Chapter 1

Chapter 2

PHYS8750, Homework 1

2.1

2.1.1

For backward difference, the finite difference scheme is:

$$\frac{d\psi}{dt} \simeq \frac{\psi_n - \psi_{n-1}}{\Delta t}$$

by Taylor expansion:

$$\psi_{n-1} = \psi_n - \Delta t \psi'(t_n) + \frac{1}{2}\psi''(t_n)(\Delta t)^2 + \mathcal{O}(\Delta t)^3$$

thus:

$$\frac{\psi_n - \psi_{n-1}}{\Delta t} - \psi'(t_n) = -\frac{1}{2}\psi''(t_n)\Delta t + \mathcal{O}(\Delta t)^2$$

So the backward scheme has the first order of accuracy.

2.1.2

For trapezoidal difference, the finite difference scheme is

$$\frac{\psi_{n+1} - \psi_n}{\Delta t} = \frac{\psi'(t_n) + \psi'(t_{n+1})}{2}$$

by Taylor expansion:

$$\psi'(t_{n+1}) = \psi'(t_n) + \psi''(t_n)\Delta t + \frac{1}{2}\psi'''(t_n)\Delta t^2 + \mathcal{O}(\Delta t)^3$$

$$\psi_{n+1} = \psi_n + \Delta t \psi'(t_n) + \frac{1}{2}\psi''(t_n)(\Delta t)^2 + \frac{1}{6}\psi'''(t_n)(\Delta t)^3 + \mathcal{O}(\Delta t)^4$$

thus:

$$\frac{\psi_{n+1} - \psi_n}{\Delta t} - \frac{\psi'(t_n) + \psi'(t_{n+1})}{2}$$

$$= \psi'(t_n) + \frac{1}{2}\psi''(t_n)(\Delta t) + \frac{1}{6}\psi'''(t_n)(\Delta t)^2 + \mathcal{O}(\Delta t)^3 - \left[\psi'(t_n) + \frac{1}{2}\psi''(t_n)\Delta t + \frac{1}{4}\psi'''(t_n)(\Delta t)^2 + \mathcal{O}(\Delta t)^3\right]$$

$$= -\frac{1}{12}\psi'''(t_n)(\Delta t)^2 + \mathcal{O}(\Delta t)^3$$

So the trapezoidal scheme has the second order of accuracy.

2.1.3

For oscillation-diffusion problem ($\lambda < 0$), the difference scheme is

$$\frac{\psi_n - \psi_{n-1}}{\Delta t} = (\lambda + \mathrm{i}\,\omega)\psi_n$$

Solve for ψ_{n-1}

$$\psi_{n-1} = \psi_n[1 - (\lambda + \mathrm{i}\,\omega)\Delta t]$$

Absolute stability criteria

$$\left|\frac{\psi_n}{\psi_{n-1}}\right| = \frac{1}{(1-\lambda\Delta t)^2 + (\omega\Delta t)^2} \leq 1$$

Then

$$(\lambda\Delta t - 1)^2 + (\omega\Delta t)^2 \geq 1$$

which is the outside region of a circle centered at 1 with radius 1.

For oscillation-amplification problem ($\lambda > 0$),

$$\left|\frac{\psi_{n-1}}{\psi_n}\right| = (1-\lambda\Delta t)^2 + (\omega\Delta t)^2 \leq 1$$

which is the inside of the circle.

For trapezoidal difference scheme, solve for ψ_{n+1}

$$\psi_{n+1} = \psi_n \frac{2 + (\lambda + \mathrm{i}\,\omega)\Delta t}{2 - (\lambda + \mathrm{i}\,\omega)\Delta t}$$

For oscillation-diffusion problem, absolute stability criterion

$$\left|\frac{\psi_{n+1}}{\psi_n}\right| = \frac{(2+\lambda\Delta t)^2 + (\omega\Delta t)^2}{(2-\lambda\Delta t)^2 + (\omega\Delta t)^2} \leq 1$$

Then

$$\lambda\Delta t \leq 0$$

which is the left half of the plane. Since λ is negative, the scheme is stable for all positive Δt.

For oscillation-amplification problem, absolute stability criterion

$$\left|\frac{\psi_n}{\psi_{n+1}}\right| = \frac{(2-\lambda\Delta t)^2 + (\omega\Delta t)^2}{(2+\lambda\Delta t)^2 + (\omega\Delta t)^2} \leq 1$$

Then

$$\lambda\Delta t \geq 0$$

which is the right half of the plane. Since λ is positive, the scheme is stable for all positive Δt. Overall, trapezoidal difference scheme would be stable for all positive Δt.

2.2

For backward time scheme (Figure 1.1), when λ is negative, the schemes using all Δt would be stable, i.e., if true solution decreases with time, the numerical solution would not increase with time.

For λ is positive, blue and red curves correspond to unstable situation since they fall into the unstable region, because

$$(\lambda\Delta t - 1)^2 + (\omega\Delta t)^2 = [1.2973, 1.0189, 0.9968, 0.9996]$$

.

For stable schemes, smaller Δt results in smaller amplitude and phase errors.

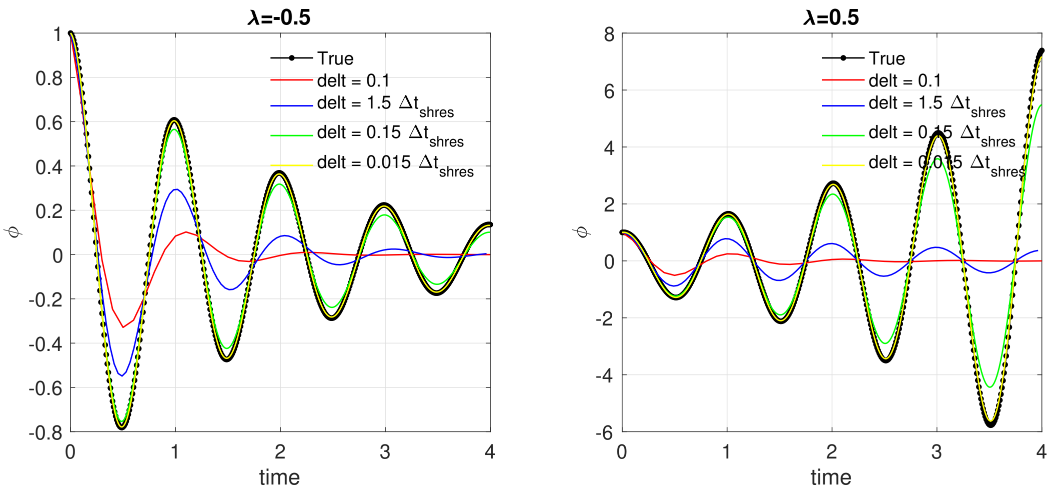

Figure 2.1: Different settings of backward difference scheme

2.3

For trapezoidal scheme (Figure 1.2), all Δt correspond to stable situation, and errors are smaller than those from backward schemes. Phase delay becomes more apparent as Δt increases.

2.4

In all three schemes, trapezoidal scheme which has second order of accuracy shows the best performance of stability, also less strict criterion for the time step Δt. Larger time step Δt usually lead to bigger errors.

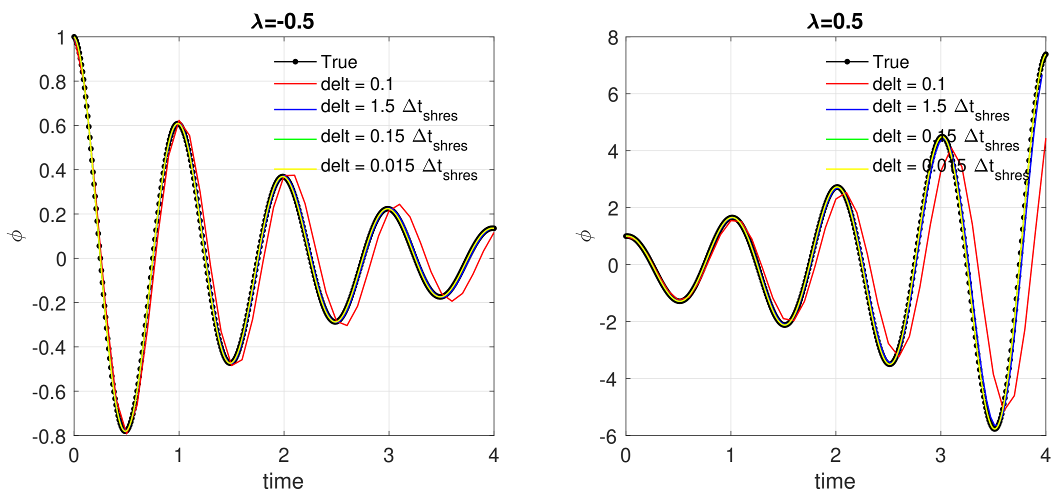

Figure 2.2: Different settings of trapezoidal difference scheme

Chapter 3

Homework 2

3.1

Consider the advection problem

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

Using von Neumann stability analysis, derive the stability condition for the following difference scheme:

$$\delta_{2t}\phi + c\left(\frac{4}{3}\delta_{2x}\phi - \frac{1}{3}\delta_{4x}\phi\right) = 0$$

Here

$$\delta_{nt}f(t) = \frac{f(t+n\Delta t/2) - f(t-n\Delta t/2)}{n\Delta t} \quad \delta_{nx}f(x) = \frac{f(x+n\Delta x/2) - f(x-n\Delta x/2)}{n\Delta x}$$

3.1.1

The finite difference form is

$$\frac{\phi(t+\Delta t, x) - \phi(t-\Delta t, x)}{2\Delta t} + c\left(\frac{4}{3}\frac{\phi(t, x+\Delta x) - \phi(t, x-\Delta x)}{2\Delta x} - \frac{1}{3}\frac{\phi(t, x+2\Delta x) - \phi(t, x-2\Delta x)}{4\Delta x}\right) = 0$$

Denote ϕ_j^n as the solution at time $n\Delta t$ and position $j\Delta x$, the above equation can be rewritten as

$$\frac{\phi_j^{n+1} - \phi_j^{n-1}}{2\Delta t} + c\left(\frac{4}{3}\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} - \frac{1}{3}\frac{\phi_{j+2}^n - \phi_{j-2}^n}{4\Delta x}\right) = 0$$

Use $\mu = c\Delta t/\Delta x$

$$6\left(\phi_j^{n+1} - \phi_j^{n-1}\right) + \mu\left[8\left(\phi_{j+1}^n - \phi_{j-1}^n\right) - \left(\phi_{j+2}^n - \phi_{j-2}^n\right)\right] = 0$$

Decompose the solution into wave components

$$\phi_j^n = \sum_{k=-N}^{N} a_k^{n\mathrm{i}\,kj\Delta x}$$

For k-th component, the above equation can be simplified as

$$6\left(a_k^{n+1\mathrm{i}\,kj\Delta x} - a_k^{n-1\mathrm{i}\,kj\Delta x}\right) + \mu\left[8\left(a_k^{n\mathrm{i}\,k(j+1)\Delta x} - a_k^{n\mathrm{i}\,k(j-1)\Delta x}\right) - \left(a_k^{n\mathrm{i}\,k(j+2)\Delta x} - a_k^{n\mathrm{i}\,k(j-2)\Delta x}\right)\right] = 0$$

Then

$$6\left(a_k^{n+1} - a_k^{n-1}\right) + \mu a_k^n \left[8\left({}^{\mathrm{i}\,k\Delta x} - {}^{-\,\mathrm{i}\,k\Delta x}\right) - \left({}^{2\,\mathrm{i}\,k\Delta x} - {}^{-2\,\mathrm{i}\,k\Delta x}\right)\right] = 0$$

$$6\left(a_k^{n+1} - a_k^{n-1}\right) + \mu a_k^n (8 \cdot 2\,\mathrm{i} \sin k\Delta x - 2\,\mathrm{i} \sin 2k\Delta x) = 0$$

The recursion relation of a_k^n is

$$a_k^{n+1} = \mathrm{i}\,\frac{\mu}{3}(8 \sin k\Delta x - \sin 2k\Delta x) a_k^n + a_k^{n-1}$$

For constant advection problem, the amplification factor is a constant, and we have

$$A_k = \frac{a_k^{n+1}}{a_k^n} = \frac{a_k^n}{a_k^{n-1}}$$

The characteristic equation of the recursion relation is

$$(A_k)^2 = \mathrm{i}\,\frac{\mu}{3}(8 \sin k\Delta x - \sin 2k\Delta x) A_k + 1$$

The roots of the quadratic equation are

$$A_k^{\pm} = \mathrm{i}\,\frac{\mu}{6}(8 \sin k\Delta x - \sin 2k\Delta x) \pm \sqrt{1 - \frac{\mu^2}{36}(8 \sin k\Delta x - \sin 2k\Delta x)^2}$$

1) If $1 - \mu^2/36(8 \sin k\Delta x - \sin 2k\Delta x)^2 < 0$, then

$$\left|A_k^{\pm}\right| = \left|\frac{\mu}{6}(8 \sin k\Delta x - \sin 2k\Delta x) \pm \sqrt{\frac{\mu^2}{36}(8 \sin k\Delta x - \sin 2k\Delta x)^2 - 1}\right|$$

In this case, if $8 \sin k\Delta x - \sin 2k\Delta x > 0$, then

$$\frac{\mu}{6}(8 \sin k\Delta x - \sin 2k\Delta x) > 1$$

then

$$\left|\frac{\mu}{6}(8 \sin k\Delta x - \sin 2k\Delta x) + \sqrt{\frac{\mu^2}{36}(8 \sin k\Delta x - \sin 2k\Delta x)^2 - 1}\right| > 1$$

Similarly, if $8 \sin k\Delta x - \sin 2k\Delta x < 0$, then

$$\frac{\mu}{6}(8 \sin k\Delta x - \sin 2k\Delta x) < -1$$

then

$$\left|\frac{\mu}{6}(8 \sin k\Delta x - \sin 2k\Delta x) - \sqrt{\frac{\mu^2}{36}(8 \sin k\Delta x - \sin 2k\Delta x)^2 - 1}\right| > 1$$

Thus for both situations, one of the roots will have an amplification factor larger than 1, and the scheme is unstable.

2) Now, if $1 - \mu^2/36(8 \sin k\Delta x - \sin 2k\Delta x)^2 > 0$, then

$$\left|A_k^{\pm}\right| = \sqrt{\left[\frac{\mu}{6}(8 \sin k\Delta x - \sin 2k\Delta x)\right]^2 + 1 - \frac{\mu^2}{36}(8 \sin k\Delta x - \sin 2k\Delta x)^2} = 1$$

In this case, a_k^n will stay bounded, and the scheme is stable. So the requirement for μ is

$$\mu \leq \frac{6}{|8\sin k\Delta x - \sin 2k\Delta x|}$$

Define $f(x) = 8\sin x - \sin 2x$, then we need to find the maximum absolute value of f(x) by looking at its derivative

$$f'(x) = 8\cos x - 2\cos 2x$$

Let $f'(x_0) = 0$

$$2\cos^2 x_0 - 4\cos x_0 - 1 = 0$$

Solve for $\cos x_0$, discard the root which is larger than 1, we get the criteria of $f(x)$'s extreme points

$$\cos x_0 = 1 - \frac{\sqrt{6}}{2}$$

Then the extreme values of $f(x)$ are

$$f(x_0) = 8\sin x_0 - \sin 2x_0 = (8 - 2\cos x_0)\sin x_0 = (6+\sqrt{6})\sin x_0 = \pm(6+\sqrt{6})\sqrt{\sqrt{6} - \frac{3}{2}}$$

Therefore the range of $f(x)$ is

$$-(6+\sqrt{6})\sqrt{\sqrt{6} - \frac{3}{2}} \leq f(x) \leq (6+\sqrt{6})\sqrt{\sqrt{6} - \frac{3}{2}}$$

The range of $6/|8\sin k\Delta x - \sin 2k\Delta x|$ is

$$\frac{6}{|8\sin k\Delta x - \sin 2k\Delta x|} \geq \frac{6}{(6+\sqrt{6})\sqrt{\sqrt{6}-\frac{3}{2}}} = \frac{\sqrt{6}}{(\sqrt{6}+1)\sqrt{\sqrt{6}-\frac{3}{2}}}$$

To satisfy the stability conditions for all wave numbers, the range of μ is

$$\mu \leq \frac{\sqrt{6}}{(\sqrt{6}+1)\sqrt{\sqrt{6}-\frac{3}{2}}} \approx 0.73$$

3.2

Read Takacs (1985) paper, derive the five coefficients (a_{-2}, a_{-1}, a_0, a_1, and a_2) for the fourth order Takacs method. Examine and understand the function `F_phin_4s_Takacs.m`. Are the coefficients correctly set up?

3.2.1

The equation set associated with the 4th order Takacs method is

$$\sum_{j'=-2}^{2} j'^m a_{j'} = (-\mu)^m \quad m = 0, \ldots, 4$$

Denote A as the coefficient matrix

$$A = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ -2 & -1 & 0 & 1 & 2 \\ 4 & 1 & 0 & 1 & 4 \\ -8 & -1 & 0 & 1 & 8 \\ 16 & 1 & 0 & 1 & 16 \end{pmatrix}$$

The equation in matrix form is:

$$A\begin{pmatrix} a_{-2} \\ a_{-1} \\ a_0 \\ a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} 1 \\ -\mu \\ \mu^2 \\ -\mu^3 \\ \mu^4 \end{pmatrix}$$

The augmented matrix of the linear system is

$$A' = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ -2 & -1 & 0 & 1 & 2 & -\mu \\ 4 & 1 & 0 & 1 & 4 & \mu^2 \\ -8 & -1 & 0 & 1 & 8 & -\mu^3 \\ 16 & 1 & 0 & 1 & 16 & \mu^4 \end{pmatrix}$$

The the matrix can be written as

$$A'\begin{pmatrix} a_{-2} \\ a_{-1} \\ a_0 \\ a_1 \\ a_2 \\ -1 \end{pmatrix} = 0$$

Apply a series of elementary operations to each row of A', A' can be reduced to upper triangular form

$$A' \to \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ & 1 & 2 & 3 & 4 & -\mu+2 \\ & & 2 & 6 & 12 & \mu^2-3\mu+2 \\ & & & 6 & 24 & -\mu^3+3\mu^2-2\mu \\ & & & & 24 & \mu^4-2\mu^3-\mu^2+2\mu \end{pmatrix}$$

Further reduce A' to triangular form

$$A' \to \begin{pmatrix} 24 & & & & & \mu^4+2\mu^3-\mu^2-2\mu \\ & 6 & & & & -\mu^4-\mu^3+4\mu^2+4\mu \\ & & 4 & & & \mu^4-5\mu^2+4 \\ & & & 6 & & -\mu^4+\mu^3+4\mu^2-4\mu \\ & & & & 24 & \mu^4-2\mu^3-\mu^2+2\mu \end{pmatrix}$$

The coefficients are

$$\begin{cases} a_{-2} & = \frac{1}{24}\left(\mu^4+2\mu^3-\mu^2-2\mu\right) \\ a_{-1} & = \frac{1}{6}\left(-\mu^4-\mu^3+4\mu^2+4\mu\right) \\ a_0 & = \frac{1}{4}\left(\mu^4-5\mu^2+4\right) \\ a_1 & = \frac{1}{6}\left(-\mu^4+\mu^3+4\mu^2-4\mu\right) \\ a_2 & = \frac{1}{24}\left(\mu^4-2\mu^3-\mu^2+2\mu\right) \end{cases}$$

3.3

Use the code “`Advection_PDE_RK_2rdSpace_LaxWen_Takacs_stability_2.m`” and answer the following questions:

1. For "waveform = 3 (select one wave component to start)", try CFL $= 0.2, 0.5, 0.9, 1.01, 1.05, 1.1$, run the model for the same amount of time (not the same amount of time step), comment on the CFL stability condition. Mark the maximum amplitudes and compare these among different schemes and different CFL numbers for each individual scheme.
   Note: you can name the time you will stop the model, as long as you can make up your story and put forward reasonings. (stopping time is flexible).

2. For "waveform = 3", turn on two waves. Comment on dispersion errors of different schemes.

3. Which scheme leads to the best amplitude performance? Comment on amplitude and phase errors, respectively?

4. Replace the wave function to triangle and step functions, refer to questions 1 and 3, and comment on what you find. Discuss shared principles among these three functions, and differences.

Some of the answers will be quantitative with respect to the settings you choose. The comments from you will learn from these exercises can be qualitative.

3.3.1

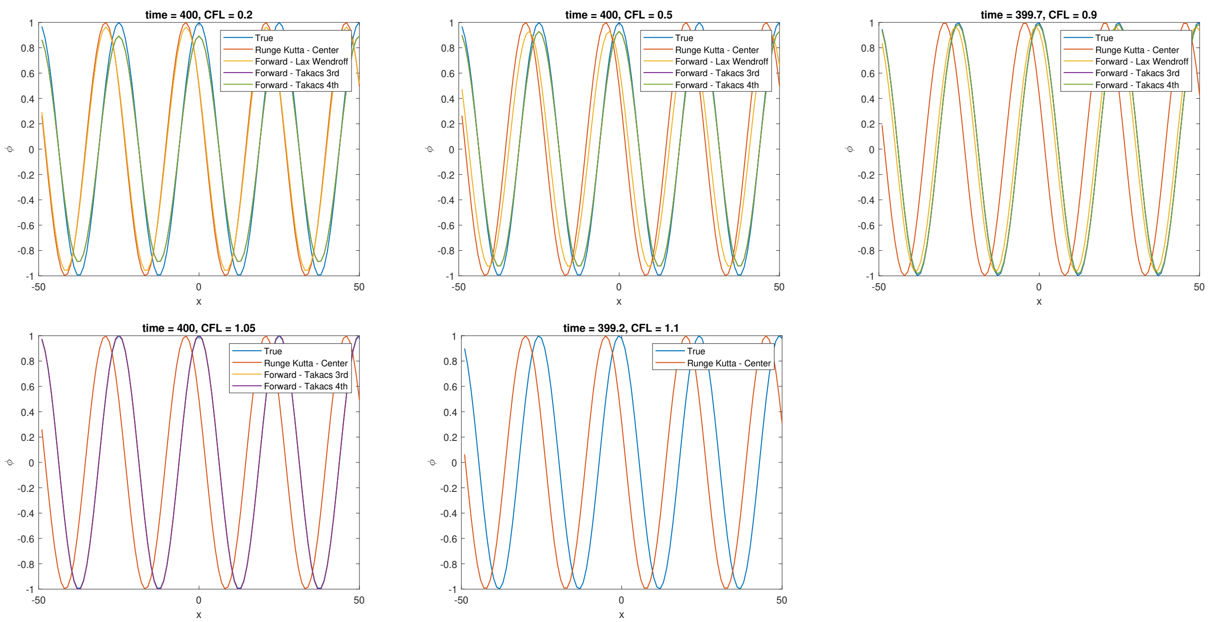

Figure 3.1: Comparison of different numerical schemes with varying CFL numbers, only stable solutions are shown.

1. In figure 3.1, for CFL < 1, all numerical schemes are stable. But for CFL > 1, only scheme with Runge-Kutta in time and centered difference in space is stable.

2. In figure 3.2, schemes with forward difference in time and Takacs methods in space are in phase with the true solution, scheme with Runge-Kutta in time, centered difference in space and scheme with forward difference in time, Lax-Wendroff method in space don't resolve the correct phase.

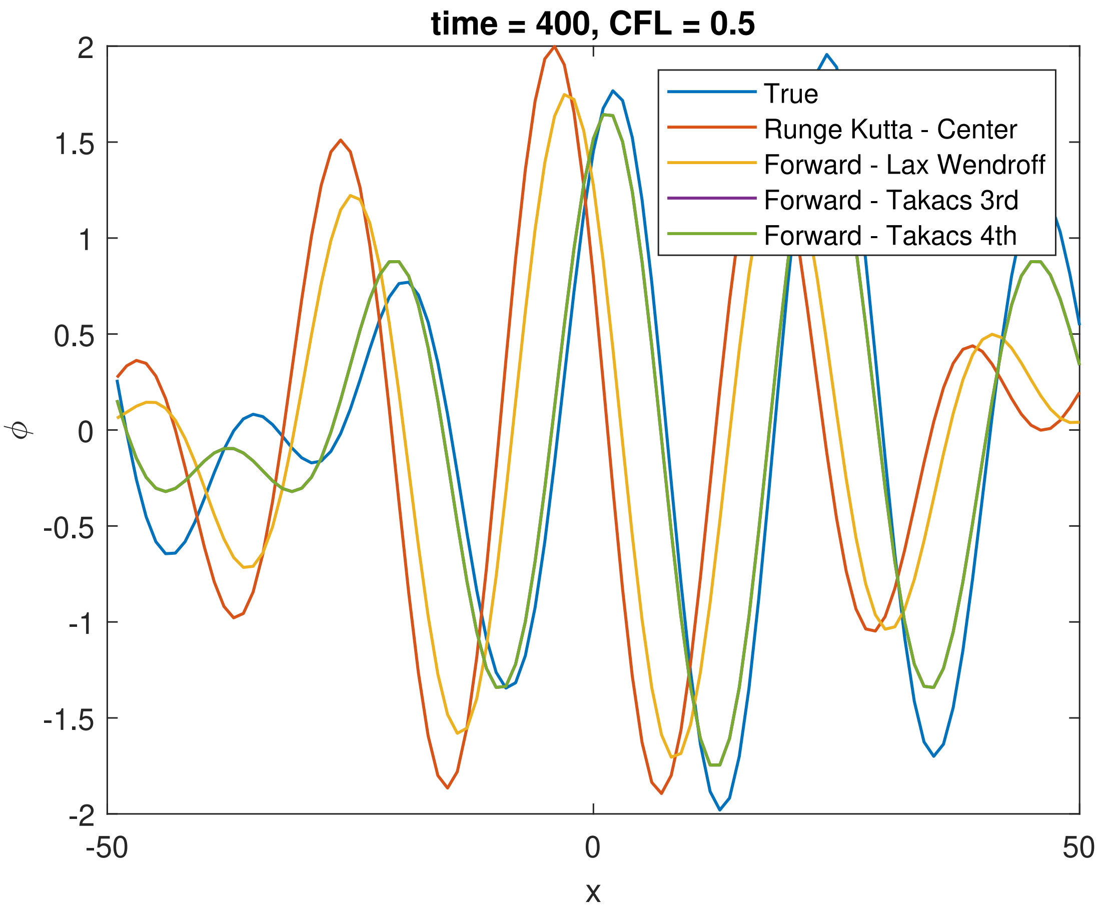

Figure 3.2: Comparison of different numerical schemes for two trigonometric waves.

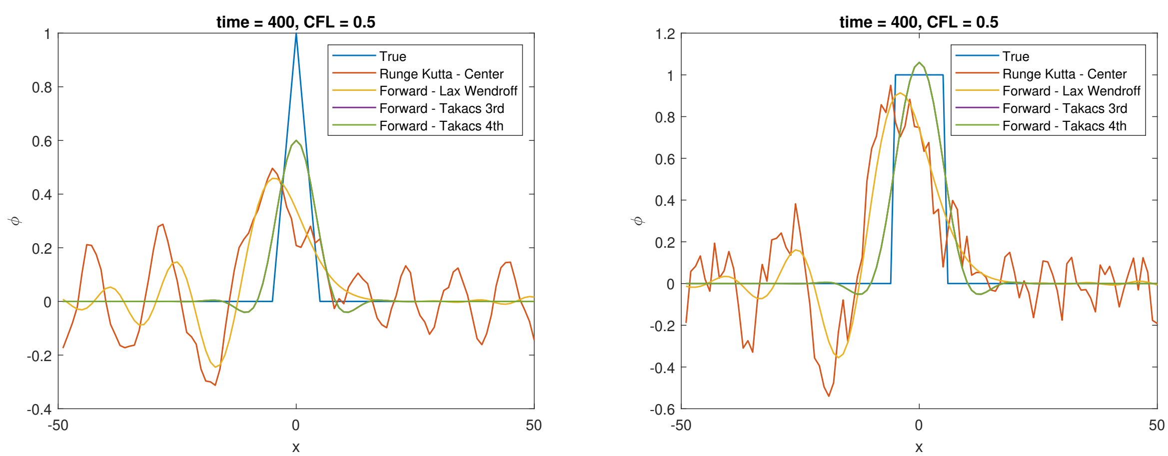

Figure 3.3: Comparison of different numerical schemes for triangle and rectangle waves.

3. Schemes with forward difference in time and Takacs methods in space have both the best amplitude and phase performance. In the situation of two trigonometric waves, during the time of simulation, two Takacs methods don't show distinguishable differences.

4. In figure 3.3, schemes with forward difference in time and Takacs methods in space perform best among four difference numerical schemes, two Takacs schemes are correct in phase, but they still underestimated amplitudes in the situation of triangle wave.