AM213B Numerical Methods for the Solution of Differential Equations

Lecture 14

List of topics in this lecture

- Behavior of solution of the modified PDE, dissipation, unbounded growth associated with negative dissipation, phase velocity, dispersion, group velocity
- Behavior of first order methods based on modified PDEs
- Behavior of second order methods based on modified PDEs

Review

Modified PDE:

Consider the upwind method for solving $u_t + au_x = 0$, $a > 0$.

$$u_i^{n+1} = u_i^n - ar\left(u_i^n - u_{i-1}^n\right), \qquad r = \frac{\Delta t}{\Delta x}, \qquad a > 0$$

Key: we view $u_i^n = w(x_i, t_n)$ and expand $w(x, t)$ in the numerical method.

The governing equation for $w(x, t)$, after neglecting $O((\Delta t)^2+(\Delta x)^2)$ term, is

$$\boxed{w_t = -aw_x + \sigma w_{xx}} \qquad \text{(E01)}$$

where the coefficient σ is given by

$$\sigma = \frac{\Delta x}{2} a(1-ar), \qquad r = \frac{\Delta t}{\Delta x}$$

(E01) is the modified PDE of the upwind method for solving $u_t + au_x = 0$

Remarks:

- The modified PDE is a perturbation of the original PDE.
- The numerical method is more consistent with the modified PDE than with the original PDE.
- Consequently, the numerical solution is better described by the behavior of the modified PDE than that of the original PDE.

(E01) is a convection-diffusion equation. When the CFL condition is satisfied, $(a\,r) \le 1$, the diffusion coefficient σ is non-negative.

$$\sigma = \frac{\Delta x}{2} a\left(1 - ar\right) \ge 0 \qquad \text{when } ar \le 1$$

Behavior of solution of $w_t = -a w_x + \sigma w_{xx}$

We try solution of the form

$$w(x,t) = e^{\sqrt{-1}\xi x + F(\xi)t}$$

This is a Fourier mode of wave number ξ.

Differentiating with respect to t and x, we have

$$w_t = F(\xi) w(x,t)$$

$$w_x = \sqrt{-1}\,\xi\, w(x,t)$$

$$w_{xx} = -\xi^2 w(x,t)$$

Substituting these derivatives into $w_t = -a w_x + \sigma w_{xx}$ yields

$$F(\xi) = -(a\sqrt{-1}\,\xi + \sigma \xi^2)$$

$$\Longrightarrow \quad w(x,t) = e^{\sqrt{-1}\xi x - (a\sqrt{-1}\xi + \sigma\xi^2)t} = e^{\sqrt{-1}\xi(x-at) - \sigma\xi^2 t}$$

This wave i) travels with velocity a and ii) decays exponentially with rate $\sigma\xi^2$.

$$w(x,t) = \underbrace{e^{\sqrt{-1}\xi(x-at)}}_{\substack{\text{convection} \\ \text{traveling wave} \\ \text{with velocity } a}} \cdot \underbrace{e^{-\sigma\xi^2 t}}_{\substack{\text{dissipation} \\ \text{exponential decay} \\ \text{of amplitude}}}$$

Since the PDE is linear, a general solution is <u>a linear superposition</u> of these modes.

$$w(x,t) = \int e^{\sqrt{-1}\xi(x-at)} \cdot e^{-\sigma\xi^2 t}\, \alpha(\xi)\, d\xi$$

where $\alpha(\xi)$ is the weight coefficient in the linear superposition.

When the diffusion coefficient σ is positive, the amplitude of each mode decays exponentially. Consequently, <u>the solution $w(x, t)$ is bounded</u>.

When the diffusion coefficient σ is negative, the amplitude grows exponentially and the growth rate is proportional to the square of wave number: $(-\sigma)\xi^2$. Consequently, the solution $w(x, t)$ is unbounded <u>even at finite time</u> because the growth rates of large wave number modes are unbounded.

The behavior of $w(x, t)$ suggests that

- When σ is negative, the numerical method is unstable.
- When σ is positive, the numerical method is stable; and because of the fast decay of large wave number modes, discontinuities are smoothed over time.

Below, we examine this assertion on several first order methods.

Behavior of first order methods based on modified PDEs

Behavior of the upwind method for $u_t + au_x = 0, \quad a > 0$

$$u_i^{n+1} = u_i^n - ar\left(u_i^n - u_{i-1}^n\right)$$

Modified PDE:

$$w_t = -aw_x + \sigma w_{xx}, \qquad \sigma = \frac{\Delta x}{2} a\left(1 - ar\right) \geq 0 \quad \text{when } ar \leq 1$$

which suggests that the upwind method is stable for $a\,r \leq 1$.

Due to the dissipation, discontinuities are smoothed out in numerical solution of upwind method. Figure 1 compares the exact solution and the numerical solution of upwind method for initial value problem (IVP01).

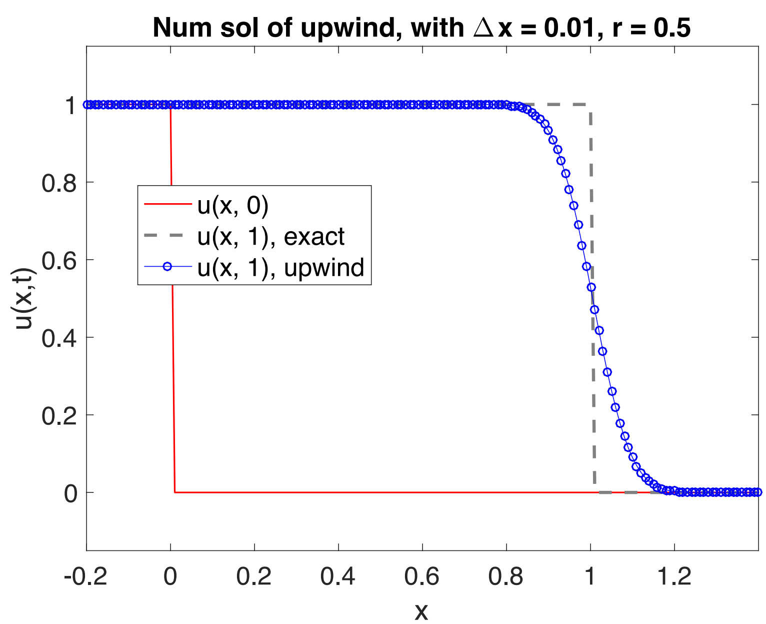

Figure 1: Exact solution of PDE and numerical solution of upwind method

$$\begin{cases} u_t + u_x = 0 \\ u(x,0) = \begin{cases} 1, & x \le 0 \\ 0, & x > 0 \end{cases} \end{cases} \qquad \text{(IVP01)}$$

<u>Behavior of the downwind method</u> for $u_t + au_x = 0$, $a > 0$

$$u_i^{n+1} = u_i^n - ar\left(u_{i+1}^n - u_i^n\right)$$

Modified PDE:

$$w_t = -aw_x + \sigma w_{xx}, \qquad \sigma = \frac{-\Delta x}{2} a\left(1 + ar\right) < 0 \text{ negative diffusion!}$$

which suggests that the downwind method is unstable for all r.

<u>Behavior of the FTCS method</u> for $u_t + au_x = 0$, ($a > 0$ or $a < 0$)

$$u_i^{n+1} = u_i^n - \frac{ar}{2}\left(u_{i+1}^n - u_{i-1}^n\right)$$

Modified PDE:

$$w_t = -aw_x + \sigma w_{xx}, \qquad \sigma = \frac{-\Delta x}{2} a^2 r < 0 \text{ negative diffusion!}$$

which suggests that the FTCS method is unstable for all r.

<u>Behavior of the Lax-Friedrichs method</u> for $u_t + au_x = 0$, ($a > 0$ or $a < 0$)

$$u_i^{n+1} = \frac{u_{i+1}^n + u_{i-1}^n}{2} - \frac{ar}{2}\left(u_{i+1}^n - u_{i-1}^n\right)$$

Modified PDE:

$$w_t = -aw_x + \sigma w_{xx}, \qquad \sigma = \frac{\Delta x}{2}\left(\frac{1}{r} - a^2 r\right) \ge 0 \text{ when } |ar| \le 1$$

which suggests that the Lax-Friedrichs method is stable for $|\,a\,r\,| \le 1$.

Lax-Friedrichs method has more dissipation than the upwind method.

$$\sigma_{\text{upwind}} = \frac{\Delta x}{2} a(1 - ar)$$

$$\sigma_{\text{L-F}} = \frac{\Delta x}{2}\left(\frac{1}{r} - a^2 r\right) = \frac{\Delta x}{2} a(1 - ar) \cdot \frac{1 + ar}{ar}$$

$$\Longrightarrow \quad \sigma_{\text{L-F}} = \sigma_{\text{upwind}} \cdot \frac{1 + ar}{ar}$$

As a result, discontinuities are smoothed out more in numerical solution of Lax-Friedrichs method. Figure 2 compares the exact solution, and numerical solutions of upwind and Lax-Friedrichs methods for initial value problem (IVP01).

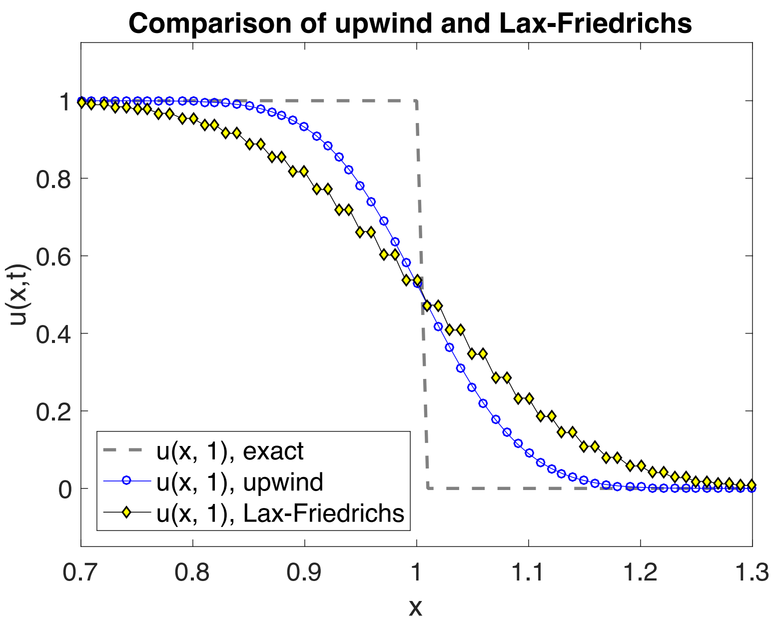

Figure 2: Comparison of upwind and Lax-Friedrichs near a discontinuity.

In the above, the modified PDEs for first order methods, have the general form

$$w_t = -a w_x + \sigma w_{xx}$$

Next, we study the modified PDEs for second order methods.

Modified PDE of Lax-Wendroff method:

<u>Lax-Wendroff method</u> for $u_t + a u_x = 0$, ($a > 0$ or $a < 0$)

$$u_i^{n+1} = u_i^n - \frac{ar}{2}\left(u_{i+1}^n - u_{i-1}^n\right) + \frac{(ar)^2}{2}\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right), \qquad r = \frac{\Delta t}{\Delta x}$$

Modified PDE:

$$w_t = -a w_x + \mu w_{xxx}$$

$$\mu = \frac{(\Delta x)^2}{6} a\left((ar)^2 - 1\right), \qquad r = \frac{\Delta t}{\Delta x}$$

(See Appendix A for the derivation of Modified PDE of Lax-Wendroff method).

Behavior of solution of $w_t = -a w_x + \mu w_{xxx}$

We try solution of the form

$$w(x,t) = e^{\sqrt{-1}\xi x + F(\xi)t}$$

Differentiating with respect to t and x, we have

$$w_t = F(\xi) w(x,t)$$

$$w_x = \sqrt{-1}\,\xi w(x,t)$$

$$w_{xx} = -\xi^2 w(x,t)$$

$$w_{xxx} = -\sqrt{-1}\,\xi^3 w(x,t)$$

Substituting these derivatives into $w_t = -a w_x + \mu w_{xxx}$ yields

$$F(\xi) = -a\sqrt{-1}\,\xi - \mu\sqrt{-1}\,\xi^3 \equiv -\sqrt{-1}\,\omega(\xi), \qquad \omega(\xi) \equiv (a\xi + \mu\xi^3)$$

$F(\xi)$ has only the imaginary part. We write $w(x, t)$ as

$$w(x,t) = e^{\sqrt{-1}\xi x + F(\xi)t} = \exp\left(\sqrt{-1}\,(\xi x - \omega(\xi)t)\right)$$

where $\omega(\xi)$ is the angular frequency of the mode of wave number ξ.

We discuss phase velocity, dispersion, and group velocity for general $\omega(\xi)$.

Phase velocity

Consider the mode of wave number ξ with angular frequency $\omega(\xi)$

$$w(x,t) = \exp\left(\sqrt{-1}\,(\xi x - \omega(\xi)t)\right) = \exp\left(\sqrt{-1}\,\xi\left(x - \frac{\omega(\xi)}{\xi}t\right)\right)$$

$w(x, t)$ is a traveling wave. $v_p(\xi) = \dfrac{\omega(\xi)}{\xi}$ is called the *phase velocity*.

Dispersion:

Note that the phase velocity varies with the wave number ξ. Modes of different wave numbers travel with different phase velocities. This phenomenon is called *dispersion*.

Group velocity

We look at a cluster of modes. The cluster forms an envelope. While each mode in the cluster travels with its individual phase velocity, the envelope of the cluster travels with the *group velocity*. In general, the *group velocity* is different from the *phase velocity*, and could even be in the opposite direction of the phase velocity.

Consider a cluster of modes near wave number $\xi = \xi_0$.

$$w(x,t) \equiv \int_{\substack{\text{near} \\ \xi=\xi_0}} \exp\left(\sqrt{-1}\,(\xi x - \omega(\xi)t)\right)\alpha(\xi)d\xi$$

where $\omega(\xi)$ is the angular frequency of wave number ξ, and $\alpha(\xi)$ is the weight coefficient of wave number ξ.

We calculate the group velocity, the traveling velocity of the envelope.

We expand $\omega(\xi)$ around ξ_0 to re-write $w(x, t)$

$$w(x,t) \equiv \int_{\substack{\text{near} \\ \xi=\xi_0}} \exp\left(\sqrt{-1}\,(\xi x - \omega(\xi)t)\right)\alpha(\xi)d\xi$$

$$= \exp\left(\sqrt{-1}\,(\xi_0 x - \omega(\xi_0)t)\right) \int_{\substack{\text{near} \\ \xi=\xi_0}} \exp\left(\sqrt{-1}\,((\xi-\xi_0)x - (\omega(\xi)-\omega(\xi_0))t)\right)\alpha(\xi)d\xi$$

Taylor expansion: $\quad \omega(\xi)-\omega(\xi_0) = \omega'(\xi_0)(\xi-\xi_0)+\cdots$

$$= \underbrace{\exp\left(\sqrt{-1}\,\xi_0\left(x - \frac{\omega(\xi_0)}{\xi_0}t\right)\right)}_{\text{wave number } \xi_0} \int_{\substack{\text{near} \\ \xi=\xi_0}} \underbrace{\exp\left(\sqrt{-1}(\xi-\xi_0)(x-\omega'(\xi_0)t)+\cdots\right)}_{\text{wave number } (\xi-\xi_0)}\alpha(\xi)d\xi$$

The factor outside the integral has wave number ξ_0. The integrand has a much smaller wave number $(\xi - \xi_0)$. Thus, the integral describes the envelope of the cluster. Notice that in the integrand, the time dependence is via the term $z \equiv x - \omega'(\xi_0)t$, which is independent of ξ. We write the integral as a function of z.

$$w(x,t) = \exp\left(\sqrt{-1}\,\xi_0\left(x - \frac{\omega(\xi_0)}{\xi_0}t\right)\right)\cdot \phi(z)\Big|_{z=x-\omega'(\xi_0)t}$$

where $\phi(z)$ is defined below.

$$\phi(z) \equiv \int_{\substack{\text{near}\\ \xi=\xi_0}} \exp\left(\sqrt{-1}(\xi-\xi_0)z\right)\alpha(\xi)d\xi$$

As a function of z, $\phi(z)$ has no dependence on t.

The time evolution of the cluster is described by

$$w(x,t) = \underbrace{\exp\left(\sqrt{-1}\,\xi_0\left(x-\frac{\omega(\xi_0)}{\xi_0}t\right)\right)}_{\substack{\text{Fast varying in space,}\\ \text{traveling with}\\ \text{phase velocity}}} \cdot \underbrace{\phi\left(x-\omega'(\xi_0)t\right)}_{\substack{\text{Envelope of the wave,}\\ \text{slow varying in space,}\\ \text{traveling with}\\ \text{group velocity}}}$$

The group velocity is

$$v_g(\xi_0) = \omega'(\xi_0)$$

where $\omega(\xi)$ is the angular frequency of wave number ξ.

<u>Example</u> of phase velocity and group velocity

A cluster of 2 modes with $\omega(\xi) = \omega_0$ (constant).

$$\sin\left((\xi_0-\Delta\xi)x-\omega_0 t\right)+\sin\left((\xi_0+\Delta\xi)x-\omega_0 t\right) = 2\sin(\xi_0 x-\omega_0 t)\cos(\Delta\xi\, x)$$

$$= \underbrace{2\sin\left(\xi_0\left(x-\frac{\omega_0}{\xi_0}t\right)\right)}_{\substack{\text{Fast varying in space,}\\ \text{traveling with}\\ \text{phase velocity } \omega_0/\xi_0}} \cdot \underbrace{\cos(\Delta\xi\, x)}_{\substack{\text{Envelope of the wave,}\\ \text{slow varying in space,}\\ \text{traveling with 0 velocity}\\ \text{(a standing wave)}}}$$

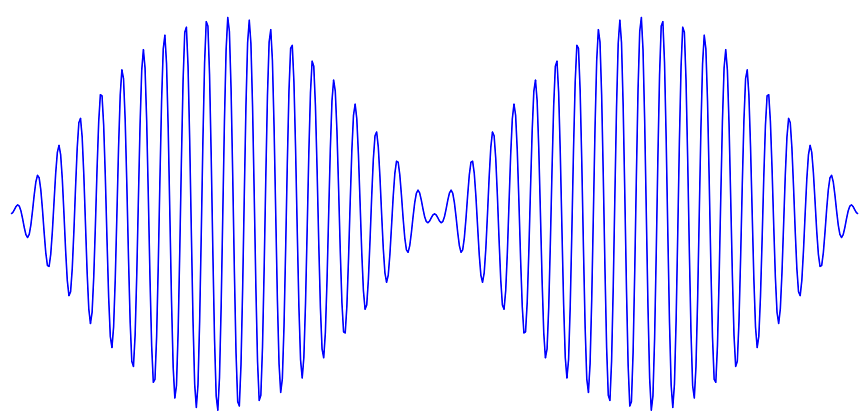

Figure 3: Internal oscillations and the slow-varying envelope of the wave

Figure 3 illustrates the internal oscillations and the slow-varying envelope of the wave.

Phase velocity is the traveling velocity of $\sin(\xi x - \omega_0 t)$:

$$v_p(\xi) = \omega_0/\xi$$

Group velocity is the traveling velocity of the envelope $\cos(\Delta\xi x)$:

$$v_g = \omega'(\xi_0) = 0, \qquad \text{which is a standing wave}$$

We now apply the general result to $\omega(\xi) = a\xi + \mu\xi^3$.

<u>Behavior of solution of</u> $w_t = -aw_x + \mu w_{xxx}$

The mode of wave number ξ travels with its *phase velocity*.

$$w(x,t) = \exp\left(\sqrt{-1}\,\xi\left(x - \frac{\omega(\xi)}{\xi}t\right)\right), \qquad \omega(\xi) = \left(a\xi + \mu\xi^3\right)$$

Phase velocity: $\quad v_p(\xi) = \dfrac{\omega(\xi)}{\xi} = a + \mu\xi^2$

<u>The envelope</u> of a cluster near wave number ξ_0 travels with the <u>*group velocity*</u>.

$$w(x,t) \equiv \int_{\substack{\text{near}\\ \xi=\xi_0}} \exp\left(\sqrt{-1}\,(\xi x - \omega(\xi)t)\right)\alpha(\xi)d\xi$$

$$= \underbrace{\exp\left(\sqrt{-1}\,\xi_0\left(x - \frac{\omega(\xi_0)}{\xi_0}t\right)\right)}_{\substack{\text{Fast varying in space,}\\ \text{traveling with}\\ \text{phase velocity}}} \cdot \underbrace{\phi\left(x - \omega'(\xi_0)t\right)}_{\substack{\text{Envelope of the wave,}\\ \text{slow varying in space,}\\ \text{traveling with}\\ \text{group velocity}}}, \qquad \omega(\xi) = \left(a\xi + \mu\xi^3\right)$$

Group velocity: $\quad v_g(\xi_0) = \omega'(\xi_0) = a + 3\mu\xi_0^2$

Behavior of second order methods based on modified PDEs

<u>Behavior of the Lax-Wendroff method</u> for $u_t + au_x = 0$

Modified PDE:

$$w_t = -aw_x + \mu w_{xxx}, \qquad \mu = \frac{(\Delta x)^2}{6}a\left((ar)^2 - 1\right), \qquad r = \frac{\Delta t}{\Delta x}$$

- Near a discontinuity, due to dispersion, Lax-Wendroff method will produce <u>numerical oscillations</u>.

- The envelope of numerical oscillations travels with the group velocity

$$v_g(\xi_0)=\omega'(\xi_0)=a+3\mu\xi_0^2=\begin{cases} >a & \text{for } \mu>0 \\ <a & \text{for } \mu<0 \end{cases}$$

- For $a > 0$ and when $(a\,r) < 1$ (the CLF condition), we have

$$\mu=\frac{(\Delta x)^2}{6}a\left((ar)^2-1\right)<0$$

==> group velocity $v_g(\xi_0) < a$

==> numerical oscillations are lagging the propagation of solution.

Figure 4 shows the exact solution and the numerical solution of Lax-Wendroff method for initial value problem (IVP01).

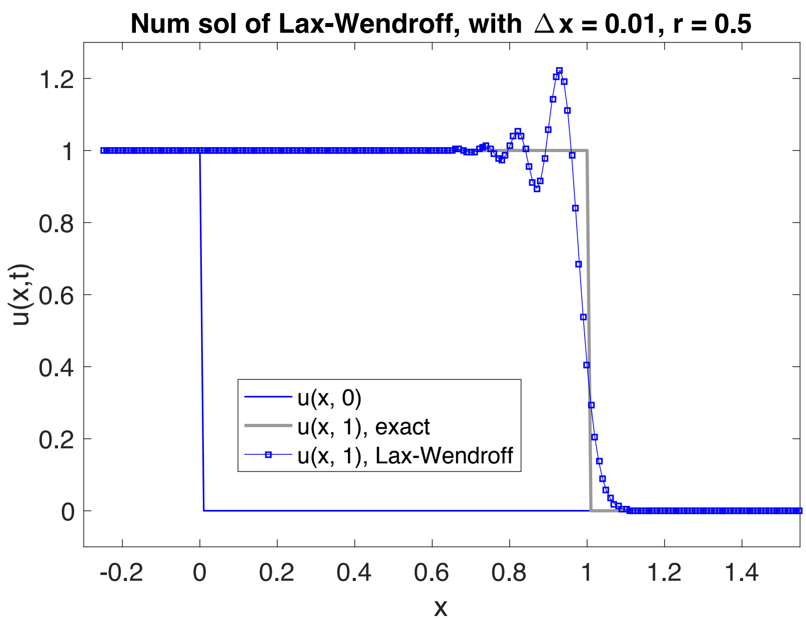

Figure 4: Exact solution of PDE and numerical solution of Lax-Wendroff method

Behavior of the Beam-Warming method for $u_t + au_x = 0$, $a > 0$

$$u_i^{n+1}=u_i^n-\frac{ar}{2}\left(3u_i^n-4u_{i-1}^n+u_{i-2}^n\right)+\frac{(ar)^2}{2}\left(u_i^n-2u_{i-1}^n+u_{i-2}^n\right), \qquad r=\frac{\Delta t}{\Delta x}$$

Modified PDE:

$$w_t=-aw_x+\mu w_{xxx}, \qquad \mu=\frac{(\Delta x)^2}{6}a\left((ar)^2-3(ar)+2\right), \qquad r=\frac{\Delta t}{\Delta x}$$

- Near a discontinuity, due to dispersion, Beam-Warming method will produce numerical oscillations.
- The envelope of numerical oscillations travels with the group velocity

$$v_g(\xi_0) = \omega'(\xi_0) = a + 3\mu\xi_0^2 = \begin{cases} > a & \text{for } \mu > 0 \\ < a & \text{for } \mu < 0 \end{cases}$$

- For $a > 0$ and when $(a\,r) < 1$, we have

$$\mu = \frac{(\Delta x)^2}{6} a\left((ar)^2 - 3(ar) + 2\right) = \frac{(\Delta x)^2}{6} a\left((ar) - 2\right)\left((ar) - 1\right) > 0$$

==> group velocity $v_g(\xi_0) > a$

==> numerical oscillations are leading the propagation of solution.

Figure 5 displays the exact solution and the numerical solution of Beam-Warming method for initial value problem (IVP01).

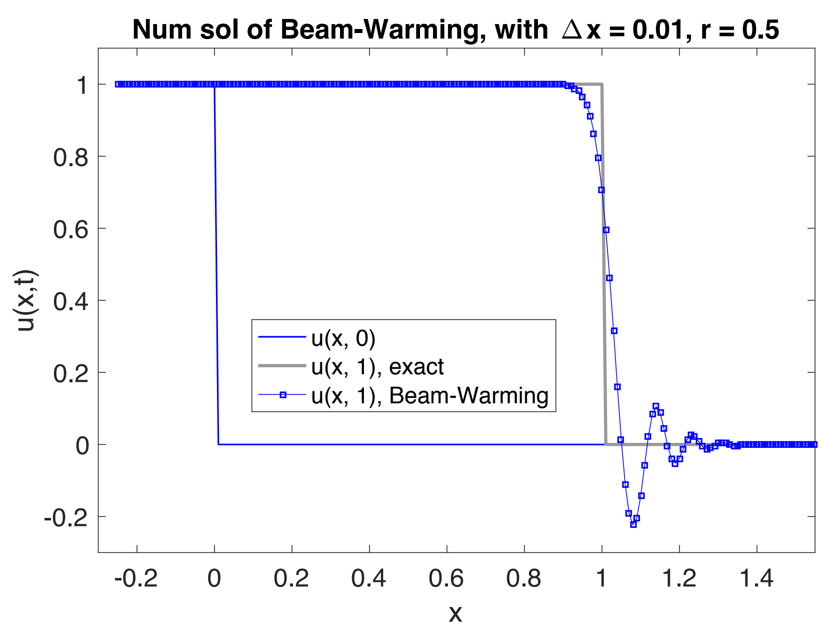

Figure 5: Exact solution of PDE and numerical solution of Beam-Warming method

Appendix A: Derivation of modified PDE of Lax-Wendroff method

Lax-Wendroff method:

$$u_i^{n+1} = u_i^n - \frac{ar}{2}\left(u_{i+1}^n - u_{i-1}^n\right) + \frac{(ar)^2}{2}\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right), \qquad r = \frac{\Delta t}{\Delta x}$$

Suppose $u_i^n = w(x_i, t_n)$ for an unknown smooth function $w(x, t)$.

Substituting $u_i^n = w(x_i, t_n)$ into the Lax-Wendroff method, we have

$$w(x_i, t_{n+1}) - w(x_i, t_n) = -\frac{a}{2}\cdot\frac{\Delta t}{\Delta x}\Big(w(x_{i+1}, t_n) - w(x_{i-1}, t_n)\Big)$$
$$+\frac{a^2}{2}\cdot\frac{(\Delta t)^2}{(\Delta x)^2}\Big(w(x_{i+1}, t_n) - 2w(x_i, t_n) + w(x_{i-1}, t_n)\Big)$$

Expanding every term around (x_i, t_n) and using $r = \dfrac{\Delta t}{\Delta x}$ yields

$$w_t\Big|_{(x_i,t_n)}\Delta t + w_{tt}\Big|_{(x_i,t_n)}\frac{(\Delta t)^2}{2} + w_{ttt}\Big|_{(x_i,t_n)}\frac{(\Delta t)^3}{6} + O\Big((\Delta t)^4\Big)$$
$$= -a\frac{\Delta t}{\Delta x}\left[w_x\Big|_{(x_i,t_n)}\Delta x + w_{xxx}\Big|_{(x_i,t_n)}\frac{(\Delta x)^3}{6} + O\Big((\Delta x)^4\Big)\right]$$
$$+\frac{a^2}{2}\cdot\frac{(\Delta t)^2}{(\Delta x)^2}\left[w_{xx}\Big|_{(x_i,t_n)}(\Delta x)^2 + O\Big((\Delta x)^4\Big)\right]$$

Dividing by Δt, and moving w_{tt} and w_{ttt} to the right side, we get

$$w_t = -aw_x - \frac{\Delta t}{2}w_{tt} + \frac{\Delta t}{2}a^2 w_{xx} - \frac{(\Delta t)^2}{6}w_{ttt} - \frac{(\Delta x)^2}{6}a w_{xxx} + O\Big((\Delta t)^3 + (\Delta x)^3\Big) \qquad \text{(T02)}$$

We convert w_{tt} and w_{ttt} to spatial derivatives using an iterative approach.

We start with the leading term of (T02) and differentiate with respect to t.

$$w_t = -a w_x + O(\Delta t + \Delta x)$$

$$w_{tt} = a^2 w_{xx} + O(\Delta t + \Delta x)$$

$$w_{ttt} = -a^3 w_{xxx} + O(\Delta t + \Delta x)$$

The leading term approximation for w_{ttt} is good for our purpose. The next step is to calculate the O(Δt+Δx) term of w_{tt}. We keep up to O(Δt+Δx) terms in (T02).

$$w_t = -a w_x - \frac{\Delta t}{2} w_{tt} + \frac{\Delta t}{2} a^2 w_{xx} + O\left((\Delta t)^2 + (\Delta x)^2\right)$$

Using the approximation $w_{tt} = a^2 w_{xx} + O(\Delta t + \Delta x)$, we get

$$w_t = -a w_x + O\left((\Delta t)^2 + (\Delta x)^2\right)$$

Differentiating with respect to *t*, we have

$$\begin{aligned} w_{tt} &= -a(w_x)_t + O\left((\Delta t)^2 + (\Delta x)^2\right) = -a(w_t)_x + O\left((\Delta t)^2 + (\Delta x)^2\right) \\ &= a^2 w_{xx} + O\left((\Delta t)^2 + (\Delta x)^2\right) \end{aligned}$$

Substituting these expressions of w_{tt} and w_{ttt} into (T02), we obtain

$$w_t = -a w_x + \frac{(\Delta x)^2}{6} a \left(a^2 \frac{(\Delta t)^2}{(\Delta x)^2} - 1 \right) w_{xxx} + O\left((\Delta t)^3 + (\Delta x)^3\right)$$

Neglecting the $O((\Delta t)^3+(\Delta x)^3)$ term, we write the equation for $w(x, t)$ as

$$w_t = -a w_x + \mu w_{xxx}, \qquad \mu = \frac{(\Delta x)^2}{6} a\left((ar)^2 - 1\right), \qquad r = \frac{\Delta t}{\Delta x}$$

This completes the derivation.