Numerical solution of the heat equation

«The Book of Nature is written in the language of mathematics».
Galileo Galilei

1 Short theoretical excursion

Mathematical physics is a branch of mathematics in which physical problems are studied at the mathematical level of rigour. As it happens that a quite huge amount of real processes are described by partial differential equations (PDE). In this regard, PDE are one of the main objects of study of mathematical physics. Within this tutorial, we will talk about the heat equation. Let $u(t, x, y, z)$ be the desired function then we can write a heat equation

$$\frac{\partial u}{\partial t} = a^2 \Delta u, \tag{1}$$

where a — some coefficient, $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ — Laplace operator written in the Cartesian coordinate system. Equations like (1) describes how the distribution of some quantity evolves in time and space.

First of all, we will talk about the simplest variant of the heat equation – linear homogeneous one-dimensional equation. Let meaning of $u(t, x)$ be a temperature $T(t, x)$, let's rewrite (1) for our case

$$\frac{\partial T}{\partial t} = a^2 \frac{\partial^2 T}{\partial x^2}, \tag{2}$$

where $a^2 = \sqrt{\frac{\lambda}{\rho c}}$ — coefficient of thermal diffusivity (ρ — density, c — coefficient of heat capacity). This coefficient is determined by the properties of the material. Those who have previously dealt with differential equations know that to obtain a single solution, it is necessary to specify the initial condition. Because the order of time derivative is first we have to specify only one initial condition for our function. Let suppose that our initial moment of time $t_0 = 0$. Otherwise, we can always replace variables and achieve this. So, we may write

$$T(0, x) = \varphi(x), \tag{3}$$

where $\varphi(x)$ — some known function. Generally speaking, we are already able to solve equation (2) with initial condition (3). This solution is known and is called Poisson formula

$$T(t, x) = \frac{1}{2a\sqrt{\pi t}} \int\limits_{-\infty}^{+\infty} \exp\left[-\frac{(x-\xi)^2}{4a^2 t}\right] \varphi(\xi) d\xi. \tag{4}$$

And all in this formula is cool except fact that it's correct only for infinite space. In practical tasks, we are dealing with limited areas ($x \in [a, b]$). To settle this moment it is necessary to set the boundary conditions (on bound $x = a$ and on bound $x = b$). There are three main types of boundary conditions

- Dirichlet condition

$$
\begin{aligned}
T(t, a) &= \psi_1(t), \\
T(t, b) &= \psi_2(t),
\end{aligned}
$$

- Neumann condition

$$
\begin{aligned}
\left.\frac{\partial T}{\partial x}\right|_{x=a} &= f_1(t), \\
\left.\frac{\partial T}{\partial x}\right|_{x=b} &= f_2(t),
\end{aligned}
$$

- Robin condition

$$
\begin{aligned}
\left.\left(\alpha T + \beta \frac{\partial T}{\partial x}\right)\right|_{x=a} &= g_1(t), \\
\left.\left(\alpha T + \beta \frac{\partial T}{\partial x}\right)\right|_{x=b} &= g_2(t).
\end{aligned}
$$

Boundary conditions may be mixed: for example on the left side we have Dirichlet condition but on the right side, we have Neumann condition.

For convenience, we will consider the specific problem

$$
\begin{cases}
\dfrac{\partial T}{\partial t} = a^2 \dfrac{\partial^2 T}{\partial x^2}, \quad x \in (a, b), \quad t \in (0, t^*); \\
T(0, x) = \varphi(x); \\
\left.\dfrac{\partial T}{\partial x}\right|_{x=a} = g(t); \\
T(t, b) = f(t).
\end{cases}
\tag{5}
$$

2 Computational solution

There are lots of methods for calculating the problem such (5). We going to tell about finite difference method. The main idea of this method is to replace derivatives with their differential analogues. This can be done in many different ways. First of all, let's look at the first order derivative at the point x^* (we suppose that it's exist). By definition we may write

$$
f'(x^*) = \lim_{\Delta x \to 0} \frac{f(x^* + \Delta x) - f(x^*)}{\Delta x}.
$$

The idea of finite difference method is to approximate derivatives by their finite analogues

$$f'(x^*) \approx \frac{f(x^* + \Delta x) - f(x^*)}{\Delta x}.$$

However, this can be done in different ways, for example

$$f'(x^*) \approx \frac{f(x^*) - f(x^* - \Delta x)}{\Delta x},$$

or

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

If we want calculate the second-ordinary derivative we may use the same idea

$$f''(x^*) = \frac{\frac{f(x^*+\Delta x) - f(x^*)}{\Delta x} - \frac{f(x^*) - f(x^*-\Delta x)}{\Delta x}}{\Delta x} = \frac{f(x^* + \Delta x) - 2f(x^*) + f(x^* - \Delta x)}{(\Delta x)^2}.$$

Surely we can use whatever formula what we want (accuracy may depend on it, but in this tutorial, we won't talk about the intricacies of computational mathematics).

So, let's back to our problem. First of all, we have to create a grid – split the area $[a, b]$ into N sub-areas and the same for the time. We will create a uniform grids with step h for space and τ for time

$$\{x_i\}_{i=0}^{N}: \quad x_0 = a, \quad x_N = b, \quad x_{k+1} = x_k + h;$$
$$\{t_i\}_{i=0}^{M}: \quad t_0 = 0, \quad t_M = t^*, \quad t_{k+1} = t_k + \tau.$$

let's use the following notation

$$T_i^n \triangleq T(x_i, t_n).$$

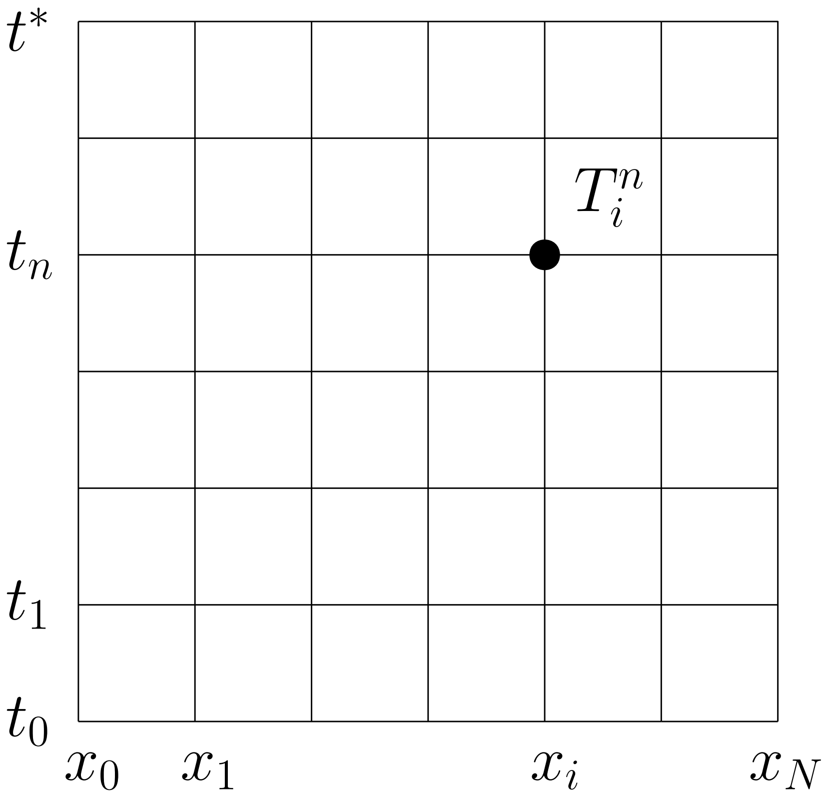

Figure 1: Grid.

Now let's replace derivatives with their finite difference analogues

$$\frac{\partial T}{\partial t} \approx \frac{T_i^{n+1} - T_i^n}{\tau},$$

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}}{h^2}.$$

The same idea for initial and boundary conditions. But previously let's choose specific parameters (all values are written in International System of Units) — it's going to be steel

$$[a, b] = [0, 0.1], \;\; \lambda = 0.7, \;\; \rho = 7800, \;\; c = 460;$$

$$\varphi(x) = 27, \;\; \forall x \in [0, 0.1];$$

$$g(t) = 0, \;\; f(t) = 50, \;\; \forall t \in [0, t^*].$$

$$T(0, x) = \varphi(x) \to T_i^0 = 27, \;\; \forall i = \overline{0, N};$$

$$T(t, 0.1) = 50 \to T_N^n = 50, \;\; \forall n = \overline{0, M};$$

$$\left.\frac{\partial T}{\partial x}\right|_{x=a} = 0 \to \frac{T_1^n - T_0^n}{h} = 0 \Rightarrow T_0^n = T_1^n, \;\; \forall n = \overline{0, M}.$$

Now let's rewrite the heat equation in (5) in our new terms

$$c\rho\frac{T_i^{n+1} - T_i^n}{\tau} = \lambda\frac{T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}}{h^2}. \tag{6}$$

We can see that (6) - it's a linear equation for unknown T_i^{n+1}. First of all, we will write it in a slightly different form

$$A_i T_{i+1}^{n+1} - B_i T_i^{n+1} + C_i T_{i-1}^{n+1} = F_i, \tag{7}$$

where

$$A_i = C_i = \frac{\lambda}{h}, \;\; B_i = \frac{2\lambda}{h^2} + \frac{\rho c}{\tau}, \;\; F_i = -\frac{\rho c}{\tau}T_i^n.$$

We may rewrite (7) in matrix form

$$\begin{pmatrix} B_1 & C_1 & 0 & 0 & \dots & 0 \\ A_2 & -B_2 & C_2 & 0 & \dots & 0 \\ 0 & A_3 & -B_3 & C_3 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & A_{N-1} & -B_{N-1} & C_{N-1} \\ 0 & 0 & \dots & 0 & A_N & -B_N \end{pmatrix} \begin{pmatrix} T_1^{n+1} \\ T_2^{n+1} \\ T_3^{n+1} \\ \vdots \\ T_{N-1}^{n+1} \\ T_N^{n+1} \end{pmatrix} = \begin{pmatrix} F_1 \\ F_2 \\ F_3 \\ \vdots \\ F_{N-1} \\ F_N \end{pmatrix} \tag{7$'$}$$

Systems like (7′) call tridiagonal and there are many methods how to solve this system. We will use one of the most useful – Tridiagonal matrix algorithm.

The idea of the Tridiagonal matrix algorithm is to find the solution in the form

$$T_i^{n+1} = \alpha_i T_{i+1}^{n+1} + \beta_i.$$

We have to put this in (7) and as a a result we may write

$$\alpha_i = \frac{A_i}{B_i - C_i\alpha_{i-1}}, \quad \beta_i = \frac{C_i\beta_{i-1} - F_i}{B_i - C_i\alpha_{i-1}}.$$

From the left side boundary condition, we can find

$$T_0 = T_1 \Rightarrow \alpha_0 = 1, \quad \beta_0 = 0.$$

Now we can realize our algorithm.

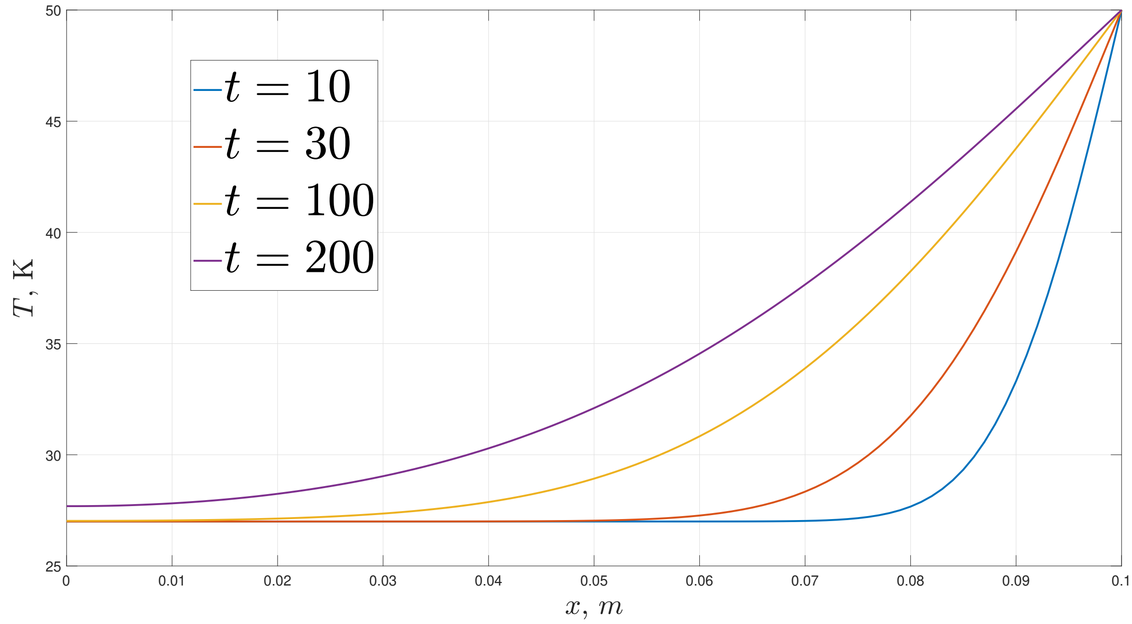

Figure 2: Temperature distribution for different moments in time (sec).