

# Numerical Solutions to Partial Differential Equations

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School of Mathematical Sciences  
Peking University

# The Crank-Nicolson scheme

$$\frac{U_j^{m+1} - U_j^m}{\tau} = \frac{1}{2} \left[ \frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{h^2} + \frac{U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}}{h^2} \right]; \quad (2.2.56)$$

$$(1 + \mu)U_j^{m+1} = (1 - \mu)U_j^m + \frac{\mu}{2} \left( U_{j-1}^m + U_{j+1}^m + U_{j-1}^{m+1} + U_{j+1}^{m+1} \right) \quad (2.2.60)$$

$$\textcircled{1} \quad T_j^{m+\frac{1}{2}} = -\frac{1}{12} \left[ u_{ttt}(x_j, \eta) \tau^2 + u_{xxxx}(\xi, t_{m+\frac{1}{2}}) h^2 \right]; \quad (2.2.57)$$

$$\textcircled{2} \quad \lambda_k = \left[ 1 - 2\mu \sin^2 \frac{k\pi\Delta x}{2} \right] / \left[ 1 + 2\mu \sin^2 \frac{k\pi\Delta x}{2} \right], \text{ thus} \quad (2.2.59)$$

unconditionally  $\mathbb{L}^2$  stable.

③ The computational cost is about twice that of the explicit scheme if solved by the Thompson method.

④ The maximum principle holds for  $\mu \leq 1$ .

⑤ Convergence rate is  $O(\tau^2 + h^2)$ , efficient if  $\tau = O(h)$ .

# The $\theta$ -scheme ( $0 < \theta < 1$ , $\theta \neq 1/2$ )

$$\frac{U_j^{m+1} - U_j^m}{\tau} = (1 - \theta) \frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{h^2} + \theta \frac{U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}}{h^2}; \quad (2.2.61)$$

$$(1 + 2\mu\theta)U_j^{m+1} = (1 - 2\mu(1 - \theta))U_j^m + \mu(1 - \theta)(U_{j-1}^m + U_{j+1}^m) + \mu\theta(U_{j-1}^{m+1} + U_{j+1}^{m+1}). \quad (2.2.64)$$

①  $T_j^{m+\frac{1}{2}} = O(\tau^2 + h^4)$ , if  $\theta = \frac{1}{2} - \frac{1}{12\mu}$ ;  $= O(\tau + h^2)$ , otherwise. (2.2.66)

②  $\lambda_k = \left[ 1 - 4(1 - \theta)\mu \sin^2 \frac{k\pi\Delta x}{2} \right] / \left[ 1 + 4\theta\mu \sin^2 \frac{k\pi\Delta x}{2} \right]$ , thus (2.2.62)

$\mathbb{L}^2$  stable for  $2\mu(1 - 2\theta) \leq 1$  (unconditional for  $\theta \geq 1/2$ ). (2.2.63)

③ The maximum principle holds for  $2\mu(1 - \theta) \leq 1$ . (2.2.65)

# The maximum principle and $L^\infty$ stability and convergence

**Remark 1:** For a finite difference scheme,  $L^2$  stability conditions are generally weaker than  $L^\infty$  stability conditions.

**Remark 2:** The maximum principle is only a sufficient condition for  $L^\infty$  stability. A finite difference scheme can be  $L^\infty$  stable, but does not satisfy the maximum principle.

**Remark 3:** Under certain circumstances, for parabolic problems,  $L^2$  stability and convergence can lead to  $L^\infty$  stability and convergence (see page 45-46, conclusion 2.6 for an example).

# The maximum principle and $L^\infty$ stability and convergence

**Remark 4:** In applications, it is safe to use  $L^2$  stability if the data involved is smooth with high frequencies modes decay fast, otherwise, use the maximum principle conditions until it is such.

在计算中，如果数据平滑且高频模式衰减快，则使用 $L^2$ 稳定性是安全的；否则，使用最大原则条件，直到它是这样的。

**Remark 5:** In general applications, it should be safe to use the Crank-Nicolson scheme with  $\mu = 1/2$  initially, since then, for the high frequency modes,  $\lambda_k \sim \frac{\pi^2}{4} \left(\frac{N-k}{N}\right)^2$ , and the high frequency modes will decay fast in limited steps, and it will be safe to use arbitrary  $\mu$  afterwards. Notice also that,  $\lambda_{\frac{N}{2}} = \frac{1}{3}$  and  $0 \leq \lambda_k < \lambda_{\frac{N}{2}}$  if  $\frac{N}{2} < k \leq N$ .

# The Variable-coefficient Linear Heat Equation

## 2.3.1节, P52

Consider the variable-coefficient linear heat equation:

$$u_t = a(x, t)u_{xx}, \quad (2.3.1)$$

with the homogeneous Dirichlet boundary condition, where  $a(x, t) \geq a_0 > 0$  is a given real function.

The 1st order forward explicit scheme:

$$\frac{U_j^{m+1} - U_j^m}{\tau} = a_j^m \frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{h^2}, \quad (2.3.2)$$

where  $a_j^m = a(x_j, t_m)$ , or equivalently

$$U_j^{m+1} = (1 - 2\mu_j^m)U_j^m + \mu_j^m (U_{j+1}^m + U_{j-1}^m), \quad (2.3.3)$$

where  $\mu_j^m = a_j^m \tau / h^2$ .

# Explicit Scheme for Variable-coefficient Heat Equation

- ① The **truncation operator** of the explicit scheme is

$$T(x, t) = \left[ \frac{\Delta_{+t}}{\Delta t} - a(x, t) \frac{\delta_x^2}{(\Delta x)^2} \right] - [\partial_t - a(x, t) \partial_x^2].$$

- ② The **local truncation error** is

$$Tu(x, t) = \frac{1}{2} u_{tt}(x, \eta) \tau - a(x, t) \frac{1}{12} u_{xxxx}(\xi, t) h^2 = O(\tau + h^2).$$

- ③ Denote  $\mu_j^m = a_j^m \tau / h^2$ , the **error equation** is

$$e_j^{m+1} = (1 - 2\mu_j^m) e_j^m + \mu_j^m (e_{j+1}^m + e_{j-1}^m) - \tau T_j^m. \quad (2.3.4)$$

- ④ The **maximum principle** holds on  $\bar{\Omega}_{t_{\max}} = [0, 1] \times [0, t_{\max}]$ , if

$$\mu(x, t) \equiv a(x, t) \frac{\tau}{h^2} \leq \frac{1}{2}, \quad \forall (x, t) \in \bar{\Omega}_{t_{\max}}. \quad (2.3.5)$$

- ⑤ Variable-coefficient schemes **do not have Fourier modes solutions**, so, the **Fourier analysis method does not apply**. However, necessary conditions for  $\mathbb{L}^2$  stability can be derived by **local Fourier analysis**.

# $\theta$ -scheme for Variable-coefficient Heat Equation

①  $U_j^{m+1} = U_j^m + \mu_j^{m*} \left[ \theta \delta_x^2 U_j^{m+1} + (1 - \theta) \delta_x^2 U_j^m \right] + \tau f_j^{m*}$ , where (2.3.7)  
 $\mu_j^{m*} = \mu_j^{m+\theta}$ , if  $\theta = 0, 1$ ; and  $\mu_j^{m*} = \mu_j^{m+\frac{1}{2}}$ , if  $0 < \theta < 1$ .

② The local truncation error is

$$T_j^{m+*} = \begin{cases} O(\tau^2 + h^2), & \text{if } \theta = \frac{1}{2}, \\ O(\tau + h^2), & \text{if } \theta \neq \frac{1}{2}. \end{cases} \quad (2.3.8)$$

③ The maximum principle holds on  $\overline{\Omega}_{t_{\max}} = [0, 1] \times [0, t_{\max}]$ , if  $\mu(x, t) (1 - \theta) \equiv a(x, t) \frac{\tau}{h^2} (1 - \theta) \leq \frac{1}{2}$ ,  $\forall (x, t) \in \overline{\Omega}_{t_{\max}}$ . (2.3.9)



## $\theta$ -Scheme for $u_t = (a(x, t)u_x)_x$ — in Conservation Form

(2.3.10)  $\Rightarrow$

① The integral form of the equation

$$\int_{x_l}^{x_r} [u(x, t_a) - u(x, t_b)] dx = \int_{t_b}^{t_a} [a(x_r, t)u_x(x_r, t) - a(x_l, t)u_x(x_l, t)] dt, \quad (2.3.12)$$
$$\forall 0 \leq x_l < x_r, \quad \forall t_a > t_b \geq 0,$$

② Take the control volume  $x_l = x_{j-\frac{1}{2}}$ ,  $x_r = x_{j+\frac{1}{2}}$ ,  $t_b = t_m$ ,  $t_a = t_{m+1}$ , and apply middle point quadrature rules;

③ The corresponding  $\theta$ -scheme

$$U_j^{m+1} = U_j^m + \theta \left[ \mu_{j+\frac{1}{2}}^{m+*} (U_{j+1}^{m+1} - U_j^{m+1}) - \mu_{j-\frac{1}{2}}^{m+*} (U_j^{m+1} - U_{j-1}^{m+1}) \right] \\ + (1 - \theta) \left[ \mu_{j+\frac{1}{2}}^{m+*} (U_{j+1}^m - U_j^m) - \mu_{j-\frac{1}{2}}^{m+*} (U_j^m - U_{j-1}^m) \right]. \quad (2.3.11)$$

# Explicit Scheme for $u_t = a(u)u_{xx}$ (with $a(\cdot) \geq a_0 > 0$ )

(2.3.13) ==&gt;

- ① The 1st order forward explicit difference scheme is given as

$$U_j^{m+1} = U_j^m + \bar{\mu} a(U_j^m) (U_{j+1}^m - 2U_j^m + U_{j-1}^m), \quad (2.3.14)$$

where  $\bar{\mu} = \tau/h^2$  is the coefficient independent grid ratio.

- ② The maximum principle holds, if

$$\bar{\mu} \left[ \max_{(x_j, t_m) \in \Omega_{t_{\max}}} a(U_j^m) \right] \leq \frac{1}{2}. \quad (2.3.15)$$

- ③ Substituting the real solution  $u$  into the scheme, we have

$$u_j^{m+1} = u_j^m + \bar{\mu} a(u_j^m) (u_{j+1}^m - 2u_j^m + u_{j-1}^m) + \tau T_j^m. \quad (2.3.16)$$

where the local truncation error is again  $T_j^m = O(\tau + h^2)$ .

# Error Equation of Explicit Scheme in Nonlinear Case

④ Taylor expanding  $a(u_j^m)$  at  $U_j^m$  leads to  
$$a(u_j^m) = a(U_j^m) + a'(\eta_j^m)(u_j^m - U_j^m) = a(U_j^m) - a'(\eta_j^m) e_j^m.$$

⑤ The error equation

$$e_j^{m+1} = e_j^m + \bar{\mu} a(U_j^m) (e_{j+1}^m - 2e_j^m + e_{j-1}^m) - \tau T_j^m \\ + \bar{\mu} a'(\eta_j^m) e_j^m (u_{j+1}^m - 2u_j^m + u_{j-1}^m). \quad (2.3.17)$$

Nonlinear  $\theta$ -scheme and its consistency and stability can also be established in a similar way.

Note, because of the extra term in the error equation, the stability and consistency are not sufficient to guarantee convergence.


Under certain additional conditions, the difference schemes for the nonlinear equations do converge, but the errors can often be significantly larger than in the linear case (see Exercise 2.16).

# Semi-discrete Methods of Parabolic Equations

## 2.3.2节, P56

The idea of **semi-discrete methods** (or the **method of lines**) is to discretize the equation  $-L(u) = f - u_t$  as if it is an elliptic equation, *i.e.* for a fixed  $t$ , we

- ① introduce a spatial grid  $J_\Omega$  on  $\Omega$ ;
- ② introduce spatial grid functions  $U_h(t) = \{U_j(t)\}_{j \in J_\Omega}$  and  $f_h = \{f_j(t)\}_{j \in J_\Omega}$ ;
- ③ approximate the differential operator  $L$  by a corresponding difference operator  $L_h$ .

The method of lines (MOL, NMOL, NUMOL) is a technique for solving partial differential equations (PDEs) in which all but one dimension is discretized as a system of ODEs or DAEs. A significant advantage of the method is that it allows the solution to take advantage of the sophisticated general-purpose methods and software that  been developed for numerically integrating ODEs and DAEs.

# Semi-discrete Methods of Parabolic Equations

The procedure transforms an initial-boundary value problem of the parabolic partial differential equation into an initial problem of a system of ordinary differential equations on the grid nodes  $J_\Omega$ :

$$U'_j(t) = L_h(U_h(t))_j + f_j(t), \quad \forall j \in J_\Omega, \quad (2.3.19)$$

$$U_j(0) = u(x_j, 0), \quad \forall j \in J_\Omega. \quad (2.3.20)$$

# Convergence Analysis of Semi-discrete Methods

For linear problems, the convergence analysis of semi-discrete methods is similar **as** that of the finite difference methods, *i.e.*

- ① analyze the **consistency** of the approximation by calculating the local truncation error via Taylor series expansions;
- ② analyze the **stability** of the semi-discrete system of the ordinary differential equations (the uniformly well-posedness of the semi-discrete problem).

## An Example of the Semi-discrete Method

Consider the 1D heat equation on  $(0, 1)$  with homogeneous Dirichlet boundary condition.

- Let  $h = 1/N$ , on the spatial grid  $x_j = j/N$ ,  $j = 0, 1, \dots, N$ ;
- substitute  $\partial^2/\partial x^2$  by  $\delta_x^2/h^2$ .

The corresponding initial problem of a system of ordinary differential equations:

$$U_j'(t) = N^2 [U_{j+1}(t) - 2U_j(t) + U_{j-1}(t)], \quad t > 0, \quad 1 \leq j \leq N-1, \quad (2.3.21)$$

$$U_0(t) = U_N(t) = 0, \quad t > 0, \quad (2.3.22)$$

$$U_j(0) = u(x_j, 0), \quad 1 \leq j \leq N-1. \quad (2.3.23)$$

# An Example of the Semi-discrete Method

The initial problem of a system of ordinary differential equations:

$$\begin{aligned} U'_j(t) &= N^2 [U_{j+1}(t) - 2U_j(t) + U_{j-1}(t)], \quad t > 0, \quad 1 \leq j \leq N-1, \\ U_0(t) &= U_N(t) = 0, \quad t > 0, \\ U_j(0) &= u(x_j, 0), \quad 1 \leq j \leq N-1. \end{aligned} \tag{2.3.21}$$

The matrix form of the equation is

$$U'_h(t) = -N^2 A_h U_h(t), \tag{2.3.24}$$

where  $A_h$  is a tridiagonal, positive definite and symmetric matrix with diagonal elements 2, subdiagonal and superdiagonal nonzero elements  $-1$ . The eigenvalues and corresponding eigenvectors of  $A_h$  are  $\lambda_k = 4 \sin^2 \frac{k\pi}{2N}$ ,  $V^k = (V_j^k) = (\sin \frac{kj\pi}{N})$ ,  $1 \leq k \leq N-1$ .



## Semi-discrete Method + ODE Solver $\Rightarrow$ Fully Discrete Scheme

Discretize the ODE system obtained by the semi-discretization by

- ① forward Euler method leads to the forward explicit scheme;
- ② backward Euler method leads to the backward implicit scheme;
- ③ a linear combination of the two yields the  $\theta$ -scheme;

Note that the ODE system obtained is generally a stiff system, special care should be taken in choosing ODE solvers.

Recommended solvers including Gear and Runge-Kutta methods.

# The 3rd Type Boundary Condition for 1D Problems

## 2.3.3节, P60

We consider at  $x = 0$  the 3rd type boundary condition:

$$u_x(0, t) = \alpha(t)u(0, t) + g_0(t), \quad \alpha(t) \geq 0, \quad \forall t > 0. \quad (2.3.35)$$

The simplest finite difference approximation of the boundary condition:

$$\frac{U_1^m - U_0^m}{\Delta x} = \alpha^m U_0^m + g_0^m, \quad m \geq 1, \quad (2.3.36)$$

or equivalently

$$U_0^m = \beta^m U_1^m - \beta^m g_0^m \Delta x, \quad m \geq 1, \quad (2.3.37)$$

where

$$\beta^m = \frac{1}{1 + \alpha^m \Delta x}. \quad (2.3.38)$$

# The Effective Difference Scheme on the Node $(x_1, t_m)$

By the Taylor series expansion, the local truncation error of the numerical boundary condition is

$$\tau_b^m = \left[ \frac{\Delta_{+x}}{\Delta x} - \frac{\partial}{\partial x} \right] u_0^m = \left[ \frac{1}{2} \Delta x u_{xx} + \dots \right]_0^m = O(\Delta x).$$

Since  $U_0^m$  will be used to calculate  $U_1^m$ , the truncation error at the boundary will spread into the interior nodes.

# The Effective Difference Scheme on the Node $(x_1, t_m)$

To see how this will affect the local truncation error there, we substitute the boundary condition  $U_0^m = \beta^m U_1^m - \beta^m g_0^m \Delta x$  into the **1st order forward explicit** scheme to obtain the effective difference scheme on the node  $(x_1, t_m)$

$$\frac{U_1^{m+1} - U_1^m}{\Delta t} = \frac{U_2^m - 2U_1^m + (\beta^m U_1^m - \beta^m g_0^m \Delta x)}{(\Delta x)^2}. \quad (2.3.39)$$

# Truncation Error of the Effective Difference Scheme

Remember  $g_0^m = u_x(0, t_m) - \alpha^m u_0^m$  and  $\beta^m = (1 + \alpha^m \Delta x)^{-1}$ , we have

$$\begin{aligned}
 & \frac{u_2^m - 2u_1^m + (\beta^m u_1^m - \beta^m g_0^m \Delta x)}{(\Delta x)^2} - u_{xx}(x_1, t_m) \\
 (2.3.35) \quad &= \left[ \frac{u_2^m - 2u_1^m + u_0^m}{(\Delta x)^2} - u_{xx}(x_1, t_m) \right] + \frac{\beta^m}{\Delta x} \left[ \frac{u_1^m - u_0^m}{\Delta x} - u_x(x_0, t_m) \right] \\
 &= \left[ \frac{\delta_x^2}{(\Delta x)^2} - \frac{\partial^2}{\partial x^2} \right] u_1^m + \frac{\beta^m}{\Delta x} \left[ \frac{\Delta_{+x}}{\Delta x} - \frac{\partial}{\partial x} \right] u_0^m \\
 &= \left[ \frac{1}{12} (\Delta x)^2 u_{xxxx} + \cdots \right]_1^m + \frac{\beta^m}{\Delta x} \left[ \frac{1}{2} \Delta x u_{xx} + \cdots \right]_0^m \\
 &= \frac{1}{2} \beta^m u_{xx}(x_0, t_m) + O(\Delta x) = O(1). \tag{2.3.40}
 \end{aligned}$$

# Truncation Error of the Effective Difference Scheme

Thus the local truncation error  $T_1^m$  of the effective scheme is

$$\begin{aligned}
 & \left[ \frac{u_1^{m+1} - u_1^m}{\tau} - \frac{u_2^m - 2u_1^m + (\beta^m u_1^m - \beta^m g_0^m h)}{h^2} \right] - [u_t - u_{xx}](x_1, t_m) \\
 &= \left[ \frac{u_1^{m+1} - u_1^m}{\tau} - \frac{u_2^m - 2u_1^m + u_0^m}{h^2} - (u_t - u_{xx})(x_1, t_m) \right] \\
 & \quad - \frac{(\beta^m u_1^m - \beta^m g_0^m h) - u_0^m}{h^2} \\
 &= \left[ \frac{1}{2} \tau u_{tt} - \frac{1}{12} h^2 u_{xxxx} + \dots \right]_1^m - \frac{\beta^m}{h} \left[ \frac{1}{2} h u_{xx} + \dots \right]_0^m = O(1). \tag{2.3.43}
 \end{aligned}$$

In other words, we have  $T_1^m = \hat{T}_1^m - \frac{\beta^m}{h} T_b^m$ .

# $\mathbb{L}^\infty$ Stability of the Effective Difference Scheme

Compare the standard 1st order forward explicit scheme on  $(j, m)$

$$U_j^{m+1} = (1 - 2\mu)U_j^m + \mu(U_{j+1}^m + U_{j-1}^m), \quad \forall j > 1, \quad (2.2.26)$$

and the effective scheme on  $(1, m)$

$$U_1^{m+1} = (1 - \mu(2 - \beta^m))U_1^m + \mu U_2^m - \mu \beta^m g_0^m h, \quad (2.3.41)$$

we see that the conditions for the maximum principle to hold are  $2\mu \leq 1$  and  $(2 - \beta^m)\mu \leq 1$ . Since  $0 < \beta^m < 1$ , the condition for the maximum principle to hold is still  $\mu \leq 1/2$ .

# Convergence Rate of the Effective Difference Scheme

By taking a properly defined **comparison function** and applying the **maximum principle**, we can prove that the error of the overall scheme obtained by combining the 1st order forward explicit scheme with the 1st order forward approximation boundary condition is  **$O(\tau + h)$**  (see Exercise 2.18).  
Page 85

The overall convergence rate is jeopardized by the numerical boundary condition, which has a local truncation error  $O(h)$ .  
危害

To decrease the local truncation error, especially to cope with the **finite volume approximations**, which create **conservative schemes for conservative equations**, we must consider other kinds of numerical boundary conditions.



# A Numerical Boundary Condition with a Ghost Node

- ① set  $h = \Delta x = (N - \frac{1}{2})^{-1}$ , and let  $x_j = (j - \frac{1}{2})h$ ,  $j = 0, 1, \dots, N$ , where  $x_0 = -h/2$  is a **ghost node**;

- ② boundary condition:

$$\frac{U_1^m - U_0^m}{\Delta x} = \frac{1}{2} \alpha^m (U_1^m + U_0^m) + g_0^m, \quad (2.3.47)$$

or equivalently  $U_0^m = \xi^m U_1^m - \eta^m g_0^m \Delta x, \quad (2.3.48)$

where  $\xi^m = \frac{1 - \frac{1}{2} \alpha^m \Delta x}{1 + \frac{1}{2} \alpha^m \Delta x}$  and  $\eta^m = \frac{1}{1 + \frac{1}{2} \alpha^m \Delta x}$ ; (2.3.49)

- ③ local truncation error of the numerical boundary condition  $T_b^m = O(h^2)$ ;

# A Numerical Boundary Condition with a Ghost Node

- ④ the effective scheme:

$$\frac{U_1^{m+1} - U_1^m}{\tau} = \frac{U_2^m - (2 - \xi^m)U_1^m - \eta^m g_0^m h}{h^2}; \quad (2.3.50)$$

- ⑤ local truncation error of the effective scheme:

$$T_1^m = \hat{T}_1^m - \frac{\eta^m}{h} T_b^m = O(\tau + h); \quad (2.3.52)$$

- ⑥ the condition for the maximum principle:  $\mu \leq 1/2$ ;

- ⑦ overall convergence rate can be shown to be  $O(\tau + h^2)$ .

# Another Numerical Boundary Condition with a Ghost Node

- ① set  $h = \Delta x = N^{-1}$ , and let  $x_j = jh$ ,  $j = -1, 0, \dots, N$ , where  $x_{-1} = -h$  is a ghost node,  $[x_{-1}, x_0]$  is a ghost cell;

- ② boundary condition:

$$\frac{U_1^m - U_{-1}^m}{2\Delta x} = \alpha^m U_0^m + g_0^m, \quad (2.3.55)$$

or equivalently

$$U_{-1}^m = U_1^m - 2\alpha^m U_0^m \Delta x - 2g_0^m \Delta x; \quad (2.3.56)$$

- ③ local truncation error of the numerical boundary condition  
 $T_b^m = O(h^2);$

# Another Numerical Boundary Condition with a Ghost Node

- ④ the effective scheme:

$$\frac{U_0^{m+1} - U_0^m}{\tau} = \frac{2 U_1^m - 2(1 + \alpha^m h) U_0^m - 2 g_0^m h}{h^2}; \quad (2.3.57)$$

- ⑤ local truncation error of the effective scheme:

$$T_0^m = \hat{T}_0^m - \frac{2}{h} T_b^m = O(\tau + h); \quad (2.3.59)$$

- ⑥ the condition for the maximum principle:  $(1 + \alpha^m h)\mu \leq 1/2$ . (2.3.62)

- ⑦ overall convergence rate can be shown to be  $O(\tau + h^2)$ .

# Dissipation and Stability of Difference Schemes

## 2.3.4节, P65

For the heat equation  $u_t = u_{xx}$  defined on  $(0, 1)$ ,

- ① analytical Fourier mode solutions  $e^{-k^2\pi^2 t} e^{ik\pi x}$  decay fast;
- ② discrete Fourier modes  $\lambda_k^m e^{ik\pi jh}$ ;
- ③ for 1st order forward explicit scheme,  $\lambda_k = 1 - 4\mu \sin^2 \frac{k\pi h}{2}$ ,  
 $h = \frac{1}{N}$ ,  $k = 1, 2, \dots, N$ , all Fourier modes decay if  $\mu < 1/2$ ;
- ④ for any  $N \geq 1$ ,  $\lambda_N = 1 - 4\mu = -1$ , if  $\mu = 1/2$ , the corresponding Fourier mode does not decay (nor grow).

# Dissipation and Stability of Difference Schemes

- ⑤  $\lim_{h \rightarrow 0} \lambda_k^m e^{k^2 \pi^2 m \tau} = \lim_{h \rightarrow 0} (1 - k^2 \pi^2 \tau)^m e^{k^2 \pi^2 m \tau} = 1,$   
 $0 < m\tau \leq t_{\max}$  and any fixed  $k$ ,  $\Rightarrow$  convergence of mode  $k$ ;  
 $\Rightarrow$  差分解的确正确反映了真解的衰减特性.
- ⑥ for any  $N \geq 1$ ,  $\lambda_N = 1 - 4\mu < -1$ , if  $\mu > 1/2$ ,  $\Rightarrow$  unstable;
- ⑦ a necessary and sufficient condition for  $\mathbb{L}^2$  stability:  $\mu \leq 1/2$ .

## Local $\mathbb{L}^2$ Stability of Variable-coefficient Difference Schemes

For variable-coefficient heat equation  $u_t = a(x)u_{xx}$  defined on  $(0, 1)$ , we can apply the Fourier method to study the necessary stability conditions of a scheme by analyzing its local dissipation property.

- ① discrete Fourier modes  $\lambda_k^m e^{ik\pi jh}$ ;
- ② for the forward explicit scheme

$$U_j^{m+1} = U_j^m + \bar{\mu} a(\xi) (U_{j+1}^m - 2U_j^m + U_{j-1}^m), j = 1, 2, \dots, N. \quad (2.3.64)$$

$$\lambda_k = 1 - 4\bar{\mu} a(\xi) \sin^2 \frac{k\pi h}{2}, h = \frac{1}{N}, k = 1, 2, \dots, N, \quad (2.3.65)$$

$$\Rightarrow \text{all Fourier modes decay, if } \bar{\mu} \max_{\xi \in [0,1]} a(\xi) < 1/2; \quad (2.3.66)$$

- ③ for any  $N \geq 1$ , if  $\bar{\mu} \max_{\xi \in [0,1]} a(\xi) > 1/2$ , then  $\lambda_N < -1$ ,  
 $\Rightarrow$  unstable;

# Parabolic Equation in Conservation Form

Parabolic equations with the differential operator  $L$  being of the **divergence form** can be written into a conservative integral form:

$$\int_{x_l}^{x_r} u(x, t_a) dx = \int_{x_l}^{x_r} u(x, t_b) dx + \int_{t_b}^{t_a} [a u_x(x_r, t) - a u_x(x_l, t)] dt, \\ \forall 0 \leq x_l < x_r \leq 1, \quad \forall t_a > t_b \geq 0. \quad (2.3.67)$$

In a heat flow problem,

- ①  $h([x_l, x_r]; t) \triangleq \int_{x_l}^{x_r} u(x, t) dx$  is the **total heat** of the system on the interval  $(x_l, x_r)$  at time  $t$ ;
- ②  $f(u) \triangleq -a u_x(x, t)$  is the heat flux on  $x$  at time  $t$ ;
- ③  $u_x(0, t) = g_0(t), u_x(1, t) = g_1(t)$  (the Neumann boundary condition) given inflow heat rate at the boundary; (2.3.68)

**Remark:** The equation describes the local heat conservation (or balance) property of a source free heat flow problem.



# Finite Volume Method and Conservative Schemes

We would like to establish a scheme which preserves the property.

- ①  $U_j^m$ : the heat density of the discrete system on the grid cell  $(x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}})$  at time  $t_m$ ;
- ②  $H([x_{j_l-\frac{1}{2}}, x_{j_r+\frac{1}{2}}]; t_{m+k}) \triangleq \sum_{j=j_l}^{j_r} U_j^{m+k} h$ : the total heat of the discrete system on the interval  $(x_{j_l-\frac{1}{2}}, x_{j_r+\frac{1}{2}})$  at time  $t_{m+k}$ ;
- ③  $F(U_j^{m+1}, U_j^m, U_{j-1}^{m+1}, U_{j-1}^m)$ : the numerical heat flux on  $x_{j-\frac{1}{2}}$  in the time period  $(t_m, t_{m+1})$ ;

# Finite Volume Method and Conservative Schemes

④ a general conservative scheme

$$U_j^{m+1} = U_j^m - \frac{\tau}{h} \left[ F(U_{j+1}^{m+1}, U_{j+1}^m, U_j^{m+1}, U_j^m) - F(U_j^{m+1}, U_j^m, U_{j-1}^{m+1}, U_{j-1}^m) \right], \quad (2.3.70)$$

⑤ local heat conservation of the discrete system

$$\sum_{j=j_l}^{j_r} U_j^{m+k} h = \sum_{j=j_l}^{j_r} U_j^m h + \sum_{l=1}^k \left[ -F(U_{j_r+1}^{m+l}, U_{j_r+1}^{m+l-1}, U_{j_r}^{m+l}, U_{j_r}^{m+l-1}) \right. \\ \left. + F(U_{j_l+1}^{m+l}, U_{j_l+1}^{m+l-1}, U_{j_l}^{m+l}, U_{j_l}^{m+l-1}) \right] \tau, \quad 0 \leq j_l < j_r < N, m \geq 0, k > 0. \quad (2.3.72)$$

**Remark:** To preserve the global conservation of the system, the initial and boundary data must also be properly handled.

## Numerical Initial and Boundary Data for Conservative Schemes

① a grid with ghost nodes  $x_j = (j - \frac{1}{2})h$ ,  $0 \leq j \leq N$ , (2.3.73)

$h = 1/(N - 1)$ ,  $t_m = m\tau$ ,  $m \geq 0$ ,  $\tau = \mu(h^2)$ ; (2.3.74)

②  $F(U_j^{m+1}, U_j^m, U_{j-1}^{m+1}, U_{j-1}^m) = -a \frac{U_j^m - U_{j-1}^m}{h} \Leftrightarrow$  explicit scheme;

③ numerical Neumann boundary conditions:

$$\frac{U_1^m - U_0^m}{h} = \bar{g}_0^m, \quad \frac{U_N^m - U_{N-1}^m}{h} = \bar{g}_1^m, \quad (2.3.75)$$

where  $\bar{g}_0^m = \frac{1}{\tau} \int_{t_m}^{t_{m+1}} g_0(t) dt$ ,  $\bar{g}_1^m = \frac{1}{\tau} \int_{t_m}^{t_{m+1}} g_1(t) dt$ , (2.3.76)

$\Rightarrow$  ④ global numerical boundary flux equals global boundary flux

$$\tau \sum_{l=0}^m \left[ \left( a \frac{U_N^l - U_{N-1}^l}{h} \right) - \left( a \frac{U_1^l - U_0^l}{h} \right) \right] = \int_0^{t_{m+1}} a(g_1(t) - g_0(t)) dt;$$

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## Numerical Initial and Boundary Data for Conservative Schemes

- ⑤ numerical initial data:

$$U_j^0 = \frac{1}{h} \int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} u(x, 0) dx, \quad j = 1, \dots, N-1; \quad (2.3.78)$$

- ⑥ the initial heat of the system:

$$H([0, 1]; 0) = \sum_{j=1}^{N-1} U_j^0 h = \sum_{j=1}^{N-1} \int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} u(x, 0) dx = h([0, 1]; 0);$$

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- ⑦ the heat of the system at  $t_{m+1}$ :

$$\begin{aligned} H([0, 1]; t_{m+1}) &= h([0, 1]; 0) + \int_0^{t_{m+1}} a(g_1(t) - g_0(t)) dt \\ &= h([0, 1]; t_{m+1}), \quad \forall m \geq 0. \end{aligned} \quad (2.3.77)$$

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习题 2: 18, 19; 上机作业 2 Page 83

**Thank You!**