

Compact finite difference schemes for solving Partial differential equations

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by

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- A general form of Quasi linear/Semi linear PDEs

$$Au_{xx} + Bu_{xy} + Cu_{yy} + F(x, y, u_x, u_y, u) = G(x, y) \quad (1)$$

Further equation (1) can be classified based on $\Delta = B^2 - 4AC$, as elliptic, parabolic and hyperbolic.

- Parabolic PDEs describe time-dependent processes involving diffusion, transport, and reactions. **General 1D form:**

$$\frac{\partial u}{\partial t} + \beta \frac{\partial u}{\partial x} + \gamma u = \alpha \frac{\partial^2 u}{\partial x^2} \quad (2)$$

Special cases of equation (2) based on α, β and γ :

- Diffusion Equation
- Advection-Diffusion Equation
- Advection-Diffusion-Reaction Equation

Concept	Description
Truncation Error	Difference between the exact differential operator and its discrete approximation.
Stability	Ensures errors do not grow uncontrollably during iterations or time evolution.
Consistency	Truncation error tends to zero as grid spacing tends to zero.
Numerical Convergence	Numerical solution tends to the exact solution as grid is refined.
Order of Convergence	Rate at which numerical solution approaches the exact one (e.g., error h^p).
Finite Difference Method (FDM)	Numerical technique to approximate derivatives using discrete difference formulas.
Compact Finite Difference Method (CFDM)	High-order scheme with implicit stencil using fewer grid points for better accuracy.

Method	Stability	Order of Convergence
FTCS (Explicit)	Conditionally stable	$\mathcal{O}(h^2 + k)$
BTCS (Implicit)	Unconditionally stable	$\mathcal{O}(h^2 + k)$
Crank–Nicolson	Unconditionally stable	$\mathcal{O}(h^2 + k^2)$

Traditional FDMs are simple but limited to second-order accuracy, so Compact Finite Difference Methods (CFDMs) provide fourth-order accuracy using compact stencils, making them efficient for solving 1D parabolic PDEs.

Motivating research studies:

- M. Dehghan [3, 2]
- D. A. Spalding [5]
- A. Mohebbi & M. Dehghan [4]
- A. Chemedda et al. [1]
- Z. Sun & X. Zhang [6]

- On Considering equation (2) with $\gamma = 0$ and $\beta = 0$.
- In space we use operator $\mathcal{Z}$ to approximate the second-order spatial derivative with fourth order approximation:

$$\mathcal{Z}(S_i) = \frac{1}{12} [S''(x_{i+1}) + 10S''(x_i) + S''(x_{i-1})] \quad (3)$$

- The fully discrete form becomes:

$$\mathcal{Z} \frac{u_i^{j+1} - u_i^j}{k} = \frac{\alpha}{2} \left(\mathcal{Z} \delta_x^2 u_i^{j+1} + \mathcal{Z} \delta_x^2 u_i^j \right) \quad (4)$$

- This leads to the fourth-order compact finite difference scheme:

$$Wu_{i+1}^{j+1} + Xu_i^{j+1} + Yu_{i-1}^{j+1} = \tilde{W}u_{i+1}^j + \tilde{X}u_i^j + \tilde{Y}u_{i-1}^j \quad (5)$$

Where $x_i = x_{\min} + ih$, $i = 0, 1, 2, \dots, m$; $t_j = jk$, $j = 0, 1, 2, \dots, n$. and

$$Y = \frac{1}{12k} - \frac{\alpha}{2h^2}, \quad X = \frac{10}{12k} + \frac{\alpha}{h^2}, \quad W = \frac{1}{12k} - \frac{\alpha}{2h^2},$$
$$\tilde{Y} = \frac{1}{12k} + \frac{\alpha}{2h^2}, \quad \tilde{X} = \frac{10}{12k} - \frac{\alpha}{h^2}, \quad \tilde{W} = \frac{1}{12k} + \frac{\alpha}{2h^2}$$

The numerical scheme using operator method is given by equation (4), then the local truncation error is given by equation (6)-(7)

$$\tau_i^j = \mathcal{Z} \frac{u(x_i, t_{j+1}) - u(x_i, t_j)}{k} - \frac{\alpha}{2} \left(\mathcal{Z} \delta_x^2 u(x_i, t_{j+1}) + \mathcal{Z} \delta_x^2 u(x_i, t_j) \right) \quad (6)$$

$$\tau_i^j = \frac{\alpha k^2}{6} u_{xxtt} + \mathcal{O}(k^2) + \mathcal{O}(h^4) \quad (7)$$

showing that the scheme is fourth-order accurate in space, hence the scheme is consistent.

- On Considering equation (2) with $\gamma \neq 0$ and $\beta \neq 0$.

- **Semi-Discrete Scheme**

Let us consider the differential equation,

$$\alpha \frac{d^2 V}{dx^2} - \beta \frac{dV}{dx} - \gamma V = f(x), \quad 0 < x < l. \quad (8)$$

with $V(0) = v_0$, $V(l) = v_l$.

using central finite difference approximation we get

$$\alpha \delta_x^2 V_i - \beta \delta_x V_i - \gamma V_i = f_i + \mathcal{T}_i, \quad (9)$$

- Now on expressing V_i''' and $V_i^{(iv)}$ in terms of known quantities from equation (8)

$$V_i''' = \frac{1}{\alpha} \left(\delta_x f_i + \beta \delta_x^2 V_i + \gamma V_i' \right) + \mathcal{O}(h^2). \quad (10)$$

$$V_i^{(iv)} = \delta_x^2 V_i \left(\frac{\beta^2}{\alpha^2} + \frac{\gamma}{\alpha} \right) + \delta_x V_i \left(\frac{\gamma\beta}{\alpha^2} \right) + \delta_x f_i \left(\frac{\beta}{\alpha^2} \right) + \frac{\delta_x^2 f_i}{\alpha^2} + \mathcal{O}(h^2). \quad (11)$$

- Derivation of Error term, From equation (10) and (11)

$$\mathcal{T}_i = \delta_x^2 V_i \left(\frac{h^2 \gamma}{12} - \frac{\beta^2 h^2}{12\alpha} \right) + \delta_x V_i \left(-\frac{\gamma\beta h^2}{12\alpha} \right) + \delta_x f_i \left(-\frac{\beta h^2}{12\alpha} \right) + \delta_x^2 f_i \left(\frac{h^2}{12} \right) + \mathcal{O}(h^4) \quad (12)$$

This equation (7) shows the truncation error due to derivative approximation and ensures that the derivatives is fourth order accurate in space discretization.

Using equation (26) in equation (9), we get,

$$\begin{aligned} & -(K_1 + K_2)u_{i+1}(t) + (2K_1 - \gamma)u_i(t) - (K_1 - K_2)u_{i-1}(t) \\ & = (K_3 + K_4)u'_{i+1}(t) + (1 - 2K_3)u'_i(t) + (K_3 - K_4)u'_{i-1}(t) \end{aligned} \quad (13)$$

where $K_1 = -\left(\frac{\alpha}{h^2} + \frac{\beta^2}{12\alpha} - \frac{\gamma}{12}\right)$, $K_2 = \frac{\beta}{2h} - \frac{\gamma\beta h}{24\alpha}$, $K_3 = \frac{1}{12}$, $K_4 = -\frac{\beta h}{24\alpha}$

• Fully-Discrete Scheme

Now we apply the crank-nicolson scheme, we get,

$$Fu_{i+1}^{j+1} + Gu_i^{j+1} + Hu_{i-1}^{j+1} = \tilde{F}u_{i+1}^j + \tilde{G}u_i^j + \tilde{H}u_{i-1}^j \quad (14)$$

Where $x_i = x_{\min} + ih$, $i = 0, 1, 2, \dots, m$; $t_j = jk$, $j = 0, 1, 2, \dots, n$. and coefficients are given by:

$$\begin{aligned} F &= -\frac{(K_1 + K_2)}{2} - \frac{(K_3 + K_4)}{k}, & G &= \frac{2K_1 - \gamma}{2} - \frac{(1 - 2K_3)}{k}, & H &= -\frac{(K_1 - K_2)}{2} - \frac{(K_3 - K_4)}{k}, \\ \tilde{F} &= \frac{(K_1 + K_2)}{2} - \frac{(K_3 + K_4)}{k}, & \tilde{G} &= -\frac{2K_1 - \gamma}{2} - \frac{(1 - 2K_3)}{k}, & \tilde{H} &= \frac{(K_1 - K_2)}{2} - \frac{(K_3 - K_4)}{k} \end{aligned}$$

In Method -I and Method - II we will have a tri-diagonal system of the form

$$\mathcal{A}U^{j+1} = \mathcal{B}U^j + \mathcal{C} \quad (15)$$

where $\mathcal{A}$ and $\mathcal{B}$ are tri-diagonal matrices of dimension $m-1 \times m-1$, $\mathcal{C}$ is the vector of dimension $m-1 \times 1$ due to boundary conditions and

$$U^{j+1} = \begin{bmatrix} u_1^{j+1} \\ u_2^{j+1} \\ \vdots \\ \vdots \\ \vdots \\ u_{m-2}^{j+1} \\ u_{m-1}^{j+1} \end{bmatrix}_{m-1 \times 1}, \quad U^j = \begin{bmatrix} u_1^j \\ u_2^j \\ \vdots \\ \vdots \\ \vdots \\ u_{m-2}^j \\ u_{m-1}^j \end{bmatrix}_{m-1 \times 1}$$

Lemma (Fourier Mode Stability Condition)

For a numerical scheme to be stable under von Neumann (Fourier) stability analysis, it is required that

$$|\mathcal{X}(\xi)| \leq 1, \quad \forall \xi, \quad (16)$$

where $\mathcal{X}(\xi)$ is the amplification factor corresponding to the Fourier mode with wavenumber ξ .

The method assumes a solution of the form:

$$u_m^n = \xi^n e^{i\beta m h} \quad (17)$$

Is it sufficient?

Not always. Von Neumann analysis assumes linearity and periodic boundaries.

Sufficient Condition: According to the **Lax Equivalence Theorem**, a consistent finite difference scheme is stable *if and only if* it is convergent (for linear problems). i.e.

$$\text{Consistency} + \text{Stability} \Leftrightarrow \text{Convergence}$$

On substituting the Fourier mode form in equation (5), we get

$$\begin{aligned} Y \xi^{n+1} e^{i\beta(m-1)h} + X \xi^{n+1} e^{i\beta mh} + W \xi^{n+1} e^{i\beta(m+1)h} \\ = \tilde{Y} \xi^n e^{i\beta(m-1)h} + \tilde{X} \xi^n e^{i\beta mh} + \tilde{W} \xi^n e^{i\beta(m+1)h} \end{aligned} \quad (18)$$

we have $W = Y = \frac{1}{12k} - \frac{\alpha}{2h^2}$, $X = \frac{10}{12k} + \frac{\alpha}{h^2}$ and $\tilde{W} = \tilde{Y} = \frac{1}{12k} + \frac{\alpha}{2h^2}$, $\tilde{Q} = \frac{10}{12k} - \frac{\alpha}{h^2}$.
we can write

$$\begin{aligned} \xi &= \frac{\tilde{X} + 2\tilde{W} \cos(\beta h)}{X + 2W \cos(\beta h)}. \\ |\xi| &= \left| \frac{\mathcal{I}_1 - \mathcal{I}_2}{\mathcal{I}_1 + \mathcal{I}_2} \right| < 1 \end{aligned} \quad (19)$$

where

$$\mathcal{I}_1 = \frac{10 + 2 \cos(\beta h)}{12k} > 0, \quad \mathcal{I}_2 = \frac{\alpha}{h^2} (1 - \cos(\beta h)) \geq 0,$$

i.e. from equation (19), The method is unconditionally stable for all mesh sizes h and time steps k .

On substituting the Fourier mode form in equation (14), we get

$$\begin{aligned} F\hat{u}^{n+1}e^{i\xi x_{m+1}} + G\hat{u}^{n+1}e^{i\xi x_m} + H\hat{u}^{n+1}e^{i\xi x_{m-1}} \\ = \tilde{F}\hat{u}^n e^{i\xi x_{m+1}} + \tilde{G}\hat{u}^n e^{i\xi x_m} + \tilde{H}\hat{u}^n e^{i\xi x_{m-1}} \end{aligned} \quad (20)$$

On using Euler's identities $e^{i\xi h} = \cos(\xi h) + i \sin(\xi h)$, $e^{-i\xi h} = \cos(\xi h) - i \sin(\xi h)$, we have

$$\mathcal{X} = \frac{(\tilde{F} + \tilde{H}) \cos \xi h + i(\tilde{F} - \tilde{H}) \sin \xi h + \tilde{G}}{(F + H) \cos \xi h + i(F - H) \sin \xi h + G} \quad (21)$$

we can write as

$$|\mathcal{X}|^2 = \frac{N}{D} = \frac{\mathcal{J}_1 - \mathcal{J}_2}{\mathcal{J}_1 + \mathcal{J}_2} < 1 \quad (22)$$

$$\begin{aligned} \mathcal{J}_1 = & \alpha^2 h^4 (204 + 80 \cos(h\xi) + 4 \cos(2h\xi)) + \alpha^4 k^2 (432 - 576 \cos(h\xi) + 144 \cos(2h\xi)) \\ & + \beta^2 h^6 (1 - \cos(2h\xi)) + \alpha^2 \beta^2 h^2 k^2 (108 - 96 \cos(h\xi) - 12 \cos(2h\xi)) \\ & + \beta^4 h^4 k^2 (3 - 4 \cos(h\xi) + \cos(2h\xi)) \end{aligned}$$

$$\mathcal{J}_2 = h^2 k \alpha^3 (432 - 384 \cos(h\xi) - 48 \cos(2h\xi)) + h^4 k \alpha \beta^2 (24 - 32 \cos(h\xi) + 8 \cos(2h\xi))$$

i.e. from equation (22), The method is unconditionally stable for all mesh sizes h and time steps k .

Example

Consider 1-D diffusion equation, with $\alpha = \frac{1}{\pi^2}$, $L = 1$ and $t > 0$. The Exact solution is for this example is given by $u(x, t) = e^{-t} \sin(\pi x)$. and initial and boundary condition are given by

$$\begin{cases} u(x, 0) = \sin(\pi x) & \text{Initial Condition} \\ u(0, t) = u(1, t) = 0 & \text{Boundary Condition} \end{cases}$$

Numerical Solution

h	CN-Error	CN-Order	CF-1 Error	CF-1 Order	CF-2 Error	CF-2 Order
1/5	2.5764e-2	*	1.8398e-4	*	1.8399e-4	*
1/10	6.7221e-3	1.94	1.1923e-5	3.95	1.1923e-5	3.95
1/20	1.6772e-3	2.00	7.4250e-7	4.00	7.4250e-7	4.00
1/40	4.1909e-4	2.00	4.6364e-8	4.00	4.6364e-8	4.00
1/80	1.0476e-4	2.00	2.8970e-9	4.00	2.8970e-9	4.00
1/160	2.6190e-5	2.00	1.8059e-10	4.00	1.8059e-10	4.00

Table: Max Absolute Error and Order of Convergence

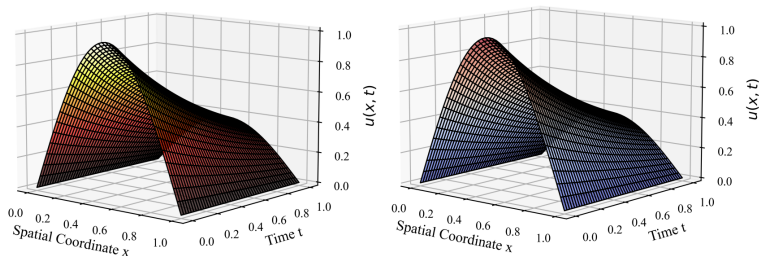
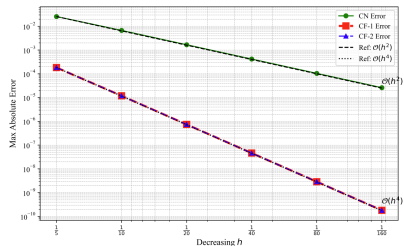
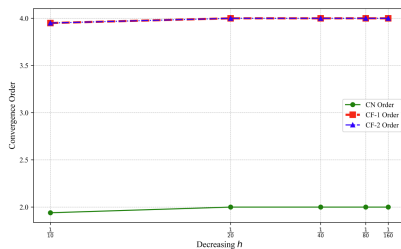


Figure: Numerical and Exact Solutions at $h=1/40$ and $k=h^2$

Error and Order of Convergence Plot



(a) CN, CF-1, and CF-2 Errors vs h



(b) CN, CF-1, and CF-2 Orders vs h

Figure: Error and Order of Convergence with varying h

Example

Consider 1-D advection-diffusion equation, with initial condition $\phi(x) = a \exp(-\bar{c}x)$.

where $\bar{c} = \frac{-\beta + \sqrt{\beta^2 + 4\alpha b}}{2\alpha}$

The exact solution for this example is given by $u(x, t) = a \exp(bt - \bar{c}x)$.

We are finding the solution for $a = 1, b = 0.1, \beta = -1$ and comparing with different Péclet number $(P_e) = \left| \frac{\beta}{\alpha} \right|$

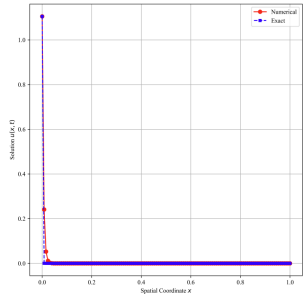
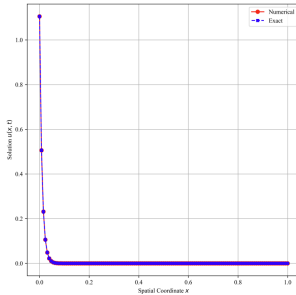
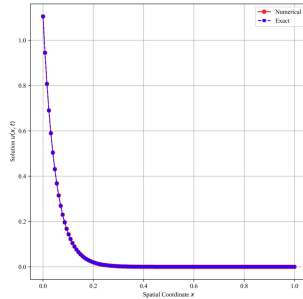
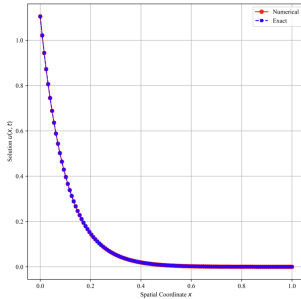
h	$P_e = 10$		$P_e = 20$	
	CF-2 Error	CF-2 Order	CF-2 Error	CF-2 Order
1/16	8.8239×10^{-5}	*	1.4970×10^{-3}	*
1/32	5.5792×10^{-6}	3.98	8.7430×10^{-5}	4.00
1/64	3.4715×10^{-7}	4.00	5.5135×10^{-6}	4.00
1/128	2.1691×10^{-8}	4.00	3.4308×10^{-7}	4.00

Table: Max Absolute Error and Order of Convergence for CF-2 Scheme at smaller P_e Values

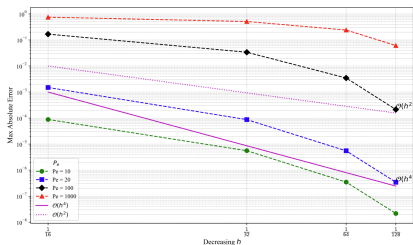
h	$P_e = 100$		$P_e = 1000$	
	CF-2 Error	CF-2 Order	CF-2 Error	CF-2 Order
1/16	1.6741×10^{-1}	*	7.5202×10^{-1}	*
1/32	3.3796×10^{-2}	2.38	5.1300×10^{-1}	0.55
1/64	3.4567×10^{-3}	3.30	2.4073×10^{-1}	1.09
1/128	2.1290×10^{-4}	4.00	6.1102×10^{-2}	2.00

Table: Max Absolute Error and Order of Convergence for CF-2 Scheme at Higher P_e Values

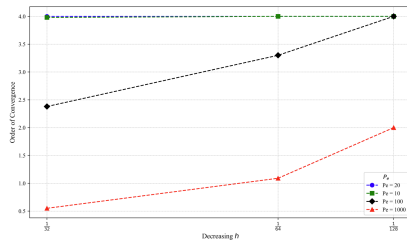
Exact and Numerical Solution for $Pe = 10, 20, 100, 1000$ at $h = 1/128$



Error and Order of Convergence Plot



(a) Behavior of CF-2 Error for with different Pe



(b) Behavior of CF-2 Order for with different Pe

Figure: Error and Order of Convergence with varying h

Example

Consider 1-D diffusion equation

$$\frac{\partial u}{\partial t}(x, t) + \frac{\partial u}{\partial x}(x, t) - 3u(x, t) = \frac{\partial^2 u}{\partial x^2}(x, t), \quad (x, t) \in [0, 2\pi] \times \left[0, \frac{1}{2}\right],$$

with initial Condition $u(x, 0) = \sin(x)$ and boundary conditions are $u(0, t) = e^{2t} \sin(-t)$ and $u(2\pi, t) = e^{2t} \sin(2\pi - t)$

h	CF-2 Error	CF-2 Order
1/8	3.0497×10^{-4}	*
1/16	1.9066×10^{-5}	3.98
1/32	1.1919×10^{-6}	4.00
1/64	7.4495×10^{-8}	4.00
1/128	4.6559×10^{-9}	4.00

Table: Max Absolute Error and Order of Convergence

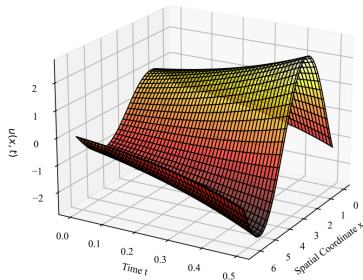
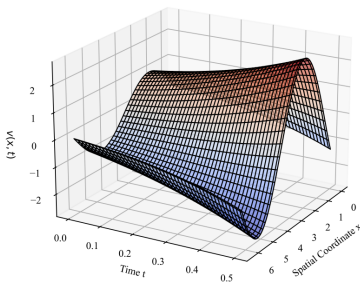


Figure: Numerical and Exact Solutions at $h=1/40$ and $k=h^2$

- A high-order accurate scheme was developed using a fourth-order Compact Finite Difference Method (CFDM) in space and the Crank–Nicolson method in time.
- The proposed scheme achieved global accuracy of $\mathcal{O}(k^2 + h^4)$ and outperformed traditional FDMs in terms of solution smoothness and accuracy with fewer grid points.
- Numerical experiments on diffusion, advection-diffusion, and ADR equations confirmed the efficiency and stability of the compact method.

- **Application to Variable Coefficient Problems**
- **Application to Nonlinear Problems**
- **Extension to Non-Uniform Grids**

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- [5] D. B. Spalding: A novel finite difference formulation for differential expressions involving both first and second derivatives. *International Journal for Numerical Methods in Engineering* Vol. 4 (1972), pp. 551–559.
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Thank you!

Derivation of Operator Z

Starting from the Taylor series expansion for a smooth function $S(x)$:

$$S(x_{i+1}) = S(x_i) + hS'(x_i) + \frac{h^2}{2}S''(x_i) + \frac{h^3}{6}S^{(3)}(x_i) + \frac{h^4}{24}S^{(4)}(x_i) + \frac{h^5}{120}S^{(5)}(x_i) \\ + \frac{h^5}{120} \int_0^1 [S^{(6)}(x_i + \nu h) - S^{(6)}(x_i)](1 - \nu)^5 d\nu$$

$$S(x_{i-1}) = S(x_i) - hS'(x_i) + \frac{h^2}{2}S''(x_i) - \frac{h^3}{6}S^{(3)}(x_i) + \frac{h^4}{24}S^{(4)}(x_i) - \frac{h^5}{120}S^{(5)}(x_i) \\ + \frac{h^5}{120} \int_0^1 [S^{(6)}(x_i - \nu h) - S^{(6)}(x_i)](1 - \nu)^5 d\nu$$

Adding both:

$$\frac{1}{h^2}[S(x_{i+1}) - 2S(x_i) + S(x_{i-1})] - S''(x_i) + \frac{h^2}{12}S^{(4)}(x_i) + \frac{h^4}{120} \int_0^1 \Delta_6^{(a)}(\nu)(1 - \nu)^5 d\nu$$

where $\Delta_6^{(a)}(\nu) = S^{(6)}(x_i + \nu h) + S^{(6)}(x_i - \nu h) - 2S^{(6)}(x_i)$

Now expand $S''(x)$ at x_{i+1} and x_{i-1} :

$$\begin{aligned}
 S''(x_{i+1}) &= S''(x_i) + hS^{(3)}(x_i) + \frac{h^2}{2}S^{(4)}(x_i) + \frac{h^3}{6}S^{(5)}(x_i) + \frac{h^4}{24}S^{(6)}(x_i) \\
 &\quad + \frac{h^4}{24} \int_0^1 [S^{(6)}(x_i + vh) - S^{(6)}(x_i)](1-v)^3 dv \\
 S''(x_{i-1}) &= S''(x_i) - hS^{(3)}(x_i) + \frac{h^2}{2}S^{(4)}(x_i) - \frac{h^3}{6}S^{(5)}(x_i) + \frac{h^4}{24}S^{(6)}(x_i) \\
 &\quad + \frac{h^4}{24} \int_0^1 [S^{(6)}(x_i - vh) - S^{(6)}(x_i)](1-v)^3 dv
 \end{aligned}$$

Then,

$$\frac{1}{12} [S''(x_{i+1}) + 10S''(x_i) + S''(x_{i-1})] - S''(x_i) + \frac{h^2}{12}S^{(4)}(x_i) + \frac{h^4}{72} \int_0^1 \Delta_6^{(b)}(v)(1-v)^3 dv$$

Subtracting the two results:

$$\frac{1}{12} [S''(x_{i+1}) + 10S''(x_i) + S''(x_{i-1})] - \frac{1}{h^2} [S(x_{i+1}) - 2S(x_i) + S(x_{i-1})] = \frac{h^4}{360} \int_0^1 \Delta_6^{(c)}(v) dv$$

Using the mean value theorem:

$$\frac{1}{12} [S''(x_{i+1}) + 10S''(x_i) + S''(x_{i-1})] - \frac{1}{h^2} [S(x_{i+1}) - 2S(x_i) + S(x_{i-1})] = \frac{h^4}{240} S^{(6)}(\xi_i),$$

We define the operator as:

$$\mathcal{Z}(S_i) = \frac{1}{12} [S''(x_{i+1}) + 10S''(x_i) + S''(x_{i-1})]$$

This gives a fourth-order accurate compact finite difference representation of the second derivative.

Derivation of Truncation Error of General CFDM

From the equation,

$$\alpha V'' - \beta V' - \gamma V = f \quad (23)$$

$$\alpha \delta_x^2 V_i - \beta \delta_x V_i - \gamma V_i = f_i + \tau_i \quad (24)$$

$$V' = \delta_x V_i - \frac{h^2}{6} V_i''' + \mathcal{O}(h^4)$$

and

$$V'' = \delta_x^2 V_i - \frac{h^2}{12} V_i^{(iv)} + \mathcal{O}(h^4)$$

On using the fourth order approximating derivative, we have

$$\alpha \delta_x^2 V_i - \beta \delta_x V_i - \gamma V_i - \left[\alpha \frac{h^2}{12} V_i^{(iv)} - \beta \frac{h^2}{6} V_i''' \right] = f_i + \mathcal{O}(h^4)$$

where

$$\tau_i = \frac{h^2}{12} \left[\alpha V_i^{(iv)} - 2\beta V_i''' \right] + \mathcal{O}(h^4) \quad (25)$$

On differentiating equation (23) for higher order, we have,

$$V''' = \frac{1}{\alpha} [f' + \beta V'' + \gamma V']$$

$$V^{(iv)} = \frac{1}{\alpha^2} [\alpha f'' + \beta f' + \gamma \beta V' + (\beta^2 + \alpha \gamma) V'']$$

on using higher order derivative in equation (25),

$$\tau_i = \delta_x^2 V_i \left(\frac{h^2 \gamma}{12} - \frac{\beta^2 h^2}{12 \alpha} \right) + \delta_x V_i \left(-\frac{\gamma \beta h^2}{12 \alpha} \right) + \delta_x f_i \left(-\frac{\beta h^2}{12 \alpha} \right) + \delta_x^2 f_i \left(\frac{h^2}{12} \right) + \mathcal{O}(h^4) \quad (26)$$