16. Modified Eqns.

→ So far, given a PDE, we've derived the corresponding difference eqn (DE) ;

PDE → DE

→ Now, we are doing the reverse ;

DE → PDE

→ Modified eqns allow us to understand ;

(i) dissipation errors, &

(ii) dispersion errors.

→ For example, we can see why there are

(i) dissipations in first-order schemes ;

(ex) upwind, Lax-Friedrichs

(ii) oscillations in second-order schemes ;

(ex) Lax-Wendroff, Beam-Warming, Fromm's.

(1) Dissipation errors in first-order methods.

→ Consider $u_t + a u_x = 0$, $a > 0$, and let's use the upwind method (or FTBS):

$$v_i^{n+1} = v_i^n - \frac{a\Delta t}{\Delta x}\left[v_i^n - v_{i-1}^n\right] \quad \cdots \text{①}$$

→ For now, let's assume that the analytical soln $u(x,t)$ exactly satisfies ① at the discrete pts (x_i, t^n);

i.e, $\underline{u(x_i,t^n) = v(x_i,t^n)}$, rather than

$$u(x_i,t^n) = v(x_i,t^n) + O(\Delta t + \Delta x).$$

→ $$u(x,t+\Delta t) = u(x,t) - \frac{a\Delta t}{\Delta x}\left[u(x,t) - u(x-\Delta x,t)\right] \quad \cdots \text{②}$$

→ Taylor series expansion of ②;

$$\cancel{u(x,t)} + \Delta t\, u_t(x,t) + \frac{\Delta t^2}{2} u_{tt}(x,t) + O(\Delta t^3)$$
$$= \cancel{u(x,t)} - \frac{a\Delta t}{\Delta x}\left[\cancel{u(x,t)} - \left\{\cancel{u(x,t)} - \Delta x\, u_x(x,t) + \frac{\Delta x^2}{2} u_{xx}(x,t) + O(\Delta x^3)\right\}\right]$$

→ Dividing by Δt and rearranging;

$$u_t + a u_x = \frac{1}{2}\left(a u_{xx}\Delta x - u_{tt}\Delta t\right) - \frac{1}{6}\left(a u_{xxx}\Delta x^2 + u_{ttt}\Delta t^2\right) + \cdots \quad \cdots \text{③}$$

→ Therefore, in ③, we now have

$$\boxed{u_t + a u_x \neq 0}$$

→ But instead, we have

$$u_t + a u_x = \mathcal{O}(\Delta t + \Delta x). \quad \cdots \text{④}$$

→ If we keep the $\mathcal{O}(\Delta t + \Delta x)$ term;

$$u_t + a u_x = \frac{1}{2}(\Delta x \, a u_{xx} - \Delta t \, u_{tt}) \quad \cdots \text{⑤}$$

then

$$\begin{cases} u_{tt} = -a u_{xt} + \frac{1}{2}(\Delta x \, a u_{xxt} - \Delta t \, u_{ttt}) & \cdots \text{⑥} \\ u_{tx} = -a u_{xx} + \frac{1}{2}(\Delta x \, a u_{xxx} - \Delta t \, u_{ttx}) & \cdots \text{⑦} \end{cases}$$

→ ⑥ becomes, when combining with ⑦;

$$\begin{aligned} u_{tt} &= -a(-a u_{xx} + \mathcal{O}(\Delta t + \Delta x)) + \mathcal{O}(\Delta t + \Delta x) \\ &= a^2 u_{xx} + \mathcal{O}(\Delta t + \Delta x) \end{aligned} \quad \cdots \text{⑧}$$

→ ③ + ⑧;

$$\begin{aligned} u_t + a u_x &= \frac{1}{2}(\Delta x \, a u_{xx} - \Delta t \, a^2 u_{xx}) + \mathcal{O}(\Delta t^2 + \Delta x^2) \\ &= \frac{a \Delta x}{2}\left[1 - \frac{a \Delta t}{\Delta x}\right] u_{xx} + \mathcal{O}(\Delta t^2 + \Delta x^2) \end{aligned} \quad \cdots \text{⑨}$$

→ If we let $k = \frac{a\Delta x}{2}\left[1 - \frac{a\Delta t}{\Delta x}\right]$, then ⑨ becomes

$$u_t + a u_x = k u_{xx} + \mathcal{O}(\Delta t^2 + \Delta x^2). \quad \cdots \text{⑩}$$

→ If we drop $\mathcal{O}(\Delta t^2 + \Delta x^2)$, we get a new PDE;

$$\boxed{u_t + a u_x = k u_{xx}} \quad \cdots \text{⑪}$$

→ Note (11) is an advection – diffusion eqn which is different from the original pure advection PDE.

→ This new eqn (11) is called the modified eqn of the upwind method when solving the pure advection PDE, $u_t + a u_x = 0$.

→ This means that, when the upwind method is used for $u_t + a u_x = 0$, the actual corresponding PDE the upwind method solves is (11), instead of the pure advection eqn.

→ Since (11) has the diffusion term κu_{xx} with

$$\kappa = \frac{a\Delta x}{2}\left(1 - \frac{a\Delta t}{\Delta x}\right), \qquad (a>0)$$

the upwind method becomes "diffusive".   5/16/2016

→ Also note that as long as the CFL condition satisfies, i.e., $0 < \frac{a\Delta t}{\Delta x} \le 1$, then $\kappa \ge 0$, which is necessary for diffusion.

Rmk $\kappa = \frac{\Delta x^2}{2\Delta t}\left(1 - \left(\frac{a\Delta t}{\Delta x}\right)^2\right)$ for Lax-Friedrichs (HW)

Summary (1) All first-order methods yield their modified eqns in the form of (11).

(ii) First-order methods are diffusive.

(2) Note that, for $C_a =$ constant,

$$K = \begin{cases} \frac{a\Delta x}{2}(1 - C_a) & \text{for upwind} \\ \frac{\Delta x^2}{2\Delta t}(1 - C_a^2) = \frac{1}{C_a}\frac{\Delta x}{2}(1 - C_a^2) & \text{for LF} \end{cases}$$

is $O(\Delta x)$ and hence $k \to 0$ as $\Delta x \to 0$.

This is called "the vanishing viscosity".

(3) In real calculation, for example, let's assume

$C_a = 0.8$ (e.g., $a = 1$, $\Delta x = 1$, $\Delta t = 0.8$).

Then we see that

$$K = \begin{cases} 0.1 & \text{for upwind} \\ 0.1152 & \text{for LF.} \end{cases}$$

$\Rightarrow$ The LF method is slightly more diffusive than the upwind method.

(2) Dispersion errors in second-order methods

→ One can show that the modified eqn for Lax-Wendroff is

$$u_t + a u_x = \underbrace{\frac{a\Delta x^2}{6}\left[\left(\frac{a\Delta t}{\Delta x}\right)^2 - 1\right]}_{\equiv \mu} u_{xxx} \equiv \mu u_{xxx} \quad \text{(HW)} \quad \text{--- (12)}$$

→ We are going to take Fourier transform of (12) to understand the behavior of μu_{xxx}.

→ dispersion error with dispersion coeff. μ.

→ First, recall that Fourier Transform;

(i) $u(x,t) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \hat{u}(\xi,t)\, e^{I\xi x}\, d\xi$, --- (13)

(ii) $\hat{u}(\xi,t) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} u(x,t)\, e^{-I\xi x}\, dx$.

→ We will see that, using Fourier analysis, the Fourier components with different wave number ξ propagate at diferent wave speeds, i.e, disperse in time.

→ This is called the dispersion error, producing unwanted numerical oscillations.

→ Since Fourier transform is linear, we only consider a single Fourier component with ξ.

→ From (13),

$$\begin{cases} u_t = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \hat{u}_t(\xi,t)\, e^{I\xi x}\, dx, \\ u_x = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \hat{u}(\xi,t)\, I\xi\, e^{I\xi x}\, dx \end{cases}$$

$\Rightarrow$ $\begin{cases} \widehat{(u_t)} = (\hat{u})_t \\ \widehat{(u_x)} = I\xi \hat{u} \end{cases}$

$\Rightarrow$ Take Fourier transform of (13) ;

$$\widehat{(u_t)} + \widehat{(a u_x)} = \widehat{(\mu u_{xxx})}$$

$$\Leftrightarrow \quad \hat{u}_t + a I\xi \hat{u} = \mu (I\xi)^3 \hat{u}$$

$$\Leftrightarrow \quad \hat{u}_t = -I \underbrace{(a\xi + \mu\xi^3)}_{\equiv \omega} \hat{u} \equiv -I\omega\hat{u} \quad \cdots (14)$$

$\Rightarrow$ the exact soln of the ODE (14) ;

$$\hat{u}(\xi,t) = e^{-I\omega t} \hat{\eta}(\xi), \quad \hat{\eta}(\xi) = \hat{u}(\xi,0)$$

$$\Rightarrow \quad u(x,t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{u}(\xi,t) e^{I\xi x} d\xi$$

$$= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{\eta}(\xi) e^{-I\omega t} e^{I\xi x} d\xi$$

$$= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{\eta}(\xi) e^{I\xi\left(x - \frac{\omega}{\xi} t\right)} d\xi$$

$\Rightarrow$ The speed at which the oscillating wave propagates is given by $\frac{\omega}{\xi}$, called the phase velocity, c_p.

$$\Rightarrow \quad c_p(\xi) \equiv \frac{\omega(\xi)}{\xi} = \frac{1}{\xi}(a\xi + \mu\xi^3) = a + \mu\xi^2.$$

$\Rightarrow$ $\left[\begin{array}{l} c_p \text{ varies with } \xi, \ \& \\ c_p \approx a \text{ when } \xi \text{ is small (i.e, } \xi \ll 1). \end{array}\right.$

$\Rightarrow$ If $\xi > 1$, then $c_p \not\approx a$.

$\Rightarrow$ Note that, for pure advection $u_t + a u_x = 0$, everything should propagate with the velocity a.

$\Rightarrow$ However, what we see here is that $c_p \not\approx a$ when $\xi > 1$.

$\Rightarrow$ This is why we see <u>oscillations</u> in Lax-Wendroff, and, in general, in all 2nd-order methods.

$\rightarrow$ We also define, so-called, <u>the group velocity</u>, by

$$c_g(\xi) = \frac{d\omega}{d\xi}$$

$\Rightarrow$ $c_g(\xi) = a + 3\mu\xi^2$; the velocity at which the <u>"wave packet"</u> as a group propagates.

Rmk. We can find that the dispersion coeff. μ is

$$\mu = \begin{cases} \dfrac{a\,\Delta x^2}{6}\left(C_a^2 - 1\right) & \text{for Lax-Wendroff (LW)} \\[2ex] \dfrac{a\,\Delta x^2}{6}\left(C_a^2 - 3C_a + 2\right) & \text{for Beam-Warming (BW)} \end{cases}$$

Note that, for $0 < C_a \leq 1$,

$$\begin{cases} \mu \leq 0 & \text{for LW}, \\ \mu \geq 0 & \text{for BW}. \end{cases}$$

(HW)

$\Rightarrow$ For $a > 0$,

$$C_g = \begin{cases} a + 3\mu\xi^2 < a & \text{for LW} \\ a + 3\mu\xi^2 > a & \text{for BW} \end{cases}$$

$\Rightarrow$
- LW : oscillations are slower than the advection velocity and they appear behind anything that advects (e.g. shocks)
- BW : oscillations are faster than the advection velocity and they appear ahead of anything that advects (e.g. shocks)

Rmk Beam–Warming method $\sim \mathcal{O}(\Delta t^2 + \Delta x^2)$

(i) $a > 0$;

$$U_i^{n+1} = U_i^n - \frac{a\Delta t}{2\Delta x}\left[3U_i^n - 4U_{i-1}^n + U_{i-2}^n\right] + \frac{a^2\Delta t^2}{2\Delta x^2}\left[U_i^n - 2U_{i-1}^n + U_{i-2}^n\right]. \quad \text{--- (15)}$$

(ii) $a < 0$;

$$U_i^{n+1} = U_i^n - \frac{a\Delta t}{2\Delta x}\left[-3U_i^n + 4U_{i+1}^n - U_{i+2}^n\right] + \frac{a^2\Delta t^2}{2\Delta x^2}\left[U_i^n - 2U_{i+1}^n + U_{i+2}^n\right] \quad \text{--- (16)}$$

→ Note that these are one-sided differencing approximations to the spatial derivatives.

→ (i) (15) is stable for $0 \le C_a \le 2$,
  (ii) (16) is stable for $-2 \le C_a \le 0$,

Where $C_a = \frac{a\Delta t}{\Delta x}$, (HW)