Lecture 5

Finite difference methods for parabolic problems. The pure initial value problem

$$\begin{cases} \frac{\partial u}{\partial t} = a^2 \Delta u \text{ in } \mathbb{R}^n \times \mathbb{R}_+, \ (n = 1, 2, 3) \\ u(x, 0) = v(x) \quad \text{in } \mathbb{R}^n \end{cases}$$

where $v(x)$ is a given smooth bounded function. The meaning of the symbol Δu (the laplacian of u) is as follows:

$$\Delta u = \begin{cases} \frac{\partial^2 u}{\partial x^2}(x, t), \ (n = 1), \\ \frac{\partial^2 u}{\partial x^2}(x, y, t) + \frac{\partial^2 u}{\partial y^2}(x, y, t), \ (n = 2), \\ \frac{\partial^2 u}{\partial x^2}(x, y, z, t) + \frac{\partial^2 u}{\partial y^2}(x, y, z, t) + \frac{\partial^2 u}{\partial z^2}(x, y, z, t), \ (n = 3) \end{cases}$$

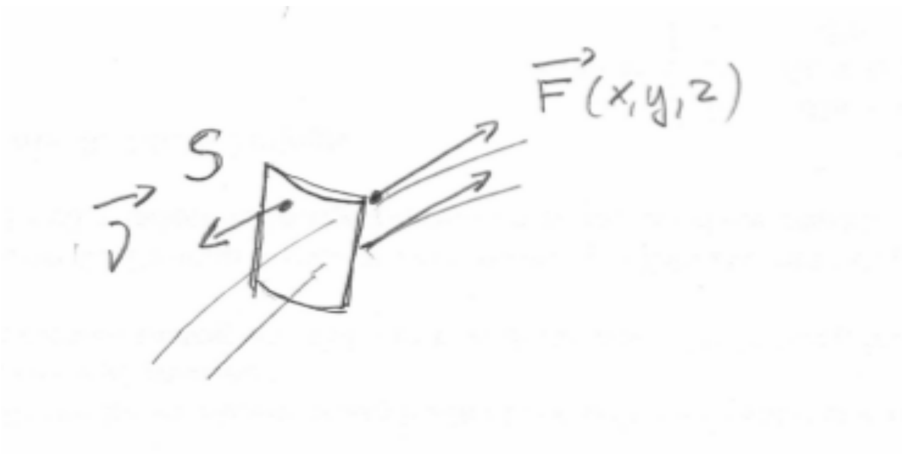
Physical interpretation. The equation above is known as the heat equation or also as the diffusion equation. It describes in typical applications the evolution in time of the density $u(x, y, z, t)$ of some quantity such as heat, chemical concentration, etc. If $V \subset U$ is any smooth subregion, the rate of change of the total quantity within V equals the negative of the net flux $\vec{F}(x, y, z, t)$ through $S = \partial V$: let us consider

some interval of time $[t, t + \Delta t]$, Δt,

Δm - mass of medium flowing through the area S within Δt,

$\vec{\nu}$ - the unit normal vector to the surface S. Then we have the relation

$$\Delta m \approx -(\vec{F} \cdot \vec{\nu}) \cdot S \cdot \Delta t$$



Thus the total change of mass m in the region V within Δt is given as

$$m(t + \Delta t) - m(t) = \int\limits_V (u(x, t + \Delta t) - u(x, t))dV = \sum \Delta m = -\Delta t \int\limits_{\partial V} (\vec{F} \cdot \vec{\nu})dS.$$

Hence the rate of change is given as

$$\lim_{\Delta \to 0} \frac{m(t + \Delta t) - m(t)}{\Delta t} = \frac{d}{dt} \int_V u dV = \int_V u_t dV = -\int\limits_{\partial V} (\vec{F} \cdot \vec{\nu})dS$$

The change of the surface integral into the volume integral (integration by parts)

$$\int_{\partial V} \vec{F} \cdot \vec{\nu} dS = \int_V \text{div}\, \vec{F}\, dV$$

gives

$$\frac{d}{dt} \int_V u\, dV = \int_V u_t\, dV = -\int_V \text{div}\, \vec{F}\, dV.$$

where

$$\vec{F}(x, y, z, t) = [P(x, y, z, t), Q(x, y, z, t), R(x, y, z, t)]$$

is the flux of the medium density, i.e. it is the amount of medium flowing through the unit of area in unit of time and

$$\text{div}\, \vec{F}(x, y, z, t) = (P_x + Q_y + R_z)(x, y, z, t),$$

As this integral relation is satisfied in any subregion V we get the equality

$$u_t = -\text{div}\, \vec{F},$$

In many situations $\vec{F}$ is proportional to the gradient of u (this is the Fourier or Fick law):

(1) $\quad \vec{F} = -a^2\, \nabla u \ \ (a > 0),$

where

$$\nabla u(x, y, z, t) = [u_x, u_y, u_z],$$

but points in the opposite direction (since the flow is always from the regions of higher concentration to the regions of lower concentration).
Substituting (1) into equation above, we obtain the PDE

(2) $\quad u_t = a^2 \text{div}(\nabla u) = a^2 \Delta u,$

which is called the heat equation.

The heat equation appears as well in the study of the Brownian motion.
The heat conduction problem has a unique solution, many properties of which follow from the representation of the solution to the problem

$$\begin{cases} u_t = a^2 u_{xx} \\ u(x, 0) = v(x), \quad x \in \mathbb{R},\ t > 0 \end{cases}$$

Its solution is given in the following formula

$$u(x, t) = \frac{1}{a\sqrt{4\pi t}} \int_{-\infty}^{\infty} e^{-\frac{y^2}{4a^2 t}} v(x - y) dy.$$

In particular, we note that this solution is bounded

$$\max_x |u(x,t)| \le \frac{1}{a\sqrt{4\pi t}} \int_{-\infty}^{\infty} e^{-\frac{y^2}{4a^2t}} |v(x-y)| dy \le$$

$$\max_x |v(x)| \frac{1}{a\sqrt{4\pi t}} \int_{-\infty}^{\infty} e^{-\frac{y^2}{4a^2t}} dy = \max_x |v(x)| = ||v||_\infty$$

Parabolic problems in bounded domains. The model problem

1a. differential equation

$$\frac{\partial u}{\partial t} = a^2 \frac{\partial^2 u}{\partial x^2} + f(x,t) \quad \text{in } (a,b) \times (0,T)$$

1b. additional conditions

an initial condition:

$$u(x,0) = v(x), \quad x \in (a,b)$$

a boundary condition (of the Dirichlet Type):

$$u(a,t) = \phi(t), \quad u(b,t) = \psi(t), \quad t \in (0,T).$$

Further, for simplicity we assume that $\phi(t) \equiv 0$, $\psi(t) \equiv 0$.

2. Approximation by the difference method

2a. Discretization

$$a = x_0 < x_1 < x_2 < \cdots < x_N = b, \quad h = (b-a)/N,$$
$$0 = t_0 < t_1 < t_2 < \cdots < t_M = T, \quad k = (T-0)/M.$$

2b. Approximate solution

a series: $\{u_i^j\}$, $u_i^j \approx u(x_i, t_j)$, $i = 0,1,2,\ldots,N$, $j = 0,1,2,\ldots,N$

2c. Basic relations (depending on the approximate method)

Explicit method

$$\frac{U_i^{j+1} - U_i^j}{k} = a^2 \frac{U_{i+1}^j - 2U_i^j + U_{i-1}^j}{h^2} + f_{i,j},$$

$i = 1,2,\ldots,M-1$, $j = 0,1,2,\ldots,N-1$

Implicit method

$$\frac{U_i^{j+1} - U_i^j}{k} = a^2 \frac{U_{i+1}^{j+1} - 2U_i^{j+1} + U_{i-1}^{j+1}}{h^2} + f_{i,j+1},$$

$i = 1,2,\ldots,M-1$, $j = 0,1,2,\ldots,N-1$

The Crank-Nicolson method

$$\frac{U_i^{j+1}-U_i^j}{k}=\frac{1}{2}a^2\frac{U_{i+1}^j-2U_i^j+U_{i-1}^j}{h^2}+\frac{1}{2}a^2\frac{U_{i+1}^{j+1}-2U_i^{j+1}+U_{i-1}^{j+1}}{h^2}+f_{i,j+\frac{1}{2}},$$
$$f_{i,j+\frac{1}{2}}=f(x_i,t_{j+\frac{1}{2}k}),\quad i=1,2,\dots,M-1,\quad j=0,1,2,\dots,N-1$$

2d. Additional information

$$u_{i,0}=v_i,\quad v_i=v(x_i),\quad i=0,1,2,\dots,N$$
$$u_{0,j}=\phi_j,\quad \phi_j=\phi(t_j),\quad u_{M,j}=\psi_j,\quad \psi_j=\psi(t_j),\quad j=0,1,2,\dots,M-1$$

3. Algorithms in the matrix form

Explicit method

$$\begin{bmatrix} U_1^{j+1}\\ U_2^{j+1}\\ U_3^{j+1}\\ \vdots\\ U_{M-2}^{j+1}\\ U_{M-1}^{j+1}\end{bmatrix}=\begin{bmatrix}1-2\lambda & \lambda & 0 & \dots & 0 & 0\\ \lambda & 1-2\lambda & \lambda & \dots & 0 & 0\\ 0 & \lambda & 1-2\lambda & \lambda & \dots & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ 0 & 0 & 0 & \lambda & 1-2\lambda & \lambda\\ 0 & 0 & 0 & 0 & \lambda & 1-2\lambda\end{bmatrix}\begin{bmatrix} U_1^{j}\\ U_2^{j}\\ U_3^{j}\\ \vdots\\ U_{M-2}^{j}\\ U_{M-1}^{j}\end{bmatrix}+k\begin{bmatrix} f_1^{j}\\ f_2^{j}\\ f_3^{j}\\ \vdots\\ f_{M-2}^{j}\\ f_{M-1}^{j}\end{bmatrix}+\lambda\begin{bmatrix}\phi_j\\ 0\\ 0\\ \vdots\\ 0\\ \psi_j\end{bmatrix}$$

for $j=0,1,2,\dots,N-1$.

The method is stable if

$$(3)\qquad \lambda=a^2\frac{k}{h^2}\le\frac{1}{2}.$$

Implicit method

$$B\begin{bmatrix} U_1^{j+1}\\ U_2^{j+1}\\ \vdots\\ U_{M-1}^{j+1}\end{bmatrix}=\begin{bmatrix} U_1^{j}\\ U_2^{j}\\ \vdots\\ U_{M-1}^{j}\end{bmatrix}+k\begin{bmatrix} f_1^{j+1}\\ f_2^{j+1}\\ \vdots\\ f_{M-1}^{j+1}\end{bmatrix}+\lambda\begin{bmatrix}\phi_{j+1}\\ 0\\ \vdots\\ 0\\ \psi_{j+1}\end{bmatrix}$$

where

$$B=\begin{bmatrix}1+2\lambda & -\lambda & 0 & 0 & \dots & 0\\ -\lambda & 1+2\lambda & -\lambda & 0 & \dots & 0\\ \vdots & \vdots & \vdots & \vdots & \dots & \vdots\\ 0 & 0 & 0 & \dots & -\lambda & 1+2\lambda\end{bmatrix},\quad \lambda=a^2\frac{k}{h^2}$$

B is diagonally dominant, symmetric and tridiagonal. Thus it is invertible and the vector $\left[\; U_1^{n+1},\; U_2^{n+1},\; \ldots,\; U_{M-1}^{n+1} \;\right]$ can be determined

The stability of the method.

The stability of the method does not require any relation between k and h.

The convergence results for the implicit method

Theorem 4

$$||U^n - u^n||_\infty \leq C \cdot n \cdot k(h^2 + k) \max_{t \leq T} |u(\cdot, t)|_{C^4}$$

Comments

The above convergence result for the backward Euler method is satisfactory in that it requires no restrictions on the mesh ratio $k/h^2 = \lambda$. On the other hand, since it is only first order accurate in time, the error in the time discretization will dominate unless k is chosen much smaller than h.

3. The Crank-Nicolson scheme

Introducing the matrices

$$B = \begin{bmatrix} 1+\lambda & -\frac{1}{2}\lambda & 0 & 0 & \ldots & 0 \\ -\frac{1}{2}\lambda & 1+\lambda & -\frac{1}{2}\lambda & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ldots & \vdots \\ 0 & 0 & 0 & \ldots & -\frac{1}{2}\lambda & 1+\lambda \end{bmatrix}$$

$$A = \begin{bmatrix} 1-\lambda & \frac{1}{2}\lambda & 0 & 0 & \ldots & 0 \\ \frac{1}{2}\lambda & 1-\lambda & \frac{1}{2}\lambda & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ldots & \vdots \\ 0 & 0 & 0 & \ldots & \frac{1}{2}\lambda & 1-\lambda \end{bmatrix}$$

the Crank-Nicolson scheme can be written in the form

$$B \begin{bmatrix} U_1^{j+1} \\ U_2^{j+1} \\ \vdots \\ U_{M-1}^{j+1} \end{bmatrix} = A \begin{bmatrix} U_1^{j} \\ U_2^{j} \\ \vdots \\ U_{M-1}^{j} \end{bmatrix} + k \begin{bmatrix} f_1^{j+\frac{1}{2}} \\ f_2^{j+\frac{1}{2}} \\ \vdots \\ f_{M-1}^{j+\frac{1}{2}} \end{bmatrix} + \lambda \begin{bmatrix} \phi_{j+\frac{1}{2}} \\ 0 \\ \vdots \\ \psi_{j+\frac{1}{2}} \end{bmatrix}$$

The method is stable if

$$(4) \quad \lambda = a^2 \frac{k}{h^2} \leq 1.$$

Remark

It can be shown that in the case of the L_2 norm $||\cdot||_2$ no restrictions on λ are needed.

The convergence result.

Theorem 5

For $\lambda \leq 1$

$$||U^n - u^n||_\infty \leq C \cdot nk(h^2 + k^2) \max_{t \leq T} |u(\cdot, t)|_{C^4}$$

For any $\lambda > 0$

$$||U^n - u^n||_{2,h} \leq C \cdot nk(h^2 + k^2) \max_{t \leq T} |u(\cdot, t)|_{C^4}$$

definitions:

- of the discrete L_2 - norm $||\cdot||_{2,h}$:

$$||w||_{2,h} = \left(h \sum_{j=0}^{M} w_j^2 \right)^{1/2}$$

- $\max_{t \leq T} |u(\cdot, t)|_{C^4} = \max_{0 \leq k \leq 4} m_k,$

where

$$m_0 = \max_{t \leq T} |u(\cdot, t)|, \quad m_1 = \max_{t \leq T} |u_x(\cdot, t)|, \quad m_2 = \max_{t \leq T} |u_{xx}(\cdot, t)|,$$
$$m_3 = \max_{t \leq T} |u_{xxx}(\cdot, t)|, \quad m_4 = \max_{t \leq T} |u_{xxxx}(\cdot, t)|.$$

4. The Fourier method for solution of the problem

$$\begin{cases} (1) \quad u_t = a^2 u_{xx} \\ (2) \quad u(0, t) = u(l, t) = 0 \\ (3) \quad u(x, 0) = v(x) \end{cases}$$

1. We observe that the functions

$$e^{-\frac{\pi^2 a^2}{l^2} t} \sin \frac{\pi x}{l}, \; e^{-\frac{4\pi^2 a^2}{l^2} t} \sin \frac{2\pi x}{l}, \; e^{-\frac{9\pi^2 a^2}{l^2} t} \sin \frac{3\pi x}{l},$$

$$e^{-\frac{16\pi^2 a^2}{l^2} t} \sin \frac{4\pi x}{l}, \; \ldots, \; e^{-\frac{k^2\pi^2 a^2}{l^2} t} \sin \frac{k\pi x}{l}, \; \ldots$$

satisfy equations (1) and (2). Hence the solution to the whole problem (1) – (3) is sought in the following form

$$u(x,t) = \sum_{k=1}^{\infty} a_k e^{-\frac{k^2\pi^2a^2}{l^2}t} \sin\frac{k\pi x}{l}$$

the coefficients a_k are to be determined. To find them we first observe that

$$v(x) = u(x,0) = \sum_{k=1}^{\infty} a_k \sin\frac{k\pi x}{l}$$

The presentation of $v(x)$ in the above series is called the Fourier expansion of $v(x)$.

2. We find the expansion of the function $v(x)$ in the Fourier series

$$v(x) = \sum_{k=1}^{\infty} a_k \sin\frac{k\pi x}{l}$$

The coefficients a_k are given as

$$a_k = \int_0^l v(x)\sin\frac{k\pi x}{l}dx \Big/ \int_0^l \sin^2\frac{k\pi x}{l}dx = \frac{2}{l}\int_0^l v(x)\sin\frac{k\pi x}{l}dx.$$

3. Finally, the solution of the whole problem (1), (2), (3) is a function $u(x,t)$ given as

$$u(x,t) = \sum_{k=1}^{\infty} a_k e^{-\frac{\pi^2k^2a^2}{l^2}t} \sin\frac{k\pi x}{l}$$

4. We define approximate solutions as finite sums, $n = 1, 2, 3, \ldots$

$$u_p(x,t) = \sum_{k=1}^{n} a_k e^{-\frac{\pi^2k^2a^2}{l^2}t} \sin\frac{k\pi x}{l}$$