Numerical Solutions to Partial Differential Equations

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A Model Problem of the Advection-Diffusion Equation

- An initial value problem of a 1D constant-coefficient advection-diffusion equation ($a > 0$, $c > 0$): $u_t + au_x = cu_{xx}$, $x \in \mathbb{R}$, $t > 0$; $\quad u(x,0) = u^0(x)$, $x \in \mathbb{R}$.
- By a change of variables $y = x - at$ and $v(y,t) \triangleq u(y + at, t)$, $v_t = cv_{yy}$, $\;y \in \mathbb{R}$, $\;t > 0$; $v(x,0) = u^0(x)$, $x \in \mathbb{R}$.

Characteristic global properties of the solution u:

1. There is a characteristic speed as in the advection equation, which plays an important role to the solution, especially when $|a| \gg c$ (advection dominant).
2. Along the characteristic, the solution behaves like a parabolic solution (dissipation and smoothing).

Classical Difference Schemes and Their Stability Conditions

Classical explicit difference schemes:

$$\left[\tau^{-1}\triangle_{t+} + a(2h)^{-1}\triangle_{0x}\right] U_j^m = \tilde{c}h^{-2}\delta_x^2 U_j^m,$$

($\tilde{c} = c$, central; $c + \frac{a^2\tau}{2}$, modified central; $c + \frac{1}{2}ah$, upwind).

1. Maximum principle $\Leftrightarrow \frac{\tilde{c}\tau}{h^2} \le \frac{1}{2}$, $h \le \frac{2\tilde{c}}{a}$.
2. $\mathbb{L}^2$ strongly stable $\Leftrightarrow \frac{\tilde{c}\tau}{h^2} \le \frac{1}{2}$ and $\tau \le \frac{2\tilde{c}}{a^2}$.

The Crank-Nicolson scheme

$$\tau^{-1}\delta_t U^{m+\frac{1}{2}} + a\,(4h)^{-1}\triangle_{0x}\left[U_j^m + U_j^{m+1}\right] = c\,(2h^2)^{-1}\delta_x^2\left[U_j^m + U_j^{m+1}\right],$$

1. Maximum principle $\Leftrightarrow \mu \le 1$, $h \le \frac{2c}{a}$.
2. Unconditionally $\mathbb{L}^2$ strongly stable.

What Do We See Along a Characteristic Line?

For constant-coefficient advection-diffusion equation:

1. The characteristic equation for the advection part: $\frac{\mathrm{d}x}{\mathrm{d}t} = a$.
2. Unit vector in characteristic direction: $\mathbf{n}_s = (\frac{a}{\sqrt{1+a^2}}, \frac{1}{\sqrt{1+a^2}})$.
3. Let s be the length parameter for the characteristic lines.
4. $$\frac{\partial u}{\partial s} = \mathbf{grad}(u) \cdot \mathbf{n}_s = \left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial t}\right) \cdot \mathbf{n}_s = \frac{1}{\sqrt{1+a^2}} \left(\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x}\right).$$
5. This yields $\frac{\partial u}{\partial s} = \tilde{c}\frac{\partial^2 u}{\partial x^2}$, (*i.e.* along the characteristics $\frac{\mathrm{d}x}{\mathrm{d}t} = a$, the solution u to the constant-coefficient advection-diffusion equation $\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = c\frac{\partial^2 u}{\partial x^2}$ behaves like a solution to a diffusion equation with diffusion coefficient $\tilde{c} = \frac{c}{\sqrt{1+a^2}}$.)

Operator Splitting and Characteristic Difference Schemes

For general variable coefficients advection-diffusion equations:

1. The idea of the characteristic difference schemes for the advection-diffusion equation is to approximate the process by applying the operator splitting method.

2. Every time step will be separated into two sub-steps.

3. In the first sub-step, approximate the advection process by the characteristic method: $\tilde{u}_j^{m+1} \triangleq u(\bar{x}_j^m) = u(x_j - a_j^{m+1}\tau)$, along the characteristics.

Operator Splitting and Characteristic Difference Schemes

4. In the second sub-step, approximate the diffusion process with $\tilde{u}_j^{m+1}$ as the initial data at t_m by, say, the implicit scheme:

$$\frac{u_j^{m+1} - u(\bar{x}_j^m)}{\tau} = c_j^{m+1} \frac{u_{j+1}^{m+1} - 2u_j^{m+1} + u_{j-1}^{m+1}}{h^2} + \bar{T}_j^m,$$

5. The local truncation error $\bar{T}_j^m = O(\tau + h^2)$.

6. Replacing $u(\bar{x}_j^m)$ by certain interpolations of the nodal values leads to characteristic difference schemes.

A Characteristic Difference Scheme by Linear Interpolation

Suppose $\bar{x}_j^m \in [x_{i-1}, x_i)$ and $|\bar{x}_j^m - x_{i-1}| < h$. Approximate $u(\bar{x}_j^m)$ by the linear interpolation of u_{i-1}^m and u_i^m leads to:

$$\frac{U_j^{m+1} - \alpha_j^m U_i^m - (1-\alpha_j^m) U_{i-1}^m}{\tau} = c_j^{m+1} \frac{U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}}{h^2},$$

where $\alpha_j^m = h^{-1}(\bar{x}_j^m - x_{i-1}) \in [0, 1)$, or equivalently

$$(1+2\mu_j^{m+1}) U_j^{m+1} = \alpha_j^m U_i^m + (1-\alpha_j^m) U_{i-1}^m + \mu_j^{m+1} (U_{j+1}^{m+1} + U_{j-1}^{m+1}),$$

where $\mu_j^{m+1} = c_j^{m+1} \tau \, h^{-2}$.

A Characteristic Difference Scheme by Linear Interpolation

1. $T_j^m = O(\tau + \tau^{-1} h^2)$. $\left(u(\bar{x}_j^m) = \alpha_j^m u_i^m + (1 - \alpha_j^m) u_{i-1}^m + O(h^2)\right)$.
2. Maximum principle holds. (Note $\alpha_j^m \in [0, 1)$, $\mu_j^{m+1} > 0$.)
3. Since $e^{-\mathrm{i}k(j-i+1)h} = e^{-\mathrm{i}k(\alpha_j^m h + a_j^{m+1}\tau)}$, we have
   $$\lambda_k = \frac{1-\alpha_j^m(1-\cos kh)+\mathrm{i}\,\alpha_j^m \sin kh}{1+4\mu_j^{m+1}\sin^2\frac{1}{2}kh}\, e^{-\mathrm{i}k(\alpha_j^m h + a_j^{m+1}\tau)}, \ |\lambda_k| \le 1, \ \forall k,$$
   $$\because \ |1 - \alpha_j^m(1 - \cos kh) + \mathrm{i}\,\alpha_j^m \sin kh|^2 = 1 - 2\alpha_j^m(1 - \alpha_j^m)(1 - \cos kh).$$
4. Unconditionally locally $\mathbb{L}^2$ stable.
5. Optimal convergence rate is $O(h)$, when $\tau = O(h)$.

A Characteristic Difference Scheme by Quadratic Interpolation

Suppose $\alpha_j^m = h^{-1}(\bar{x}_j^m - x_{i-1}) \in [-\frac{1}{2}, \frac{1}{2}]$. Approximate $u(\bar{x}_j^m)$ by the quadratic interpolation of u_{i-2}^m, u_{i-1}^m and u_i^m leads to:

$$\frac{U_j^{m+1} - \frac{1}{2}\alpha_j^m(1+\alpha_j^m)U_i^m - (1-\alpha_j^m)(1+\alpha_j^m)U_{i-1}^m + \frac{1}{2}\alpha_j^m(1-\alpha_j^m)U_{i-2}^m}{\tau} = c_j^{m+1}\frac{U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}}{h^2}.$$

1. $T_j^m = O(\tau + \tau^{-1}h^3 + h^2)$. (quadratic interpolation error $O(h^3)$).
2. Maximum principle does not hold. (Note $\alpha_j^m \in [-\frac{1}{2}, \frac{1}{2}]$.)
3. $\lambda_k = \frac{1-(\alpha_j^m)^2(1-\cos kh)+\mathrm{i}\,\alpha_j^m \sin kh}{1+4\mu_j^{m+1}\sin^2\frac{1}{2}kh}\, e^{-\mathrm{i}k(\alpha_j^m h + a_j^{m+1}\tau)}$, $|\lambda_k| \le 1$, $\forall k$.
   ($\because\ |1-(\alpha_j^m)^2(1-\cos kh)+\mathrm{i}\,\alpha_j^m\sin kh|^2 = 1-(\alpha_j^m)^2(1-(\alpha_j^m)^2)(1-\cos kh)$.)
4. Unconditionally locally $\mathbb{L}^2$ stable.
5. Optimal convergence rate is $O(h^{3/2})$, when $\tau = O(h^{3/2})$.

Dissipation, Dispersion and Group Speed of the Scheme

In the case of the constant-coefficient, $u(x,t) = e^{-ck^2 t} e^{\mathrm{i}k(x-at)}$ are the Fourier mode solutions for the advection-diffusion equation.

1. Dissipation speed: e^{-ck^2}; dispersion relation: $\omega(k) = -ak$; group speed: $C(k) = a$; for all k.
2. For the Fourier mode $U_j^m = \lambda_k^m e^{\mathrm{i}kjh}$,
$$\lambda_k = \frac{1 - (\alpha_j^m)^2(1-\cos kh) + \mathrm{i}\,\alpha_j^m \sin kh}{1 + 4\mu_j^{m+1} \sin^2 \frac{1}{2}kh} e^{-\mathrm{i}k(\alpha_j^m h + a_j^{m+1}\tau)}, \quad \forall k.$$
3. The errors on the amplitude, phase shift and group speed can be worked out (see Exercise 3.12).

Initial and Initial-Boundary Value Problems of the Wave Equation

1. 1D wave equation $u_{tt} = a^2 u_{xx}, \quad x \in I \subset \mathbb{R}, \quad t > 0.$
2. Initial conditions

$$\begin{aligned} u(x,0) &= u^0(x), \qquad x \in I \subset \mathbb{R}, \\ u_t(x,0) &= v^0(x), \qquad x \in I \subset \mathbb{R}. \end{aligned}$$

3. Boundary conditions, when I is a finite interval, say $I = (0,1)$,

$$\begin{aligned} \alpha_0(t)u(0,t) - \beta_0(t)u_x(0,t) &= g_0(t), \quad t > 0, \\ \alpha_1(t)u(1,t) + \beta_1(t)u_x(1,t) &= g_1(t), \quad t > 0, \end{aligned}$$

where $\alpha_i \geq 0$, $\beta_i \geq 0$, $\alpha_i + \beta_i \neq 0$, $i = 0, 1$.

Equivalent First Order Hyperbolic System of the Wave Equation

1. Let $v = u_t$ and $w = -au_x$ $(a > 0)$. The wave equation is transformed to

$$\begin{bmatrix} v \\ w \end{bmatrix}_t + \begin{bmatrix} 0 & a \\ a & 0 \end{bmatrix} \begin{bmatrix} v \\ w \end{bmatrix}_x = 0.$$

2. The eigenvalues of the system are $\pm a$.
3. The two families of characteristic lines of the system

$$\begin{cases} x + at = c, \\ x - at = c, \end{cases} \qquad \forall c \in \mathbb{R}.$$

4. The solution to the initial value problem of the wave equation:

$$u(x,t) = \frac{1}{2}\left[u^0(x+at) + u^0(x-at)\right] + \frac{1}{2a}\int_{x-at}^{x+at} v^0(\xi)\, d\xi.$$

The Explicit Difference Scheme for the Wave Equation

1. $$\frac{U_j^{m+1} - 2U_j^m + U_j^{m-1}}{\tau^2} - a^2\,\frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{h^2} = 0.$$
2. The local truncation error:
$$\left[\left(\tau^{-2}\delta_t^2 - h^{-2}a^2\delta_x^2\right) - \left(\partial_t^2 - a^2\partial_x^2\right)\right] u_j^m = O(\tau^2 + h^2).$$
3. By $u(x,\tau) = u(x,0) + \tau\, u_t(x,0) + \frac{1}{2}\tau^2 u_{tt}(x,0) + O(\tau^3)$,
$$u(x,\tau) = u^0(x) + \tau\, v^0(x) + \frac{1}{2}\nu^2\big(u^0(x+h) - 2u^0(x) + u^0(x-h)\big) + O(\tau^3 + \tau^2 h^2).$$
4. The discrete initial conditions (local truncation error $O(\tau^3 + \tau^2 h^2)$), denote $\nu = a\tau/h$:
$$U_j^0 = u_j^0; \quad U_j^1 = \frac{1}{2}\nu^2\left(U_{j+1}^0 + U_{j-1}^0\right) + (1-\nu^2)U_j^0 + \tau v_j^0.$$

Remark: If an additional term $\frac{1}{6}\tau\nu^2\delta_x^2 v^0(x)$ is used in (3), then the truncation error is $O(\tau^4 + \tau^2 h^2)$.

Boundary Conditions for the Explicit Scheme of the Wave Equation

1. For $\beta = 0$, use the Dirichlet boundary condition of the problem directly;
2. For $\beta \neq 0$, say $\beta_0 = 1$, $\alpha_0 > 0$, introduce a ghost node x_{-1}, and a discrete boundary condition with truncation error $O(h^2)$:
$$\alpha_0^m U_0^m - \frac{U_1^m - U_{-1}^m}{2h} = g_0^m.$$
3. Eliminating U_{-1}^m leads to an equivalent difference scheme with truncation error $O(\tau^2 + h)$ (see Exercise 3.13) at x_0:

$$\frac{U_0^{m+1} - 2U_0^m + U_0^{m-1}}{\tau^2} - 2a^2 \frac{U_1^m - (1 + \alpha_0^m h)U_0^m + g_0^m h}{h^2} = 0.$$

Fourier Analysis for the Explicit Scheme of the Wave Equation

1. Initial value problem of constant-coefficient wave equation.
2. Characteristic equation of the discrete Fourier mode $U_j^m = \lambda_k^m e^{\mathrm{i}kjh}$: $\lambda_k^2 - 2\lambda_k + 1 = \lambda_k \nu^2 \left(e^{\mathrm{i}kh} - 2 + e^{-\mathrm{i}kh}\right)$.
3. The corresponding amplification factors are given by
$$\lambda_k^{\pm} = 1 - 2\nu^2 \sin^2 \frac{1}{2}kh \pm \mathrm{i}2\nu \sin \frac{1}{2}kh\sqrt{1 - \nu^2 \sin^2 \frac{1}{2}kh}.$$
4. If the CFL condition, *i.e.* $\nu \leq 1$, is satisfied, $|\lambda_k^{\pm}| = 1$;
5. there is phase lag, and the relative phase error is $O(k^2h^2)$,
$$\arg \lambda_k^{\pm} = \pm ak\tau \left(1 - \frac{1-\nu^2}{24}k^2h^2 + \cdots\right), \ \ \forall kh \ll 1, \ \ (\nu \leq 1).$$
6. Group speed $C^{\pm}(k) = \pm a$, $C_h^{\pm}(k)\tau = -\frac{\mathrm{d}}{\mathrm{d}k} \arg \lambda_k^{\pm}$.

The θ-Scheme of the Wave Equation

1. For $\theta \in (0,1]$, θ-scheme of the wave equation ($O(\tau^2+h^2)$):

$$\frac{U_j^{m+1}-2U_j^m+U_j^{m-1}}{\tau^2} = a^2\left[\theta\,\frac{U_{j+1}^{m+1}-2U_j^{m+1}+U_{j-1}^{m+1}}{h^2}\right.$$
$$\left.+(1-2\theta)\,\frac{U_{j+1}^{m}-2U_j^{m}+U_{j-1}^{m}}{h^2}+\theta\,\frac{U_{j+1}^{m-1}-2U_j^{m-1}+U_{j-1}^{m-1}}{h^2}\right].$$

2. Characteristic equation of the Fourier mode $U_j^m = \lambda_k^m e^{\mathrm{i}kjh}$:

$$\lambda_k^2-2\lambda_k+1 = \left(\theta\nu^2\lambda_k^2+(1-2\theta)\nu^2\lambda_k+\theta\nu^2\right)\left(e^{\mathrm{i}kh}-2+e^{-\mathrm{i}kh}\right).$$

3. The corresponding amplification factors are given by

$$\lambda_k^{\pm} = 1-\frac{2\nu^2\sin^2\frac{1}{2}kh}{1+4\theta\nu^2\sin^2\frac{1}{2}kh}\pm\frac{\sqrt{-4\nu^2\sin^2\frac{1}{2}kh\left(1+\nu^2(4\theta-1)\sin^2\frac{1}{2}kh\right)}}{1+4\theta\nu^2\sin^2\frac{1}{2}kh}.$$

$\mathbb{L}^2$ Stability Conditions for the θ-Scheme of the Wave Equation

4. The $\mathbb{L}^2$ stability condition of the θ-scheme:

$$\begin{cases} (1-4\theta)\nu^2 \leq 1, & \text{if } \theta < \frac{1}{4}; \\ \text{unconditionally stable}, & \text{if } \theta \geq \frac{1}{4}. \end{cases}$$

5. When the θ-scheme is $\mathbb{L}^2$ stable, $\lambda_k^+ = \bar{\lambda}_k^-$, $|\lambda_k^\pm| = 1$, $\forall k$;

6. the relative phase error is $O(k^2h^2)$, if $kh \ll 1$ or $\pi - kh \ll 1$, there is always a phase lag

$$\arg \lambda_k^\pm = \pm ak\tau \left(1 - \frac{1}{24}(1 + (12\theta - 1)\nu^2)k^2h^2 + \cdots \right).$$

Remark 1: We may calculate the group speed to see how the scheme works on superpositions of Fourier modes.

Remark 2: For many physical problems, the energy stability analysis can be a better alternative approach.

The Wave Equation and Its Mechanical Energy Conservation

For the initial-boundary value problem of the wave equation:

$$\begin{aligned} u_{tt} = (a^2 u_x)_x, &\qquad x \in (0,1), &\qquad t > 0, \\ u(0,t) = 0, &\qquad u(1,t) = 0, &\qquad t > 0, \\ u(x,0) = u^0(x), &\quad u_t(x,0) = v^0(x), &\quad x \in [0,1], \end{aligned}$$

if $a > 0$ is a constant, it follows from integral by parts, and

$$\int_0^1 \left(u_{tt} - (a^2 u_x)_x\right) u_t \, \mathrm{d}x = 0, \quad u_t(0,t) = u_t(1,t) = 0,$$

that the mechanical energy of the system is a constant, *i.e.*

$$E(t) \triangleq \int_0^1 \frac{1}{2} \left(u_t^2 + a^2 u_x^2\right) \mathrm{d}x = \mathrm{const.}$$

The above result also holds for $a = a(x) > a_0 > 0$.

Variable-coefficient θ-Scheme and the Idea of the Energy Method

Let $0 < A_0 \leq a(x,t) \leq A_1$, consider the θ-scheme

$$\tau^{-2}\delta_t^2 U_j^m = h^{-2}\triangle_{-x}\left[a^2\triangle_{+x}\right]\left(\theta\, U_j^{m+1} + (1-2\theta)\, U_j^m + \theta\, U_j^{m-1}\right),$$

where

$$\triangle_{-x}\left[a^2\triangle_{+x}\right] U_j^m = (a_j^m)^2\left(U_{j+1}^m - U_j^m\right) - (a_{j-1}^m)^2\left(U_j^m - U_{j-1}^m\right).$$

Variable-coefficient θ-Scheme and the Idea of the Energy Method

The idea of the energy method is to find a discrete energy norm $\|U^m\|_E \equiv En(U^m, U^{m-1})$, and a function $S(U^m, U^{m-1})$, so that

1. $S_{m+1} = S_m = \cdots = S_1$ $(S_k \triangleq S(U^k, U^{k-1}))$ by the scheme;
2. There exist constants $0 < C_0 \leq C_1$, such that

   $$C_0 En(U^m, U^{m-1}) \leq S(U^m, U^{m-1}), \quad S(U^1, U^0) \leq C_1 En(U^1, U^0);$$

3. Thus, the solution U^m of the θ-scheme is proved to satisfy the energy inequality: $C_0\|U^m\|_E \leq C_1\|U^1\|_E$, for all $m > 0$.

Establish $\|\triangle_{-t} U^{m+1}\|_2^2 - \|\triangle_{-t} U^{m}\|_2^2$ by Manipulating the θ-Scheme

Remember in the continuous problem, the mechanical energy has a term $\int_0^1 u_t^2 \,\mathrm{d}x$, and notice that in the θ-scheme the term $\delta_t^2 U_j^m = (U_j^{m+1} - U_j^m) - (U_j^m - U_j^{m-1}) = \triangle_{-t} U_j^{m+1} - \triangle_{-t} U_j^m$.

Multiplying

$$h\left(U_j^{m+1} - U_j^{m-1}\right) = h\triangle_{-t} U_j^{m+1} + h\triangle_{-t} U_j^m,$$

on the both sides of the θ-scheme

$$\tau^{-2}\delta_t^2 U_j^m = h^{-2}\triangle_{-x}\left[a^2\triangle_{+x}\right]\left(\theta\, U_j^{m+1} + (1-2\theta)\, U_j^m + \theta\, U_j^{m-1}\right),$$

and summing up with respect to $j = 1, 2, \cdots, N-1$,

Establish $\|\triangle_{-t}U^{m+1}\|_2^2 - \|\triangle_{-t}U^m\|_2^2$ by Manipulating the θ-Scheme

we are lead to

$$\begin{aligned}
&\tau^{-2}\|\triangle_{-t}U^{m+1}\|_2^2 - \tau^{-2}\|\triangle_{-t}U^m\|_2^2 \\
&\quad = \theta h^{-2}\left\langle \triangle_{-x}\left[a^2\triangle_{+x}\right](U^{m+1}+U^{m-1}), U^{m+1}-U^{m-1}\right\rangle_2 \\
&\qquad\qquad + (1-2\theta)h^{-2}\left\langle \triangle_{-x}\left[a^2\triangle_{+x}\right]U^m, U^{m+1}-U^{m-1}\right\rangle_2,
\end{aligned}$$

where $\|U\|_2^2 = \langle U, U\rangle_2$ is the $\mathbb{L}^2$ norm of the grid function U and

$$\langle U, V\rangle_2 = \sum_{j=1}^{N-1} U_j V_j h = \int_0^1 UV\,dx.$$

Summation by Parts and a Discrete Version of $(\|u_t\|_2^2)_t = -(\|u_x\|_2^2)_t$

Corresponding to the integral by parts, we have the formula of summation by parts

$$
\begin{aligned}
\langle \triangle_{-x} U, V \rangle_2 &= h \sum_{j=1}^{N-1} U_j V_j - h \sum_{j=1}^{N-1} U_{j-1} V_j \\
&= h \sum_{j=1}^{N-1} U_j V_j - h \sum_{j=1}^{N-1} U_j V_{j+1} = -\langle U, \triangle_{+x} V \rangle_2 .
\end{aligned}
$$

Summation by Parts and a Discrete Version of $(\|u_t\|_2^2)_t = -(\|u_x\|_2^2)_t$

Thus, the two terms on the right can be rewritten respectively as

$$
\begin{aligned}
-\theta h^{-2}\left\langle a\triangle_{+x}U^{m+1}, a\triangle_{+x}U^{m+1}\right\rangle_2 &+ \theta h^{-2}\left\langle a\triangle_{+x}U^{m-1}, a\triangle_{+x}U^{m-1}\right\rangle_2 \\
&= -\theta h^{-2}\left(\|a\triangle_{+x}U^{m+1}\|_2^2 - \|a\triangle_{+x}U^{m-1}\|_2^2\right),
\end{aligned}
$$

$$
\begin{aligned}
&-(1-2\theta)h^{-2}\left[\left\langle a\triangle_{+x}U^{m}, a\triangle_{+x}U^{m+1}\right\rangle_2 - \left\langle a\triangle_{+x}U^{m}, a\triangle_{+x}U^{m-1}\right\rangle_2\right] \\
= \ &\frac{1-2\theta}{4}h^{-2}\left[-\|a\triangle_{+x}(U^m - U^{m-1})\|_2^2 + \|a\triangle_{+x}(U^{m+1} - U^m)\|_2^2\right. \\
&\left.+\|a\triangle_{+x}(U^m + U^{m-1})\|_2^2 - \|a\triangle_{+x}(U^{m+1} + U^m)\|_2^2\right].
\end{aligned}
$$

S_m and the Discrete Energy Norm $\|U^m\|_e$

The above analysis show that $S_{m+1} = S_m$, if we define

$$S_m = \tau^{-2}\|\triangle_{-t}U^m\|_2^2 + \theta h^{-2}\left[\|a\triangle_{+x}U^m\|_2^2 + \|a\triangle_{+x}U^{m-1}\|_2^2\right]$$
$$+\frac{1-2\theta}{4}h^{-2}\left[\|a\triangle_{+x}(U^m + U^{m-1})\|_2^2 - \|a\triangle_{+x}(U^m - U^{m-1})\|_2^2\right].$$

Notice that

$$\|a\triangle_{+x}U^m\|_2^2 + \|a\triangle_{+x}U^{m-1}\|_2^2 =$$
$$\frac{1}{2}\left[\|a\triangle_{+x}(U^m + U^{m-1})\|_2^2 + \|a\triangle_{+x}(U^m - U^{m-1})\|_2^2\right],$$

we can equivalently rewrite S_m as

$$S_m = \left\|\frac{\triangle_{-t}}{\tau}U^m\right\|_2^2 + \frac{1}{4}\left\|a\frac{\triangle_{+x}}{h}(U^m + U^{m-1})\right\|_2^2 + \frac{4\theta-1}{4}\left\|a\frac{\triangle_{+x}}{h}(U^m - U^{m-1})\right\|_2^2.$$

Establishment of the Energy Inequality for $0 \le \theta < 1/4$

If $0 \le \theta < 1/4$, denote $\bar{\nu} = \tau h^{-1}$, by $0 < A_0 \le a(x,t) \le A_1$ and

$$\|a\triangle_{+x}(U^m - U^{m-1})\|_2^2 \le 4A_1^2\|U^m - U^{m-1}\|^2 = 4A_1^2\|\triangle_{-t}U^m\|^2,$$

we have

$$S_m \ge \left(1 - A_1^2(1-4\theta)\bar{\nu}^2\right)\left\|\frac{\triangle_{-t}}{\tau}U^m\right\|_2^2 + \frac{A_0^2}{4}\left\|\frac{\triangle_{+x}}{h}(U^m + U^{m-1})\right\|_2^2.$$

Furthermore, if $0 \le \theta < 1/4$, we have

$$S_1 \le \left\|\frac{\triangle_{-t}}{\tau}U^1\right\|_2^2 + \frac{A_1^2}{4}\left\|\frac{\triangle_{+x}}{h}(U^1 + U^0)\right\|_2^2.$$

Establishment of the Energy Inequality for $0 \leq \theta < 1/4$

Define

$$\|U^m\|_E^2 = \left\| \frac{\triangle_{-t}}{\tau} U^m \right\|_2^2 + \left\| \frac{\triangle_{+x}}{h} (U^m + U^{m-1}) \right\|_2^2,$$

then, we have

$$\|U^m\|_E^2 \leq K_1 \|U^1\|_E^2, \quad \forall m > 0 \quad \text{if} \quad A_1 \sqrt{(1-4\theta)}\, \bar{\nu} < 1,$$

where $K_1 = \max\{1, A_1^2/4\} / \min\{1 - A_1^2(1-4\theta)\bar{\nu}^2, A_0^2/4\}$.

Establishment of the Energy Inequality for $1/4 \leq \theta \leq 1$

If $1/4 \leq \theta \leq 1$, by $0 < A_0 \leq a(x,t) \leq A_1$, we have

$$S_m \geq \left\| \frac{\triangle_{-t}}{\tau} U^m \right\|_2^2 + \frac{A_0^2}{4} \left[\left\| \frac{\triangle_{+x}}{h} (U^m + U^{m-1}) \right\|_2^2 + (4\theta - 1) \left\| \frac{\triangle_{+x}}{h} (U^m - U^{m-1}) \right\|_2^2 \right],$$

$$S_1 \leq \left\| \frac{\triangle_{-t}}{\tau} U^1 \right\|_2^2 + \frac{A_1^2}{4} \left[\left\| \frac{\triangle_{+x}}{h} (U^1 + U^0) \right\|_2^2 + (4\theta - 1) \left\| \frac{\triangle_{+x}}{h} (U^1 - U^0) \right\|_2^2 \right].$$

Establishment of the Energy Inequality for $1/4 \leq \theta \leq 1$

Thus, if we define the energy norm $\|\cdot\|_{E(\theta)}$ as

$$\|U^m\|_{E(\theta)} = \left\|\frac{\triangle_{-t}}{\tau} U^m\right\|_2^2 + \left\|\frac{\triangle_{+x}}{h}(U^m + U^{m-1})\right\|_2^2 + [4\theta - 1]^+ \left\|\frac{\triangle_{+x}}{h}(U^m - U^{m-1})\right\|_2^2,$$

where $[\alpha]^+ = \max\{0, \alpha\}$, then the following energy inequality holds:

$$\|U^m\|_{E(\theta)}^2 \leq K_2 \|U^1\|_{E(\theta)}^2, \qquad \forall\, m > 1.$$

where $K_2 = \max\{1, A_1^2/4\} / \min\{1, A_0^2/4\}$.

Summary of the Stability of the θ-Scheme for the Wave Equation

The θ-scheme for the wave equation ($0 \le \theta \le 1$):

$$\tau^{-2}\delta_t^2 U_j^m = h^{-2}\triangle_{-x}\left[a^2\triangle_{+x}\right]\left(\theta\, U_j^{m+1} + (1-2\theta)\, U_j^m + \theta\, U_j^{m-1}\right),$$

The energy norm $\|\cdot\|_{E(\theta)}$:

$$\|U^m\|_{E(\theta)} = \left\|\frac{\triangle_{-t}}{\tau}U^m\right\|_2^2 + \left\|\frac{\triangle_{+x}}{h}(U^m + U^{m-1})\right\|_2^2 + [4\theta-1]^+\left\|\frac{\triangle_{+x}}{h}(U^m - U^{m-1})\right\|_2^2.$$

The energy norm stability: $\|U^m\|_{E(\theta)}^2 \le K(\theta)\|U^1\|_{E(\theta)}^2$, $\forall\, m > 1$,

$$\begin{cases} (1-4\theta)A_1^2\bar{\nu}^2 \le 1, & \text{if } \theta < \frac{1}{4}; \\ \text{unconditionally stable}, & \text{if } \theta \ge \frac{1}{4}, \end{cases}$$

where $K(\theta) = \max\{1, A_1^2/4\}/\min\{1 - A_1^2[1-4\theta]^+\bar{\nu}^2, A_0^2/4\}$.

The First Order Hyperbolic System and Its Difference Approximation

1. Let $\mathbf{u} = (v, w)^T$ with $v = u_t$ and $w = -au_x$ ($a > 0$ constant). The wave equation is transformed to $\mathbf{u}_t + A\,\mathbf{u}_x = 0$, or
$$\begin{bmatrix} v \\ w \end{bmatrix}_t + \begin{bmatrix} 0 & a \\ a & 0 \end{bmatrix} \begin{bmatrix} v \\ w \end{bmatrix}_x = 0.$$
2. Expanding $\mathbf{u}_j^{m+1}$ at (x_j, t_m) in Taylor series
$$\mathbf{u}_j^{m+1} = \left[\mathbf{u} + \tau\,\mathbf{u}_t + \frac{1}{2}\tau^2\mathbf{u}_{tt}\right]_j^m + O(\tau^3),$$
3. Since $\mathbf{u}_t = -A\,\mathbf{u}_x$, $\mathbf{u}_{tt} = A^2\,\mathbf{u}_{xx}$,
$$\mathbf{u}_j^{m+1} = \left[\mathbf{u} - \tau\,A\mathbf{u}_x + \frac{1}{2}\tau^2 A^2\mathbf{u}_{xx}\right]_j^m + O(\tau^3).$$
4. Various difference schemes can be obtained by replacing the differential operators by appropriate difference operators.

The Lax-Wendroff Scheme and Its Stability Analysis

The Lax-Wendroff scheme (denote $\bar{\nu} = \tau / h$)

$$\mathbf{U}_j^{m+1} = \mathbf{U}_j^m - \frac{1}{2}\bar{\nu}\, A \left[\mathbf{U}_{j+1}^m - \mathbf{U}_{j-1}^m\right] + \frac{1}{2}\bar{\nu}^2 A^2 \left[\mathbf{U}_{j+1}^m - 2\mathbf{U}_j^m + \mathbf{U}_{j-1}^m\right].$$

1. Local truncation error $O(\tau^2 + h^2)$.
2. The Fourier mode: $\mathbf{U}_j^m = \lambda_k^m \begin{bmatrix} V \\ W \end{bmatrix} e^{\mathrm{i}kjh}$.
3. The characteristic equation:
$$\lambda_k \begin{bmatrix} V \\ W \end{bmatrix} = \left(I - 2\bar{\nu}^2 \sin^2 \frac{1}{2}kh\, A^2 - \mathrm{i}\bar{\nu} \sin kh\, A \right) \begin{bmatrix} V \\ W \end{bmatrix},$$
4. $\lambda_k = 1 - 2\nu^2 \sin^2 \frac{1}{2}kh \pm \mathrm{i}\nu \sin kh.$ (where $\nu = a\bar{\nu} = a\tau / h$)
5. $|\lambda_k|^2 = 1 - 4\nu^2(1-\nu^2)\sin^4 \frac{1}{2}kh \le 1 \Leftrightarrow |\nu| \le 1 \Leftrightarrow \mathbb{L}^2$ stable.
6. Dissipation, dispersion and group speed are the same as the Lax-Wendroff scheme for the scalar advection equation.

The Staggered Leap-frog Scheme

- The staggered leap-frog scheme:

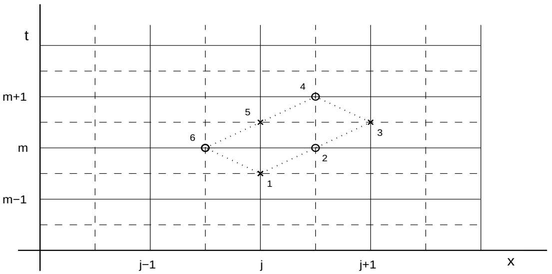
$$\frac{V_j^{m+\frac{1}{2}} - V_j^{m-\frac{1}{2}}}{\tau} + a\,\frac{W_{j+\frac{1}{2}}^m - W_{j-\frac{1}{2}}^m}{h} = 0, (\Leftrightarrow \delta_t V_j^m + \nu\,\delta_x W_j^m = 0)$$

$$\frac{W_{j+\frac{1}{2}}^{m+1} - W_{j+\frac{1}{2}}^m}{\tau} + a\,\frac{V_{j+1}^{m+\frac{1}{2}} - V_j^{m+\frac{1}{2}}}{h} = 0, (\Leftrightarrow \delta_t W_{j+\frac{1}{2}}^{m+\frac{1}{2}} + \nu\,\delta_x V_{j+\frac{1}{2}}^{m+\frac{1}{2}} = 0).$$

$$V_j^{m+\frac{1}{2}} = \tau^{-1}\delta_t U_j^{m+\frac{1}{2}},\ W_{j+\frac{1}{2}}^m = -a\,h^{-1}\delta_x U_{j+\frac{1}{2}}^m,\ \Rightarrow \left[\delta_t^2 - \nu^2\delta_x^2\right]\ U_j^m = 0.$$

$\circ$ for W

$\times$ for V



The Fourier Analysis of the Staggered Leap-frog Scheme

1. The Fourier mode for the staggered leap-frog scheme:

$$\begin{bmatrix} V_j^{m-\frac{1}{2}} \\ W_{j-\frac{1}{2}}^m \end{bmatrix} = \lambda_k^m \begin{bmatrix} \widehat{V}_k \\ \widehat{W}_k e^{-\mathrm{i}\frac{1}{2}kh} \end{bmatrix} e^{\mathrm{i}kjh}, \qquad \text{(where } \widehat{V}_k \text{ and } \widehat{W}_k \text{ are real numbers.)}$$

2. The characteristic equation:

$$\begin{bmatrix} \lambda_k - 1 & \mathrm{i}2\nu \sin \frac{1}{2}kh \\ \mathrm{i}2\lambda_k \nu \sin \frac{1}{2}kh & \lambda_k - 1 \end{bmatrix} \begin{bmatrix} \widehat{V}_k \\ \widehat{W}_k \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

3. $\lambda_k^2 - 2\left(1 - 2\nu^2 \sin^2 \frac{1}{2}kh\right)\lambda_k + 1 = 0.$ (Exactly as (3.5.18))

4. $\mathbb{L}^2$ stable $\Leftrightarrow |\nu| \le 1.$ There is no dissipation. If $|\nu| < 1$, there is a phase lag, and phase error is $O(k^2h^2)$.

5. Nothing special so far.

Local Energy Conservation of the Wave Equation

1. The mechanical energy of the system on (x_l, x_r):

$$E(x_l, x_r; t) = \int_{x_l}^{x_r} E(x,t)\,dx \triangleq \int_{x_l}^{x_r} \left[\frac{1}{2}v^2(x,t) + \frac{1}{2}w^2(x,t)\right] dx,$$

2. The only external forces exerted on (x_l, x_r) are $-a^2u_x(x_l,t) = aw(x_l,t)$ and $a^2u_x(x_r,t) = -aw(x_r,t)$.

3. The local energy conservation law (recall $v = u_t$):

$$\frac{dE(x_l, x_r; t)}{dt} = -av(x_r,t)w(x_r,t) + av(x_l,t)w(x_l,t).$$

Local Energy Conservation of the Wave Equation

Equivalently,

$$\left[\frac{1}{2}v^2(x,t)+\frac{1}{2}w^2(x,t)\right]_t+[av(x,t)w(x,t)]_x=0;$$

or $$\int_{\partial\omega}[f(v,w)\,dt-E(x,t)\,dx]=\int_{\omega}[E_t+f(v,w)_x]\,(x,t)\,dx\,dt=0,$$

where $E(x,t)=\frac{1}{2}(v^2(x,t)+w^2(x,t))$ is the mechanical energy of the system, and $f(v,w)=avw$ is the energy flux.

We will see that the staggered leap-frog scheme somehow inherits this property.

How Does the Discrete Mechanical Energy Change?

- The average operators σ_t and σ_x:

$$\sigma_t V_j^m = \frac{1}{2}\left(V_j^{m+\frac{1}{2}} + V_j^{m-\frac{1}{2}}\right),\ \sigma_x V_{j+\frac{1}{2}}^{m+\frac{1}{2}} = \frac{1}{2}\left(V_{j+1}^{m+\frac{1}{2}} + V_j^{m+\frac{1}{2}}\right).$$

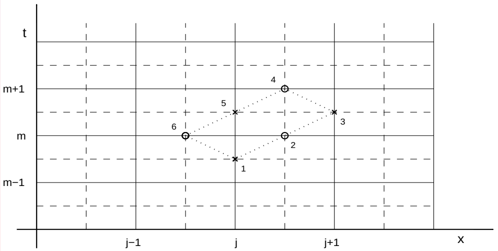
- Then, the solution of the staggered leap-frog scheme satisfies:

$$\delta_t\left[\frac{1}{2}\left(V_j^m\right)^2\right] + \nu\left[\left(\sigma_t V_j^m\right)\left(\delta_x W_j^m\right)\right] = 0,$$

$$\delta_t\left[\frac{1}{2}\left(W_{j+\frac{1}{2}}^{m+\frac{1}{2}}\right)^2\right] + \nu\left[\left(\sigma_t W_{j+\frac{1}{2}}^{m+\frac{1}{2}}\right)\left(\delta_x V_{j+\frac{1}{2}}^{m+\frac{1}{2}}\right)\right] = 0.$$

$\circ$ for W

$\times$ for V



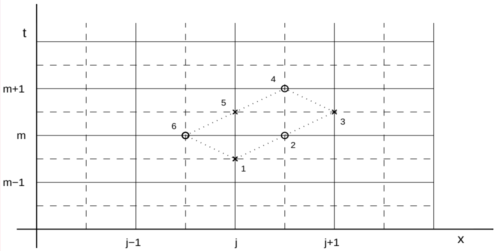
The Enclosed Path Integral of the Discrete Kinetic Energy $\int_{\partial\omega_j^m} \frac{1}{2} V^2 \, dx$

- The control volume ω_j^m is enclosed by the line segments connecting the nodes $\mathbf{j}_1$, $\mathbf{j}_2$, $\mathbf{j}_3$, $\mathbf{j}_4$, $\mathbf{j}_5$, $\mathbf{j}_6 = \mathbf{j}_0$ (as shownin figure).
- Calculate $-\int_{\partial\omega_j^m} \frac{1}{2} V^2 \, dx$ by applying the middle point quadrature rule on three broken line segments $\widehat{\mathbf{j}_0\mathbf{j}_1\mathbf{j}_2}$, $\widehat{\mathbf{j}_2\mathbf{j}_3\mathbf{j}_4}$ and $\overline{\mathbf{j}_4\mathbf{j}_5\mathbf{j}_6}$, yields

$$-\int_{\partial\omega_j^m} \frac{1}{2} V^2 \, dx = \frac{1}{2} h \left(V_j^{m+\frac{1}{2}} \right)^2 - \frac{1}{2} h \left(V_j^{m-\frac{1}{2}} \right)^2 = h\delta_t \left[\frac{1}{2} \left(V_j^m \right)^2 \right].$$

$\circ$ for W

$\times$ for V



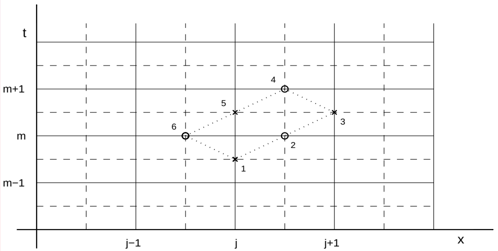
The Enclosed Path Integral of the Discrete Elastic Energy $\int_{\partial\omega_j^m} \frac{1}{2} W^2 \, dx$

- Calculate $-\int_{\partial\omega_j^m} \frac{1}{2} W^2 \, dx$ by applying the middle point quadrature rule on three broken line segments $\overline{\mathbf{j}_1\mathbf{j}_2\mathbf{j}_3}$, $\widehat{\mathbf{j}_3\mathbf{j}_4\mathbf{j}_5}$ and $\widehat{\mathbf{j}_5\mathbf{j}_6\mathbf{j}_1}$, yields

$$-\int_{\partial\omega_j^m} \frac{1}{2} W^2 \, dx = \frac{1}{2} h \left(W_{j+\frac{1}{2}}^{m+1} \right)^2 - \frac{1}{2} h \left(W_{j+\frac{1}{2}}^{m} \right)^2 = h\delta_t \left[\frac{1}{2} \left(W_{j+\frac{1}{2}}^{m+\frac{1}{2}} \right)^2 \right].$$

$\circ$ for W

$\times$ for V



The Enclosed Path Integral of the Discrete Energy Flux $\int_{\partial\omega_j^m} aVW\,dx$

Calculate $\int_{\partial\omega_j^m} aVW\,dx$ by applying the numerical quadrature rule on six broken line segments $\overline{\mathbf{j}_i\mathbf{j}_{i+1}}$, $i = 0, 1, 2, 3,\ 4, 5$, using node values of V and W on the broken line segments, yields

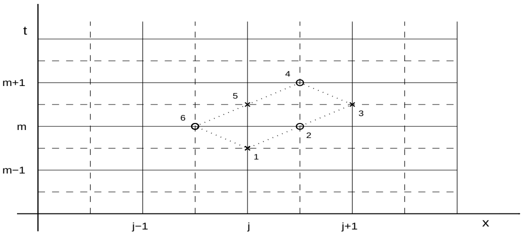
$$\int_{\partial\omega_j^m} aVW\,dt = \frac{1}{2}a\tau\left[V_j^{m-\frac{1}{2}}W_{j+\frac{1}{2}}^m + V_{j+1}^{m+\frac{1}{2}}W_{j+\frac{1}{2}}^m + V_{j+1}^{m+\frac{1}{2}}W_{j+\frac{1}{2}}^{m+1}\right]$$

$$-\frac{1}{2}a\tau\left[V_j^{m+\frac{1}{2}}W_{j+\frac{1}{2}}^{m+1} + V_j^{m+\frac{1}{2}}W_{j-\frac{1}{2}}^m + V_j^{m-\frac{1}{2}}W_{j-\frac{1}{2}}^m\right]$$

$$= a\tau\left[\left(\sigma_t V_j^m\right)\left(\delta_x W_j^m\right) + \left(\sigma_t W_{j+\frac{1}{2}}^{m+\frac{1}{2}}\right)\left(\delta_x V_{j+\frac{1}{2}}^{m+\frac{1}{2}}\right)\right].$$

$\circ$ for W

$\times$ for V



The Discrete Local Energy Conservation

Combine the above three equations, we obtain

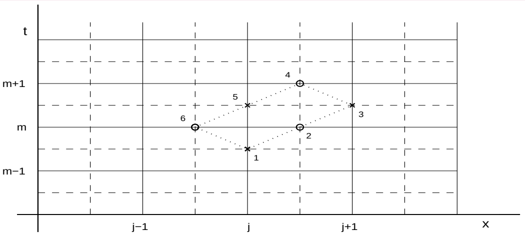
$$\int_{\partial\omega_j^m} \left[aVW\,dt - \left(\frac{1}{2}V^2 + \frac{1}{2}W^2\right)\,dx \right] = 0.$$

This is the discrete version of the local energy conservation law

$$\int_{\partial\omega} [f(v,w)\,dt - E(x,t)\,dx] = \int_{\omega} [E_t + f(v,w)_x]\,(x,t)\,dx\,dt = 0.$$

$\circ$ for W

$\times$ for V



习题 3：12，13；　上机作业 2

Thank You!