Lecture 8
Partial Differential Equations (PDE)
Heat equation

1. Finite-Difference Method

As a model problem the heat equation in its one-dimensional version together with subsidiary conditions is as follows:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + f(x,t), \tag{1}$$

with initial condition

$$u(x,0) = g(x), \qquad a \le x \le b,$$

and with boundary condition

$$u(a,t) = \phi_1(t), \qquad u(b,t) = \phi_2(t), \qquad t \ge 0,$$

where u is the temperature, which depends on x coordinate and time t, D is thermal diffusivity coefficient. For the sake of simplicity, we assume that

$$f(x,t) = 0, \qquad \phi_1(t) = \phi_2(t) = 0, \qquad D = 1, \qquad a = 0, \qquad b = 1,$$

that is, the initial-boundary problem we are going to study is given by

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \qquad u(x,0) = g(x), \qquad 0 \le x \le 1, \qquad u(0,t) = u(1,t) = 0, \qquad t \ge 0. \tag{2}$$

Using the finite-difference method involves the discretisation of the domain:

$$t_j = jk, \quad j \ge 0, \qquad x_i = ih, \quad 0 \le i \le n+1, \tag{3}$$

where the variables t and x have different step size k and h,

$$h = \frac{1}{n+1}.$$

Our objective is to compute approximate values of the solution function u at the so-called mesh points-nodes (t_j, x_i).

The next step is the replacement of the continuous derivatives with the finite-differences

$$g'(t) = \frac{1}{k}[g(t+k) - g(t)] - \frac{k}{2}g''(s), \qquad f''(x) = \frac{f(x+h) + f(x-h) - 2f(x)}{h^2} - \frac{h^2}{12}f^4(\xi).$$

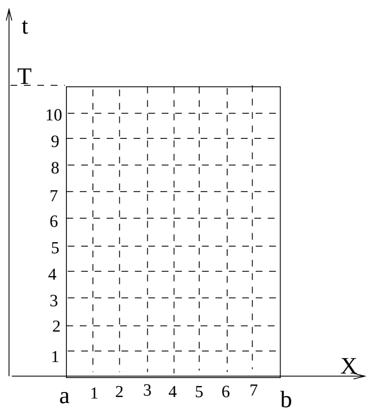

Figure 1: Initial boundary value problem for the heat transfer equation

As a result of the discretisation and replacement of $u(x_i, t_j)$ by u_{ij} we obtain the finite-difference equation

$$\frac{u_{i-1,j} - 2u_{ij} + u_{i+1,j}}{h^2} = \frac{u_{i,j+1} - u_{ij}}{k}. \tag{4}$$

The initial temperature distribution g gives us

$$g(x_i) = u(x_i, 0) = u_{i0}.$$

Boundary condition yields

$$u_{0j} = u_{n+1,j} = 0.$$

The finite-difference equation can be written in the form

$$u_{i,j+1} = \frac{k}{h^2}(u_{i-1,j} - 2u_{ij} + u_{i+1,j}) + u_{i,j},$$

or, introducing the notation $s = k/h^2$,

$$u_{i,j+1} = su_{i-1,j} + (1 - 2s)u_{ij} + su_{i+1,j}.$$

Since this equation gives the new values of $u_{i,j+1}$ explicitly in terms of previous values of $u_{i+1,j}, \;\; u_{ij}, \;\; u_{i-1,j}$, the method based on this equation is called an explicit method.

2. Stability Analysis

The finite-difference equation, which defines the numerical process, can be interpreted using matrix and vector notations. It can be written as

$$U_{j+1} = AU_j, \tag{5}$$

where

$$A = \begin{pmatrix} 1-2s & s & 0 & ... & 0 \\ s & 1-2s & s & ... & 0 \\ 0 & s & 1-2s & ... & 0 \\ ... & ... & ... & ... & ... \\ 0 & 0 & 0 & ... & 1-2s \end{pmatrix}, \qquad U_j = \begin{pmatrix} u_{1j} \\ u_{2j} \\ u_{3j} \\ ... \\ u_{nj} \end{pmatrix}.$$

Notice that boundary conditions $u_{0j} = u_{n+1,j} = 0$ have been taken into account. Hence, we have

$$U_j = AU_{j-1} = A^2 U_{j-2} = ... = A^j U_0. \tag{6}$$

From the physical point of view,

$$\lim_{t \to +\infty} u(x,t) = 0,$$

thus, we require

$$\lim_{j \to +\infty} U_j = \lim_{j \to +\infty} A^j U_0 = 0$$

for all vector U_0. If the explicit algorithm satisfies this condition it is called to be stable. On the other side, we have

$$||U_j|| = ||A^j U_0|| \leq ||A||^j ||U_0||,$$

and the mentioned above limiting condition is fulfilled if $||A|| < 1$. The matrix A is symmetric, the inequality $||A|| < 1$ is equivalent to the fact that all the eigenvalues of A must satisfy $|\lambda_m| < 1$. To complete the foregoing analysis, we use the following representation for A:

$$A = I - sB, \tag{7}$$

where I is the identity matrix, and

$$B = \begin{pmatrix} 2 & -1 & 0 & ... & 0 \\ -1 & 2 & -1 & ... & 0 \\ 0 & -1 & 2 & ... & 0 \\ ... & ... & ... & ... & ... \\ 0 & 0 & 0 & ... & 2 \end{pmatrix}.$$

The eigenvalues of A are $\lambda_m = 1 - s\mu_m$, where μ_m are the eigenvalues of B, and moreover,

$$\mu_m = 2(1 - \cos\theta_m), \qquad \theta_m = \frac{m\pi}{n+1}, \qquad 1 \leq m \leq n.$$

Hence the inequality $|\lambda_m| < 1$ holds if

$$-1 < 1 - 2s(1 - \cos\theta_m) < 1.$$

Note that $s > 0$. Thus, we obtain that $|\lambda_m| < 1$ is equivalent to

$$s < \frac{1}{1 - \cos\theta_m},$$

or

$$s < \frac{1}{2}. \tag{8}$$

This result means that if $s < 1/2$, or $k/h^2 < 1/2$, the explicit algorithm is stable. This severe restriction forces the method to be very slow, as the t-variable step k is to be chosen very small.

There is another way to derive the stability condition. This is application of the Fourier method. The basic idea is as follows. We seek solution of the difference equation in the form

$$u_{lj} = e^{i\alpha lh} q^j.$$

On substituting the trial solution in the difference equation and removing the factor $e^{i\alpha lh} q^j$, we obtain

$$q = se^{-i\alpha h} + 1 - 2s + se^{i\alpha h} = 1 - 4s\sin^2(\frac{\alpha h}{2}).$$

The explicit method is stable if the solution satisfies

$$\lim_{j\to+\infty} u_{lj} = 0.$$

Thus, require that $|q| < 1$, or

$$-1 < 1 - 4s\sin^2(\frac{\alpha h}{2}) < 1.$$

This leads to the restriction

$$s < \frac{1}{2\sin^2(\frac{\alpha h}{2})},$$

and we must have $s < 1/2$ for stability.

3. Implicit Method

We continue to study the model problem of heat equation. Using the notations introduced in the previous section, and changing the finite-difference formula approximating the continuous derivative with respect to t, we write the finite-difference equation as

$$\frac{u_{i+1,j} - 2u_{ij} + u_{i-1,j}}{h^2} = \frac{u_{i,j} - u_{i,j-1}}{k}. \tag{9}$$

This method is said to provide the implicit algorithm. This leads to

$$u_{i,j-1} = -su_{i-1,j} + (1+2s)u_{ij} - su_{i+1,j},$$

and, hence, we have

$$AU_j = U_{j-1}, \tag{10}$$

where

$$A = \begin{pmatrix} 1+2s & -s & 0 & ... & 0 \\ -s & 1+2s & -s & ... & 0 \\ 0 & -s & 1+2s & ... & 0 \\ ... & ... & ... & ... & ... \\ 0 & 0 & 0 & ... & 1+2s \end{pmatrix}, \qquad U_j = \begin{pmatrix} u_{1j} \\ u_{2j} \\ u_{3j} \\ ... \\ u_{nj} \end{pmatrix}.$$

Formally, the solution of the difference equation is given by

$$U_j = A^{-1}U_{j-1} = A^{-j}U_0.$$

The stability question for the implicit algorithm is solved easily as in this case the matrix A is represented in the form:

$$A = I + sB,$$

and its eigenvalues are

$$\lambda_m = 1 + 2s(1 - \cos\theta_m), \qquad \theta_m = \frac{m\pi}{n+1}, \qquad 1 \le m \le n.$$

Since these obviously satisfy $\lambda_m > 1$, the eigenvalues of A^{-1} lie in the interval $(0,1)$ for arbitrary $s > 0$, and as a result $||A^{-1}|| < 1$. Thus, we conclude that the proposed method is stable for all values of h and k as

$$||U_j|| = ||A^{-j}U_0|| \le ||A^{-1}||^j ||U_0||, \quad \text{and} \lim_{j\to+\infty} ||U_j|| = 0.$$

4. Crank-Nicolson Method

It is possible to combine the implicit and explicit methods into a more general formula containing a parameter θ. This formula is

$$\frac{\theta}{h^2}(u_{i-1,j} - 2u_{ij} + u_{i+1,j}) + \frac{1-\theta}{h^2}(u_{i-1,j-1} - 2u_{i,j-1} + u_{i+1,j-1}) = \frac{1}{k}(u_{i,j} - u_{i,j-1}). \tag{11}$$

We see that when $\theta = 0$, this formula yields the explicit scheme. When $\theta = 1$, the formula reduces to the implicit scheme discussed above. The case $\theta = 1/2$ leads to a numerical procedure known as Crank-Nicolson method. In this case the difference equation is given by

$$-su_{i-1,j} + (2+2s)u_{ij} - su_{i+1,j} = su_{i-1,j-1} + (2-2s)u_{i,j-1} + su_{i+1,j-1}.$$

This equation has the vector form

$$(2I + sB)U_j = (2I - sB)U_{j-1}.$$

Hence, the solution is given by

$$U_j = (2I + sB)^{-1}(2I - sB)U_{j-1}.$$

A little algebra shows that all eigenvalues λ_m of the matrix

$$(2I + sB)^{-1}(2I - sB)$$

satisfy the inequality $|\lambda_m| < 1$ for arbitrary $s > 0$. Thus, the Crank-Nicolson method is stable for all values of the ratio $s = k/h^2$.

It is worth remarking that the prevous explicit and impicit methods have the order of approximation of $O(k) + O(h^2)$, whereas the Crank-Nicolson method has the order of $O(k^2) + O(h^2)$. It is shown from the following analysis, namely, we have

$$\frac{u_{i-1,j+1} - 2u_{ij+1} + u_{i+1,j+1} + u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{2h^2} = \frac{u_{i,j+1} - u_{i,j}}{k}.$$

Then we proceed with the following approximation

$$\frac{1}{2}(u_{xx}(j+1) + \frac{h^2}{12}u_{xxxx}) + \frac{1}{2}(u_{xx}(j) + \frac{h^2}{12}u_{xxxx}) = u_t + \frac{k}{2}u_{tt}.$$

As

$$\frac{1}{2}u_{xx}(j+1) = \frac{1}{2}u_{xx}(j) + \frac{1}{2}ku_{xxt} + O(k^2),$$

and

$$u_t = u_{xx}, \qquad u_{tt} = u_{xxt},$$

one can see clear that the Crank-Nicolson method has the order of approximation $O(k^2) + O(h^2)$.

5. Error Analysis for the Explicit Method

Stability is , of course, not the only criterion used in selecting the step size k and h in these methods. In general, the smaller we take k and h, the more accurately the discretized problem will approximate the original differential equation. What is required is the theorem to guarantee that the solution of the discrete problem converges to the solution of the original problem when $k \to 0$ and $h \to 0$, that is, the error as a difference between both solutions tends to zero. We shall study the corresponding error analysis for the explicit method.

In the error analysis we introduce the error

$$e_{ij} = u_{ij} - \hat{u}_{ij},$$

where $\hat{u}_{ij} = u(x_i, y_j)$ are the values of the exact solution. Substituting

$$u_{ij} = e_{ij} + \hat{u}_{ij}$$

into the difference equation of explicit algorithm

$$u_{i,j+1} = su_{i-1,j} + (1-2s)u_{ij} + su_{i+1,j},$$

we obtain

$$e_{i,j+1} = se_{i-1,j} + (1-2s)e_{ij} + se_{i+1,j} - s[u_{i-1,j} + u_{i+1,j} - 2u_{i,j}] + [u_{i,j+1} - u_{i,j}].$$

Using the finite-difference approximation formulas

$$f''(x) = \frac{1}{h^2}[f(x+h) + f(x-h) - 2f(x)] - \frac{h^2}{12}f^{(4)}(\xi),$$

$$g'(t) = \frac{1}{k}[g(t+k) - g(t)] - \frac{k}{2}g''(\tau),$$

yields

$$e_{i,j+1} = se_{i-1,j} + (1-2s)e_{ij} + se_{i+1,j} - s[h^2 u_{xx}(x_i, t_j) + \frac{h^4}{12}u_{xxxx}(\xi_i, t_j)] +$$

$$[ku_t(x_i,t_j)+\frac{k^2}{2}u_{tt}(x_i,\tau_j)].$$

Now use the fact that $sh^2=k$ and $u_{xx}=u_t$. The last equation can be written in the form

$$e_{i,j+1}=se_{i-1,j}+(1-2s)e_{ij}+se_{i+1,j}-kh^2[\frac{1}{12}u_{xxxx}(\xi_i,t_j)-\frac{s}{2}u_{tt}(x_i,\tau_j)]. \tag{12}$$

Let us confine (x,t) to the compact set

$$S=\{(x,t):0\le x\le 1 \quad \text{and} \quad 0\le t\le T\}.$$

The put over all $(x,t)\in S$

$$M=\frac{1}{12}\sup|u_{xxxx}(\xi_i,t_j)|+\frac{s}{2}\sup|u_{tt}(x_i,\tau_j)|.$$

We also define an error vector

$$E_j=\begin{pmatrix} e_{1j}\\ e_{2j}\\ e_{3j}\\ \dots\\ e_{nj}\end{pmatrix},$$

and put

$$||E_j||=\max|e_{ij}|, \qquad 1\le i\le n.$$

Finally, we assume that $1-2s\ge 0$. Then from the equation (12), we have

$$|e_{i,j+1}|\le s|e_{i-1,j}|+(1-2s)|e_{ij}|+s|e_{i+1,j}|+kh^2M\le s||E_j||+$$

$$(1-2s)||E_j||+s||E_j||+kh^2M=||E_j||+kh^2M,$$

and, hence,

$$||E_{j+1}||\le||E_j||+kh^2M\le||E_{j-1}||+2kh^2M\le||E_0||+(j+1)kh^2M,$$

or

$$||E_j||\le||E_0||+jkh^2M.$$

Then, because $t\le T$ and $||E_0||=0$, we have

$$||E_j||\le Th^2M.$$

Thus, as $h \to 0$, $||E_j|| \to 0$, and the numerical solution converges to the exact solution provided that $s < 1/2$ and the functions u_{xxxx} and u_{tt} are continuous.

6. Wave Equation. Finite-Difference Method

As a model problem the wave equation in its one-dimensional version together with subsidiary conditions is as follows:

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} + f(x,t), \tag{13}$$

with initial condition

$$u(x,0) = u_0(x), \qquad u_t(x,0) = u_1(x), \qquad a \le x \le b,$$

and with boundary condition

$$u(a,t) = \phi_1(t), \qquad u(b,t) = \phi_2(t), \qquad t \ge 0,$$

where solution u dependent on x coordinate and time t describes wave propagating with speed c. For the sake of simplicity, we again assume that

$$f(x,t) = 0, \qquad \phi_1(t) = \phi_2(t) = 0, \qquad c = 1, \qquad a = 0, \qquad b = 1.$$

Then, the initial-boundary problem is given by

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}, \qquad u(x,0) = u_0(x), \qquad u_t(x,0) = u_1(x), \qquad 0 \le x \le 1, \tag{14}$$

$$u(0,t) = u(1,t) = 0, \qquad t \ge 0.$$

Using the finite-difference method involves the discretisation of the domain:

$$t_j = jk, \quad j \ge 0, \qquad x_i = ih, \quad 0 \le i \le n+1, \tag{15}$$

where the variables t and x have different step size k and h,

$$h = \frac{1}{n+1}.$$

Our objective is to compute approximate values of the solution function u at the so-called mesh points-nodes (t_j, x_i).

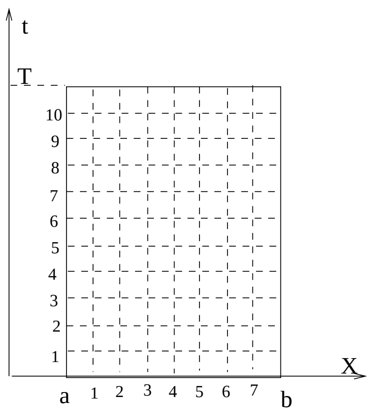

Figure 2: Initial boundary value problem for the wave equation

The next step is the replacement of the continuous derivatives with the finite-differences

$$f''(x) \approx \frac{f(x+h)+f(x-h)-2f(x)}{h^2}.$$

As a result of the discretisation and replacement of $u(x_i, t_j)$ by u_{ij} we obtain the finite-difference equation

$$\frac{u_{i-1,j} - 2u_{ij} + u_{i+1,j}}{h^2} = \frac{u_{i,j-1} - 2u_{ij} + u_{i,j+1}}{k^2}. \tag{16}$$

The initial conditions gives us

$$u_0(x_i) = u(x_i, 0) = u_{i0},$$
$$u_1(x_i) = u_t(x_i, 0) \approx \frac{u(x_i, k) - u(x_i, 0)}{k} = \frac{u_{i1} - u_{i0}}{k}.$$

This means that we know the values of

$$u_{i1} = u_1(x_i)k + u_0(x_i).$$

Boundary conditions yield

$$u_{0j} = u_{n+1,j} = 0.$$

The finite-difference equation can be written in the form

$$u_{i,j+1} = su_{i-1,j} + 2(1-s)u_{ij} + su_{i+1,j} - u_{i,j-1},$$

where $s = k^2/h^2$, and, hence, we have

$$U_{j+1} = AU_j - U_{j-1}, \tag{17}$$

where

$$A = \begin{pmatrix} 2(1-s) & s & 0 & ... & 0 \\ s & 2(1-s) & s & ... & 0 \\ 0 & s & 2(1-s) & ... & 0 \\ ... & ... & ... & ... & ... \\ 0 & 0 & 0 & ... & 2(1-s) \end{pmatrix}, \qquad U_j = \begin{pmatrix} u_{1j} \\ u_{2j} \\ u_{3j} \\ ... \\ u_{nj} \end{pmatrix}.$$

Since this equation gives the new values of $u_{i,j+1}$ explicitly in terms of previous values of $u_{i+1,j}, \quad u_{ij}, \quad u_{i-1,j}, \quad u_{i,j-1}$, the method based on this equation is called an explicit method. Taking into account the boundary and initial conditions, this algorithm enables us to evaluate numerically u_{ij} in the rectangular $0 \leq x \leq 1, \qquad 0 \leq t \leq T$.

Using the Fourier method, we derive the stability condition. We seek solution of the difference equation in the form

$$u_{lj} = e^{i\alpha l h} q^j.$$

On substituting the trial solution into the difference equation and removing the factor $e^{i\alpha l h} q^j$, we obtain

$$q^2 = q(se^{-i\alpha h} + 2(1-s) + se^{i\alpha h}) - 1 = 2q(1 - 2s\sin^2(\frac{\alpha h}{2})) - 1,$$

or

$$q^2 - 2q(1 - 2s\sin^2(\frac{\alpha h}{2})) + 1 = 0.$$

The explicit method is stable if the solution satisfies

$$\lim_{j \to +\infty} u_{lj} \neq \infty.$$

Thus, we require that the zeros of this quadratic equation $|q_{1,2}| \leq 1$. Taking into account the fact $q_1 q_2 = 1$, it is clear that the inequality $|q_{1,2}| \leq 1$ holds if both zeros $q_{1,2}$ are complex conjugate

$$q_{1,2} = e^{\pm i\gamma}.$$

This takes place if

$$[1 - 2s\sin^2(\frac{\alpha h}{2})]^2 \leq 1.$$

This leads to the restriction

$$s \leq \frac{1}{\sin^2(\frac{\alpha h}{2})},$$

and we must have $s \leq 1$ for stability, that is $k \leq h$.