MSDM5004
Numerical Methods and Modeling in Science
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Lecture 9

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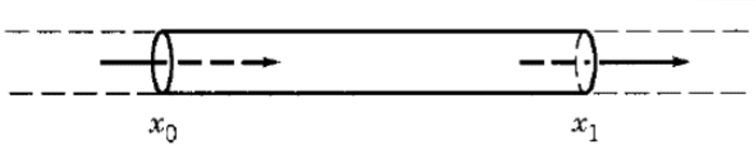
Diffusion equation in one dimension

$$u_t = ku_{xx}$$



where k>0 is the diffusion constant.

Diffusion equation in three dimensions

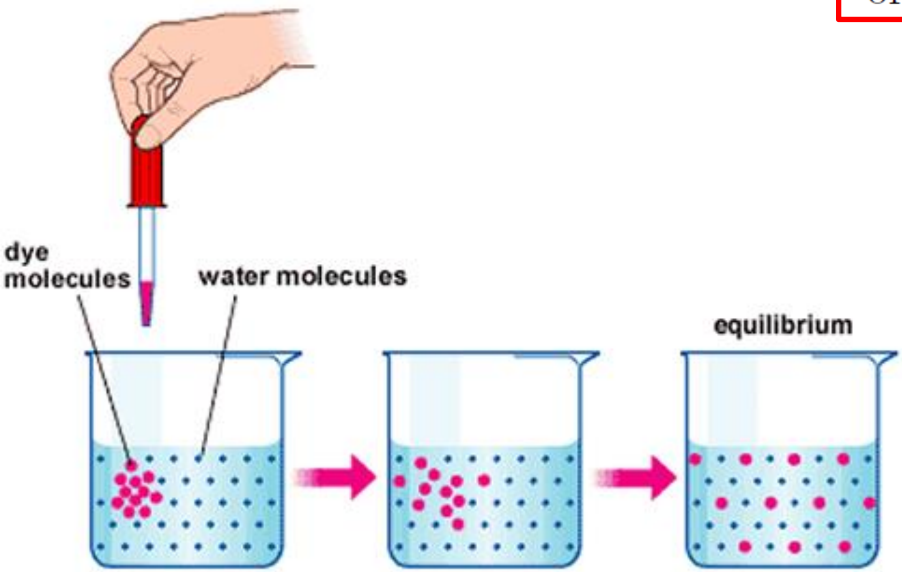
$$u_t = k(u_{xx} + u_{yy} + u_{zz}) = k\,\Delta u.$$

Laplacian operator in three dimensions

$$\triangle = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

or ∇^2

Example: Random motion of (dye) molecules



These kind of equations can also describe the heat flow, where they are called heat equations.

Solution of the diffusion equation

Diffusion on the whole line: initial value problem

$$u_t = ku_{xx} \quad (-\infty < x < \infty,\ 0 < t < \infty)$$
$$u(x,0) = \phi(x).$$

Solution

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

Once t>0, the solution depends on the initial information at all points, i.e. the initial value at a point has an immediate effect everywhere. That means the speed of propagation is infinite.

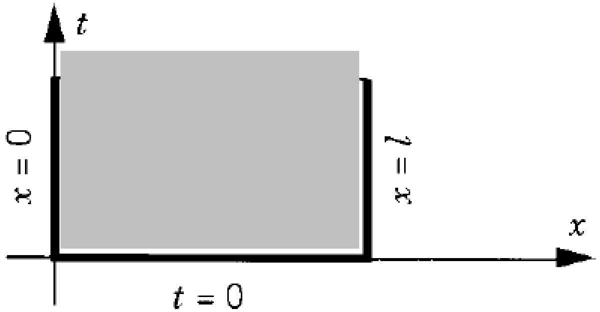
Initial-boundary value problems

of diffusion equation

$$u_t - ku_{xx} = f(x,t) \quad \text{for } 0 < x < l \text{ and } t > 0$$

$$u(0,t) = g(t) \qquad u(l,t) = h(t)$$

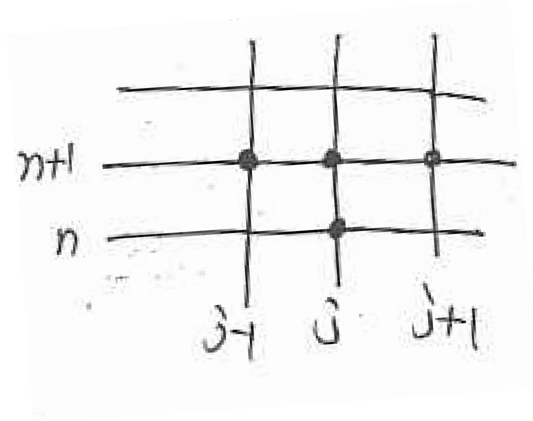
$$u(x,0) = \phi(x)$$



This problem is well-posed, i.e., the solution

1) exists,
2) is unique,
3) continuously depend on the given data.

1.5. An implicit scheme



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

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

$$j = 1, 2, \ldots, J-1.$$

a system of $J - 1$ linear equations in the $J-1$ unknowns U_j^{n+1}

$$j = 1, 2, \ldots, J-1.$$

Solving linear system

$$\begin{bmatrix} 1+2\mu & -\mu & & & 0 \\ -\mu & 1+2\mu & \mu & & \\ & \ddots & \ddots & \ddots & \\ 0 & & -\mu & 1+2\mu & -\mu \\ & & & -\mu & 1+2\mu \end{bmatrix} \begin{bmatrix} u_1^{n+1} \\ u_2^{n+1} \\ \vdots \\ u_{J-2}^{n+1} \\ u_{J-1}^{n+1} \end{bmatrix} = \begin{bmatrix} u_1^{n} \\ u_2^{n} \\ \vdots \\ u_{J-2}^{n} \\ u_{J-1}^{n} \end{bmatrix}$$

- Tridiagonal system.
- Can be solved efficiently by Thomas algorithm with *O(N)* operations. Here *N=J-1*.

Truncation error

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

expand at (x_j, t_{n+1})

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

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

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

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

Thus

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

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

$$+ O((\Delta t)^2) + O((\Delta x)^3)$$

From the PDE, $\frac{\partial u}{\partial t}(x_j, t_{n+1}) - \frac{\partial^2 u}{\partial x^2}(x_j, t_{n+1})$

We have

$$T(x_j, t_{n+1}) = -\frac{1}{2}\Delta t \frac{\partial^2 u}{\partial t^2}(x_j, t_{n+1}) - \frac{1}{12}(\Delta x)^2 \frac{\partial^4 u}{\partial x^4}(x_j, t_{n+1})$$

$$+ O((\Delta t)^2) + O((\Delta x)^3)$$

This means that the implicit scheme is also first order in t and second order in x.

Stability

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

Put it into the scheme.

$$-\mathcal{X}[\lambda(k)]^{n+1} e^{ik((j-1)\Delta x)} + (1+2\mathcal{X})[\lambda(k)]^{n+1} e^{ik(j\Delta x)} - \mathcal{X}[\lambda(k)]^{n+1} e^{ik((j+1)\Delta x)}$$

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

Divide it by $[\lambda(k)]^n e^{ik(j\Delta x)}$

$$-\mu\lambda(k)e^{-ik\Delta x} + (1+2\mu)\lambda(k) - \mu\lambda(k)e^{ik\Delta x} = 1$$

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

$$\lambda(k)(1+2\mu - 2\mu\cos k\Delta x) = 1$$

$$\lambda(k)(1+4\mu\sin^2\frac{k\Delta x}{2}) = 1$$

$$\lambda(k) = \frac{1}{1+4\mu\sin^2\frac{k\Delta x}{2}}$$

$|\lambda(k)| \leq 1$ $\quad |\lambda(k)|^n \leq 1$ for all k

Thus the implicit scheme is unconditionally stable.

1.6. Weighted average method (θ-method)

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

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

average of (1) and (2) : $0 \leq \theta \leq 1$ $\quad (1)*(1-\theta)+(2)*\theta$

weighted average method (θ-method):
$$\frac{U_j^{n+1}-U_j^n}{\Delta t} = \frac{(1-\theta)(U_{j+1}^n-2U_j^n+U_{j-1}^n)}{(\Delta x)^2} + \frac{\theta(U_{j+1}^{n+1}-2U_j^{n+1}+U_{j-1}^{n+1})}{(\Delta x)^2} \quad (3)$$

or

$$-\theta\mu U_{j-1}^{n+1} + (1+2\theta\mu)U_j^{n+1} - \theta\mu U_{j+1}^{n+1} = (1-\theta)\mu U_{j-1}^n + [1-2(1-\theta)\mu]U_j^n + (1-\theta)\mu U_{j+1}^n \quad (4)$$

$\theta = 0$, it is (1)

$\theta = 1$, it is (2)

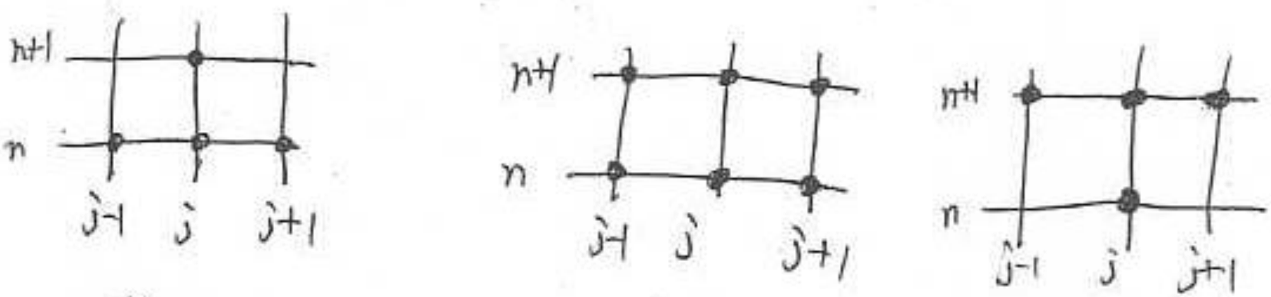
$$\theta = \frac{1}{2}: \quad -\frac{\mu}{2}u_{j-1}^{n+1} + (1+\mu)u_j^{n+1} - \frac{\mu}{2}u_{j+1}^{n+1} = \frac{\mu}{2}u_{j-1}^{n} + (1-\mu)u_j^{n} + \frac{\mu}{2}u_{j+1}^{n} \qquad (5)$$

Crank-Nicolson method

$\theta = 0$: explicit

$0 < \theta \leq 1$: implicit, tridiagonal system, solved using Thomas algorithm

Stencil :



$\theta = 0$ $\qquad$ $0 < \theta \leq 1$ $\qquad$ $\theta = 1$

Truncation error

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

Expand at $(x_j, t_{n+\frac{1}{2}})$.

Use the equation $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$

and therefore $\frac{\partial^2 u}{\partial t^2} = \frac{\partial^3 u}{\partial x^2 \partial t}$, $\frac{\partial^3 u}{\partial t^3} = \frac{\partial^4 u}{\partial x^2 \partial t^2}$

$\theta \neq \frac{1}{2}$, the scheme is first order in t, second order in x

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

$$+ O((\Delta t)^3) + O((\Delta x)^3)$$

Second order in both t and x.

Stability

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

Putting it into the θ-method (4), we have

$$\lambda(k) = \frac{1 - 4(1-\theta)\mu \sin^2\frac{k\Delta x}{2}}{1 + 4\theta\mu \sin^2\frac{k\Delta x}{2}}$$

For this $\lambda(k)$,

$$\underset{n\Delta t \le t_F}{\left|[\lambda(k)]^n\right| \text{ bounded}} \Longleftrightarrow |\lambda(k)| \le 1$$

$$\Longleftrightarrow -1 \le \lambda(k) \le -1$$

$$\Longleftrightarrow -1 \le \frac{1 - 4(1-\theta)\mu \sin^2\frac{k\Delta x}{2}}{1 + 4\theta\mu \sin^2\frac{k\Delta x}{2}} \le 1 \Longleftrightarrow 2\mu(1-2\theta)\sin^2\frac{k\Delta x}{2} \le 1$$

$\frac{1}{2} \leq \theta \leq 1$, stable for all μ (unconditionally stable)

$0 \leq \theta < \frac{1}{2}$ stable $\iff$ $\mu \leq \frac{1}{2(1-2\theta)}$

special cases:

$\theta = 0$ explicit method (1) $\mu \leq \frac{1}{2}$

$\theta = 1$ implicit method (2) unconditionally

$\theta = \frac{1}{2}$ Crank-Nicolson (5) unconditionally

Crank-Nicolson: Second order in both t and x

unconditionally stable: can keep $\nu = \frac{\Delta t}{\Delta x}$ constant

— popular

1.7. Lax equivalence theorem

For a well-posed linear evolutionary problem

and a consistent numerical scheme

stability $\Longleftrightarrow$ convergence

Well-posed problem: The solution exists, is unique, and depends continuously on the give data.