Progress Report

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Derivation of central difference formula for second derivative

We know that

$$f_{i+1} = f_i + \left.\frac{df}{dx}\right|_i (x_{i+1} - x_i) + \left.\frac{d^2f}{dx^2}\right|_i \frac{(x_{i+1} - x_i)^2}{2!} + \dots \tag{1}$$

$$f_{i-1} = f_i + \left.\frac{df}{dx}\right|_i (x_{i-1} - x_i) + \left.\frac{d^2f}{dx^2}\right|_i \frac{(x_{i-1} - x_i)^2}{2!} + \dots \tag{2}$$

Adding equations (1) and (2) and neglecting the higher order terms,

$$\begin{aligned} f_{i+1} + f_{i-1} = \quad & 2f_i + \left.\frac{df}{dx}\right|_i (x_{i+1} - x_i + x_{i-1} - x_i) \\ & + \left.\frac{d^2f}{dx^2}\right|_i \frac{(x_{i+1} - x_i)^2}{2} + \left.\frac{d^2f}{dx^2}\right|_i \frac{(x_{i-1} - x_i)^2}{2} \end{aligned} \tag{3}$$

For *equally spaced intervals*,

$$x_{i+1} - x_i = x_i - x_{i-1} = \Delta x$$

$$x_{i+1} - x_i + x_{i-1} - x_i = 0$$

Substituting in equation (3), we get

$$f_{i+1} + f_{i-1} = 2f_i + 2\left.\frac{d^2f}{dx^2}\right|_i \frac{(\Delta x)^2}{2}$$

$$\left.\frac{d^2f}{dx^2}\right|_i = \frac{f_{i+1} - 2f_i + f_{i-1}}{(\Delta x)^2} \tag{4}$$

For *unequally spaced intervals*, from equation (3), we can write

$$\begin{aligned} f_{i+1} + f_{i-1} = \quad & 2f_i + \left.\frac{df}{dx}\right|_i (x_{i+1} - x_i + x_{i-1} - x_i) \\ & + \left.\frac{d^2 f}{dx^2}\right|_i \left[\frac{(x_{i+1} - x_i)^2 + (x_{i-1} - x_i)^2}{2}\right] \end{aligned} \tag{5}$$

We also know that the central difference formula for the first derivative, neglecting the higher order terms, may be written as

$$\left.\frac{df}{dx}\right|_i = \frac{f_{i+1} - f_{i-1}}{x_{i+1} - x_{i-1}} \tag{6}$$

Substituting equation (6) in equation (5), we have

$$\begin{aligned} f_{i+1} + f_{i-1} = \quad & 2f_i + \frac{f_{i+1} - f_{i-1}}{x_{i+1} - x_{i-1}}(x_{i+1} - 2x_i + x_{i-1}) \\ & + \left.\frac{d^2 f}{dx^2}\right|_i \left[\frac{(x_{i+1} - x_i)^2 + (x_{i-1} - x_i)^2}{2}\right] \end{aligned}$$

Rearranging this equation,

$$\left.\frac{d^2 f}{dx^2}\right|_i = \quad \frac{(f_{i+1} + f_{i-1}) - 2f_i - (f_{i+1} - f_{i-1})\dfrac{(x_{i+1} - 2x_i + x_{i-1})}{x_{i+1} - x_{i-1}}}{\dfrac{(x_{i+1} - x_i)^2 + (x_{i-1} - x_i)^2}{2}}$$

$$\begin{aligned} \left.\frac{d^2 f}{dx^2}\right|_i = \quad & \frac{2(f_{i+1} + f_{i-1})}{(x_{i+1} - x_i)^2 + (x_{i-1} - x_i)^2} \\ & - \frac{4f_i}{(x_{i+1} - x_i)^2 + (x_{i-1} - x_i)^2} \\ & - \frac{2(f_{i+1} - f_{i-1})(x_{i+1} - 2x_i + x_{i-1})}{(x_{i+1} - x_{i-1})[(x_{i+1} - x_i)^2 + (x_{i-1} - x_i)^2]} \end{aligned} \tag{7}$$

For the case of of equally spaced data with $x_{i+1} - x_i = x_i - x_{i-1} = \Delta x$, this again reduces to equation (4).

Numerical solution for 2D heat transfer

A C++ code was written to solve a simple problem of 2D heat transfer in a block of pure silver (99.9%).

Initial condition was $T_i = 25°C$.

Boundary conditions were selected as follows:

1. $T_{xi} = 25°C$ at $x = 0$
2. $T_{xf} = 25°C$ at $x = L$
3. $T_{yi} = 25°C$ at $y = 0$
4. $T_{yf} = 50°C$ at $y = L$

The analytical solution to this problem is given by:

$$T(x, y) = \frac{2T_3}{\pi} \sum_{n=1}^{\infty} \left[\frac{(-1)^{n+1} + 1}{n} \right] \frac{\sin \lambda_n x \sinh \lambda_n y}{\sinh \lambda_n W} + T_1 \tag{8}$$

where

$$T_1 = T_{xi} = T_{xf} = T_{yi} \tag{9}$$

and

$$T_3 = T_{yf} - T_1 \tag{10}$$

Forward in time center in space (FTCS) method was used with the following formula:

$$T_i^{n+1} = T_i^n + \Delta t \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) \tag{11}$$

A time step of 0.001 was utilized with 200×200 grid intervals in both x and y directions.

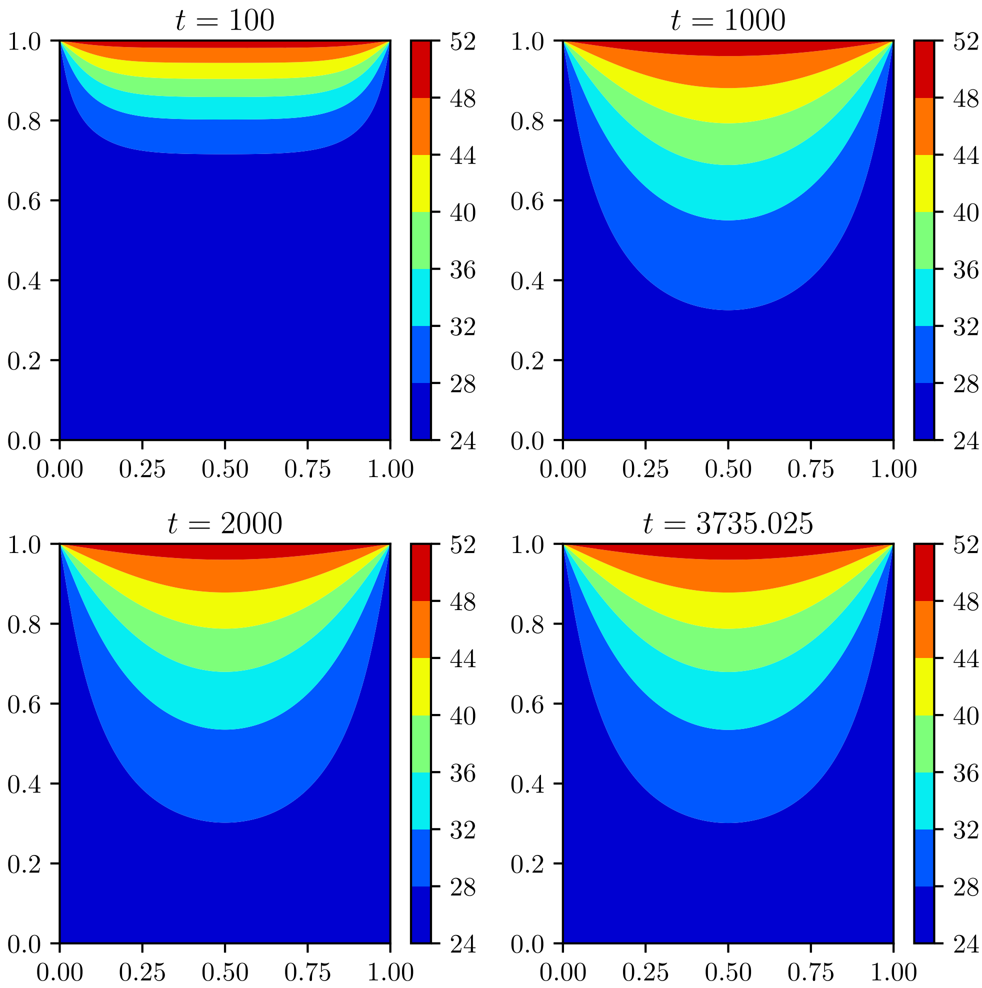

Figure 1: Plots for various values of time (time step of 0.001).