MSDM5004
Numerical Methods and Modeling in Science
Spring 2024

Lecture 8

Prof Yang Xiang
Hong Kong University of Science and Technology

Chapter 10

Numerical Methods for Partial Differential Equations (PDEs)

Numerical solution of partial differential equations: an introduction,
K.W. Morton and D. Mayers, 2nd ed., Cambridge University Press, 2005.

1. Parabolic PDEs

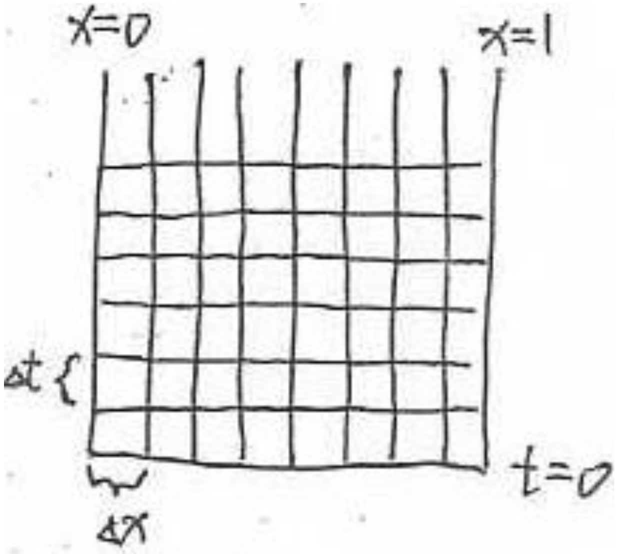
Diffusion equation, heat equation, …

1.1. Numerical scheme

An example

$$
\begin{aligned}
&\frac{\partial u}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t), \quad 0 < x < 1, \quad t > 0. \\
&u(0,t) = u(1,t) = 0, \quad t > 0 \\
&u(x,0) = u_0(x), \quad 0 \le x \le 1.
\end{aligned}
\tag{1}
$$

A grid (mesh)



Δx grid constant

Δt time step

(x_j, t_n) grid point

where $x_j = j\Delta x$, $t_n = n\Delta t$, $j = 0, 1, 2, \cdots J$, $n = 0, 1, 2, \cdots$.

Seek approximation of the solution $u(x, t)$ at grid points

$$U_j^n \approx u(x_j, t_n)$$

Approximation of derivatives

$$\frac{\partial u}{\partial t}(x_j, t_n) \approx \frac{u(x_j, t_{n+1}) - u(x_j, t_n)}{\Delta t}$$

Forward difference

$$\frac{\partial^2 u}{\partial x^2}(x_j, t_n) \approx \frac{u(x_{j+1}, t_n) - 2u(x_j, t_n) + u(x_{j-1}, t_n)}{(\Delta x)^2}$$

Central difference

Approximation of the equation

$$\frac{u(x_j, t_{n+1}) - u(x_j, t_n)}{\Delta t} \approx \frac{u(x_{j+1}, t_n) - 2u(x_j, t_n) + u(x_{j-1}, t_n)}{(\Delta x)^2}$$

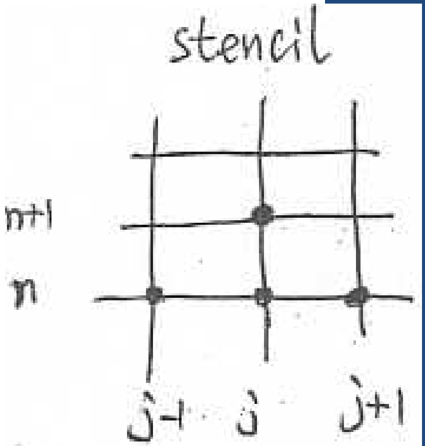
The numerical solution satisfies (numerical scheme)

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{(\Delta x)^2} \qquad (2)$$

Or

$$U_j^{n+1} = U_j^n + \mu(U_{j+1}^n - 2U_j^n + U_{j-1}^n) \qquad (3)$$

$$\mu := \frac{\Delta t}{(\Delta x)^2}$$



This is an explicit scheme.

$$U_j^0 = u^0(x_j),\ j = 1, 2, \ldots, J-1,$$

$$U_0^n = U_J^n = 0,\ n = 0, 1, 2, \ldots,$$

Compute values at time level t_{n+1} from values at time level t_n

$$U_j^0,\ 0\le j\le J \Longrightarrow U_j^1,\ 0<j<J \Longrightarrow U_j^2,\ 0<j<J \Rightarrow \cdots$$

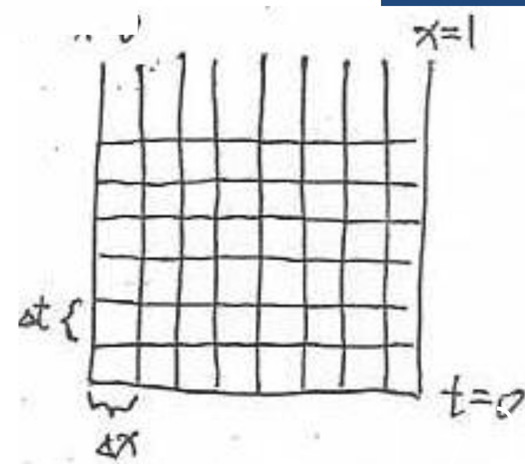
initial condition $\qquad U_0^1,\ U_J^1 \qquad U_0^2,\ U_J^2$

$$\cdots \Rightarrow U_j^n,\ 0<j<J \Longrightarrow U_j^{n+1},\ 0<j<J \Longrightarrow \cdots$$

$U_0^n,\ U_J^n \qquad U_0^{n+1},\ U_J^{n+1}$

Explicit scheme: direct calculation

(no need to solve linear system)



1.2 Truncation error and consistency

The numerical scheme
$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{(\Delta x)^2}$$

is an approximation to the PDE
$$\frac{\partial u}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t),$$

Error of this approximation: truncation error

Truncation error

$$T(x_j, t_n) = \frac{u(x_j, t_{n+1}) - u(x_j, t_n)}{\Delta t} - \frac{u(x_{j+1}, t_n) - 2u(x_j, t_n) + u(x_{j-1}, t_n)}{(\Delta x)^2}$$

-- Replace the numerical solution by the exact solution in a numerical scheme.

Using Taylor expansion at (x_j, t_n)

$$u(x_j, t_{n+1}) = u(x_j, t_n) + \frac{\partial u}{\partial t}(x_j, t_n)\Delta t + \frac{1}{2}\frac{\partial^2 u}{\partial t^2}(x_j, t_n)\Delta t^2 + O(\Delta t^3)$$

$$\frac{u(x_j, t_{n+1}) - u(x_j, t_n)}{\Delta t} = \frac{\partial u}{\partial t}(x_j, t_n) + \frac{1}{2}\frac{\partial^2 u}{\partial t^2}(x_j, t_n)\Delta t + O(\Delta t^2)$$

$$f(x) = O(g(x)),\ x \to x_0$$

$\Longleftrightarrow$ $|f(x)| \le M|g(x)|$ in a neighborhood of x_0 for some constant M

$$u(x_{j+1},t_n) = u(x_j,t_n)+\frac{\partial u}{\partial x}(x_j,t_n)\Delta x+\frac{1}{2}\frac{\partial^2 u}{\partial x^2}(x_j,t_n)\Delta x^2+\frac{1}{6}\frac{\partial^3 u}{\partial x^3}(x_j,t_n)\Delta x^3$$

$$+\frac{1}{24}\frac{\partial^4 u}{\partial x^4}(x_j,t_n)\Delta x^4 + O(\Delta x^5)$$

$$u(x_{j-1},t_n) = u(x_j,t_n)-\frac{\partial u}{\partial x}(x_j,t_n)\Delta x+\frac{1}{2}\frac{\partial^2 u}{\partial x^2}(x_j,t_n)\Delta x^2-\frac{1}{6}\frac{\partial^3 u}{\partial x^3}(x_j,t_n)\Delta x^3$$

$$+\frac{1}{24}\frac{\partial^4 u}{\partial x^4}(x_j,t_n)\Delta x^4 + O(\Delta x^5)$$

$$\frac{u(x_{j+1},t_n) - 2u(x_j,t_n) + u(x_{j-1},t_n)}{(\Delta x)^2}$$

$$= \frac{\partial^2 u}{\partial x^2}(x_j,t_n)+\frac{1}{12}\frac{\partial^4 u}{\partial x^4}(x_j,t_n)\Delta x^2+O(\Delta x^3)$$

Therefore

$$T(x_j,t_n) = \frac{\partial u}{\partial t}(x_j,t_n) - \frac{\partial^2 u}{\partial x^2}(x_j,t_n)$$

$$+\frac{1}{2}\frac{\partial^2 u}{\partial t^2}(x_j,t_n)\Delta t - \frac{1}{12}\frac{\partial^4 u}{\partial x^4}(x_j,t_n)\Delta x^2 + O(\Delta t^2) + O(\Delta x^3)$$

Since $u(x_j,t_n)$ is the exact solution, $\frac{\partial u}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t),$

$$T(x_j,t_n) = \frac{1}{2}\frac{\partial^2 u}{\partial t^2}(x_j,t_n)\Delta t - \frac{1}{12}\frac{\partial^4 u}{\partial x^4}(x_j,t_n)\Delta x^2 + O(\Delta t^2) + O(\Delta x^3).$$

- First order (accurate) in *t* (time)
- Second order (accurate) in *x* (space)

The truncation error

$$T(x_j, t_n) \to 0, \text{ as } \Delta t, \Delta x \to 0$$

We say that the numerical scheme is consistent with the PDE.

Moreover, it can be shown that

$$T(x_j, t_n) = \frac{1}{2}\frac{\partial^2 u}{\partial t^2}(x_j, \eta)\Delta t - \frac{1}{12}\frac{\partial^4 u}{\partial x^4}(\xi, t_n)(\Delta x)^2$$

$$\eta \in (t_n, t_n + \Delta t),\ \xi \in (x_j - \Delta x, x_j + \Delta x)$$

If $u(x, t)$ is smooth, there exist constants M_{tt} and M_{xxxx}, such that

$$\left|\frac{\partial^2 u}{\partial t^2}(x, t)\right| \le M_{tt}, \quad \left|\frac{\partial^4 u}{\partial x^4}(x, t)\right| \le M_{xxxx}, \quad \text{for } 0 \le x \le 1,\ 0 \le t \le t_F.$$

Therefore, we have $$T(x_j, t_n) \le \frac{1}{2}M_{tt}\Delta t + \frac{1}{12}M_{xxxx}(\Delta x)^2$$

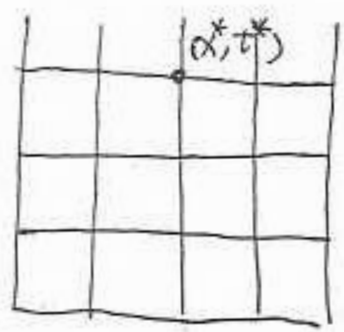
$$\text{for } 0 \le x \le 1,\ 0 \le t \le t_F.$$

1.3 Convergence

A numerical scheme is convergent if

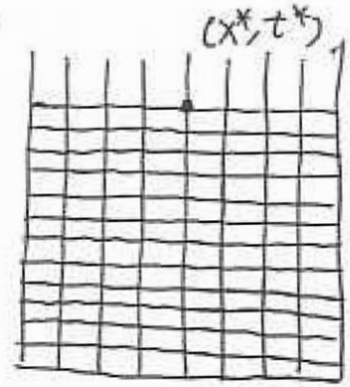
for any fixed point $(x^*, t^*) \in (0, 1) \times (0, t_F)$

$$U_j^n \to u(x^*, t^*) \quad \text{as } \Delta x \to 0,\ \Delta t \to 0 \text{ and } x_j \to x^*,\ t_n \to t^*.$$



$\Delta x_1, \Delta t_1$ $\quad \begin{cases} x^* = j_1 \Delta x_1 \\ t^* = n_1 \Delta t_1 \end{cases}$

$U_{j_1}^{n_1} \approx u(x^*, t^*)$



smaller Δx, Δt

$\Delta x_2 = \frac{1}{2}\Delta x_1$

$\Delta t_2 = \frac{1}{4}\Delta t_1$

$\begin{cases} x^* = j_2 \Delta x_2 \\ t^* = n_2 \Delta t_2 \end{cases}$

$U_{j_2}^{n_2} \approx u(x^*, t^*)$ $\quad j_2 = 2 j_1$

$n_2 = 4 n_1$

Convergence of the explicit method

Theorem

The explicit scheme
$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{(\Delta x)^2}$$

is convergent if

$$\mu = \frac{\Delta t}{(\Delta x)^2} \le \frac{1}{2}.$$

Proof

Define the error $e_j^n = U_j^n - u(x_j, t_n)$.

The numerical scheme is

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{(\Delta x)^2}$$

The exact solution satisfies

$$\frac{u(x_j, t_{n+1}) - u(x_j, t_n)}{\Delta t} - \frac{u(x_{j+1}, t_n) - 2u(x_j, t_n) + u(x_{j-1}, t_n)}{(\Delta x)^2} = T(x_j, t_n)$$

Subtract the second equation from the first one,

$$\frac{e_j^{n+1} - e_j^n}{\Delta t} - \frac{e_{j+1}^n - 2e_j^n + e_{j-1}^n}{(\Delta x)^2} = -T_j^n \qquad (T_j^n = T(x_j, t_n))$$

Multiplying both sides by Δt and using $\mu = \frac{\Delta t}{(\Delta x)^2}$,

$$\begin{aligned} e_j^{n+1} =& e_j^n + \mu\left(e_{j+1}^n - 2e_j^n + e_{j-1}^n\right) - \Delta t T_j^n \\ =& \mu e_{j+1}^n + (1-2\mu)e_j^n + \mu e_{j-1}^n - \Delta t T_j^n. \end{aligned}$$

Thus, if $\mu \le \frac{1}{2}$,

$$\begin{aligned} |e_j^{n+1}| \le& \mu|e_{j+1}^n| + |1-2\mu||e_j^n| + \mu|e_{j-1}^n| + \Delta t|T_j^n| \\ =& \mu|e_{j+1}^n| + (1-2\mu)|e_j^n| + \mu|e_{j-1}^n| + \Delta t|T_j^n| \end{aligned}$$

Let $$E^n = \max_{0\le j\le J} |e_j^n|,$$

$$\bar{T} = \max_{0\le j\le J,\ n\Delta t\le t_F} |T_j^n| = \frac{1}{2}M_{tt}\Delta t + \frac{1}{12}M_{xxxx}(\Delta x)^2$$

Then

$$\begin{aligned} |e_j^{n+1}| \le& \mu|E^n| + (1-2\mu)|E^n| + \mu|E^n| + \Delta t\bar{T} \\ =& E^n + \Delta t\bar{T}. \end{aligned}$$

Since this inequality holds for all j, we have

$$E^{n+1} \le E^n + \Delta t\bar{T}.$$

Therefore,

$$
\begin{aligned}
E^n \leq & E^{n-1} + \Delta t \bar{T} \\
\leq & (E^{n-2} + \Delta t \bar{T}) + \Delta t \bar{T} \\
= & E^{n-2} + 2\Delta t \bar{T} \\
& \cdots \\
\leq & E^0 + n\Delta t \bar{T} \\
\leq & t_F \bar{T} \quad (E^0 = 0) \\
= & t_F \left[\frac{1}{2} M_{tt} \Delta t + \frac{1}{12} M_{xxxx} (\Delta x)^2 \right] \\
\to & 0, \quad \text{as } \Delta x, \ \Delta t \to 0.
\end{aligned}
$$

This means that the numerical scheme is convergent.

If $\mu = \frac{\Delta t}{(\Delta x)^2}$ is constant,

$$|U_j^n - u(x_j, t_n)| = |e_j^n| \leq E^n \leq t_F \left[\frac{1}{2} M_{tt}\mu + \frac{1}{12} M_{xxxx}\right] (\Delta x)^2$$

Refinement path

A sequence $\{(\Delta x_i, \Delta t_i),\ i = 0, 1, 2, \cdots,\ \Delta x_i, \Delta t_i \to 0\}$

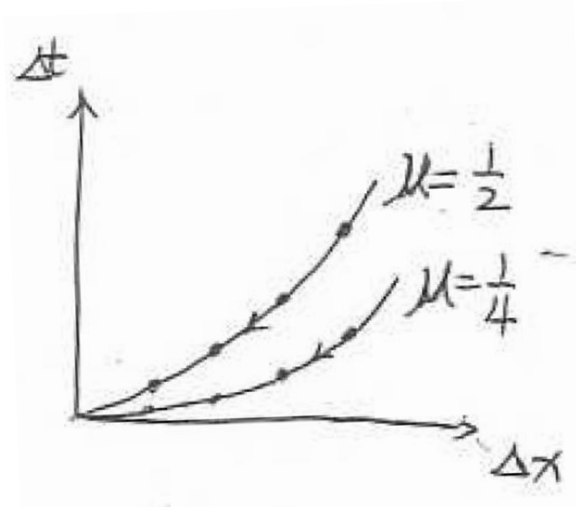
If $\mu_i = \dfrac{\Delta t_i}{(\Delta x_i)^2} \le \dfrac{1}{2}$,

then $\{U_{j_i}^{n_i}\}$, $i = 0, 1, 2, \cdots$, converges to $u(x^*, t^*)$,

where $x^* = j_i \Delta x_i$, $t^* = n_i \Delta t_i$.

Commonly used:

$$\mu = \frac{\Delta t}{(\Delta x)^2} = \text{constant} \le \frac{1}{2}.$$



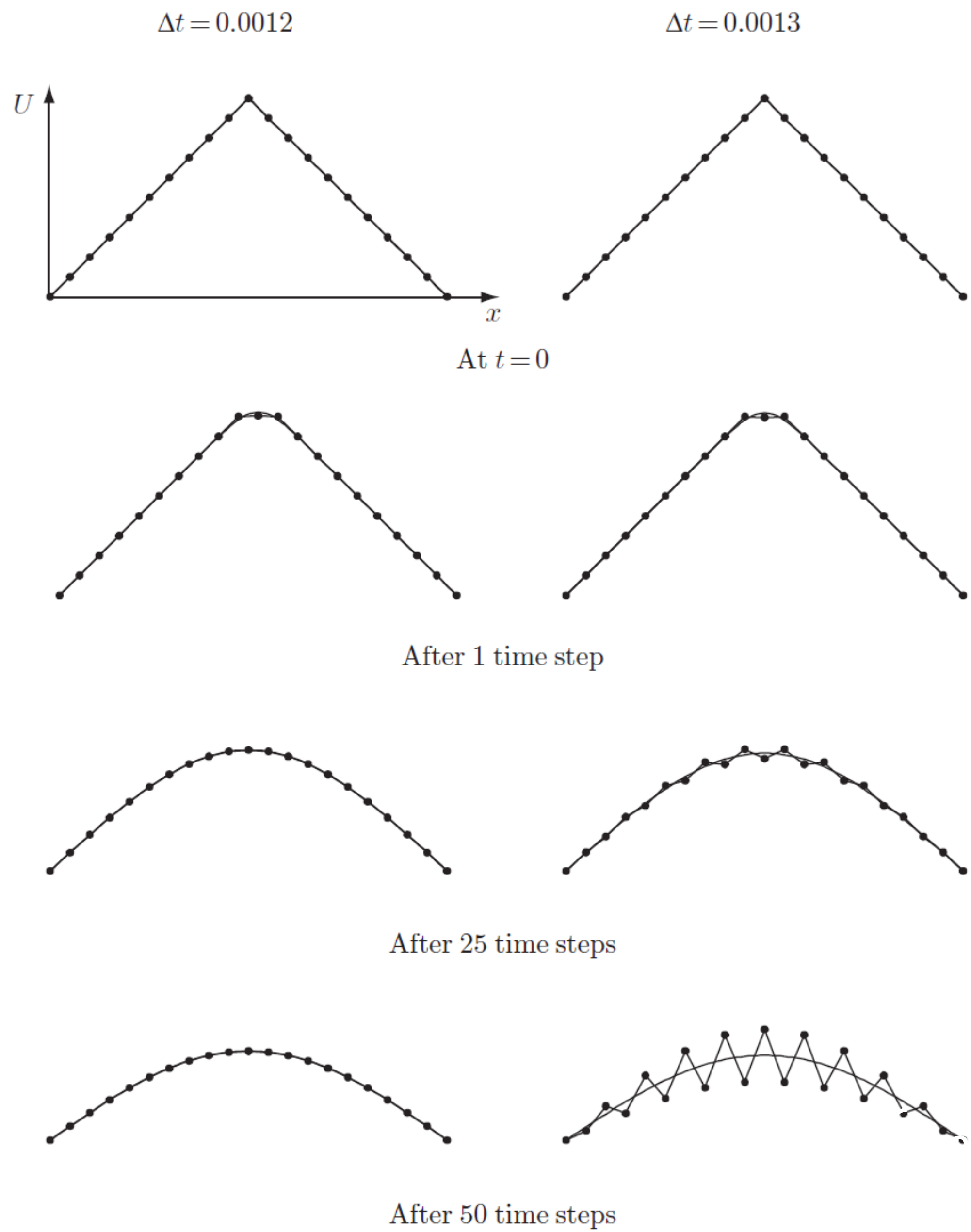
An example

$$u^0(x) = \begin{cases} 2x & \text{if} \quad 0 \le x \le \frac{1}{2}, \\ 2-2x & \text{if} \quad \frac{1}{2} \le x \le 1. \end{cases}$$

$$J = 20, \; \Delta x = 0.05.$$

$$\text{When} \qquad \mu = \frac{\Delta t}{(\Delta x)^2} = \frac{1}{2}$$

$$\Delta t = 0.00125$$



Remark

The exact solution of the problem

$$\frac{\partial u}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t), \quad 0 < x < 1, \quad t > 0.$$

$$u(0,t) = u(1,t) = 0, \quad t > 0$$

$$u(x,0) = u_0(x), \quad 0 \leq x \leq 1.$$

is (can be found by method of separation of variables)

$$u(x,t) = \sum_{m=1}^{\infty} a_m \mathrm{e}^{-(m\pi)^2 t} \sin m\pi x$$

$$a_m = 2\int_0^1 u^0(x) \sin m\pi x \, \mathrm{d}x.$$

1.4. Stability

A numerical scheme (for a linear PDE) is stable if

$$\|\mathbf{U}^n\| \leq K\|\mathbf{U}^0\| \qquad \text{(any norm)}$$

where *K* is a constant.

Here $\mathbf{U}^n$ denotes the vector formed by $\{U_j^n\}$

Fourier analysis

For the numerical scheme

$$U_j^{n+1} = U_j^n + \mu(U_{j+1}^n - 2U_j^n + U_{j-1}^n) \qquad \mu = \frac{\Delta t}{(\Delta x)^2}$$

Assume $\quad U_j^n = [\lambda(k)]^n e^{ik(j\Delta x)}$

$\lambda(k)$ is a number depending on k

Substitute it into the scheme

$$[\lambda(k)]^{n+1} e^{ik(j\Delta x)} = [\lambda(k)]^n e^{ik(j\Delta x)} +$$
$$+\mu\left([\lambda(k)]^n e^{ik((j+1)\Delta x)} - 2[\lambda(k)]^n e^{ik(j\Delta x)} + [\lambda(k)]^n e^{ik((j-1)\Delta x)}\right)$$

Dividing both sides by $[\lambda(k)]^n e^{ik(j\Delta x)}$

$$\begin{aligned}\lambda(k) &= 1 + \mu\left(\mathrm{e}^{\mathrm{i}k\Delta x} - 2 + \mathrm{e}^{-\mathrm{i}k\Delta x}\right) \\ &= 1 - 2\mu(1 - \cos k\Delta x) \\ &= 1 - 4\mu \sin^2 \tfrac{1}{2}k\Delta x;\end{aligned}$$

$\lambda(k)$ is called the *amplification factor* for the mode.

A numerical scheme (for a linear PDE) is stable if

$$|[\lambda(k)]^n| \leq K, \quad \text{for} \quad n\Delta t \leq t_F, \ \forall k.$$

where *K* is a constant.

Since

$$0 \le \sin^2 \frac{k\Delta x}{2} \le 1$$

$$0 \le 4\mu \sin^2 \frac{k\Delta x}{2} \le 4\mu$$

$$1 - 4\mu \le 1 - 4\mu \sin^2 \frac{k\Delta x}{2} \le 1$$

$$\left| 1 - 4\mu \sin^2 \frac{k\Delta x}{2} \right| \le \max\{1, |1 - 4\mu|\}$$

Note that the maximum may be achieved when $k = J\pi/L$

$$\sin \frac{k\Delta x}{2} = \sin \frac{\pi}{2} = 1$$

$$\left| 1 - 4\mu \sin^2 \frac{k\Delta x}{2} \right| = |1 - 4\mu|$$

$$\left|1 - 4\mu \sin^2 \frac{k\Delta x}{2}\right|^n \quad \text{is bounded}$$

if and only if $$\left|1 - 4\mu \sin^2 \frac{k\Delta x}{2}\right| \le 1$$

if and only if $$|1 - 4\mu| \le 1$$

if and only if $$\mu \le \frac{1}{2}.$$

Therefore, the explicit scheme is stable if and only if

$$\mu \le \frac{1}{2}.$$

For a general initial condition $u_0(x)$, we have

$$u_0(x) = \sum_k C_k e^{ikx}$$

Thus

$$u_j^0 = \sum_k C_k e^{ik(j\Delta x)}$$

Solution of a linear scheme has the form

$$u_j^n = \sum_k C_k [\lambda(k)]^n e^{ik(j\Delta x)}.$$

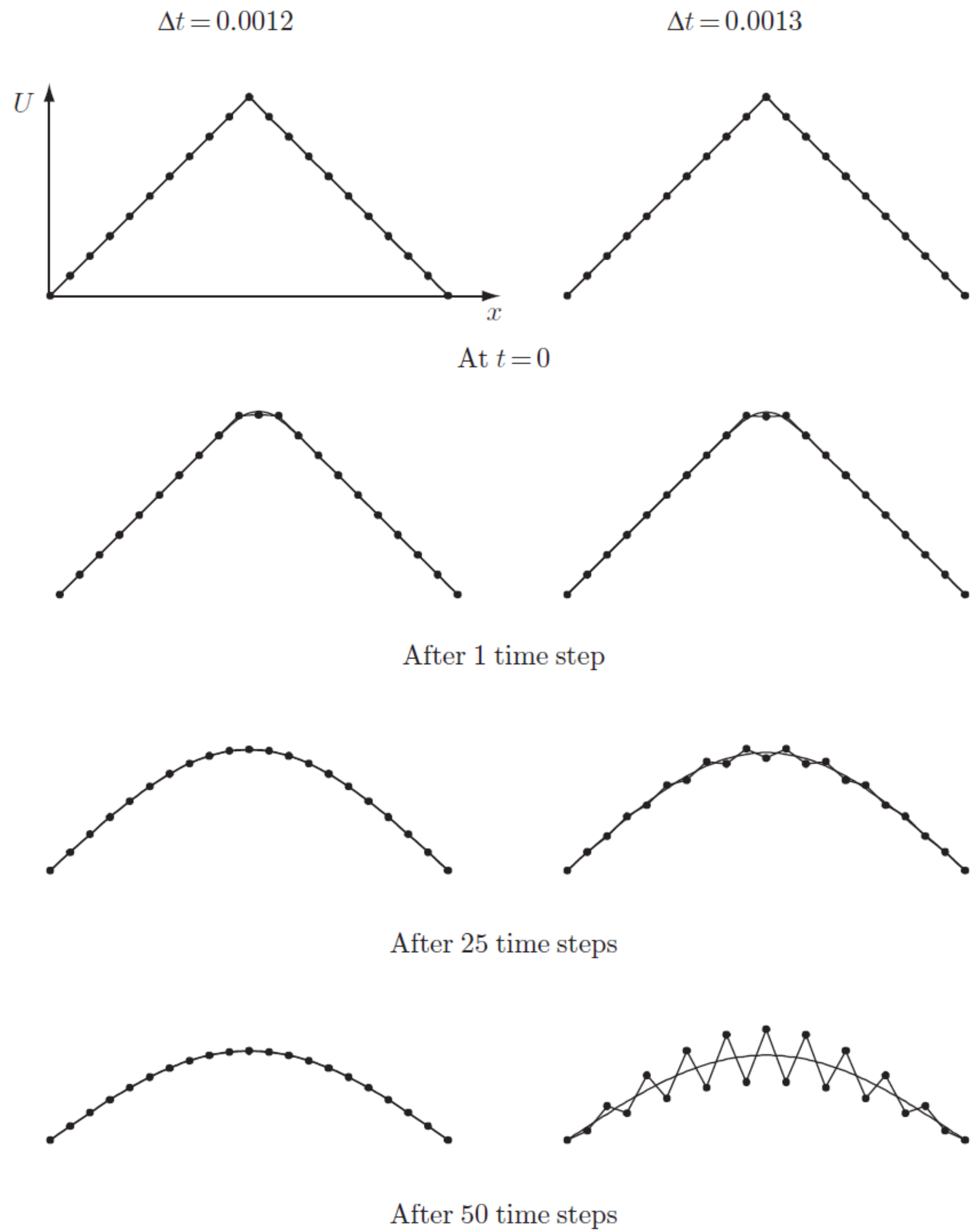
An example

$$u^0(x) = \begin{cases} 2x & \text{if} \quad 0 \le x \le \frac{1}{2}, \\ 2 - 2x & \text{if} \quad \frac{1}{2} \le x \le 1. \end{cases}$$

$$J = 20, \ \Delta x = 0.05.$$

$$\text{When} \qquad \mu = \frac{\Delta t}{(\Delta x)^2} = \frac{1}{2}$$

$$\Delta t = 0.00125$$



Stability condition is satisfied

Stability condition is not satisfied