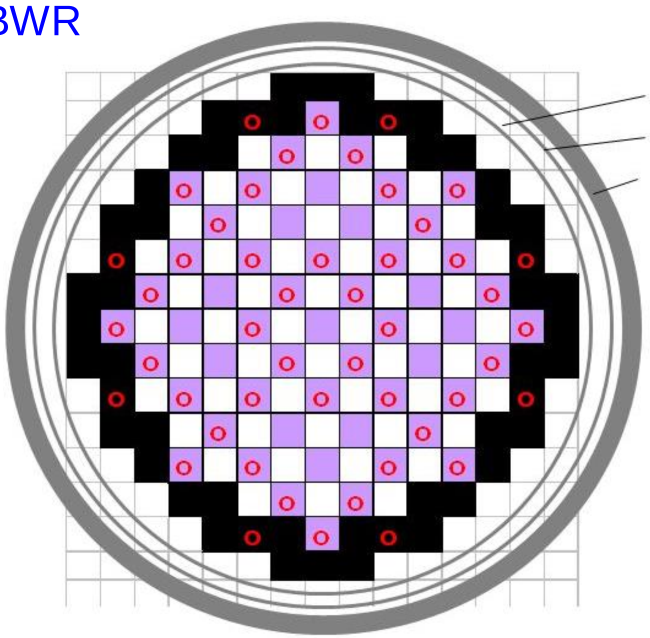


$$\mathbf{Ay} = \mathbf{s}$$

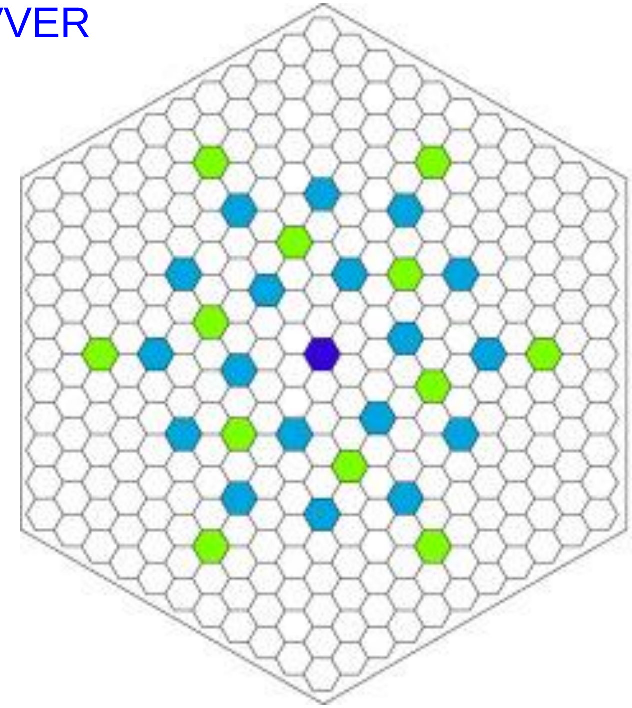
$$y_i \approx y(x_i) \qquad i = 0, 1, 2, \ldots, N+1$$

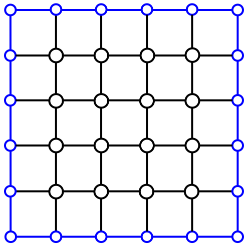
Spatial Region

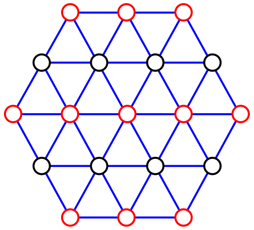
PWR/BWR



VVER

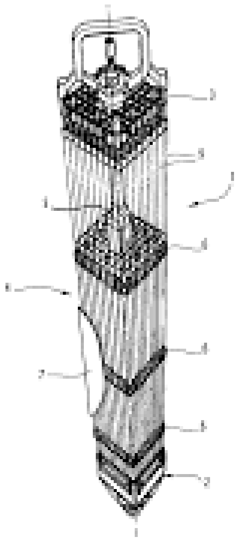




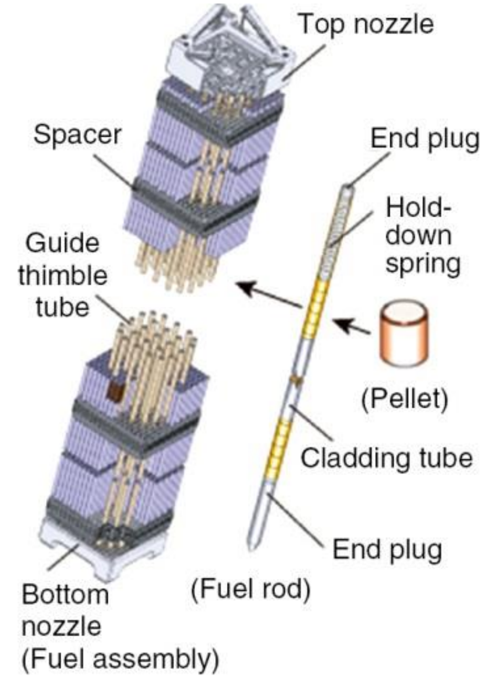


Fuel Assemblies

BWR



PWR



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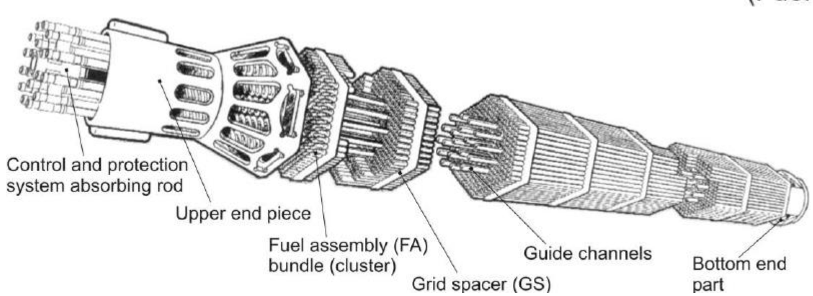
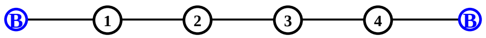
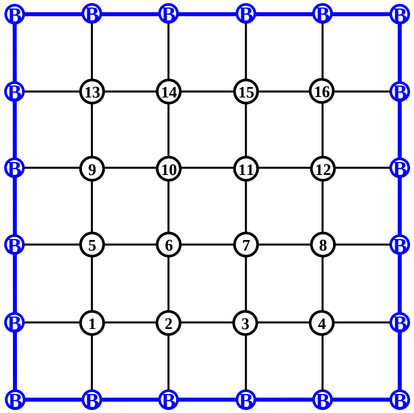


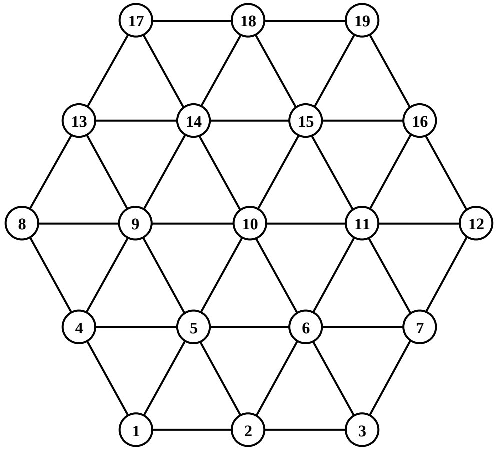
Structured Meshes

1D

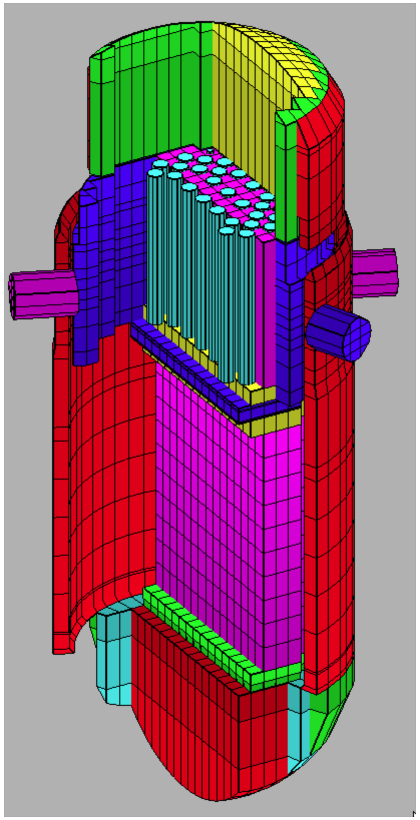


2D

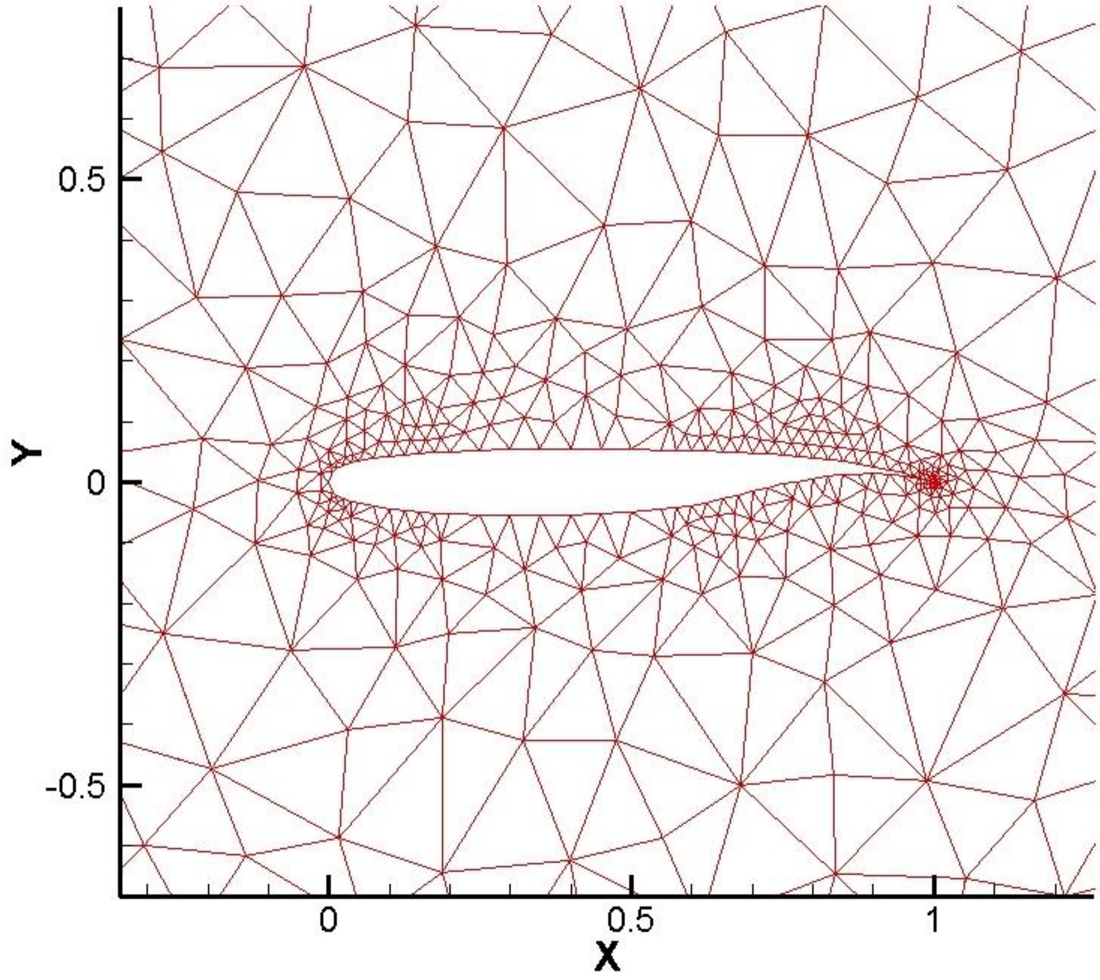




3D



Unstructured Meshes



Approximating Derivative

$$\frac{dy(x)}{dx} \approx ?$$

$$\int_a^b f(x)\,dx \approx ?$$

Difference Operator

$$y'(x) \equiv \lim_{h \to 0} \frac{y(x+h) - y(x)}{h} \approx \frac{y(x+h) - y(x)}{h}$$

$$\nabla_h^+ y(x) \equiv \frac{y(x+h) - y(x)}{h}; \qquad \nabla_h^- y(x) \equiv \frac{y(x) - y(x-h)}{h}.$$

$$y'(x) = \nabla y(x) \approx \nabla_h^+ y(x)$$

Local Truncation Error

$$y'(x) \equiv \lim_{h \to 0} \frac{y(x+h) - y(x)}{h} \approx \frac{y(x+h) - y(x)}{h}$$

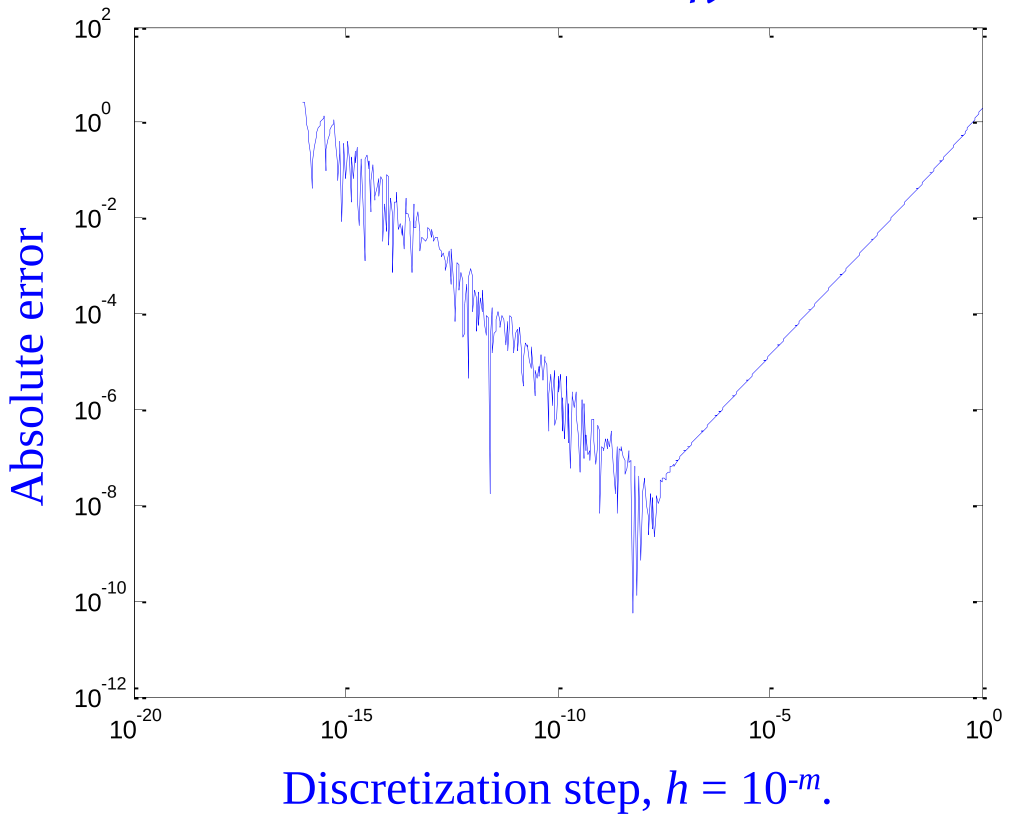
$$y(x+h) = y(x) + y'(x)h + \frac{y''(\xi)}{2!} h^2$$

$$\frac{y(x+h) - y(x)}{h} = y'(x) + \frac{y''(\xi)}{2!} h = y'(x) + O(h)$$

LTE $\left| y'(x) - \nabla_h^+ y(x) \right| = O(h); \quad \left| y'(x) - \nabla_h^- y(x) \right| = O(h).$

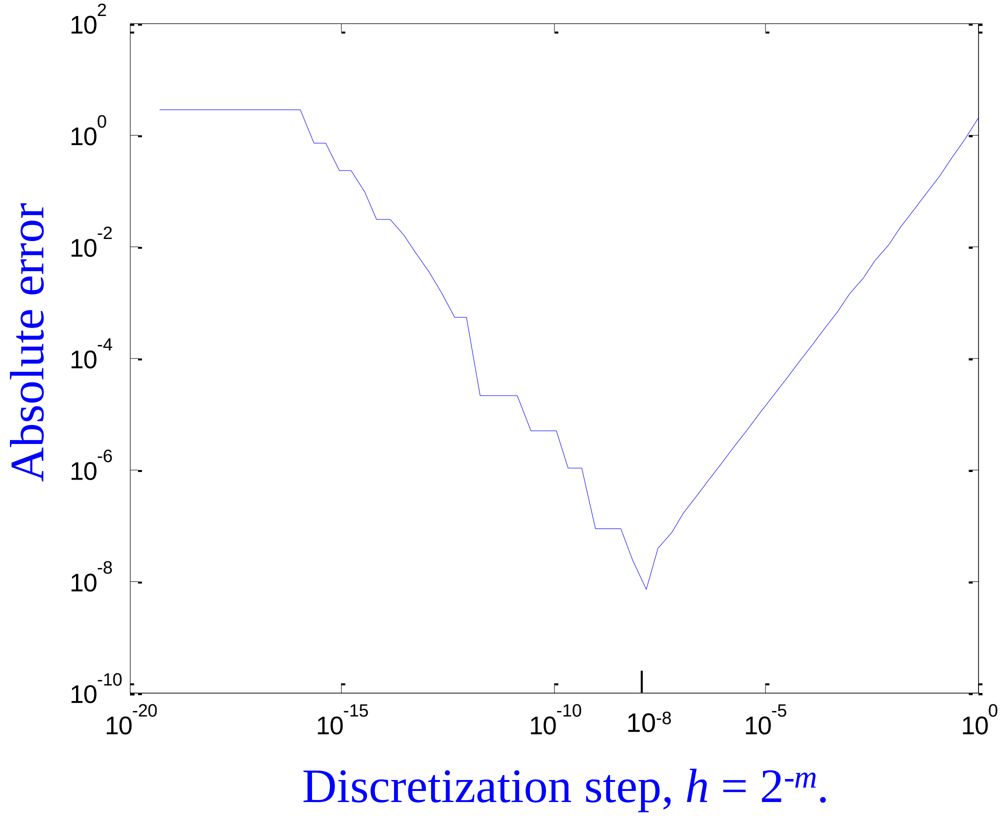
Rounding Errors

$$y(x) = e^x \qquad y'(x) \approx \frac{y(x+h) - y(x)}{h} \qquad x = 1$$



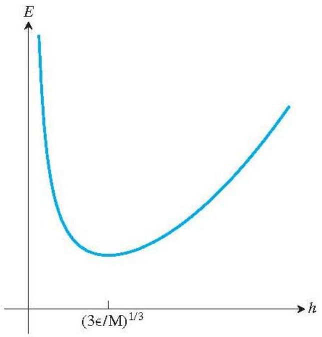
Optimal Step

$$y(x) = e^x \qquad y'(x) \approx \frac{y(x+h) - y(x)}{h} \qquad x = 1 \qquad h_{opt} = \sqrt[3]{\frac{3\varepsilon_M}{M}}$$



$$M = \left\| f''' \right\|_\infty$$

$$h_{opt} \approx 6 \times 10^{-6}$$



FD for ODE

$$\begin{cases} y'(t) = q(t) \\ y(0) = y_0 \end{cases} \longrightarrow y(t) = y_0 + \int_0^t q(\tau)d\tau$$

$$h = T/N; \quad t_i = ih;\ i = 0,1,\ldots,N$$

$$[0,T] \longrightarrow [0 = t_0, t_1, \cdots, t_N = T]$$

$$y(t) \longrightarrow [y_0, y_1, \cdots, y_N]$$

$$y'(t_i) \longrightarrow \frac{y_{i+1} - y_i}{h}$$

FD Solution

$$y'(t) = q(t) \longrightarrow \nabla_h^+ y(t) = q(t) \qquad t \in \left[t_0, t_1, \cdots, t_{N-1} \right]$$

$$\frac{y_{i+1} - y_i}{h} = q_i \qquad i = 0, 1, \cdots, N-1$$

$$y_{i+1} = y_i + hq_i \longrightarrow y_i = y_0 + \sum_{j=1}^{i-1} q(t_j) h$$

$$y(t) = y_0 + \int_0^t q(\tau) d\tau$$

Centred FD

$$y(x+h) = y(x) + y'(x)h + \frac{y''(x)}{2!}h^2 + \frac{y'''(\xi)}{3!}h^3$$

$$y(x-h) = y(x) - y'(x)h + \frac{y''(x)}{2!}h^2 - \frac{y'''(\xi)}{3!}h^3$$

$$\nabla_h^c y(x) \equiv \frac{y(x+h) - y(x-h)}{2h} = y'(x) + \frac{y'''(\xi)}{3!}h^2$$

Centred FD for ODE

$$\begin{cases} y'(t) = q(t) & t \in \left[0, T\right] \\ y(0) = y_0 \end{cases}$$

$$\nabla_h^c y(t) = q(t) \quad t \in \left[t_0, \cdots, t_N\right]$$

$$i = 1 \qquad \frac{y_2 - y_0}{2h} = q(t_1)$$

$$i = 2 \qquad \frac{y_3 - y_1}{2h} = q(t_2)$$

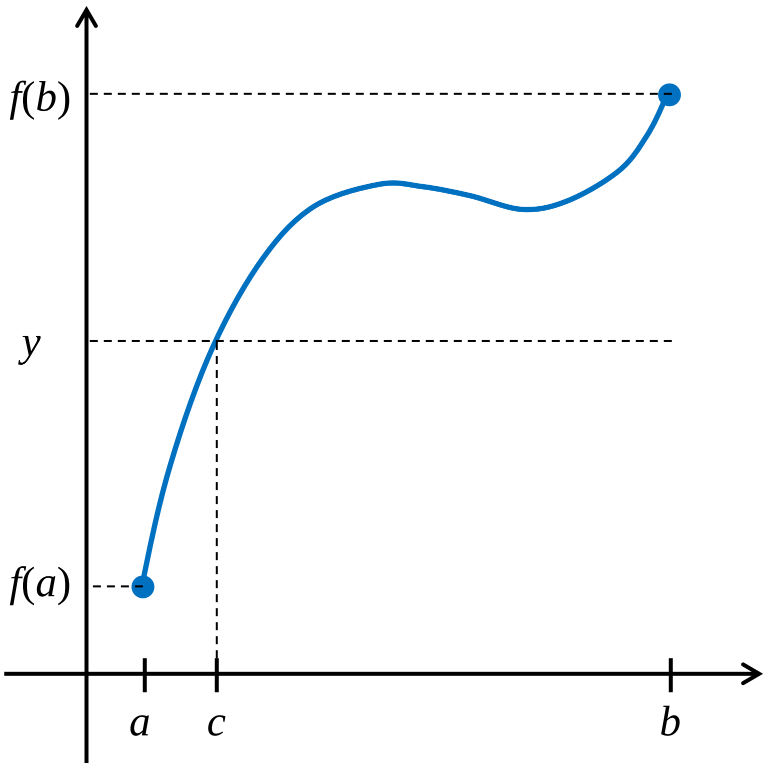
$$i = 3 \qquad \frac{y_4 - y_2}{2h} = q(t_3)$$

Intermediate Value Theorem

Continuous function

$$\lim_{x \to c} f(x) = f(c)$$

Let $f(x)$ be a continuos function on $[a,b]$ then f realises every value between $f(a)$ and $f(b)$. More precisely, if y is a number between a and b, then there exists a number c, $a \le c \le b$, such that $y = f(c)$.



Generalized IVT

There exists c such that $$\frac{f(a)+f(b)}{2}=f\left(c\right)$$

$$\frac{w_1 f(x_1)+w_2 f(x_2)+\cdots+w_n f(x_n)}{w_1+w_2+\cdots+w_n}=f\left(c\right) \qquad w_i>0$$

$$\frac{1}{3}f''(\xi_1)+\frac{2}{3}f''(\xi_2)=f''(\xi) \qquad \xi_1\le\xi\le\xi_2$$

Second Derivative

$$y(x+h) = y(x) + y'(x)h + \frac{y''(x)}{2!}h^2 + \frac{y'''(x)}{3!}h^3 + \frac{y^{(4)}(\xi_1)}{4!}h^4$$

$$y(x-h) = y(x) - y'(x)h + \frac{y''(x)}{2!}h^2 - \frac{y'''(x)}{3!}h^3 + \frac{y^{(4)}(\xi_2)}{4!}h^4$$

$$y(x+h) + y(x-h) = 2y(x) + y''(x)h^2 + \frac{y^{(4)}(\xi)}{12}h^4$$

$$\frac{y(x+h) - 2y(x) + y(x-h)}{h^2} = y''(x) + \frac{y^{(4)}(\xi)}{12}h^2$$

FD Laplace Operator

$$\nabla_h^+ y(x) \equiv \frac{y(x+h)-y(x)}{h} \qquad \nabla_h^- y(x) \equiv \frac{y(x)-y(x-h)}{h}$$

$$\nabla_h^2 y \equiv \nabla_h^- \nabla_h^+ y(x) = \nabla_h^- \frac{y(x+h)-y(x)}{h} = \frac{\nabla_h^- y(x+h) - \nabla_h^- y(x)}{h}$$

$$\nabla_h^2 y(x) = \frac{y(x+h)-2y(x)+y(x-h)}{h^2} = y''(x) + \frac{y^{(4)}(\xi)}{12} h^2$$

Extrapolation

$$\nabla_h^+ y(x) = y'(x) + \frac{y''(x)}{2} h + \frac{y'''(\xi_1)}{6} h^2$$

$$\nabla_{2h}^+ y(x) = y'(x) + y''(x) h + \frac{2y'''(\xi_2)}{3} h^2$$

$$2\nabla_h^+ y(x) - \nabla_{2h}^+ y(x) = y'(x) - \frac{y'''(\xi)}{3} h^2$$

2nd Order FD

$$2\nabla_h^+ y(x) - \nabla_{2h}^+ y(x) = 2\,\frac{y(x+h)-y(x)}{h} - \frac{y(x+2h)-y(x)}{2h} =$$

$$= \frac{2y(x+h) - 3/2\,y(x) - 1/2\,y(x+2h)}{h}$$

$$y'(x) = \frac{4y(x+h) - 3y(x) - y(x+2h)}{2h} + \frac{1}{3}y'''(\xi)h^2$$

Example

$$\cos(1) = \sin'(1) = 0.540302$$

$$\nabla^{+}_{0.25} y(x) = \frac{\sin(1.25) - \sin(1)}{0.25} = 0.430055$$

$$\nabla^{+}_{0.5} y(x) = \frac{\sin(1.5) - \sin(1)}{0.5} = 0.312048$$

$$2\nabla^{+}_{0.25} y(x) - \nabla^{+}_{0.5} y(x) = 0.548061$$

Richardson Extrapolation

$$A(h) = A + ch^n + O(h^m) \qquad m > n > 0$$

$$A(2h) = A + c2^n h^n + O(h^m)$$

$$\frac{2^n A(h) - A(2h)}{2^n - 1} = A + O(h^m)$$

$$\frac{q^n A(h) - A(qh)}{q^n - 1} = A + O(h^m)$$

Equivalent Notation

$$y(x+h) \qquad x = x_i$$

$$y(x_i) \equiv y_i \qquad y(x_i - h) \equiv y_{i-1} \qquad y(x_i + h) \equiv y_{i+1}$$

$$\nabla_h^+ y(x) \equiv \frac{y(x+h) - y(x)}{h} \longrightarrow \nabla_h^+ y(x_i) = \frac{y_{i+1} - y_i}{h}$$

$$y'(x_i) \equiv y_i' = \frac{y_i - y_{i-1}}{h} + \frac{y''(\xi)}{2} h$$

First Derivatives

$$y_i' = \frac{y_i - y_{i-1}}{h} + \frac{y''(\xi)}{2}h$$

$$y_i' = \frac{-y_i + y_{i+1}}{h} - \frac{y''(\xi)}{2}h$$

$$y_i' = \frac{3y_i - 4y_{i-1} + y_{i-2}}{2h} + \frac{y'''(\xi)}{3}h^2$$

$$y_i' = \frac{-3y_i + 4y_{i+1} - y_{i+2}}{2h} - \frac{y'''(\xi)}{3}h^2$$

$$y_i' = \frac{11y_i - 18y_{i-1} + 9y_{i-2} - 2y_{i-3}}{6h} + \frac{y^{(4)}(\xi)}{4}h^3$$

$$y_i' = \frac{-11y_i + 18y_{i+1} - 9y_{i+2} + 2y_{i+3}}{6h} - \frac{y^{(4)}(\xi)}{4}h^3$$

Matrix Representation

$$y'(x_i) \approx \nabla_h^- y_i = \frac{y_i - y_{i-1}}{h} = q_i$$

$$i = 1: \qquad \frac{y_1}{h} = q_1 + \frac{y_0}{h}$$

$$i = 2: \qquad \frac{y_2 - y_1}{h} = q_2$$

$$\frac{1}{h}\begin{bmatrix} 1 & & & 0 \\ -1 & 1 & & \\ & \ddots & \ddots & \\ 0 & & -1 & 1 \end{bmatrix}\begin{bmatrix} y_1 \\ y_2 \\ \\ y_N \end{bmatrix} = \begin{bmatrix} q_1 + y_0/h \\ q_2 \\ \\ q_N \end{bmatrix}$$

$$\nabla_h^- \mathbf{y} = \mathbf{q}$$

Two-Fold Problem

$$y'(x_i) \approx \frac{3y_i - 4y_{i-1} + y_{i-2}}{2h} = q_i$$

$$i = 2: \qquad \frac{3y_2 - 4y_1}{2h} = q_2 - \frac{y_0}{2h}$$

$$i = 3: \qquad \frac{3y_3 - 4y_2 + y_1}{2h} = q_3$$

$$\frac{1}{2h}\begin{bmatrix} ? & & & & 0 \\ -4 & 3 & & & \\ 1 & -4 & 3 & & \\ & \ddots & \ddots & \ddots & \\ 0 & & 1 & -4 & 3 \end{bmatrix}\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_N \end{bmatrix} = \begin{bmatrix} q_1 + ? \\ q_2 \\ q_3 \\ \\ q_N \end{bmatrix}$$

$$y_i = \frac{4}{3}y_{i-1} - \frac{1}{3}y_{i-2} + \frac{2}{3}hq_i$$

One-Sided Second Derivatives

$$y_i'' = \frac{y_i - 2y_{i-1} + y_{i-2}}{h^2} + y'''(\xi)h$$

$$y_i'' = \frac{y_i - 2y_{i+1} + y_{i+2}}{h^2} - y'''(\xi)h$$

$$y_i'' = \frac{2y_i - 5y_{i-1} + 4y_{i-2} - y_{i-3}}{h^2} + \frac{11y^{(4)}(\xi)}{12}h^2$$

$$y_i'' = \frac{2y_i - 5y_{i+1} + 4y_{i+2} - y_{i+3}}{h^2} + \frac{11y^{(4)}(\xi)}{12}h^2$$

Centred Second Derivatives

$$y_i'' = \frac{y_{i-1} - 2y_i + y_{i+1}}{h^2} - \frac{y^{(4)}(\xi)}{12} h^2$$

$$y_i'' = \frac{-y_{i-2} + 16y_{i-1} - 30y_i + 16y_{i+1} - y_{i+2}}{12h^2} + \frac{y^{(5)}(\xi)}{90} h^4$$

$$\nabla_h^2 \mathbf{y} = \frac{1}{h^2} \begin{bmatrix} -2 & 1 & & & 0 \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & 1 \\ 0 & & & 1 & -2 \end{bmatrix} \cdot \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \\ y_N \end{bmatrix}$$

Important

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