Numerical Solutions to Partial Differential Equations

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Amplification Factors and $\mathbb{L}^2$ stability of the Upwind Scheme

Substituting the Fourier mode $U_j^m = \lambda_k^m e^{\mathrm{i}kjh}$ into the upwind scheme $U_j^{m+1} = (1-|\nu|)U_j^m + |\nu|U_{j-\mathrm{sign}(a)}^m$ yields the characteristic equation of the scheme

$$\lambda_k = (1-|\nu|) + |\nu|\, e^{-\mathrm{sign}(a)\,\mathrm{i}kh}.$$

Hence,
$$\begin{aligned} |\lambda_k|^2 &= [(1-|\nu|) + |\nu|\cos kh]^2 + [|\nu|\sin kh]^2 \\ &= 1 - 4|\nu|(1-|\nu|)\sin^2\frac{1}{2}kh. \end{aligned}$$

consequently, for any k, $|\lambda_k| \le 1$ as long as $|\nu| \le 1$. This shows that, for the upwind scheme, CFL condition is not only a necessary but also a sufficient condition for its $\mathbb{L}^2$ stability.

(Let L be the length of the domain I, then $h = LN^{-1}$, $k = k'\pi L^{-1}$, where the frequency $-N+1 \le k' \le N$.)

Convergence of the Upwind Scheme

1. CFL condition $|\nu| \leq 1 \Rightarrow \mathbb{L}^2$ stability;
2. more precisely, $\|e^{m+1}\|_2 \leq \|e^0\|_2 + \tau \sum_{l=0}^{m} \|T^l\|_2$;
3. Further more, if $\lim_{\tau \to 0} \int_0^{t_{max}} \|Tu(\cdot, t)\|_2 \, dt = 0$, then the upwind scheme is convergent.

In applications, the regularity of the solution u is not always available. When weak solutions is involved, the truncation error above does not make much sense.

An alternative approach: Analytical properties of a difference scheme can often be explored by its errors on the amplitudes and phase angles of Fourier mode solutions.

Dispersion Relation of the Advection Equation

1. A continuous Fourier mode $u(x,t) = e^{\mathrm{i}(kx+\omega t)}$ is a solution of the advection equation $u_t + au_x = 0$, if and only if ω and k satisfies the dispersion relation $\omega(k) = -ak$, *i.e.* $\omega(k)$ is the phase speed of the Fourier mode of frequency k' $(k = k'\pi L^{-1})$;

2. The amplitude of the Fourier mode solution remains a constant in propagation, this means that there is no dissipation;

3. In each time step τ, the shift of the phase angle of the Fourier mode solution is $\omega(k)\tau = -ak\tau$.

Remark: Fourier mode solutions can be obtained by the method of separation of variables for constant coefficient evolution equations with periodic boundary conditions in general.

Dispersion Relation of the Upwind Scheme

For the corresponding discrete Fourier modes $U_j^m = \lambda_k^m e^{\mathrm{i}kjh}$,

1. $\lambda_k = (1 - |\nu|) + |\nu| \, e^{-\mathrm{sign}(a)\, \mathrm{i}kh}$;
2. $|\lambda_k|^2 = 1 - 4|\nu|(1 - |\nu|) \sin^2 \frac{1}{2} kh$, there is generally some dissipation except when $|\nu| = 1$;
3. The phase shift of the mode in one time step τ is given by $\arg \lambda_k = \arctan \frac{\mathrm{Im}(\lambda_k)}{\mathrm{Re}(\lambda_k)} = -\mathrm{sign}(a) \arctan \left[\frac{|\nu| \sin kh}{(1-|\nu|)+|\nu| \cos kh} \right]$.
4. So the phase speed, or the discrete dispersion relation is given by $\omega_h(k) = \arg \lambda_k / \tau$, or $\omega_h(k)\tau = \arg \lambda_k$.

Remark: Discrete Fourier mode solutions can also be obtained by the method of separation of variables for constant coefficient finite difference schemes with periodic boundary conditions in general.

Amplitude Errors of the Upwind Scheme

If $|\nu| < 1$ is satisfied, $|\lambda_k|^2 = 1 - 4|\nu|(1-|\nu|)\sin^2 \frac{1}{2}kh < 1, \forall k$.

1. $|\lambda_k| = 1 - O(k^2h^2)$ for low frequencies, *i.e.* $kh \ll 1$;
2. $|\lambda_k| = \sqrt{1 - 4|\nu|(1-|\nu|)}$ for the highest frequency $k = \pi/h$;
3. The higher the frequency, the faster it decays;
4. The numerical solution contains less and less high frequency modes as m increases.
5. For any fixed k, the global approximation error of the upwind scheme on the amplitude is $O(h)$, since the amplitude of the Discrete Fourier mode solution is given by $(1 - O(k^2h^2))^{\tau^{-1}t_{\max}} = 1 - \tau^{-1}t_{\max}O(k^2h^2) = 1 - O(h)$.

Phase Errors of the Upwind Scheme

Remember $\omega_h(k)\tau = \arg\lambda_k = -\mathrm{sign}(a)\arctan\left[\frac{|\nu|\sin kh}{(1-|\nu|)+|\nu|\cos kh}\right]$.

If $|\nu| = 1$, $\omega_h(k)\tau = \arg\lambda_k = -akh/|a| = -ak\tau = \omega(k)\tau$, the upwind scheme has no error on the phase angle.

If $|\nu| = 1/2$, $\omega_h(k)\tau = \arg\lambda_k = -akh/(2|a|) = -ak\tau = \omega(k)\tau$, again the upwind scheme has no error on the phase angle.

If $0 < |\nu| < 1$ and $|\nu| \neq 1/2$, the high frequency modes decay sharply, while for $kh \ll 1$, by the Taylor series expansion $\arg\lambda_k = -ak\tau\left[1 - \frac{1}{6}(1-|\nu|)(1-2|\nu|)k^2h^2 + \cdots\right]$.

- For any fixed k, $\omega_h(k) = \omega(k)(1 + O(k^2h^2)))$, the global error on the phase angle is $O(h^2)$.
- There is a phase lag (*i.e.* $|\omega_h(k)| < |\omega(k)|$), if $|\nu| < 1/2$; and a phase advance (*i.e.* $|\omega_h(k)| > |\omega(k)|$), if $|\nu| > 1/2$.

Overall Performance of the Upwind Scheme

Under the CFL condition,

1. all modes decay, the higher the frequency the faster it decays;
2. global error on the amplitude is $O(h)$, there will be significant dissipation in the numerical solution;
3. global error on the phase angle is $O(h^2)$;
4. since high frequency modes decay very fast, and low frequency modes have higher order phase error than the amplitude error, there is no obvious dispersion in the numerical solution;
5. in addition, the upwind scheme satisfies the maximum principle, hence it hardly experience any oscillations.

The obvious shortcoming: only first order approximate accuracy (in the form of $O(h)$ dissipation).

Establishment of Lax-Wendroff and Beam-Warming Schemes — 1

Method 1: Characteristic method + 2nd order interpolation.

- The Lagrange quadratic interpolation formula

$$\hat{f}(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}f(x_0)+\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}f(x_1)+\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}f(x_2).$$

- The Lax-Wendroff scheme:

$$U_j^{m+1} = -\frac{1}{2}\nu(1-\nu)U_{j+1}^m + (1-\nu^2)U_j^m + \frac{1}{2}\nu(1+\nu)U_{j-1}^m.$$

- The Beam-Warming scheme:

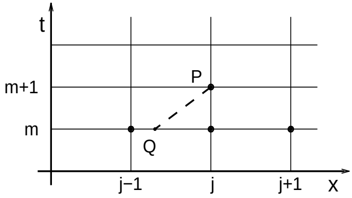
$$U_j^{m+1} = \frac{1}{2}(1-\nu)(2-\nu)U_j^m + \nu(2-\nu)U_{j-1}^m - \frac{1}{2}\nu(1-\nu)U_{j-2}^m.$$

Establishment of Lax-Wendroff and Beam-Warming Schemes — 2

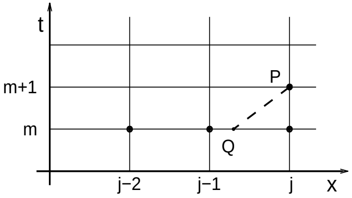
Method 2: Discrete the leading term of the truncation error.

For $a > 0$, the leading term of the truncation error of the upwind scheme is $-\frac{1}{2}ah(1-\nu)u_{xx}$,

- The Lax-Wendroff scheme: substitute $u_{xx}|_j^m$ by $h^{-2}\delta_x^2 u_j^m$.
- The Beam-Warming scheme: substitute $u_{xx}|_j^m$ by $h^{-2}\delta_x^2 u_{j-1}^m$.



Lax−Wendroff



Beam−Warming (a>0)

Establishment of Lax-Wendroff and Beam-Warming Schemes — 3

Method 3: Taylor series expansion with respect to τ + the equation + difference approximations.

1. By the Taylor series expansion

$$u_j^{m+1} = \left[u + \tau u_t + \frac{1}{2}\tau^2 u_{tt}\right]_j^m + O(\tau^3).$$

2. By the advection equation $u_t = -au_x$, $u_{tt} = a^2 u_{xx}$, etc.,

$$u_j^{m+1} = \left[u - a\tau u_x + \frac{1}{2}a^2\tau^2 u_{xx}\right]_j^m + O(\tau^3).$$

Establishment of Lax-Wendroff and Beam-Warming Schemes — 3

3. The Lax-Wendroff scheme: $\partial_x \sim \frac{\triangle_{0x}}{2h}$, $\partial_x^2 \sim \frac{\delta_x^2}{h^2}$.

4. The Beam-Warming scheme: first $\partial_x \sim \frac{\triangle_{-x}}{h}$, yields

$$u_j^{m+1} = u_j^m - a\,\tau\frac{u_j^m - u_{j-1}^m}{h} + \left[\frac{1}{2}(a^2\tau^2 - a\tau h)u_{xx}\right]_j^m + O(\tau^3).$$

then, substitute $u_{xx}|_j^m$ by $h^{-2}\delta_x^2 u_{j-1}^m$.

$\mathbb{L}^2$ Stability of Lax-Wendroff and Beam-Warming Schemes

1. Truncation error of L-W & B-W Schemes: $O(\tau^2 + h^2)$.
2. CFL condition for L-W Scheme: $|\nu| \leq 1$ (see stencil).
3. CFL condition for B-W Scheme: $|\nu| \leq 2$ (see stencil).

$\mathbb{L}^2$ Stability of Lax-Wendroff and Beam-Warming Schemes

4. Characteristic equation for L-W Scheme (see (3.2.41)):
   $\lambda_k = 1 - \mathrm{i}\nu \sin kh - 2\nu^2 \sin^2 \frac{1}{2}kh$ with its amplitude
   $|\lambda_k|^2 = 1 - 4\nu^2(1-\nu^2)\sin^4 \frac{1}{2}kh$.

5. Characteristic equation for B-W Scheme ($a > 0$, see (3.2.39)):
   $\lambda_k = 1 - \nu + \nu e^{-\mathrm{i}kh} - \frac{1}{2}\nu(1-\nu)e^{-\mathrm{i}kh}\left(e^{\mathrm{i}kh} - 2 + e^{-\mathrm{i}kh}\right)$, or
   $\lambda_k = e^{-\mathrm{i}kh}\left(1 - 2(1-\nu)^2 \sin^2 \frac{1}{2}kh + \mathrm{i}(1-\nu)\sin kh\right)$ with
   $|\lambda_k|^2 = 1 - 4\nu(2-\nu)(1-\nu)^2 \sin^4 \frac{kh}{2}$ $(= 1 - 4(\nu-1)^2(1-(\nu-1)^2)\sin^4 \frac{kh}{2})$.

6. If CFL condition is satisfied, both the Lax-Wendroff scheme and the Beam-Warming scheme are $\mathbb{L}^2$ stable.

(Let L be the length of the domain I, then $h = LN^{-1}$, $k = k'\pi L^{-1}$, where the frequency $-N+1 \le k' \le N$.)

The Leap-frog Scheme for the Advection Equation

A typical three-time-level scheme for the advection equation is the leap-frog scheme $\frac{U_j^{m+1}-U_j^{m-1}}{2\tau}+a\,\frac{U_{j+1}^m-U_{j-1}^m}{2h}=0.$ or equivalently $U_j^{m+1}=U_j^{m-1}-\nu(U_{j+1}^m-U_{j-1}^m)$.

1. CFL condition of the leap-frog scheme: $|\nu|=|a|\tau/h\le 1$.
2. Truncation error: $Tu_j^m=\frac{1}{6}ah^2(1-\nu^2)u_{xxx}|_j^m+O(h^4)$.
3. Characteristic equation: $\lambda_k^2+2\mathrm{i}\nu\lambda_k\sin kh-1=0$.
4. Amplification factors: $\lambda_{k\pm}=-\mathrm{i}\nu\sin kh\pm\sqrt{1-\nu^2\sin^2 kh}$.
5. If $|\nu|>1$, for $kh=\pi/2$, $\max\{|\lambda_{k\pm}|\}=|\nu|+\sqrt{\nu^2-1}>1$.
6. If $|\nu|\le 1$, $|\lambda_{k+}|=|\lambda_{k-}|=1$, no damping on Fourier modes.
7. The leap-frog scheme is $\mathbb{L}^2$ stable $\Leftrightarrow|\nu|\le 1$.

Dissipation and Dispersion of Solutions of Hyperbolic Equations

The solution to an initial value problem of a 1D homogeneous constant-coefficient linear system of hyperbolic equations is composed of

> a set of traveling waves, each of which propagates
>
> at a corresponding characteristic velocity of the system;
>
> without any dissipation;

regardless of whatever superpositions these waves may make.

Dissipation and Dispersion of Numerical Solutions of Hyperbolic Equations

On the other hand,

1. Dissipation and dispersion do occur in finite difference solutions.
2. The rates of dissipation and dispersion of a Fourier mode generally depend on its frequency.
3. The discrete solution is no longer composed of a set of characteristic traveling waves, because of dispersion.
4. The discrete solution may exhibits numerical oscillations.

Dissipation of Lax-Wendroff and Beam-Warming Schemes

Suppose the CFL condition is satisfied, then, the Fourier mode solutions produced by the Lax-Wendroff and Beam-Warming schemes will generally decay, if $|\nu| \neq 1$, and for B-M $|\nu| \neq 1, 2$.

1. Damping factors in each time step: $1 - O(k^4 h^4)$, for $kh \ll 1$; More damping as $kh \nearrow \pi$. $\sqrt{1 - 4\nu^2(1-\nu^2)}$ (L-W) and $\sqrt{1 - 4|\nu|(2-|\nu|)(1-|\nu|)^2}$ (B-W) respectively, for $kh = \pi$.
2. For fixed k and ν, the global decay factor at time $t_{\max}$ is $(1 - O(k^4 h^4))^{\tau^{-1} t_{\max}} = 1 - \tau^{-1} t_{\max} O(k^4 h^4) = 1 - O(h^3)$.
3. For both schemes, the global error on the amplitude of a Fourier mode solution with $kh \ll 1$ is $O(h^3)$, as $h \to 0$.
4. Relatively high frequencies on a given grid decay sharply, as $m \to \infty$.

Dispersion of Lax-Wendroff and Beam-Warming Schemes

1. $\omega(k) = -ak$: dispersion relation of Fourier mode solution $e^{\mathrm{i}(kx+\omega t)}$ for the advection equation;
2. $w_h(k) = \tau^{-1} \arg \lambda_k$: discrete dispersion relation for Fourier mode solution $U_j^m = \lambda_k^m e^{\mathrm{i}kjh}$ of a difference scheme.
3. Phase shift of the Lax-Wendroff scheme in a time step τ: $\arg \lambda_k = -ak\tau \left[1 - \frac{1}{6}(1-\nu^2)k^2h^2 + \cdots\right]$, $kh \ll 1$. (see (3.2.43))
4. Phase shift of the Beam-Warming scheme in a time step τ: $\arg \lambda_k = -ak\tau \left[1 + \frac{1}{6}(1-|\nu|)(2-|\nu|)k^2h^2 + \cdots\right]$, $kh \ll 1$.
5. Global relative phase error of both schemes: $O(k^2h^2)$, for $|\nu| \neq 1$.
6. L-W experiences phase lag, which $\nearrow$ as $k \nearrow$.
7. B-W experiences phase advance for $|\nu| < 1$, and phase lag for $1 < |\nu| < 2$, both $\nearrow$ as $k \nearrow$.

Dispersion of the Leap-frog Scheme ($kh \ll 1$)

1. Amplification factors:
$$\lambda_{k\pm} = -\mathrm{i}\nu \sin kh \pm \sqrt{1 - \nu^2 \sin^2 kh}.$$
2. Phase shift of the leap-frog scheme in a time step τ:
$$\arg \lambda_{k\pm} = \mp ak\tau \left[1 - \frac{1}{6}(1-\nu^2)k^2h^2 + \cdots \right], \quad \forall kh \ll 1.$$
3. For $kh \ll 1$, λ_+ corresponds to the real solution mode, while λ_- corresponds to a spurious solution mode.
4. Global relative phase error of the scheme: $O(k^2h^2)$, for $|\nu| \neq 1$.
5. Leap-frog scheme experiences phase lag, which $\nearrow$ as $k \nearrow$.

Dispersion of the Leap-frog Scheme ($k'h = \pi - kh$, for $kh \ll 1$)

On the high frequency end, *i.e.* $k'h = \pi - kh$, for $kh \ll 1$.

6. Amplification factors:

$$\lambda_{k'\pm} = -\mathrm{i}\nu \sin k'h \pm \sqrt{1 - \nu^2 \sin^2 k'h} = -\mathrm{i}\nu \sin kh \pm \sqrt{1 - \nu^2 \sin^2 kh}.$$

7. Phase shift of the leap-frog scheme in a time step τ:

$$\arg \lambda_{k'\pm} = \mp ak\tau \left[1 - \frac{1}{6}(1-\nu^2)k^2h^2 + \cdots \right], \quad \forall kh \ll 1.$$

8. Phase shift of the advection equation in a time step τ: $-ak'\tau = -\nu\pi + ak\tau$. The one time step phase error of the scheme on high frequency modes is $O(1)$, for $|\nu| \neq 1$.
9. Since there is no damping when CFL condition is satisfied, the dispersion as well as the spurious solution modes can cause more serious numerical oscillations.

The Group Speed and Its Geometrical and Physical Explanations

1. Group speed of Fourier mode $e^{\mathrm{i}(kx+\omega(k)t)}$: $C(k) = -\frac{d\omega(k)}{dk}$;
2. Let $k = k_0 + \triangle k$, $|\triangle k| \ll k_0$. Let $\delta = \frac{\triangle k}{k_0}$, $g(\delta) = \frac{\omega(k_0(1+\delta))}{k_0(1+\delta)}$.
3. $g(\delta) = \frac{\omega(k_0)}{k_0} + \left(\omega'(k_0) - \frac{\omega(k_0)}{k_0}\right)\delta + O(\delta^2)$. (by Taylor expansion)
4. $e^{\mathrm{i}(kx+\omega(k)t)} = e^{\mathrm{i}k(x+g(\delta)t)} = e^{\mathrm{i}(kx+(\omega(k_0)-C(k_0)\triangle k+O(\delta))t)}$.

Remark 1: In wave propagation problems, the superposition of a wave usually has important physical meaning. If accurately computing each of the Fourier mode solutions is a mission impossible, is it possible for one to accurately compute the superposition of the wave?

Remark 2: Since low frequency modes usually have small errors, the main task reduces to characterize the phase speed of the superposition of high frequency modes.

The Group Speed and Its Geometrical and Physical Explanations

5. In other words, $e^{\mathrm{i}(kx+\omega(k)t)} \approx e^{\mathrm{i}(\omega(k_0)+C(k_0)k_0)t} e^{\mathrm{i}k(x-C(k_0)t)}$.

6. Thus $\sum_{|\delta|\ll 1} a_k e^{\mathrm{i}(kx+\omega(k)t)} \approx e^{\mathrm{i}(\omega(k_0)+C(k_0)k_0)t} \sum_{|\delta|\ll 1} a_k e^{\mathrm{i}k(x-C(k_0)t)}$.

   That means the superposition of a group of waves with k close to k_0 travels approximately at the group speed $C(k_0)$.

7. In physics, the energy of a group of waves with frequencies centered at k_0 propagates approximately in the speed $C(k_0)$.

8. It makes sense to study the group speed for high frequency modes, especially for non-damping difference schemes.

The Discrete Group Speed for the Lax-Wendroff Scheme

Parallelly, we may define the discrete group speed of a finite difference scheme by $C_h(k) = -\frac{\mathrm{d}\omega_h(k)}{\mathrm{d}k}$.

Since the discrete dispersion relation of a scheme is given by $\omega_h(k) = \tau^{-1} \arg \lambda_k$, so, its discrete group speed is given by

$$C_h(k)\tau = -\frac{\mathrm{d}\omega_h(k)}{\mathrm{d}k}\tau = -\frac{\mathrm{d}}{\mathrm{d}k}\left(\arctan \frac{\mathrm{Im}(\lambda_k)}{\mathrm{Re}(\lambda_k)}\right).$$

1. For the Lax-Wendroff scheme of the advection equation:
$$C_h(k) = a\frac{(1 - 2\nu^2 \sin^2 \frac{1}{2}kh)\cos kh + \nu^2 \sin^2 kh}{(1 - 2\nu^2 \sin^2 \frac{1}{2}kh)^2 + \nu^2 \sin^2 kh}.$$
2. As $kh \to \pi$, $C_h(k) \to a/(2\nu^2 - 1)$.

The Discrete Group Speed for the Lax-Wendroff Scheme

3. Since high frequency modes decay sharply, what really matters are the modes with large k while $kh \ll 1$.

4. $C_h(k) = a(1 - \frac{1}{2}(1 - \nu^2)k^2h^2 + O(k^4h^4))$, for $kh \ll 1$.

5. $C_h(k) \approx C(k)(1 - \frac{1}{2}(1 - \nu^2)k^2h^2)$, for $kh \ll 1$, the numerical superposition of waves propagating slower than the real one.

6. On fine grids, for large k with $kh \ll 1$, the error on the group speed is about 3 times of the relative phase error.

The Discrete Group Speed for the Beam-Warming Scheme

1. For the Beam-Warming scheme ($a > 0$):

$$C_h(k) = a\frac{(1-2(1-\nu)^2\sin^2\frac{1}{2}kh)(2(2-\nu)\sin^2\frac{1}{2}kh+\cos kh)+(1-\nu)^2\sin^2 kh}{(1-2(1-\nu)^2\sin^2\frac{1}{2}kh)^2+(1-\nu)^2\sin^2 kh}.$$

2. As $kh \to \pi$, $C_h(k) \to a(3-2\nu)/(1-2(1-\nu)^2)$.
3. Since high frequency modes decay sharply, what really matters are the modes with large k while $kh \ll 1$.
4. $C_h(k) = a(1+\frac{1}{2}(1-\nu)(2-\nu)k^2h^2 + O(k^4h^4))$, for $kh \ll 1$.
5. $C_h(k) \approx C(k)(1+\frac{1}{2}(1-\nu)(2-\nu)k^2h^2)$, for $kh \ll 1$.
6. On fine grids, for large k with $kh \ll 1$, the error on the group speed is about 3 times of the relative phase error.
7. For $a < 0$, the conclusions are similar (replace ν by $|\nu|$).

The Discrete Group Speed for the Leap-frog Scheme

1. For the Leap-frog scheme:
   $\lambda_{k\pm} = -\mathrm{i}\nu \sin kh \pm \sqrt{1-\nu^2 \sin^2 kh}$, thus
   $\sin(\omega_h(k)\tau) = \sin(\arg \lambda_{k\pm}) = -\nu \sin(kh)$,
   $\cos(\omega_h(k)\tau) = \pm\sqrt{1-\nu^2 \sin^2 kh}$,
   $$C_h(k) = -\frac{\mathrm{d}\omega_h(k)}{\mathrm{d}k} = \frac{\nu h \cos(kh)}{\tau \cos(\omega_h(k)\tau)} = \frac{\pm a \cos kh}{\sqrt{1-\nu^2 \sin^2 kh}}.$$
2. Since there is no decay, all modes counts.
3. For $0 < kh < \frac{1}{2}\pi$, λ_{k+} real, λ_{k-} spurious solution.
4. $C_h(k) = \pm a(1 - \frac{1}{2}(1-\nu^2)k^2h^2 + O(k^4h^4))$, for $kh \ll 1$.
5. For $\frac{1}{2}\pi < kh < \pi$, λ_{k+} spurious, λ_{k-} real solution.
6. $C_h(\pi/h - k) = \mp a(1 - \frac{1}{2}(1-\nu^2)k^2h^2 + O(k^4h^4))$, for $kh \ll 1$.
7. On fine grids, for large k with $kh \ll 1$, the error on the group speed is about 3 times of the relative phase error.

Overall performance of the Leap-frog Scheme

1. No damping, when the CFL condition $|\nu| \leq 1$ is satisfied.
2. Relative phase error on low frequency modes are $O(k^2h^2)$.
3. For $0 < kh < \frac{1}{2}\pi$, λ_{k+} corresponds to the real solution mode.
4. For $\frac{1}{2}\pi < kh < \pi$, λ_{k-} corresponds to the real solution mode.
5. The error on the group speed is $O(h^2)$ on both high and low frequencies. Though, the one time step phase errors on high frequency modes are $O(1)$.

Proper numerical initial and boundary conditions are important in applications to reduce as much as possible the spurious modes in the numerical solution.

Inflow, Outflow Boundaries and Numerical Boundary Conditions

For initial-boundary value problems of hyperbolic equations, numerical boundary condition is also an important issue.

1. Inflow boundary: where the characteristic evolves into Ω.
2. Outflow boundary: where the characteristic goes out of Ω.
3. For the advection equation with $a > 0$, the left boundary is inflow, and the right boundary is outflow.
4. On inflow boundary, the boundary condition(s) for the PDE will naturally provide boundary condition(s) for FDM.

Inflow, Outflow Boundaries and Numerical Boundary Conditions

5. Additional numerical boundary conditions are often required on the outflow boundary point by difference schemes.

6. For example, both the Lax-Wendroff scheme and the leap-frog scheme need a numerical boundary condition at the outflow boundary.

7. Use of one sided schemes, such as the upwind scheme and the Beam-warming scheme, on the outflow boundary, can avoid the need for numerical boundary conditions there.

Zero Order Extrapolation and Non-reflection Boundary Conditions

If a numerical boundary condition is required at the outflow right boundary x_N, then, the simplest way we can do is to

- introduce a ghost node x_{N+1};
- apply the zero order extrapolation formula: $U_{N+1}^m = U_N^m$;
- couple the numerical boundary condition with the scheme used on the interior nodes.

The numerical boundary condition so obtained is called a non-reflection boundary condition or an absorbtion boundary condition. Higher order extrapolations are not recommended because of numerical oscillations.

Vertical Fourier Modes and Amplification Factors

1. Separation of variables of difference solutions: $U_j^m = \lambda^m \mu^j$.
2. Standard Fourier modes: $U_j^m = \lambda_k^m e^{\mathrm{i}kjh}$. $(\mu_k = e^{\mathrm{i}kh})$
3. Vertical Fourier modes: $U_j^m = e^{\pm \mathrm{i}amk\tau} \mu_k^j$. $(\lambda_k = e^{\pm \mathrm{i}ak\tau})$
4. Fourier mode solutions of the advection equation: $e^{\mp \mathrm{i}k(x-at)}$.
5. The amplification factors of the advection equation: $e^{\mp \mathrm{i}kh}$.
6. Substitute the vertical Fourier mode $U_j^m = e^{\pm \mathrm{i}amk\tau} \mu_k^j$ into a difference scheme to get the amplification factor $\mu_k^{\pm}$.
7. For real solution modes, we expect $\mu_k^{\pm} \approx e^{\mp \mathrm{i}kh}$.

Amplification Factor of Vertical Fourier Mode of the Lax-Wendroff Scheme

1. Substitute $U_j^m = \lambda_k^m \mu_k^j = e^{\pm \mathrm{i} amk\tau} \mu_k^j$ into the Lax-Wendroff scheme ($a > 0$, see (3.2.33)) yields the characteristic equation:
$$\frac{1}{2}\nu(1-\nu)\mu_k^2 - ((1-\nu^2) - \lambda_k)\mu_k - \frac{1}{2}\nu^2(1-\nu^2) = 0.$$
2. The amplification factor of the vertical Fourier mode:
$$\mu_k = \frac{(1-\nu^2) - \lambda_k \pm \sqrt{((1-\nu^2)-\lambda_k)^2 + \nu^2(1-\nu^2)}}{\nu(1-\nu)}.$$
3. $\lambda_k^{\pm} = e^{\pm \mathrm{i} ak\tau} \approx 1 \pm \mathrm{i} ak\tau = 1 \pm \mathrm{i}\nu kh.$

Amplification Factor of Vertical Fourier Mode of the Lax-Wendroff Scheme

4. For the two real solution modes $U_j^{\pm m} = \left(\lambda_k^{\pm}\right)^m \left(\mu_k^{r\pm}\right)^j$:

$$\mu_k^{r\pm} = \mu_k^r(\lambda_k^{\pm}) \approx \begin{cases} 1 - \mathrm{i}kh \approx e^{-\mathrm{i}kh}, \\ 1 + \mathrm{i}kh \approx e^{\mathrm{i}kh}, \end{cases}$$

5. For the two spurious solution modes $V_j^{\pm m} = \left(\lambda_k^{\pm}\right)^m \left(\mu_k^{s\pm}\right)^j$:

$$\mu_k^{s\pm} = \mu_k^s(\lambda_k^{\pm}) \approx \begin{cases} -\dfrac{1+\nu}{1-\nu}(1 + \mathrm{i}kh) \approx -\dfrac{1+\nu}{1-\nu} e^{\mathrm{i}kh}; \\ -\dfrac{1+\nu}{1-\nu}(1 - \mathrm{i}kh) \approx -\dfrac{1+\nu}{1-\nu} e^{-\mathrm{i}kh}. \end{cases}$$

Strong Damping Effect of the Lax-Wendroff Scheme to Spurious Modes

6. The two "real" solution modes satisfy $U_j^{\pm m} \approx e^{\mp \mathrm{i}k(jh-am\tau)}$, and their approximation accuracy are second order;

7. The two spurious modes satisfy, up to second order accuracy,

$$V_j^{\pm m} \approx \left(-\frac{1+\nu}{1-\nu}\right)^j e^{\pm \mathrm{i}k(jh+am\tau)}.$$

8. Exponential decay of the errors on outflow boundary ($\nu < 1$):

$$V_{j-1}^{\pm m} \approx -\frac{1-\nu}{1+\nu} e^{\mp \mathrm{i}kh} V_j^{\pm m}.$$

Strong Damping Effect of the Lax-Wendroff Scheme to Spurious Modes

In general, If the CFL condition is satisfied, the Lax-Wendroff scheme has very strong damping effect to the reversely propagating waves, so the additional numerical boundary conditions will not cause too much error pollution to the numerical results.

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Thank You!