# High Order High Resolution Finite Differential Schemes


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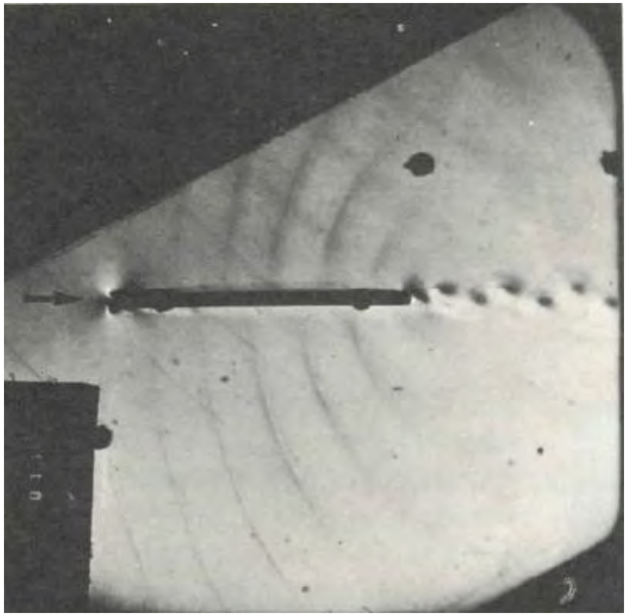
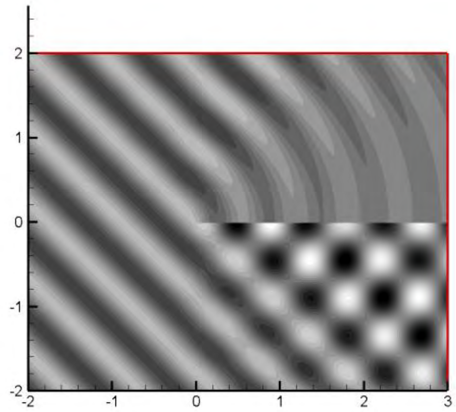
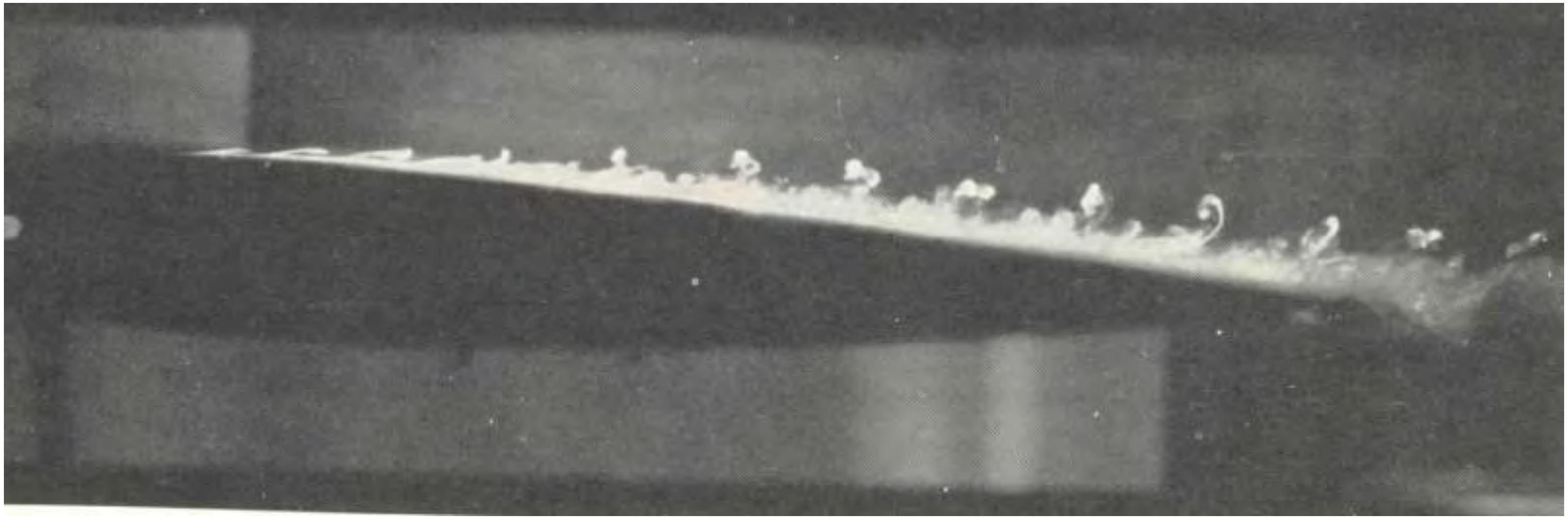
# Contents

# Application



Hermann Schlichting, “Boundary Layer Theory.”



Hermann Schlichting, “Boundary Layer Theory.”

# Acoustic Systems in Biology

- Bats use Ultrasound
  - Echo-location by using high frequency (short wavelength) sound

# Basic Concept ( Governing equation )

## ❖ Governing Equation

In order to analyze flow field, we need to solve the governing equation.

It contains temporal and spatial derivative terms. We are not able to solve this nonlinear equation analytically so we should use numerical methods.

✓ Continuity equation ( conservation of mass )

$$\frac{\partial \rho}{\partial t} + \vec{V} \cdot \nabla \rho + \rho \nabla \cdot \vec{V} = 0 \qquad \boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0}$$

✓ Momentum equation ( conservation of momentum )

$$\rho\left(\frac{\partial \vec{V}}{\partial t} + \vec{V} \cdot \nabla \vec{V}\right) = -\nabla p + \nabla \cdot \tilde{\tau} + \vec{f} \qquad \boxed{\frac{\partial (\rho \vec{V})}{\partial t} + \nabla \cdot (\rho \vec{V}\vec{V} + p) = 0}$$

Spatial term → related to resolution. ( $\Delta x$ )

Temporal term → related to stability. ( Δt )

# Basic Concept ( High order Spatial Finite Difference Method )

❖ Finite Difference Method ( Approximation of the1[st] derivative )

✓ Standard Central Differential Method

Consider Taylor series expansion.

$$f_{i\pm m} = f(x_i \pm mh) = f(x_i) + (\pm m)\frac{h}{1!}\left(\frac{\partial f}{\partial x}\right)_i + (\pm m)^2 \frac{h^2}{2!}\left(\frac{\partial^2 f}{\partial x^2}\right)_i + (\pm m)^3 \frac{h^3}{3!}\left(\frac{\partial^3 f}{\partial x^3}\right)_i + \ldots\ldots$$

**1. 2[nd] order central difference**

$$f_i' + a_{-1} f_{i-1} + a_1 f_{i+1} = 0$$

Apply Taylor series expansion

| | $f_i$ | $\left(\frac{\partial f}{\partial x}\right)_i$ | $\left(\frac{\partial^2 f}{\partial x^2}\right)_i$ | $\left(\frac{\partial^3 f}{\partial x^3}\right)_i$ |
|---|---|---|---|---|
| $f_i'$ | 0 | 1 | 0 | 0 |
| $\alpha_1 f_{i+1}$ | $a_1$ | $a_1 \frac{(\Delta x)}{1!}$ | $a_1 \frac{(\Delta x)^2}{2!}$ | $a_1 \frac{(\Delta x)^3}{3!}$ |
| $a_{-1} f_{i-1}$ | $a_{-1}$ | $a_{-1} \frac{(-\Delta x)}{1!}$ | $a_{-1} \frac{(-\Delta x)^2}{2!}$ | $a_{-1} \frac{(-\Delta x)^3}{3!}$ |

$(1)\ a_1 + a_{-1} = 0$ $(2)\ 1 + \Delta x(a_1 - a_{-1}) = 0$ 2 unknowns , 2 equations

Remain(T.E.)

$$\rightarrow a_1 = -\frac{1}{2\Delta x}, \quad a_{-1} = \frac{1}{2\Delta x}$$

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2\Delta x} + O(\Delta x^2), \qquad \mathrm{T.E.} = -2\frac{(\Delta x)^2}{3!} + \ldots$$

# Basic Concept ( Finite Difference Method )

## 2. 4th order central difference

$$f_i' + a_{-2} f_{-2} + a_{-1} f_{i-1} + a_1 f_{i+1} + a_2 f_{i+2} = 0$$

Apply Taylor series expansion

| | $f_i$ | $\left(\frac{\partial f}{\partial x}\right)_i$ | $\left(\frac{\partial^2 f}{\partial x^2}\right)_i$ | $\left(\frac{\partial^3 f}{\partial x^3}\right)_i$ | $\left(\frac{\partial^4 f}{\partial x^4}\right)_i$ | $\left(\frac{\partial^5 f}{\partial x^5}\right)_i$ |
|---|---|---|---|---|---|---|
| $f_i'$ | 0 | 1 | 0 | 0 | 0 | 0 |
| $a_2 f_{i+2}$ | $a_2$ | $a_2(2\Delta x)\frac{1}{1!}$ | $a_2(2\Delta x)^2\frac{1}{2!}$ | $a_2(2\Delta x)^3\frac{1}{3!}$ | $a_2(2\Delta x)^4\frac{1}{4!}$ | $a_2(2\Delta x)^5\frac{1}{5!}$ |
| $a_1 f_{i+1}$ | $a_1$ | $a_1(\Delta x)\frac{1}{1!}$ | $a_1(\Delta x)^2\frac{1}{2!}$ | $a_1(\Delta x)^3\frac{1}{3!}$ | $a_1(\Delta x)^4\frac{1}{4!}$ | $a_1(\Delta x)^5\frac{1}{5!}$ |
| $a_{-1} f_{i-1}$ | $a_{-1}$ | $a_{-1}(-\Delta x)\frac{1}{1!}$ | $a_{-1}(-\Delta x)^2\frac{1}{2!}$ | $a_{-1}(-\Delta x)^3\frac{1}{3!}$ | $a_{-1}(-\Delta x)^4\frac{1}{4!}$ | $a_{-1}(-\Delta x)^5\frac{1}{5!}$ |
| $a_{-2} f_{i+2}$ | $a_{-2}$ | $a_{-2}(-2\Delta x)\frac{1}{1!}$ | $a_{-2}(-2\Delta x)^2\frac{1}{2!}$ | $a_{-2}(-2\Delta x)^3\frac{1}{3!}$ | $a_{-2}(-2\Delta x)^4\frac{1}{4!}$ | $a_{-2}(-2\Delta x)^5\frac{1}{5!}$ |

**Remain(T.E.)**

4 unknowns , 4 equations

$$\left.\begin{aligned} &(1)\ a_2 + a_1 + a_{-1} + a_{-2} = 0 \\ &(2)\ 1 + \Delta x(2a_2 + a_1 - a_{-1} - 2a_{-2}) = 0 \\ &(3)\ 4a_2 + a_1 + a_{-1} + 4a_{-2} = 0 \\ &(4)\ 8a_2 + a_1 - a_{-1} - 8a_{-2} = 0 \end{aligned}\right\} \rightarrow\ a_2 = \frac{1}{12\Delta x},\ a_1 = -\frac{8}{12\Delta x},\ a_{-1} = \frac{8}{12\Delta x},\ a_{-2} = -\frac{1}{12\Delta x}$$

$$f_i' = \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12\Delta x} + O(\Delta x^4)$$

# Basic Concept ( Standard Compact Scheme )

## ❖ Standard Compact Scheme ( 4th order)

$$\alpha_{-1} f'_{i-1} + f'_i + \alpha_1 f'_{i+1} + a_{-1} f_{i-1} + a_0 f_i + a_1 f_{i+1} = 0$$

In order to determine 1st derivative of function $f$ , we use values of $f'_{i-1}$, $f'_{i+1}$, $f_{i-1}$, $f_i$ and $f_{i+1}$.

✓ Apply Taylor series expansion to above scheme

| | $f_i$ | $\left(\frac{\partial f}{\partial x}\right)_i$ | $\left(\frac{\partial^2 f}{\partial x^2}\right)_i$ | $\left(\frac{\partial^3 f}{\partial x^3}\right)_i$ | $\left(\frac{\partial^4 f}{\partial x^4}\right)_i$ | $\left(\frac{\partial^5 f}{\partial x^5}\right)_i$ |
|---|---|---|---|---|---|---|
| $\alpha_{-1} f'_{i-1}$ | 0 | $\alpha_{-1}$ | $-\alpha_{-1}\Delta x$ | $\frac{1}{2!}\alpha_{-1}\Delta x^2$ | $\frac{-1}{3!}\alpha_{-1}\Delta x^3$ | $\frac{1}{4!}\alpha_{-1}\Delta x^4$ |
| $f'_i$ | 0 | 1 | 0 | 0 | 0 | 0 |
| $\alpha_1 f'_{i+1}$ | 0 | $\alpha_1$ | $\alpha_1\Delta x$ | $\frac{1}{2!}\alpha_1\Delta x^2$ | $\frac{1}{3!}\alpha_1\Delta x^3$ | $\frac{1}{4!}\alpha_1\Delta x^4$ |
| $a_{-1} f_{i-1}$ | $a_{-1}$ | $-\Delta x a_{-1}$ | $\frac{1}{2!}\Delta x^2 a_{-1}$ | $\frac{-1}{3!}\Delta x^3 a_{-1}$ | $\frac{1}{4!}\Delta x^4 a_{-1}$ | $\frac{-1}{5!}\Delta x^5 a_{-1}$ |
| $a_0 f_i$ | $a_0$ | 0 | 0 | 0 | 0 | 0 |
| $a_1 f_{i+1}$ | $a_1$ | $\Delta x a_1$ | $\frac{1}{2!}\Delta x^2 a_1$ | $\frac{1}{3!}\Delta x^3 a_1$ | $\frac{1}{4!}\Delta x^4 a_1$ | $\frac{1}{5!}\Delta x^5 a_1$ |

**5 unknowns , 5 equations**

(1) $a_{-1} + a_0 + a_1 = 0$

(2) $\alpha_{-1} + 1 + \alpha_1 + \Delta x(-a_{-1} + a_1) = 0$

(3) $\Delta x(-\alpha_{-1} + \alpha_1) + \frac{1}{2}\Delta x^2 (a_{-1} + a_1) = 0$

(4) $\frac{1}{2}\Delta x^2(\alpha_{-1} + \alpha_1) + \frac{1}{6}\Delta x^3(-a_{-1} + a_1) = 0$

(5) $\frac{1}{6}\Delta x^3(-\alpha_{-1} + \alpha_1) + \frac{1}{24}\Delta x^4(a_{-1} + a_1) = 0$

This gives $\alpha_{-1} = \frac{1}{4},\ \alpha_1 = \frac{1}{4},\ a_{-1} = \frac{3}{4}\frac{1}{\Delta x},\ a_0 = 0,\ a_1 = -\frac{3}{4}\frac{1}{\Delta x}$

$$T.E. = \frac{1}{24}\Delta x^4(\alpha_{-1} + \alpha_1) + \frac{1}{120}\Delta x^5(-a_{-1} + a_1)$$

H. Lomax, T.H. Pulliam, D.W. Zingg, "Fundamentals of Computational Fluid Dynamics."

# Basic Concept ( Standard Compact Scheme )

$$\alpha_{-1} f'_{i-1} + f'_i + \alpha_1 f'_{i+1} + a_{-1} f_{i-1} + a_0 f_i + a_1 f_{i+1} = 0 \qquad \alpha_{-1} = \frac{1}{4},\ \alpha_1 = \frac{1}{4},\ a_{-1} = \frac{3}{4}\frac{1}{\Delta x},\ a_0 = 0,\ a_1 = -\frac{3}{4}\frac{1}{\Delta x}$$

✓ Rewrite this scheme it turns out

$$\boxed{\frac{1}{4} f'_{i-1} + f'_i + \frac{1}{4} f'_{i+1} = \frac{3}{4\Delta x}(f_{i+1} - f_{i-1}) + O(\Delta x^4)}$$

it is called 4th Standard compact scheme( Pade scheme ).

➢ **Compare standard 4th order central scheme with standard 4th order compact scheme.**

- Standard 4th order central scheme : $f'_i = \dfrac{-f_{i+2} + 8 f_{i+1} - 8 f_{i-1} + f_{i-2}}{12\Delta x} + O(\Delta x^4)$

  ( Stencil size : 5 )

- Standard 4th order compact scheme : $\dfrac{1}{4} f'_{i-1} + f'_i + \dfrac{1}{4} f'_{i+1} = \dfrac{3}{4\Delta x}(f_{i+1} - f_{i-1}) + O(\Delta x^4)$

  ( Stencil size : 3 )

# Basic Concept ( High resolution ;Modified wavenumber )

❖ Modified wave number ($\tilde{k}$)

Consider the 1-D advection equation

$$\frac{\partial f}{\partial t}+c\frac{\partial f}{\partial x}=0$$

Assume that exact solution is $f(x,t)=f(t)e^{ikx}$

Exact 1st derivative of function $f$ is $\frac{\partial f(x,t)}{\partial x}=ik\ f(t)e^{ikx}=ik\ f(x,t)$

Approximate 1st derivative of function $f$ is

$$\frac{\delta f}{\delta x}(x)\simeq\frac{1}{\Delta x}\sum_{m=-N}^{M}a_m f(x+m\Delta x,t)=\frac{1}{\Delta x}\sum_{m=-N}^{M}a_m f(t)e^{ikm\Delta x}e^{ikx}=\frac{1}{\Delta x}\sum_{m=-N}^{M}a_m e^{ikm\Delta x}f(x,t)$$

Compare exact and approximate derivative

$$\frac{\delta f}{\delta x}=\frac{1}{\Delta x}\sum_{m=-N}^{M}a_m e^{ikm\Delta x}f(x,t)\simeq ik\ f(x,t)$$

$$\frac{\partial f(x,t)}{\partial x}=ik\ f(x,t)$$

$$k=\frac{-i}{\Delta x}\sum_{m=-N}^{M}a_m e^{ikm\Delta x}f(x,t),$$

where $k$ : modified wavenumber

# Basic Concept ( Modified wavenumber )

$$k = \frac{-i}{\Delta x}\sum_{m=-N}^{M} a_m e^{ikm\Delta x} u(x,t),$$ where $k$ : modified wavenumber

Generally Modified wavenumber($\tilde{k}$) is complex number

$$k = \mathrm{Re}(k) + i\,\mathrm{Im}(k)$$

$$\frac{\delta f}{\delta x} = ik\ f(x,t) = i[\mathrm{Re}(k) + i\,\mathrm{Im}(k)]\,f(x,t)$$

Approximation of solution $\rightarrow f(x,t) = f(t)e^{ikx}$

$$= f(t)e^{i[\mathrm{Re}(k)+i\,\mathrm{Im}(k)]x} = f(t)\,\underbrace{e^{i\,\mathrm{Re}(k)x}}_{\substack{\text{phase}\\ \text{(dispersion)}}}\,\overbrace{e^{-\mathrm{Im}(k)x}}^{\substack{\text{amplitude}\\ \text{(dissipation)}}}$$

- <u>**Therefore when modified wavenumber is real number dissipation error does not occur.**</u>

# Basic Concept

❖ Modified wave number ($\tilde{k}$) of forward and central difference

$$\frac{\partial f}{\partial t} + c\frac{\partial f}{\partial x} = 0 \qquad f(x,t) = f(t)e^{ikx} \text{ (exact solution)} \qquad \frac{\partial f(x,t)}{\partial x} = ik\, f(t)e^{ikx} = ik\, f(x,t) \text{ ( exact 1}^{st}\text{ derivative )}$$

$$\frac{\partial f}{\partial t} = -c\frac{\partial f}{\partial x} = -ikcf(x,t)$$

① 1st order Forward difference method

$$\left(\frac{\partial f}{\partial x}\right)_i \simeq \frac{f_{i+1} - f_i}{\Delta x}$$

$$\frac{\partial f}{\partial t} = -\frac{c}{\Delta x}(f_{i+1} - f_i) = -\frac{c}{\Delta x}\left(e^{ik(x+\Delta x)} - e^{ikx}\right) f(t)$$

$$= -\frac{c}{\Delta x}(e^{ik\Delta x} - 1)e^{ikx} f(t) = -\frac{c}{\Delta x}(e^{ik\Delta x} - 1) f(x,t)$$

$$= -\frac{c}{\Delta x}\left\{(\cos k\Delta x - 1) + i\sin k\Delta x\right\} f(x,t)$$

$$= -ick\, f(x,t)$$

$$\rightarrow k = \frac{\left\{\sin k\Delta x - i(\cos k\,\Delta x - 1)\right\}}{\Delta x}$$

➢ <u>When we use forward difference method modified wavenumber is complex number so both dissipation and dispersion error occur.</u>

# Basic Concept

① $2^{nd}$ order central difference method

$$\left(\frac{\partial f}{\partial x}\right)_i \simeq \frac{f_{i+1} - f_{i-1}}{2\Delta x}$$

$$\frac{\partial f}{\partial t} = -\frac{c}{2\Delta x}(f_{i+1} - f_{i-1}) = -\frac{c}{2\Delta x}\left(e^{ik(x+\Delta x)} - e^{ik(x-\Delta x)}\right) f(t)$$

$$= -\frac{c}{2\Delta x}(e^{ik\Delta x} - e^{-ik\Delta x})e^{ikx} f(t)$$

$$= -\frac{c}{\Delta x} i \sin k\Delta x \; f(x,t)$$

$$= -ick \, f(x,t)$$

$$\rightarrow k = \frac{\sin k\Delta x}{\Delta x}$$

➢ <u>When we use central difference method modified wavenumber is real number so only dispersion error occur.</u>

# Spectral-Like Schemes

# (by Lele)

# Compact Scheme ( Inner nodes )

❖ Compact Scheme ( Approximation of 1st derivatives )

: Compact scheme based on **central differential** method. → **Dispersion error only!**

$$\beta f'_{i-2}+\alpha f'_{i-1}+f'_{i}+\alpha f'_{i+1}+\beta f'_{i+2}=c\frac{f_{i+3}-f_{i-3}}{6h}+b\frac{f_{i+2}-f_{i-2}}{4h}+a\frac{f_{i+1}-f_{i-1}}{2h}$$

In order to find 1st derivative of function f at x=i, we need to determine the coefficients of the formula.

Standard way to determine the coefficients is Taylor series expansion.

$$\beta f'_{i-2}+\alpha f'_{i-1}+f'_{i}+\alpha f'_{i+1}+\beta f'_{i+2}-c\frac{f_{i+3}-f_{i-3}}{6h}-b\frac{f_{i+2}-f_{i-2}}{4h}-a\frac{f_{i+1}-f_{i-1}}{2h}=0$$

Multiply the above formula with h

$$h\beta f'_{i-2}+h\alpha f'_{i-1}+hf'_{i}+h\alpha f'_{i+1}+h\beta f'_{i+2}-c\frac{f_{i+3}-f_{i-3}}{6}-b\frac{f_{i+2}-f_{i-2}}{4}-a\frac{f_{i+1}-f_{i-1}}{2}=0$$

Remind Taylor series expansion

$$f_{i+m}=f(x_i+mh)=f(x_i)+m\frac{h}{1!}\left(\frac{\partial f}{\partial x}\right)_i+m^2\frac{h^2}{2!}\left(\frac{\partial^2 f}{\partial x^2}\right)_i+m^3\frac{h^3}{3!}\left(\frac{\partial^3 f}{\partial x^3}\right)_i+........$$

$$f_{i-m}=f(x_i-mh)=f(x_i)+(-m)\frac{h}{1!}\left(\frac{\partial f}{\partial x}\right)_i+(-m)^2\frac{h^2}{2!}\left(\frac{\partial^2 f}{\partial x^2}\right)_i+(-m)^3\frac{h^3}{3!}\left(\frac{\partial^3 f}{\partial x^3}\right)_i+........$$

# Compact Scheme ( Inner nodes )

$$h\beta f'_{i-2} + h\alpha f'_{i-1} + hf'_{i} + h\alpha f'_{i+1} + h\beta f'_{i+2} - c\frac{f_{i+3} - f_{i-3}}{6} - b\frac{f_{i+2} - f_{i-2}}{4} - a\frac{f_{i+1} - f_{i-1}}{2} = 0$$

✓ Apply Taylor series expansion,

As we can see below, even order terms are automatically canceled out but odd terms remain.

| | $u_i$ | $h\left(\frac{\partial f}{\partial x}\right)_i$ | $h^2\left(\frac{\partial^2 f}{\partial x^2}\right)_i$ | $h^3\left(\frac{\partial^3 f}{\partial x^3}\right)_i$ | $h^4\left(\frac{\partial^4 f}{\partial x^4}\right)_i$ | $h^5\left(\frac{\partial^5 f}{\partial x^5}\right)_i$ |
|---|---|---|---|---|---|---|
| $h\beta\left(\frac{\partial f}{\partial x}\right)_{i-2}$ | 0 | $\beta$ | $\beta(-2)\frac{1}{1!}$ | $\beta(-2)^2\frac{1}{2!}$ | $\beta(-2)^3\frac{1}{3!}$ | $\beta(-2)^4\frac{1}{4!}$ |
| $h\alpha\left(\frac{\partial f}{\partial x}\right)_{i-1}$ | 0 | $\alpha$ | $\alpha(-1)\frac{1}{1!}$ | $\alpha(-1)^2\frac{1}{2!}$ | $\alpha(-1)^3\frac{1}{3!}$ | $\alpha(-1)^4\frac{1}{4!}$ |
| $h\left(\frac{\partial f}{\partial x}\right)_{i}$ | 0 | 1 | 0 | 0 | 0 | 0 |
| $h\alpha\left(\frac{\partial f}{\partial x}\right)_{i+1}$ | 0 | $\alpha$ | $\alpha(1)\frac{1}{1!}$ | $\alpha(1)^2\frac{1}{2!}$ | $\alpha(1)^3\frac{1}{3!}$ | $\alpha(1)^4\frac{1}{4!}$ |
| $h\beta\left(\frac{\partial f}{\partial x}\right)_{i+2}$ | 0 | $\beta$ | $\beta(2)\frac{1}{1!}$ | $\beta(2)^2\frac{1}{2!}$ | $\beta(2)^4\frac{1}{4!}$ | $\beta(2)^4\frac{1}{4!}$ |
| $-\frac{c}{6}f_{i+3}$ | $-\frac{c}{6}$ | $-\frac{c}{6}(3)\frac{1}{1!}$ | $-\frac{c}{6}(3)^2\frac{1}{2!}$ | $-\frac{c}{6}(3)^3\frac{1}{3!}$ | $-\frac{c}{6}(3)^4\frac{1}{4!}$ | $-\frac{c}{6}(3)^5\frac{1}{5!}$ |
| $-\frac{b}{4}f_{i+2}$ | $-\frac{b}{4}$ | $-\frac{b}{4}(2)\frac{1}{1!}$ | $-\frac{b}{4}(2)^2\frac{1}{2!}$ | $-\frac{b}{4}(2)^3\frac{1}{3!}$ | $-\frac{b}{4}(2)^4\frac{1}{4!}$ | $-\frac{b}{4}(2)^5\frac{1}{5!}$ |
| $-\frac{a}{2}f_{i+1}$ | $-\frac{a}{2}$ | $-\frac{a}{2}(1)\frac{1}{1!}$ | $-\frac{a}{2}(1)^2\frac{1}{2!}$ | $-\frac{a}{2}(1)^3\frac{1}{3!}$ | $-\frac{a}{2}(1)^4\frac{1}{4!}$ | $-\frac{a}{2}(1)^5\frac{1}{5!}$ |
| $\frac{a}{2}f_{i-1}$ | $\frac{a}{2}$ | $\frac{a}{2}(-1)\frac{1}{1!}$ | $\frac{a}{2}(-1)^2\frac{1}{2!}$ | $\frac{a}{2}(-1)^3\frac{1}{3!}$ | $\frac{a}{2}(-1)^4\frac{1}{4!}$ | $\frac{a}{2}(-1)^5\frac{1}{5!}$ |
| $\frac{b}{4}f_{i-2}$ | $\frac{b}{4}$ | $\frac{b}{4}(-2)\frac{1}{1!}$ | $\frac{b}{4}(-2)^2\frac{1}{2!}$ | $\frac{b}{4}(-2)^3\frac{1}{3!}$ | $\frac{b}{4}(-2)^4\frac{1}{4!}$ | $\frac{b}{4}(-2)^5\frac{1}{5!}$ |
| $\frac{c}{6}f_{i-3}$ | $\frac{c}{6}$ | $\frac{c}{6}(-3)\frac{1}{1!}$ | $\frac{c}{6}(-3)^2\frac{1}{2!}$ | $\frac{c}{6}(-3)^3\frac{1}{3!}$ | $\frac{c}{6}(-3)^4\frac{1}{4!}$ | $\frac{c}{6}(-3)^5\frac{1}{5!}$ |
| | | ① | Cancel out | ② | | ③ |

# Compact Scheme

We can control the truncation error by selecting the equations sequentially

✓ ① $a+b+c=1+2\alpha+2\beta$ ( 2nd order )

② $a+2^2b+3^2c=2\frac{3!}{2!}(\alpha+2^2\beta)$ ( 4th order )

③ $a+2^4b+3^4c=2\frac{5!}{4!}(\alpha+2^4\beta)$ ( 6th order )

④ $a+2^6b+3^6c=2\frac{7!}{6!}(\alpha+2^6\beta)$ ( 8th order )

⑤ $a+2^8b+3^8c=2\frac{9!}{8!}(\alpha+2^8\beta)$ ( 10th order )

For example, if we take equation ① the order of error is $O(h)^2$

and take ① and ② equation the order of error is $O(h)^4$

Standard 4th order compact scheme $\alpha, a, b=c=\beta=0$

# Compact Scheme

❖ Modified wavenumber

Compact Scheme

$$\beta f'_{i-2} + \alpha f'_{i-1} + f'_i + \alpha f'_{i+1} + \beta f'_{i+2} = c\frac{f_{i+3} - f_{i-3}}{6h} + b\frac{f_{i+2} - f_{i-2}}{4h} + a\frac{f_{i+1} - f_{i-1}}{2h}$$

The Fourier transform of the left and right sides

$$ik(\beta e^{-2ik\Delta x} + \alpha e^{-ik\Delta x} + 1 + \alpha e^{ik\Delta x} + \beta e^{2ik\Delta x})u = [\frac{c}{6\Delta x}(e^{3ik\Delta x} - e^{-3ik\Delta x}) + \frac{b}{4\Delta x}(e^{2ik\Delta x} - e^{-2ik\Delta x}) + \frac{a}{2\Delta x}(e^{ik\Delta x} - e^{-ik\Delta x})]u$$

$$k\Delta x = \frac{a\sin(k\Delta x) + \frac{b}{2}\sin(2k\Delta x) + \frac{c}{3}\sin(3k\Delta x)}{1 + 2\alpha\cos(k\Delta x) + 2\beta\cos(2k\Delta x)}$$

➢ **Modified wavenumber of compact scheme is real so only dispersion error occurs.**

# Compact Scheme (Lele)

❖ How to improve the resolution of compact scheme ( Lele )

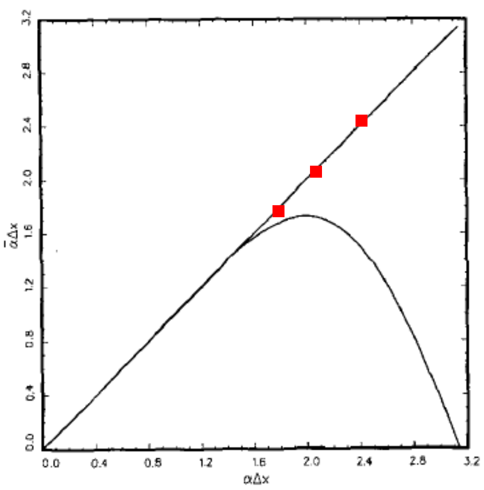
- $4^{th}$ order spectral-like scheme

$$\beta f'_{i-2} + \alpha f'_{i-1} + f'_{i} + \alpha f'_{i+1} + \beta f'_{i+2} = c\frac{f_{i+3} - f_{i-3}}{6h} + b\frac{f_{i+2} - f_{i-2}}{4h} + a\frac{f_{i+1} - f_{i-1}}{2h}$$

There are 5 unknown coefficients but 2equations only . So we need 3 more equations

① $a + b + c = 1 + 2\alpha + 2\beta$ ② $a + 2^2 b + 3^2 c = 2\frac{3!}{2!}(\alpha + 2^2\beta)$ From Taylor series

In order to get 3 more equations,



$$k\Delta x = \frac{a\sin(k\Delta x) + \frac{b}{2}\sin(2k\Delta x) + \frac{c}{3}\sin(3k\Delta x)}{1 + 2\alpha\cos(k\Delta x) + 2\beta\cos(2k\Delta x)}$$

$k$ is funtion of $k$

$k(k_1) = k_1,\ k(k_2) = k_2,\ k(k_3) = k_3$ ← **other 3 equations**

where $k$ : wave number, $k$ : modified wave number

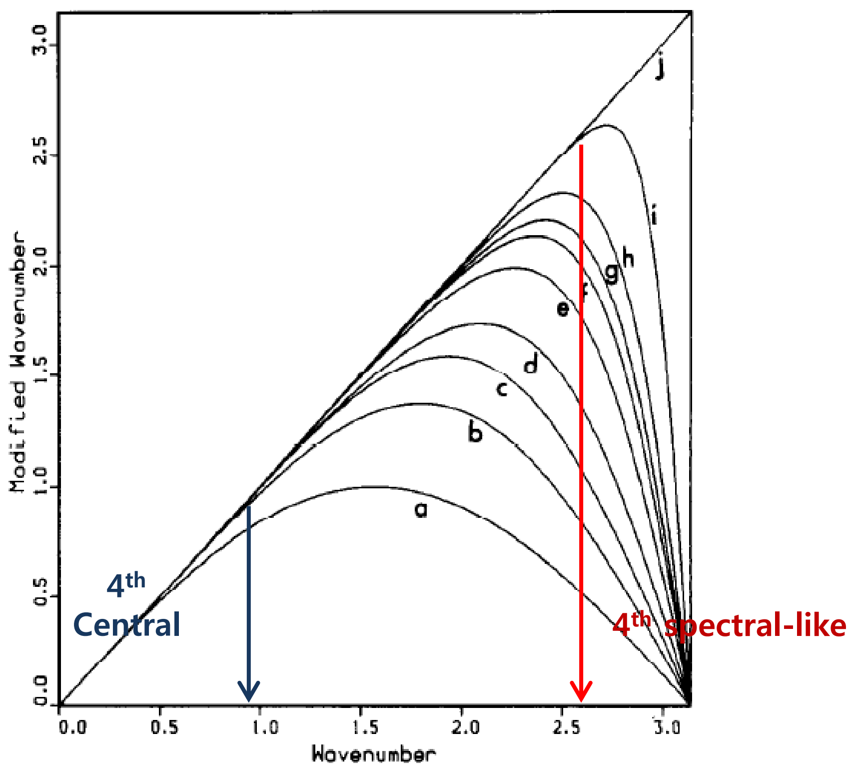
# Compact Scheme (Lele)

$$a+b+c=1+2\alpha+2\beta, \quad a+2^2b+3^2c=2\frac{3!}{2!}(\alpha+2^2\beta), \; k(k_1)=k_1, \; k(k_2)=k_2, \; k(k_3)=k_3$$

**4th spectral-like scheme : 5 unknown coefficients & 5 equations**

These equations provide a system of linear algebraic equations by which the coefficients can be determined.

$$\rightarrow \alpha=0.5771439, \; \beta=0.0896406, \; a=1.3025166, \; b=0.9935500, \; c=0.03750245$$



# Dispersion-Relation-Preserving Finite Difference Scheme (Tam & Web)

# DRP Scheme

❖ The approximation of the 1st derivative

$$(\frac{\partial f}{\partial x})_i \simeq \frac{1}{\Delta x}(a_{-n} f_{i-n} + a_{-n-1} f_{i-n-1} + \ldots + a_{n-1} f_{i+n-1} + a_n f_{i+n})$$

The way to determine the coefficient ($a_j$)

- Standard way : Using a truncation error in Taylor series.
- DRP Scheme : Using the Fourier transform and Taylor series.

$$\frac{\partial f}{\partial x}(x) \simeq \frac{1}{\Delta x}\sum_{m=-N}^{N} a_j f(x + m\Delta x) \qquad (1.1)$$

Fourier transform and its inverse of a function

$$f(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(x) e^{ikx} dx \qquad f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(\mathrm{k}) e^{-ikx} dk$$

The Fourier transform of the LHS and RHS of (1.1)

$$ik\, f(\mathrm{k}) \simeq (\frac{1}{\Delta x}\sum_{j=-N}^{N} \alpha_j e^{ikj\Delta x}) f \equiv ik\, f(\mathrm{k}) \qquad (1.2)$$

By comparing the two sides of (1.2),

$$k = \frac{-i}{\Delta x}\sum_{j=-N}^{N} \alpha_j e^{ikj\Delta x}$$

where $k$ : wave number, $k$ : modified wave number

$\tilde{k}\Delta x$ is a periodic function of $\mathrm{k}\Delta x$ with period $2\pi$

# DRP Scheme

❖ For Example ( 4th order DRP scheme based on central difference )

$$\left(\frac{\partial f}{\partial x}\right)_i \simeq \frac{1}{\Delta x}(a_{-3}f_{i-3}+a_{-2}f_{i-2}+a_{-1}f_{i-1}+a_1 f_{i+1}+a_2 f_{i+2}+a_3 f_{i+3}) \;\rightarrow\; \left(\frac{\partial f}{\partial x}\right)_i - \frac{1}{\Delta x}(a_{-3}f_{i-3}+a_{-2}f_{i-2}+a_{-1}f_{i-1}+a_1 f_{i+1}+a_2 f_{i+2}+a_3 f_{i+3}) = 0$$

✓ Apply Taylor series expansion

| | $f_i$ | $\left(\frac{\partial f}{\partial x}\right)_i$ | $\left(\frac{\partial^2 f}{\partial x^2}\right)_i$ | $\left(\frac{\partial^3 f}{\partial x^3}\right)_i$ | $\left(\frac{\partial^4 f}{\partial x^4}\right)_i$ | $\left(\frac{\partial^5 f}{\partial x^5}\right)_i$ |
|---|---|---|---|---|---|---|
| $f_i'$ | 0 | 1 | 0 | 0 | 0 | 0 |
| $-\frac{a_3}{\Delta x}f_{i+3}$ | $-\frac{a_3}{\Delta x}$ | $-\frac{a_3}{\Delta x}(3\Delta x)\frac{1}{1!}$ | $-\frac{a_3}{\Delta x}(3\Delta x)^2\frac{1}{2!}$ | $-\frac{a_3}{\Delta x}(3\Delta x)^3\frac{1}{3!}$ | $-\frac{a_3}{\Delta x}(3\Delta x)^4\frac{1}{4!}$ | $-\frac{a_3}{\Delta x}(3\Delta x)^5\frac{1}{5!}$ |
| $-\frac{a_2}{\Delta x}f_{i+2}$ | $-\frac{a_2}{\Delta x}$ | $-\frac{a_2}{\Delta x}(2\Delta x)\frac{1}{1!}$ | $-\frac{a_2}{\Delta x}(2\Delta x)^2\frac{1}{2!}$ | $-\frac{a_2}{\Delta x}(2\Delta x)^3\frac{1}{3!}$ | $-\frac{a_2}{\Delta x}(2\Delta x)^4\frac{1}{4!}$ | $-\frac{a_2}{\Delta x}(2\Delta x)^5\frac{1}{5!}$ |
| $-\frac{a_1}{\Delta x}f_{i+1}$ | $-\frac{a_1}{\Delta x}$ | $-\frac{a_1}{\Delta x}(\Delta x)\frac{1}{1!}$ | $-\frac{a_1}{\Delta x}(\Delta x)^2\frac{1}{2!}$ | $-\frac{a_1}{\Delta x}(\Delta x)^3\frac{1}{3!}$ | $-\frac{a_1}{\Delta x}(\Delta x)^4\frac{1}{4!}$ | $-\frac{a_1}{\Delta x}(\Delta x)^5\frac{1}{5!}$ |
| $-\frac{a_{-1}}{\Delta x}f_{i-1}$ | $-\frac{a_{-1}}{\Delta x}$ | $-\frac{a_{-1}}{\Delta x}(-\Delta x)\frac{1}{1!}$ | $-\frac{a_{-1}}{\Delta x}(-\Delta x)^2\frac{1}{2!}$ | $-\frac{a_{-1}}{\Delta x}(-\Delta x)^3\frac{1}{3!}$ | $-\frac{a_{-1}}{\Delta x}(-\Delta x)^4\frac{1}{4!}$ | $-\frac{a_{-1}}{\Delta x}(-\Delta x)^5\frac{1}{5!}$ |
| $-\frac{a_{-2}}{\Delta x}f_{i-2}$ | $-\frac{a_{-2}}{\Delta x}$ | $-\frac{a_{-2}}{\Delta x}(-2\Delta x)\frac{1}{1!}$ | $-\frac{a_{-2}}{\Delta x}(-2\Delta x)^2\frac{1}{2!}$ | $-\frac{a_{-2}}{\Delta x}(-2\Delta x)^3\frac{1}{3!}$ | $-\frac{a_{-2}}{\Delta x}(-2\Delta x)^4\frac{1}{4!}$ | $-\frac{a_{-2}}{\Delta x}(-2\Delta x)^5\frac{1}{5!}$ |
| $-\frac{a_{-3}}{\Delta x}f_{i-3}$ | $-\frac{a_{-3}}{\Delta x}$ | $-\frac{a_{-3}}{\Delta x}(-3\Delta x)\frac{1}{1!}$ | $-\frac{a_{-3}}{\Delta x}(-3\Delta x)^2\frac{1}{2!}$ | $-\frac{a_{-3}}{\Delta x}(-3\Delta x)^3\frac{1}{3!}$ | $-\frac{a_{-3}}{\Delta x}(-3\Delta x)^4\frac{1}{4!}$ | $-\frac{a_{-3}}{\Delta x}(-3\Delta x)^5\frac{1}{5!}$ |

**Remain(T.E.)**

In order to satisfy 4th order, we take 5equation but unknown coefficients are 6.

➢ **1 more equation is needed**

# DRP Scheme ( Central difference )

❖ Integrated Error

$a_m$ be chosen to minimize the integrated error $E$

$$E = \int_{-\pi/2}^{\pi/2} \left| k\Delta x - k\Delta x \right|^2 d(\mathrm{k}\,\Delta x) \qquad \text{( Fourier analysis )}$$

$$\left(\frac{\partial f}{\partial x}\right)_i \simeq \frac{1}{\Delta x}(a_{-3} f_{i-3} + a_{-2} f_{i-2} + a_{-1} f_{i-1} + a_1 f_{i+1} + a_2 f_{i+2} + a_3 f_{i+3})$$

To determine three coefficients ( 4th order DRP )

the truncated Taylor series method + the Fourier analysis ( minimize the integrated error )

↓ 5 equations

↓ 1 equations $\frac{\partial E}{\partial a_1} = 0$ ( by Fourier transform optimized method )

**4th order DRP scheme : 6 unknown coefficients & 6 equations**

This gives the following values

$$a_1 = -a_{-1} = 0.79926643, \quad a_2 = -a_{-2} = -0.18941314, \quad a_3 = -a_{-3} = 0.02651995$$

# DRP Scheme ( Central difference )

❖ Comparison with standard central schemes

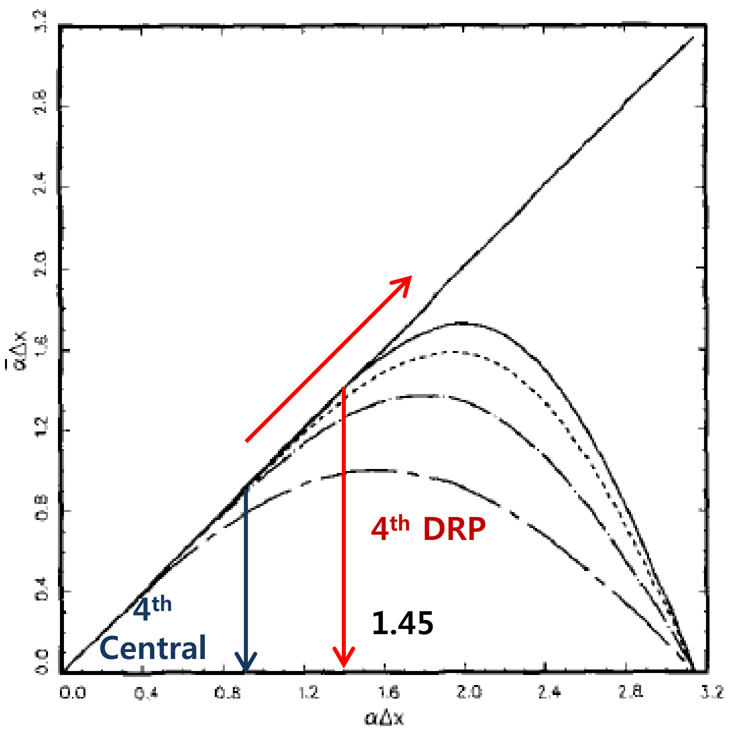



FIG. 2. $\bar{\alpha}\Delta x$ versus $\alpha\Delta x$; ——— optimized fourth-order scheme; – – – standard sixth-order scheme; —·— standard fourth-order scheme; —– – standard second-order scheme.

Ref) K. W. Tam, Jay C. Webb, " Dispersion-Relation-Preserving Finite Difference Schemes for Computational Acoustics."

$$k\Delta x = \frac{2\pi}{\lambda}\cdot\Delta x \approx 1.45$$

$$\lambda \approx \frac{2\pi}{1.45}\cdot\Delta x = 4.33\Delta x$$

✓ This scheme(DRP) provides an adequate approximation for waves with wave lengths 4.5 times longer than its mesh size.

✓ <u>High order optimized schemes should be used for short wave length ( high frequency ) cases.</u>

# Optimized High Order Compact Schemes (J.W. Kim & D.J. Lee )

# Optimized High Order Compact Scheme ( Inner nodes )

❖ J.W. Kim & D.J. Lee( Optimized High Order Compact Scheme ; OHOC )

$$\beta f'_{i-2} + \alpha f'_{i-1} + f'_{i} + \alpha f'_{i+1} + \beta f'_{i+2} = c\frac{f_{i+3} - f_{i-3}}{6h} + b\frac{f_{i+2} - f_{i-2}}{4h} + a\frac{f_{i+1} - f_{i-1}}{2h}$$

For example , Optimized 4th order pentadiagonal scheme

$$a + b + c = 1 + 2\alpha + 2\beta, \qquad a + 2^2 b + 3^2 c = 2\frac{3!}{2!}(\alpha + 2^2\beta)$$

( From Taylor series expansion )

There are 5 unknown coefficients so we need 5 equations

In order to get 3 equations, introduce the integrand-error added weighting function.

$$E \equiv \int_0^{r\pi} (k\Delta x - k\Delta x)^2 W(k\Delta x)\, d(k\Delta x)$$

$$= \int_0^{r\pi} \left( k\Delta x - \frac{a\sin(k\Delta x) + \frac{b}{2}\sin(2k\Delta x) + \frac{c}{3}\sin(3k\Delta x)}{1 + 2\alpha\cos(k\Delta x) + 2\beta\cos(2k\Delta x)} \right)^2 W(k\Delta x)\, d(k\Delta x)$$

where $W(k)$ is weighting function

$$W(k) = [(1 + 2\alpha\cos(k) + 2\beta\cos(2k))e^{k}]^2$$

$r$ is a factor to determine the optimization range $(0 < r < 1)$ under the consider

In the weighting function there is exponential term ( $e^k$ )

so it is possible to correspond modified wave number to real wave number.

# Optimized High Order Compact Scheme ( Inner nodes )

$a+b+c=1+2\alpha+2\beta,\qquad a+2^2b+3^2c=2\frac{3!}{2!}(\alpha+2^2\beta)$ ( From Taylor series expansion )

$\frac{\partial E}{\partial \alpha}=0\qquad \frac{\partial E}{\partial \beta}=0\qquad \frac{\partial E}{\partial a}=0$ ( From minimizing Integrated error )

Solve the equations

$\rightarrow \alpha=0.5889595521,\ \beta=0.097512355,\ a=1.280440844,\ b=1.049309076,\ c=0.044465832$

# Optimized High Order Compact Scheme ( Inner nodes )

$$\beta f'_{i-2} + \alpha f'_{i-1} + f'_{i} + \alpha f'_{i+1} + \beta f'_{i+2} = c\frac{f_{i+3}-f_{i-3}}{6h} + b\frac{f_{i+2}-f_{i-2}}{4h} + a\frac{f_{i+1}-f_{i-1}}{2h}$$

We can choose stencil size of LHS

✓ $\beta = 0$ : Tridiagonal

$$\begin{pmatrix} 1 & \alpha & 0 & \cdot & & \cdot & & \cdot & & 0 \\ \alpha & 1 & \alpha & 0 & & & & & \cdot & \\ 0 & \alpha & 1 & \alpha & 0 & & & & & \\ \cdot & 0 & \alpha & 1 & \alpha & 0 & & & \cdot & \\ & & \cdot & \cdot & \cdot & \cdot & \cdot & & & \\ \cdot & & & \cdot & \cdot & \cdot & \cdot & \cdot & & \\ & & & & \cdot & \cdot & \cdot & \cdot & \cdot & \\ & & & & & 0 & \alpha & 1 & \alpha & 0 \\ \cdot & & & & & & 0 & \alpha & 1 & \alpha \\ 0 & \cdot & & \cdot & & \cdot & & 0 & \alpha & 1 \end{pmatrix} \begin{bmatrix} f'_0 \\ f'_1 \\ f'_2 \\ \cdot \\ \\ \cdot \\ \\ \\ \cdot \\ f'_{i\max} \end{bmatrix} = [A] \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ \cdot \\ \\ \cdot \\ \\ \\ \cdot \\ f_{i\max} \end{pmatrix}$$

✓ $\beta \neq 0$ : Pentadiagonal

$$\begin{pmatrix} 1 & \alpha & \beta & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ \alpha & 1 & \alpha & \beta & 0 & & & & & \cdot \\ \beta & \alpha & 1 & \alpha & \beta & 0 & & & & \cdot \\ 0 & \beta & \alpha & 1 & \alpha & \beta & 0 & & & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot \\ \cdot & & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & & & 0 & \beta & \alpha & 1 & \alpha & \beta & 0 \\ \cdot & & & & 0 & \beta & \alpha & 1 & \alpha & \beta \\ \cdot & & & & & 0 & \beta & \alpha & 1 & \alpha \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot & 0 & \beta & \alpha & 1 \end{pmatrix} \begin{bmatrix} f'_0 \\ f'_1 \\ f'_2 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ f'_{imax} \end{bmatrix} = [A] \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ f_{imax} \end{pmatrix}$$

# Optimized High Order Compact Scheme ( Inner nodes )

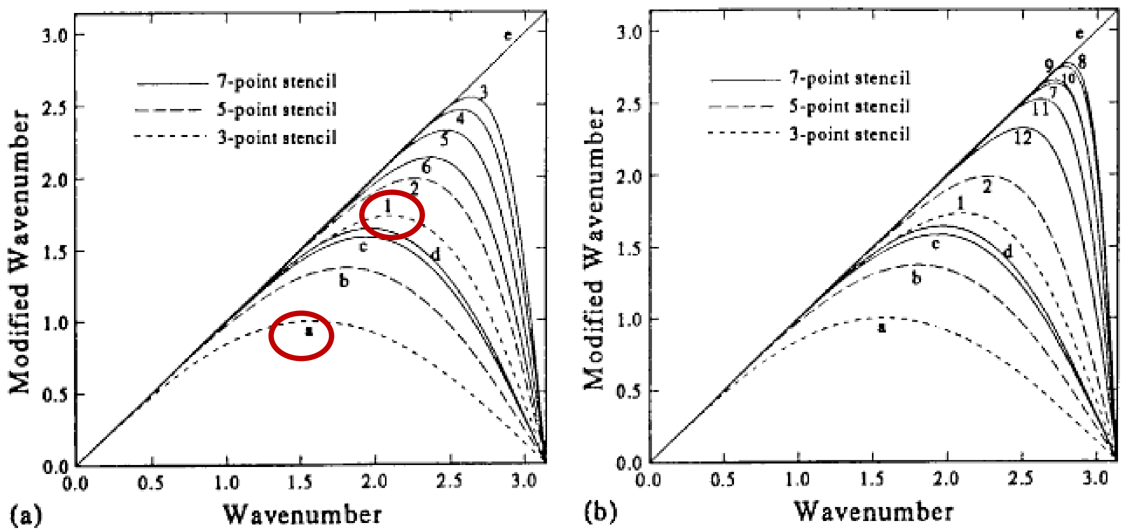



Fig. 3 Plots of the modified wavenumber vs. true wavenumber with the coefficients optimized for maximum resolution characteristics

(a) comparison of the tridiagonal schemes with others

(b) comparison of the pentadiagonal schemes with others

a : second-order central differences
b : fourth-order central differences
c : sixth-order central differences
d : Tam's DRP scheme in space
e : exact differentiation
1 : standard Pade' scheme
2 : sixth-order tridiagonal scheme ( $c = 0$ )
3 : optimized second-order tridiagonal scheme
4 : optimized fourth-order tridiagonal scheme
5 : optimized sixth-order tridiagonal scheme
6 : eighth-order tridiagonal scheme
7 : Lele's fourth-order spectral-like pentadiagonal scheme
8 : optimized second-order pentadiagonal scheme
9 : optimized fourth-order pentadiagonal scheme
10 : optimized sixth-order pentadiagonal scheme
11 : optimized eighth-order pentadiagonal scheme
12 : tenth-order pentadiagonal scheme

# Optimized Compact Scheme (Near and at the Boundary )

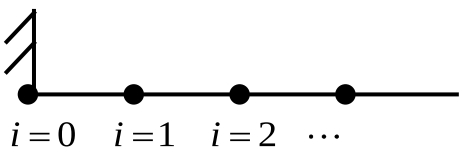
✓ High-Order Compact Discretizations ( inner nodes )

: At inner node compact scheme is base on central differential method.

$$\beta f'_{i-2} + \alpha f'_{i-1} + f'_{i} + \alpha f'_{i+1} + \beta f'_{i+2} = c\frac{f_{i+3} - f_{i-3}}{6h} + b\frac{f_{i+2} - f_{i-2}}{4h} + a\frac{f_{i+1} - f_{i-1}}{2h}$$

✓ High-Order Compact Discretizations ( near and at the boundary )

: Cannot apply central differential method




→ when $i = 0,\ i = 1\ and\ \ i = 2$ we don't have any information about $i = -1,\ i = -2\ and\ \ i = -3$

➢ The compact discretizations are formulated near and at the boundary by using <u>**the one-sided or mixed difference near and at boundary**</u>

# High Order Optimized Compact Scheme (Near and at the Boundary )

( inner nodes ) $$\beta f'_{i-2}+\alpha f'_{i-1}+f'_i+\alpha f'_{i+1}+\beta f'_{i+2}=c\frac{f_{i+3}-f_{i-3}}{6h}+b\frac{f_{i+2}-f_{i-2}}{4h}+a\frac{f_{i+1}-f_{i-1}}{2h}$$

( Near & at the boundary) $$f'_i+\alpha_{i+1}f'_{i+1}+\beta_{i+2}f'_{i+2}=\frac{1}{\Delta x}(e_i f_i+e_{i+1}f_{i+1}+e_{i+2}f_{i+2}+e_{i+3}f_{i+3}),\qquad i=0,1,2$$

- Tridiagonal discretizations $\beta = 0$

$i=0:$

$$f_0'+\alpha_1 f_1'=\frac{1}{\Delta x}(e_0 f_0+e_1 f_1+e_2 f_2+e_3 f_3)$$

$i=1:$

$$\alpha_0 f_0'+f_1'+\alpha_2 f_2'=\frac{1}{\Delta x}(e_0 f_0+e_1 f_1+e_2 f_2+e_3 f_3+e_4 f_4)$$

$i=2:$

$$\alpha_1 f_1'+f_2'+\alpha_3 f_3'=\frac{1}{\Delta x}(e_0 f_0+e_1 f_1+e_2 f_2+e_3 f_3+e_4 f_4+e_5 f_5)$$

- Pentadiagonal discretizations $\beta \neq 0$

$i=0:$

$$f_0'+\alpha_1 f_1'+\beta_2 f_2'=\frac{1}{\Delta x}(e_0 f_0+e_1 f_1+e_2 f_2+e_3 f_3)$$

$i=1:$

$$\alpha_0 f_0'+f_1'+\alpha_2 f_2'+\beta_3 f_3'=\frac{1}{\Delta x}(e_0 f_0+e_1 f_1+e_2 f_2+e_3 f_3+e_4 f_4)$$

$i=2:$

$$\beta_0 f_0'+\alpha_1 f_1'+f_2'+\alpha_3 f_3'+\beta_4 f_4'=\frac{1}{\Delta x}(e_0 f_0+e_1 f_1+e_2 f_2+e_3 f_3+e_4 f_4+e_5 f_5)$$

➢ Similarly, finding coefficients through the optimization procedures

Truncation error ( Taylor expansion ) & Minimize integrand error

# Optimized High Order Compact Scheme (Near and at the Boundary )

- OSOT Scheme ( Optimized Sixth Order Tridiagonal Scheme) $\beta = 0$

$$\begin{pmatrix} 1 & \alpha_{01} & 0 & \cdot & & \cdot & & \cdot & & 0 \\ \alpha_{10} & 1 & \alpha_{12} & 0 & & & & & \cdot & \\ 0 & \alpha & 1 & \alpha & 0 & & & & & \\ \cdot & 0 & \alpha & 1 & \alpha & 0 & & & \cdot & \\ & & \cdot & \cdot & \cdot & \cdot & \cdot & & & \\ \cdot & & & \cdot & \cdot & \cdot & \cdot & \cdot & & \\ & & & & \cdot & \cdot & \cdot & \cdot & \cdot & \\ & & & & & 0 & \alpha & 1 & \alpha & 0 \\ \cdot & & & & & & 0 & \alpha_{12} & 1 & \alpha_{10} \\ 0 & \cdot & & \cdot & & \cdot & & 0 & \alpha_{01} & 1 \end{pmatrix} \begin{bmatrix} f_0' \\ f_1' \\ f_2' \\ \cdot \\ \\ \cdot \\ \\ \\ \cdot \\ f_{imax}' \end{bmatrix} = \begin{pmatrix} e_{00} & e_{01} & e_{02} & e_{03} & 0 & \cdot & \cdot & \cdot & \cdot & 0 \\ e_{10} & e_{11} & e_{12} & e_{13} & e_{14} & 0 & & & & \cdot \\ e_{20} & e_{21} & e_{22} & e_{23} & e_{24} & e_{25} & 0 & & & \cdot \\ c & b & a & 0 & a & b & c & 0 & & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ \cdot & & 0 & c & b & a & 0 & a & b & c \\ \cdot & & & 0 & e_{25} & e_{24} & e_{23} & e_{22} & e_{21} & e_{20} \\ \cdot & & & & 0 & e_{14} & e_{13} & e_{12} & e_{11} & e_{10} \\ 0 & & & & & 0 & e_{03} & e_{02} & e_{01} & e_{00} \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ \cdot \\ \\ \cdot \\ \\ \\ \cdot \\ f_{imax} \end{pmatrix}$$

- OFOP Scheme ( Optimized Sixth Order Pentadiagonal Scheme) $\beta \neq 0$

$$\begin{pmatrix} 1 & \alpha_{01} & \beta_{02} & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ \alpha_{10} & 1 & \alpha_{12} & \beta_{13} & 0 & & & & & \cdot \\ \beta_{20} & \alpha_{21} & 1 & \alpha_{23} & \beta_{24} & 0 & & & & \cdot \\ 0 & \beta & \alpha & 1 & \alpha & \beta & 0 & & & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot \\ \cdot & & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & & & 0 & \beta & \alpha & 1 & \alpha & \beta & 0 \\ \cdot & & & & 0 & \beta_{24} & \alpha_{23} & 1 & \alpha_{21} & \beta_{20} \\ \cdot & & & & & 0 & \beta_{13} & \alpha_{12} & 1 & \alpha_{10} \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot & 0 & \beta_{02} & \alpha_{01} & 1 \end{pmatrix} \begin{bmatrix} f_0' \\ f_1' \\ f_2' \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ f_{imax}' \end{bmatrix} = \begin{pmatrix} e_{00} & e_{01} & e_{02} & e_{03} & 0 & \cdot & \cdot & \cdot & \cdot & 0 \\ e_{10} & e_{11} & e_{12} & e_{13} & e_{14} & 0 & & & & \cdot \\ e_{20} & e_{21} & e_{22} & e_{23} & e_{24} & e_{25} & 0 & & & \cdot \\ c & b & a & 0 & a & b & c & 0 & & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ \cdot & & 0 & c & b & a & 0 & a & b & c \\ \cdot & & & 0 & e_{25} & e_{24} & e_{23} & e_{22} & e_{21} & e_{20} \\ \cdot & & & & 0 & e_{14} & e_{13} & e_{12} & e_{11} & e_{10} \\ 0 & \cdot & \cdot & \cdot & \cdot & 0 & e_{03} & e_{02} & e_{01} & e_{00} \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ f_{imax} \end{pmatrix}$$

# Optimized High Order Compact Scheme ( Near and at the Boundary )

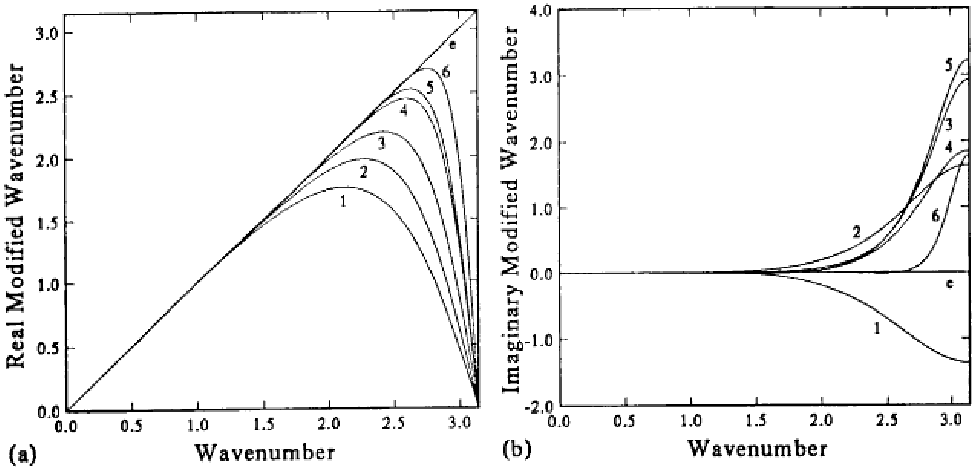



Fig. 6 Resolution and dissipation characteristics of the compact discretization near and at boundary

(a) resolution characteristics

(b) dissipation characteristics

1 : fourth-order tridiagonal discretization for $i = 0$

2 : sixth-order tridiagonal discretization for $i = 1$

3 : sixth-order tridiagonal discretization for $i = 2$

4 : second-order pentadiagonal discretization for $i = 0$

5 : fourth-order pentadiagonal discretization for $i = 1$

6 : fourth-order pentadiagonal discretization for $i = 2$

→ As we cannot apply central differential method near and at the boundary so imaginary part of modified wavenumber is not zero.

→ Dissipation error occurs near and at boundary.

# Optimized High Order Compact Scheme ( Approximation of 2nd derivative )

❖ Approximation of 2nd derivative

$$\beta f''_{i-2} + \alpha f''_{i-1} + f''_i + \alpha f''_{i+1} + \beta f''_{i+2} = c\frac{f_{i+3} - 2f_i + f_{i-3}}{9\Delta x^2} + b\frac{f_{i+2} - 2f_i + f_{i-2}}{4\Delta x^2} + a\frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}$$

Apply Taylor series expansion

① $a + b + c = 1 + 2\alpha + 2\beta$ ( 2nd order )

② $a + 2^2 b + 3^2 c = \frac{4!}{2!}(\alpha + 2^2\beta)$ ( 4th order )

③ $a + 2^4 b + 3^4 c = \frac{6!}{4!}(\alpha + 2^4\beta)$ ( 6th order )

④ $a + 2^6 b + 3^6 c = \frac{8!}{6!}(\alpha + 2^6\beta)$ ( 8th order )

⑤ $a + 2^8 b + 3^8 c = \frac{10!}{8!}(\alpha + 2^8\beta)$ ( 10th order )

We can apply same procedure as before

① corresponding modified wavenumber to wavenumber (Lele)

② minimizing integrand error ( Tam, Web )

③ Minimizing integrand error with weighting function ( J.W. Kim & D.J. Lee )

# Runge-Kutta Scheme

# LDDRK Scheme

# for time difference

# Single Time Step Method ( Runge-Kutta Scheme )

❖ Standard 4th order Runge-Kutta scheme

: Based on Taylor series truncation

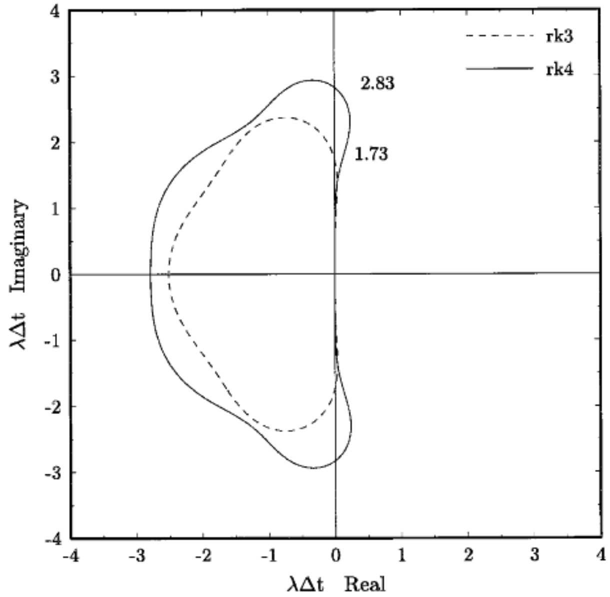
$$\frac{\partial \vec{U}}{\partial t} = \vec{F}(\vec{U})$$

where $\vec{U}$ and $\vec{F}$ are vectors, and time level $n$ is known.

To find the solution at the next time level(n+1)

$$U^{(1)} = U^n - \frac{1}{4}\Delta t F^n, \quad U^{(2)} = U^n - \frac{1}{3}\Delta t F^{(1)}, \quad U^{(3)} = U^n - \frac{1}{2}\Delta t F^{(2)}, \quad U^{n+1} = U^n - \Delta t F^{(3)}$$

✓ The choice of the time step is an important issue for stability in time stepping.




Consider the advection equation

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0 \quad \rightarrow \quad \frac{\partial u}{\partial t} + icku = 0$$

The $4^{th}$ order RK scheme should be stable if $\Delta t$ is chosen such that

$$ck_{max}\Delta t \le 2.83$$

where $\alpha_{max}$ is the maximum modified wavenumber for the spatial difference scheme.

Ref) F.Q. Hu, "Low-Dissipation and Low-Dispersion Runge-Kutta Schemes for Computational Acoustics", JCP, 1995

# Single Time Step Method ( Runge-Kutta Scheme )

❖ Analysis of the numerical error in the RK schemes

Consider the convective wave equation

$$\frac{\partial u}{\partial t} + ic\alpha u = 0 \qquad \rightarrow \qquad u^{n+1} = u^{n}\left(1 + \sum_{j=1}^{p} c_j(-ic\alpha\Delta t)^j\right)$$

✓ Amplification factor of the scheme

$$r = \frac{u^{n+1}}{u^{n}} = 1 + \sum_{j=1}^{p} c_j(-i\sigma)^j \qquad \text{where} \quad \sigma = c\alpha\Delta t$$

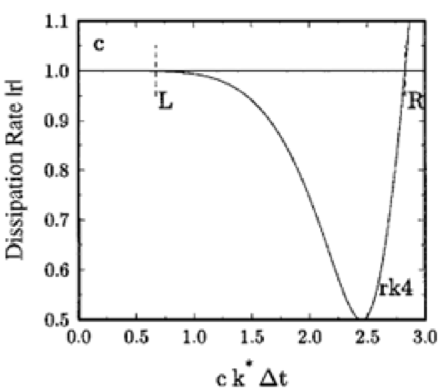
The exact amplification factor

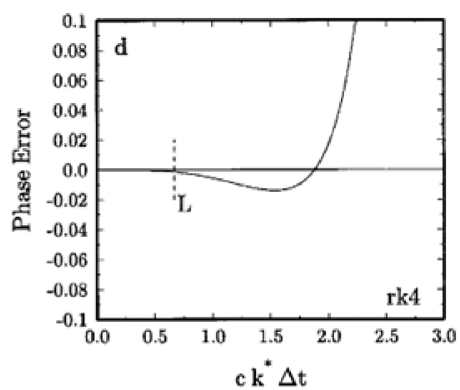
$$r_e = e^{-ic\alpha\Delta t} = e^{-i\sigma}$$

To compare the numerical and exact amplification factor

$$\frac{r}{r_e} = |r|e^{-i\delta}$$

$|r|$ represent the dissipation rate and $\delta$ represent the dispersion error




$R$ denote stablity limit of $c\alpha\Delta t$ and L denote accuracy limit

$$c\alpha_c\Delta t \le L, \qquad c\alpha_{max}\Delta t \le R$$

# LDDRK ( F.Q. Hu)

❖ Minimizing the Dissipation and Dispersion Errors

Modify the coefficients $c_j$ in the amplification factor

so that the dissipaiton & dispersion errors are minimized and the accuracy limit L is extended.

✓ Optimization is carried out by minimizing $|r - r_e|^2$ as a function of $ck^* \Delta t$.

$$\int_0^{\Gamma} \left| 1 + \sum_{j=1}^{p} c_j (-i\sigma)^j - e^{-i\sigma} \right|^2 d\sigma = MIN$$

✓ Optimized two-step alternating schemes

- The advantage of the alternating schemes
  : Dissipation and dispersion error can be further reduced
  : Higher order of accuracy can be maintained.

Let the amplification factors of the 1st and the 2nd step be

$$r_1 = 1 + \sum_{j=1}^{p_1} a_j (-i\sigma)^j$$

$$r_2 = 1 + \sum_{j=1}^{p_2} b_j (-i\sigma)^j$$

where $p_1, p_2$ are the number of stages of the two steps, respectively

The amplification factor for two steps combined = $r_1 r_2$

The exact amplification factor = $r_e^2$

To determine the coefficients $a_j$ and $b_j$

$$\int_0^{\Gamma} \left| \left(1 + \sum_{j=1}^{p_1} a_j (-i\sigma)^j\right)\left(1 + \sum_{j=1}^{p_2} b_j (-i\sigma)^j\right) - e^{-2i\sigma} \right|^2 d\sigma = MIN$$

# LDDRK ( F.Q. Hu)

- 4 – 6 Alternating LDDRK scheme

G.E. $\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{F}}{\partial x} = 0 \quad \rightarrow \quad \frac{\partial \vec{U}}{\partial t} = -\frac{\partial \vec{F}}{\partial x}$

$\rightarrow$ Step 1 ( Classical 4th order RK )

$$U^{(1)} = U^n - \frac{1}{4}\Delta t f^n$$

$$U^{(2)} = U^n - \frac{1}{3}\Delta t f^{(1)}$$

$$U^{(3)} = U^n - \frac{1}{2}\Delta t f^{(2)}$$

$$U^{n+1} = U^n - \Delta t f^{(3)}$$

$\rightarrow$ Step 2

$$U^{(1)} = U^n - 0.0.00290488096728162 0\Delta t f^n$$

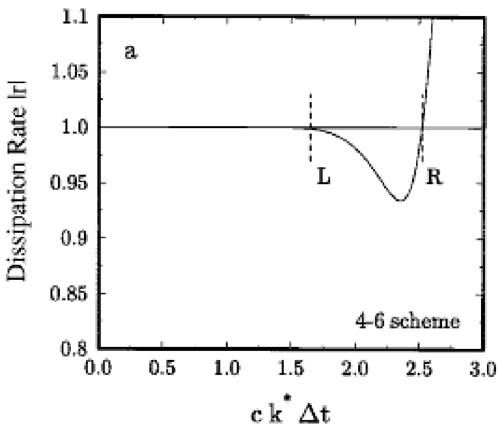
$$U^{(2)} = U^n - 0.016846105778281 67\Delta t f^n$$

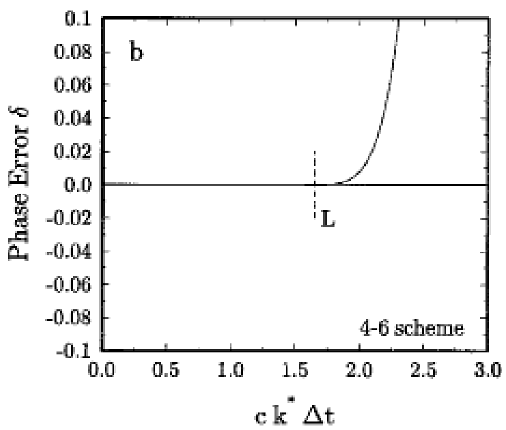
$$U^{(3)} = U^n - \frac{1}{4}\Delta t f^n$$

$$U^{(4)} = U^n - \frac{1}{3}\Delta t f^{(1)}$$

$$U^{(5)} = U^n - \frac{1}{2}\Delta t f^{(2)}$$

$$U^{(n+1)} = U^n - \Delta t f^{(3)}$$



# LDDRK ( J.W.Kim & D.J.Lee)

- 1-D Advection equation

  - Accuracy Limits ( Combined with standard 4th order RK Scheme )

    OSOT Scheme : $(u+c)\dfrac{\Delta t}{\Delta x} \le 0.375$

    OFOP Scheme : $(u+c)\dfrac{\Delta t}{\Delta x} \le 0.30$

  - Accuracy Limits ( Combined with 4-6 Stage LDDRK Scheme )

    OSOT Scheme : $(u+c)\dfrac{\Delta t}{\Delta x} \le 0.841$

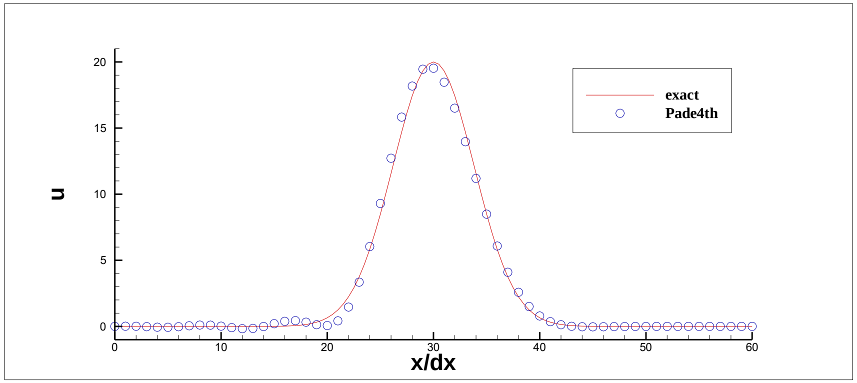
    OFOP Scheme : $(u+c)\dfrac{\Delta t}{\Delta x} \le 0.672$

→ When we use LDDRK scheme, it is possible to take lager time step than that of standard RK4 scheme

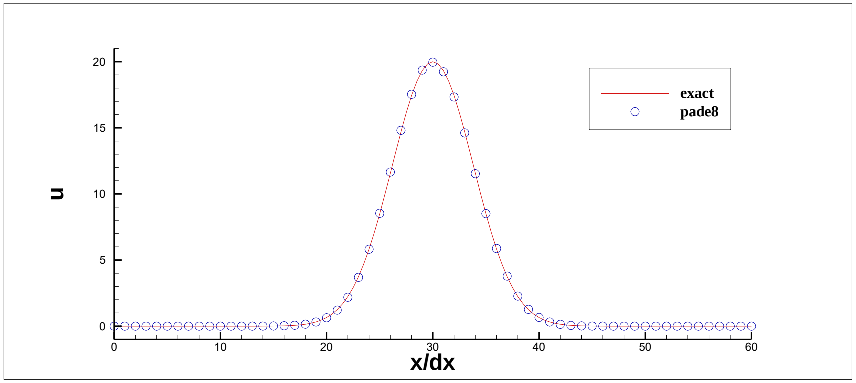
# Application

# 1D Advection equation ( bell-shaped curve )

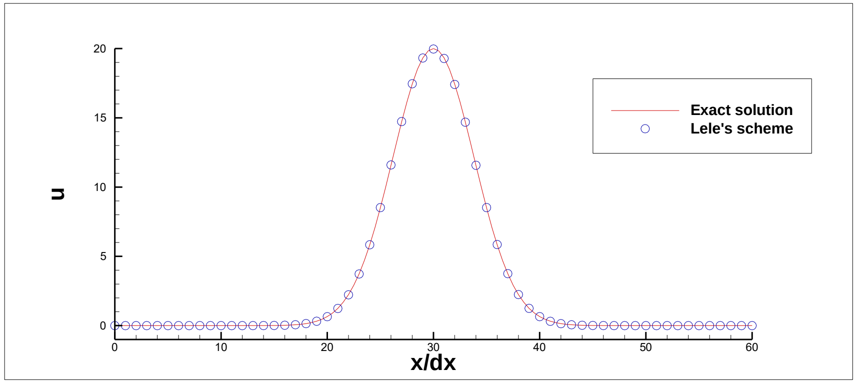
4th order Pade scheme (tridiagonal)



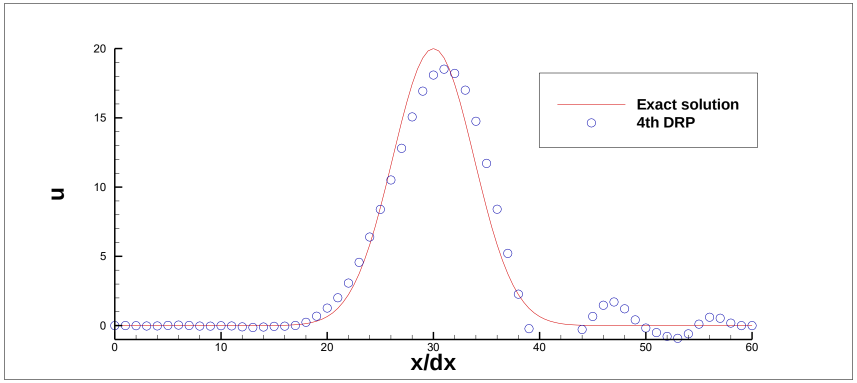

8th order pade scheme (tridiagonal)




Lele, Spectral-like Scheme (pentadiagonal)

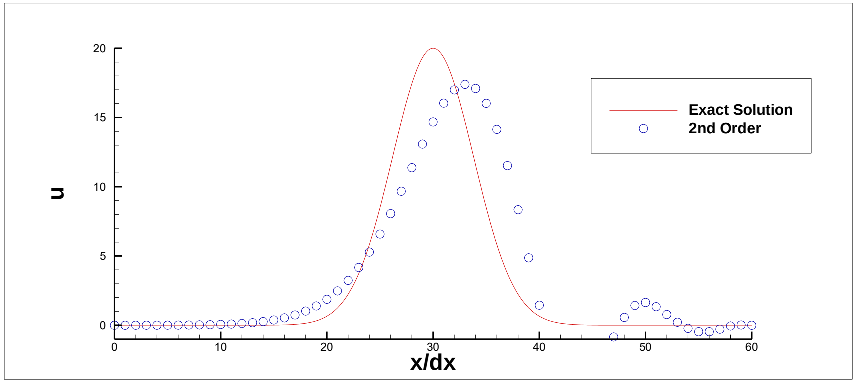



4th DRP Scheme

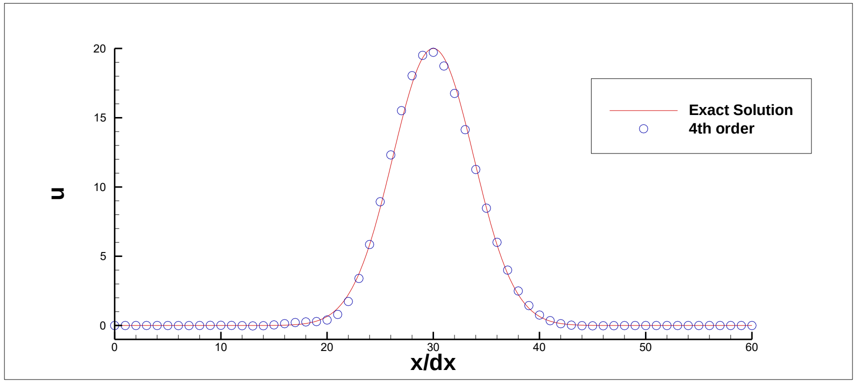


# 1D Advection equation ( bell-shaped curve , J.W. Kim & D.J. Lee)

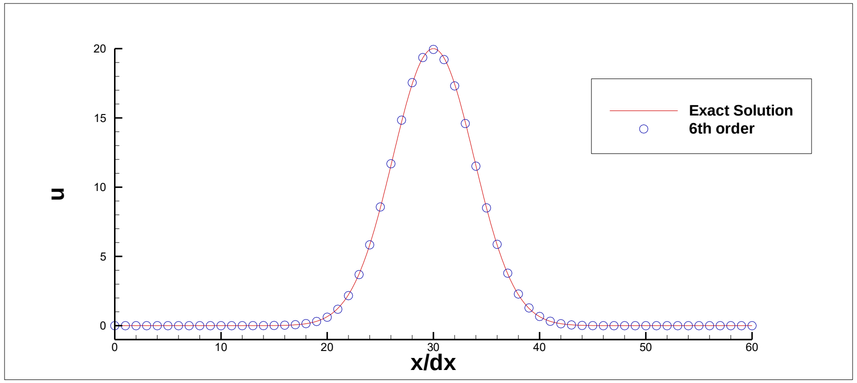
optimized $2^{nd}$ order tridiagonal scheme



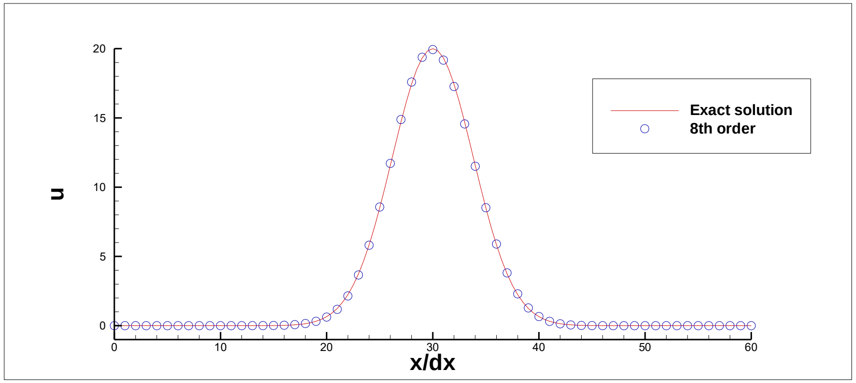

optimized $4^{th}$ order tridiagonal scheme




optimized $6^{th}$ order tridiagonal scheme

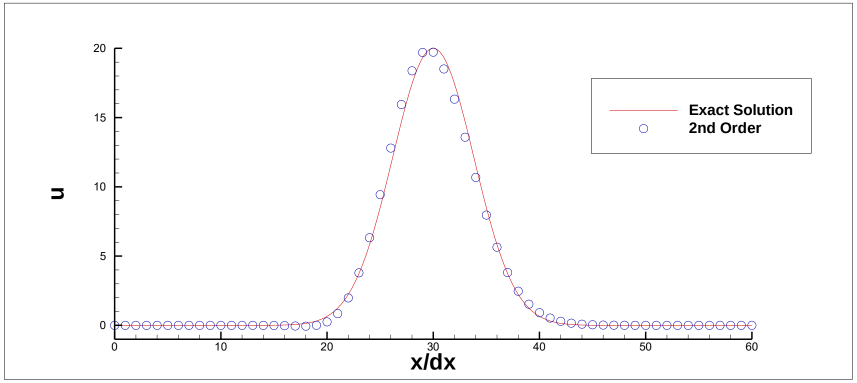



optimized $8^{th}$ order tridiagonal scheme

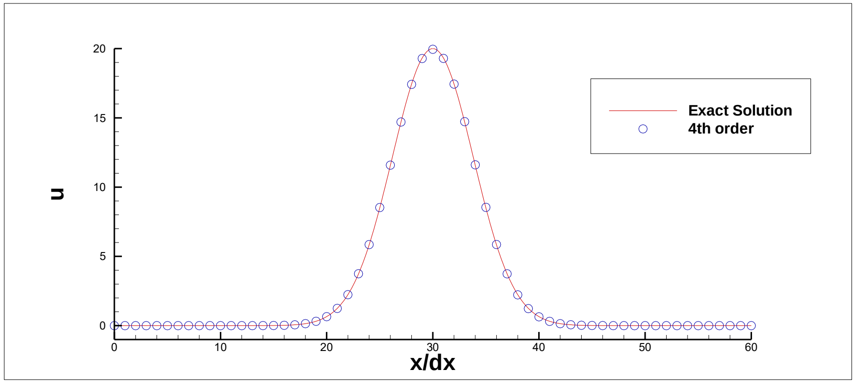


# 1D Advection equation ( bell-shaped curve, J.W.Kim & D.J. LEE)

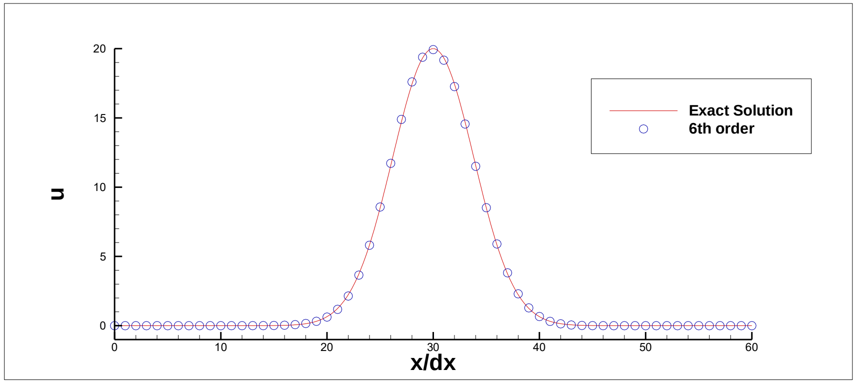
optimized 2nd order pentadiagonal scheme



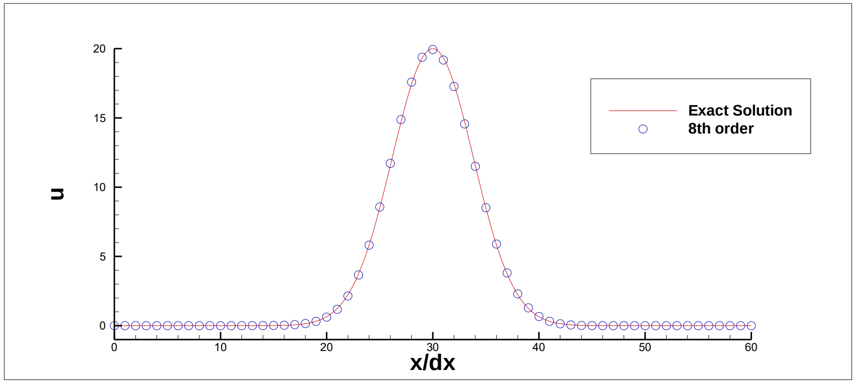

optimized 4th order pentadiagonal scheme




optimized 6th order pentadiagonal scheme




optimized 8th order pentadiagonal scheme



# 1D Riemann Problem ( Shock tube )

✓ Conservation of mass

$$\frac{\partial \rho}{\partial t} + \vec{V} \cdot \nabla \rho + \rho \nabla \cdot \vec{V} = 0$$

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0}$$ ( Conservative form )

✓ Conservation of momentum ( neglect gravity )

$$\rho \frac{\partial \vec{V}}{\partial t} + \rho(\vec{V} \cdot \nabla \vec{V}) = -\nabla p$$

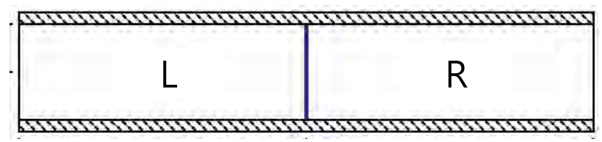
$$\boxed{\frac{\partial (\rho \vec{V})}{\partial t} + \nabla \cdot (\rho \vec{V}\vec{V} + p) = 0}$$ ( Conservative form )

So Governing equations ( conservation of mass, momentum and energy ) are expressed in vector form

For example 1-D Euler equation

$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{F}}{\partial x} = 0 \qquad \text{where} \quad \vec{U} = \begin{pmatrix} \rho \\ \rho u \\ E_t \end{pmatrix}, \quad \vec{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u(E_t + p) \end{pmatrix}$$

# 1D Riemann Problem ( Shock tube )




- Initial Condition (Air , r=1.4)

$$p_L = 7.0,\ \rho_L = 10,\ u_L = 0$$

$$p_R = 0.5,\ \rho_R = 1.0,\ u_R = 0$$

- Governing Equation

$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{F}}{\partial x} = 0 \quad \text{where} \quad \vec{U} = \begin{pmatrix} \rho \\ \rho u \\ E_t \end{pmatrix}, \quad \vec{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u(E_t + p) \end{pmatrix}, \quad E_t = \rho(e + \frac{1}{2}u^2), \quad \mathrm{e} = \frac{p}{(\gamma - 1)\rho}$$

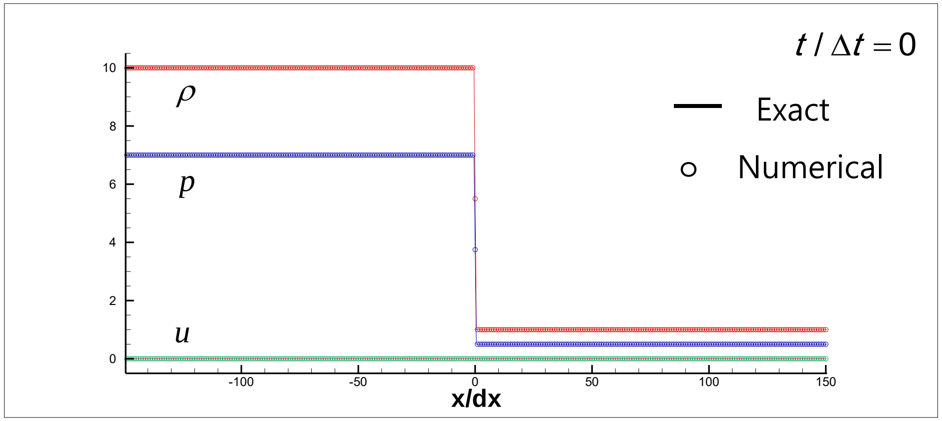
- Numerical Schemes in space

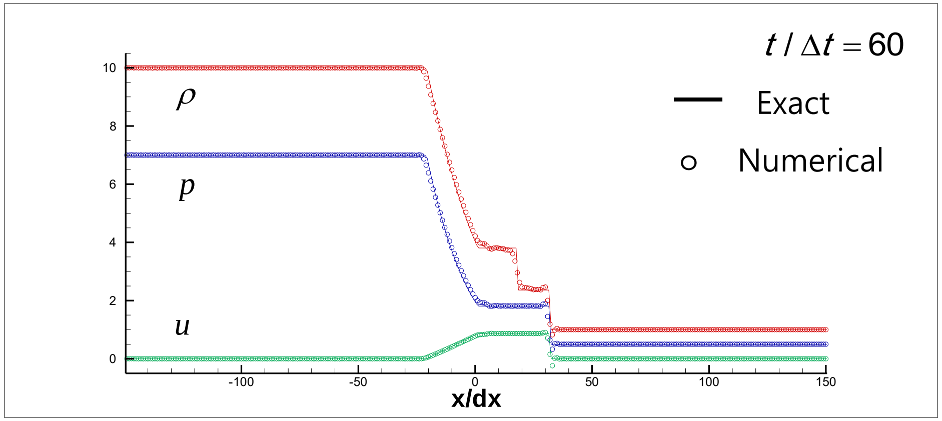
① Optimized 6th order tridiagonal scheme (D.J. LEE & J.W. Kim )

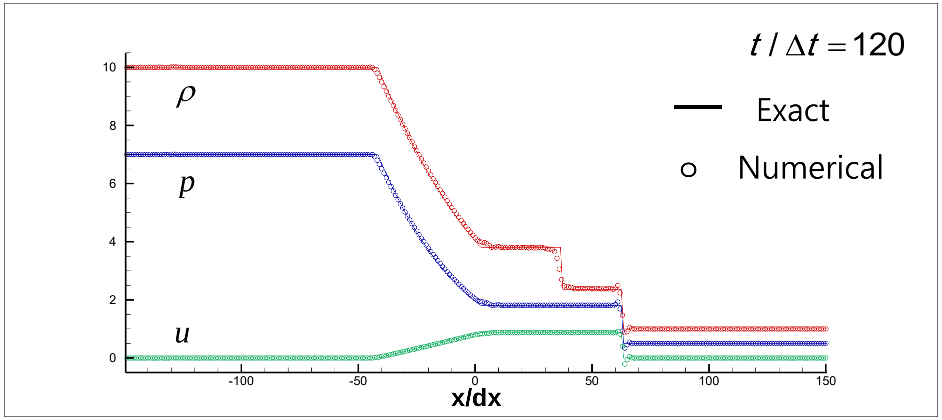
② Optimized 4th order pentadiagonal scheme (D.J. LEE & J.W. Kim )

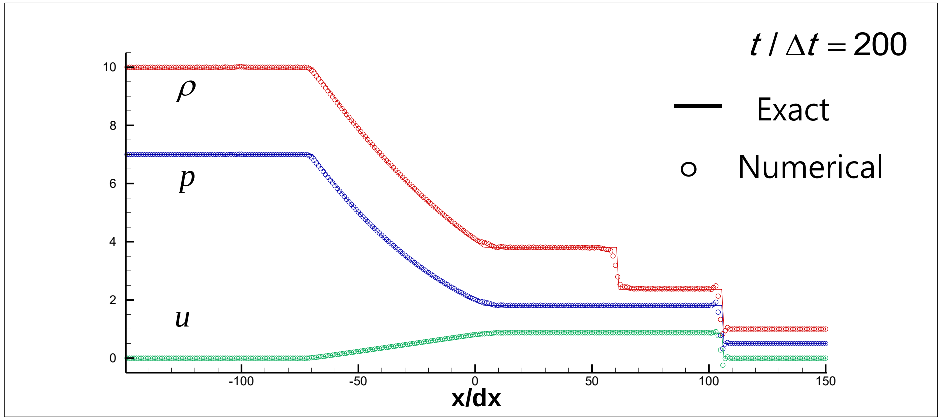
# 1D Riemann Problem ( Shock tube )

- Optimized 6th order tridiagonal scheme



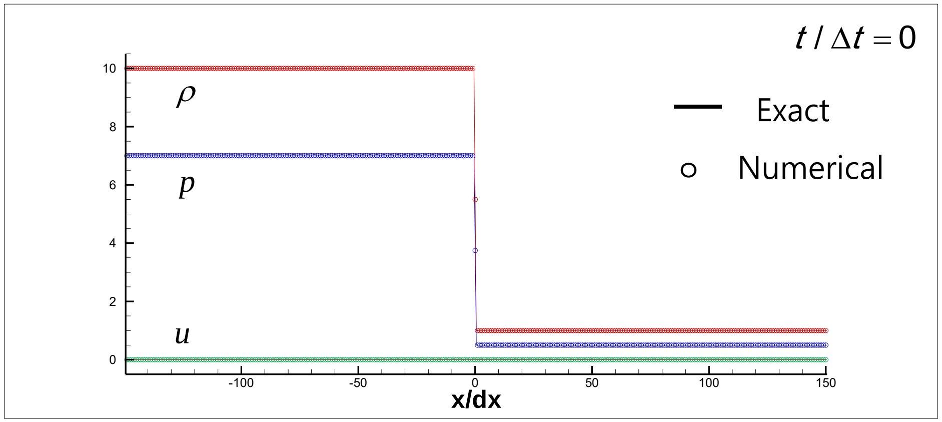



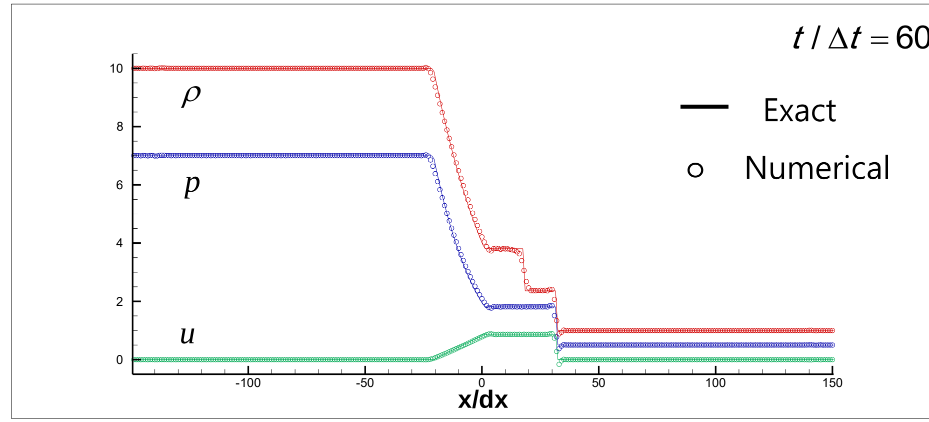



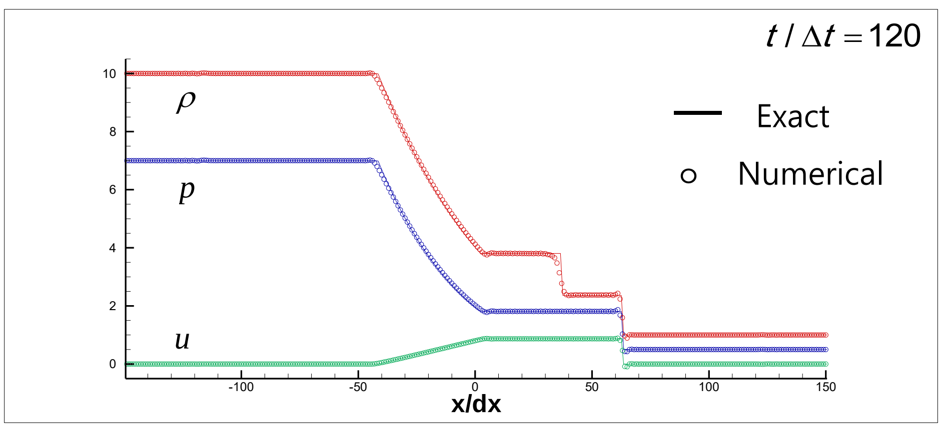



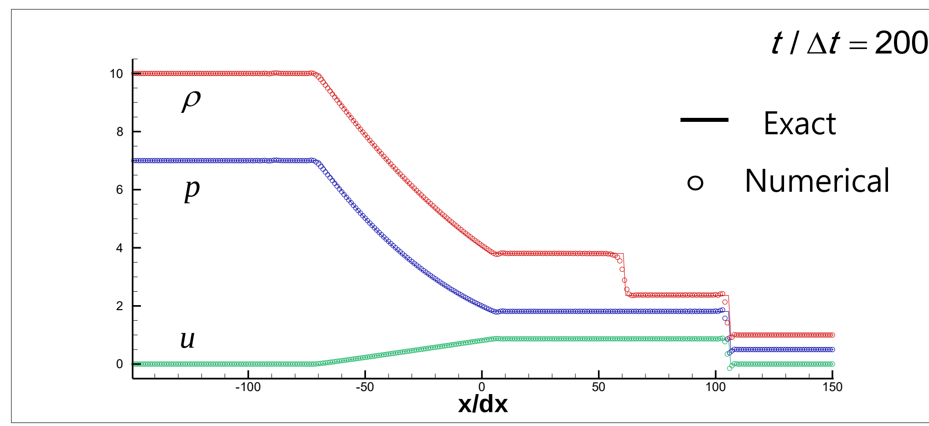
# 1D Riemann Problem ( Shock tube )

- Optimized 4th order pentadiagonal scheme



# Thank You

# Basic Concept ( Error Analysis )

## ❖ Error Analysis

✓ Consider 1-D Advection equation

$$\frac{\partial f}{\partial t} + c\frac{\partial f}{\partial x} = 0$$

the function $f$ is periodic in time and in space it can express $f = Ae^{i\omega t}e^{ikx}$ where A= constant, k=wavenumber

Exact solution of 1-D advection equation is $f(x,\mathrm{t}) = Ae^{i\omega t}e^{ikx} = e^{(\alpha + i\omega)t}e^{ikx}$

$$\frac{\partial f}{\partial t} = -c\frac{\partial f}{\partial x} \simeq -\frac{c}{2\Delta x}\left[-(1+\beta) f_{i-1} + 2\beta f_i + (1-\beta) f_{i+1}\right],$$

*where* $\beta = -1$ :forward difference (1st order )

$\beta = 0$ :central difference (2nd order)

$\beta = 1$ :backward difference (1st order )

Apply Taylor series expansion

$$\left(\frac{\delta f}{\delta x}\right)_i = \frac{1}{2\Delta x}\left[2\Delta x\left(\frac{\partial f}{\partial x}\right)_i - \beta\Delta x^2\left(\frac{\partial^2 f}{\partial x^2}\right)_i + \frac{\Delta x^3}{3}\left(\frac{\partial^3 f}{\partial x^3}\right)_i - \frac{\beta\Delta x^4}{12}\left(\frac{\partial^4 f}{\partial x^4}\right)_i + \dots\right]$$

Substituting this into 1-D advection equation

$$\frac{\partial f}{\partial t} = -c\frac{\partial f}{\partial x} + \frac{c\beta\Delta x^2}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i - \frac{c\Delta x^3}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i + \frac{c\beta\Delta x^4}{24}\left(\frac{\partial^4 f}{\partial x^4}\right)_i + \dots$$

# Basic Concept ( Error Analysis )

$$\frac{\partial f}{\partial t} = -c\frac{\partial f}{\partial x} + \frac{c\beta\Delta x^2}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i - \frac{c\Delta x^3}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i + \frac{c\beta\Delta x^4}{24}\left(\frac{\partial^4 f}{\partial x^4}\right)_i + \dots$$

$$\rightarrow \frac{\partial f}{\partial t} = -a\frac{\partial f}{\partial x} + \nu\frac{\partial^2 f}{\partial x^2} + \gamma\frac{\partial^3 f}{\partial x^3} + \tau\frac{\partial^4 f}{\partial x^4} \qquad (a)$$

Consider the solution $f(x,\mathrm{t}) = Ae^{i\omega t}e^{ikx} = e^{(\alpha+i\omega)t}e^{ikx}$

(a) $\rightarrow \alpha + i\omega = -iak - \nu k^2 - i\gamma k^3 + \tau k^4$

$$\alpha = -k^2(\nu - \tau k^2), \quad \omega = -k(a + \gamma k^2)$$

The solution is composed of both amplitude and phase terms. Thus

$$\boxed{f = \underbrace{e^{-k^2(\nu-\tau k^2)t}}_{amplitude}\underbrace{e^{ik[x-(a+\gamma k^2)t]}}_{phase}}$$

The amplitude of the solution depends only $\nu$ and $\tau$ ,the coefficients of the even derivatives

and the phase of the solution depends only a and $\gamma$ ,the coefficients of the odd derivatives

- **Therefore the even derivative terms effect amplitude and the odd derivative terms effect phase.**