

Numerical solution of partial differential equations: a very basic introduction

Partial differential equations (PDEs) are differential equations with more than one independent variable. We shall consider the simplest PDEs that have just two independent variables—one of which represents time t and the other a spatial coordinate x —and one (scalar) dependent variable u . Examples of such PDEs include the following:

$$\frac{\partial u}{\partial t} = c \frac{\partial u}{\partial x} \quad (\text{convection equation or one-way wave equation})$$

$$\frac{\partial u}{\partial t} = c \frac{\partial^2 u}{\partial x^2} \quad (\text{heat equation or diffusion equation})$$

$$\frac{\partial u}{\partial t} = c \frac{\partial^2 u}{\partial x^2} + R(u) \quad (\text{reaction–diffusion equation})$$

$$i \frac{\partial u}{\partial t} = \frac{1}{2} \frac{\partial^2 u}{\partial x^2} + V(x)u \quad (\text{Schrödinger equation})$$

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + (\kappa - 1) \frac{\partial u}{\partial x} - \kappa u \quad (\text{Black–Scholes equation})$$

To solve such a PDE means to find a function $u(t, x)$ that satisfies the PDE along with an initial condition

$$u(0, x) = g(x) \quad \text{for } a \leq x \leq b \quad (\text{initial distribution or profile at } t = 0)$$

and boundary conditions at $x = a$ and $x = b$, which are typically

$$\begin{aligned} u(t, a) = \alpha, \quad u(t, b) = \beta \quad & \text{for all } t > 0 && (\text{Dirichlet BCs}) \\ \text{or } \frac{\partial u}{\partial x}(t, a) = 0, \quad \frac{\partial u}{\partial x}(t, b) = 0 \quad & \text{for all } t > 0 && (\text{zero Neumann BCs}) \end{aligned}$$

The approach we take to compute an approximation of the solution $u(t, x)$ is to *approximate the spatial derivatives* $\frac{\partial u}{\partial x}$ and $\frac{\partial^2 u}{\partial x^2}$ *using finite difference formulas* (i.e. “spatial discretization by finite differences”).

Thus these spatial derivatives will be replaced by algebraic expressions involving $u_1, u_2, \dots, u_N$, where each u_j is the approximation of the solution u at a spatial grid point x_j . In this way, we can rewrite the original PDE in the form

$$\frac{\partial \mathbf{u}}{\partial t} = F(\mathbf{u}) \quad \text{where } \mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{pmatrix}$$

Then we use a *time-stepping algorithm* to compute $\mathbf{u}$ at a sequence of t -values up to some final time T . We can choose a fixed-time-step method such as one of the codes we wrote in class and Homework #8, or use a built-in Matlab ODE solver such as `ode45`.

Just like for the boundary value problem $y'' = f(x, y, y')$ with boundary conditions given at $x = a$ and $x = b$, we divide the interval $[a, b]$ into $N + 1$ subintervals of equal length $\Delta x = \frac{b - a}{N + 1}$, so that

$$\begin{aligned} x_0 &= a, & x_{N+1} &= b \\ x_j &= a + j\Delta x & \text{for } j &= 1, 2, \dots, N \end{aligned}$$

At each interior grid point x_j with $j = 1, 2, \dots, N$, use the $O(\Delta x^2)$ centered difference approximations

$$\begin{aligned} \frac{\partial u}{\partial x}(t, x_j) &\approx \frac{u(t, x_j + \Delta x) - u(t, x_j - \Delta x)}{2\Delta x} = \frac{u(t, x_{j+1}) - u(t, x_{j-1})}{2\Delta x} \\ \frac{\partial^2 u}{\partial x^2}(t, x_j) &\approx \frac{u(t, x_j + \Delta x) - 2u(t, x_j) + u(t, x_j - \Delta x)}{\Delta x^2} = \frac{u(t, x_{j+1}) - 2u(t, x_j) + u(t, x_{j-1}))}{\Delta x^2} \end{aligned}$$

and hence

$$\begin{aligned} \frac{\partial u}{\partial x}(t, x_j) &\approx \frac{u_{j+1} - u_{j-1}}{2\Delta x} = \frac{1}{2\Delta x}(-u_{j-1} + u_{j+1}) \\ \frac{\partial^2 u}{\partial x^2}(t, x_j) &\approx \frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2} = \frac{1}{\Delta x^2}(u_{j-1} - 2u_j + u_{j+1}) \end{aligned}$$

where u_j denotes the approximate value of $u(t, x_j)$ that we aim to compute (so each u_j is actually a function of t).

Therefore, the first derivative $\frac{\partial u}{\partial x}(t, x_j)$ for $j = 2, \dots, N - 1$ becomes an array of expressions $\frac{1}{2\Delta x}A_1\mathbf{u}$ where

$$A_1 = \begin{pmatrix} -1 & 0 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & -1 & 0 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & & & \ddots & & & \vdots \\ \vdots & \vdots & & & & \ddots & & \vdots \\ 0 & 0 & 0 & \cdots & 0 & -1 & 0 & 1 \end{pmatrix}, \quad \mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ \vdots \\ \vdots \\ u_{N-2} \\ u_{N-1} \\ u_N \end{pmatrix}$$

The second derivative $\frac{\partial^2 u}{\partial x^2}(t, x_j)$ for $j = 2, \dots, N - 1$ becomes an array of expressions $\frac{1}{\Delta x^2}A_2\mathbf{u}$ where

$$A_2 = \begin{pmatrix} 1 & -2 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & & & \ddots & & & \vdots \\ \vdots & \vdots & & & & \ddots & & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 & -2 & 1 \end{pmatrix}, \quad \mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ \vdots \\ \vdots \\ u_{N-2} \\ u_{N-1} \\ u_N \end{pmatrix}$$

The boundary conditions will appear in the $j = 1$ and $j = N$ expressions for $\frac{\partial u}{\partial x}(t, x_j)$ or $\frac{\partial^2 u}{\partial x^2}(t, x_j)$, and will be incorporated into the first and last (N th) rows of A .

Dirichlet boundary conditions

$$u|_{x=a} = \alpha, \quad u|_{x=b} = \beta$$

This means we must have $u_0 = \alpha$ and $u_{N+1} = \beta$.

For the first derivative $\frac{\partial u}{\partial x}$, the $j = 1$ expression is

$$\frac{1}{2\Delta x}(-u_0 + u_2) = \frac{1}{2\Delta x}(u_2 - \alpha)$$

so the first row of A_1 should be $(0 \ 1 \ 0 \ \cdots \ 0)$, and we need to add on an extra term $-\alpha$.

The $j = N$ expression is

$$\frac{1}{2\Delta x}(-u_{N-1} + u_{N+1}) = \frac{1}{2\Delta x}(-u_{N-1} + \beta)$$

so the N th row of A_1 should be $(0 \ \cdots \ 0 \ -1 \ 0)$, and we need to add on an extra term β .

Therefore, $\frac{\partial u}{\partial x}(t, x_j)$ for $j = 1, \dots, N$ becomes an array of expressions $\frac{1}{2\Delta x}(A_1 \mathbf{u} + B)$ where

$$A_1 = \begin{pmatrix} 0 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ -1 & 0 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & -1 & 0 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & & & \ddots & & & \vdots \\ \vdots & \vdots & & & & \ddots & & \vdots \\ 0 & \cdots & \cdots & \cdots & 0 & -1 & 0 & 1 \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & -1 & 0 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} -\alpha \\ 0 \\ \vdots \\ 0 \\ \beta \end{pmatrix}$$

For the second derivative $\frac{\partial^2 u}{\partial x^2}$, the $j = 1$ expression is

$$\frac{1}{\Delta x^2}(u_0 - 2u_1 + u_2) = \frac{1}{\Delta x^2}(-2u_1 + u_2 + \alpha)$$

so the first row of A_2 should be $(-2 \ 1 \ 0 \ \cdots \ 0)$, and we need to add on an extra term α .

The $j = N$ expression is

$$\frac{1}{\Delta x^2}(u_{N-1} - 2u_N + u_{N+1}) = \frac{1}{\Delta x^2}(u_{N-1} - 2u_N + \beta)$$

so the N th row of A_2 should be $(0 \ \cdots \ 0 \ 1 \ -2)$, and we need to add on an extra term β .

Therefore, $\frac{\partial^2 u}{\partial x^2}(t, x_j)$ for $j = 1, \dots, N$ becomes an array of expressions $\frac{1}{\Delta x^2}(A_2 \mathbf{u} + B)$ where

$$A_2 = \begin{pmatrix} -2 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & & & \ddots & & & \vdots \\ \vdots & \vdots & & & & \ddots & & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 & -2 & 1 \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & 1 & -2 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} \alpha \\ 0 \\ \vdots \\ 0 \\ \beta \end{pmatrix}$$

Zero Neumann boundary conditions

$$\left. \frac{\partial u}{\partial x} \right|_{x=a} = 0, \quad \left. \frac{\partial u}{\partial x} \right|_{x=b} = 0$$

If we use an $\boxed{O(\Delta x)}$ forward difference formula at the left end, then $\left. \frac{\partial u}{\partial x} \right|_{x=a}$ is approximated by the difference quotient $\frac{u_1 - u_0}{\Delta x}$, and the boundary condition becomes

$$\frac{u_1 - u_0}{\Delta x} = 0, \quad \text{so that } \boxed{u_0 = u_1}$$

Substituting this into the $j = 1$ expressions gives

$$\text{for the first derivative } \frac{\partial u}{\partial x} : \quad \frac{1}{2\Delta x}(-u_0 + u_2) = \frac{1}{2\Delta x}(-u_1 + u_2)$$

$$\text{for the second derivative } \frac{\partial^2 u}{\partial x^2} : \quad \frac{1}{\Delta x^2}(u_0 - 2u_1 + u_2) = \frac{1}{\Delta x^2}(u_1 - 2u_1 + u_2) = \frac{1}{\Delta x^2}(-u_1 + u_2)$$

Similarly, if we use an $\boxed{O(\Delta x)}$ backward difference formula at the right end, then $\left. \frac{\partial u}{\partial x} \right|_{x=b}$ is approximated by $\frac{u_{N+1} - u_N}{\Delta x}$, and the boundary condition becomes

$$\frac{u_{N+1} - u_N}{\Delta x} = 0, \quad \text{so that } \boxed{u_{N+1} = u_N}$$

Substituting this into the $j = N$ expressions gives

$$\text{for the first derivative } \frac{\partial u}{\partial x} : \quad \frac{1}{2\Delta x}(-u_{N-1} + u_{N+1}) = \frac{1}{2\Delta x}(-u_{N-1} + u_N)$$

$$\text{for the second derivative } \frac{\partial^2 u}{\partial x^2} : \quad \frac{1}{\Delta x^2}(u_{N-1} - 2u_N + u_{N+1}) = \frac{1}{\Delta x^2}(u_{N-1} - 2u_N + u_N) = \frac{1}{\Delta x^2}(u_{N-1} - u_N)$$

In summary, if we use $\boxed{O(\Delta x)}$ forward and backward differences to approximate the boundary conditions:

$\boxed{\frac{\partial u}{\partial x}(t, x_j)}$ for $j = 1, \dots, N$ becomes an array of expressions $\frac{1}{2\Delta x} A_1 \mathbf{u}$ where

$$A_1 = \begin{pmatrix} -1 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ -1 & 0 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & -1 & 0 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & & & \ddots & & & \vdots \\ \vdots & \vdots & & & & \ddots & & \vdots \\ 0 & \cdots & \cdots & \cdots & 0 & -1 & 0 & 1 \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & -1 & 1 \end{pmatrix}$$

$\boxed{\frac{\partial^2 u}{\partial x^2}(t, x_j)}$ for $j = 1, \dots, N$ becomes an array of expressions $\frac{1}{\Delta x^2} A_2 \mathbf{u}$ where

$$A_2 = \begin{pmatrix} -1 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & & & \ddots & & & \vdots \\ \vdots & \vdots & & & & \ddots & & \vdots \\ 0 & \cdots & \cdots & \cdots & 0 & 1 & -2 & 1 \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & 1 & -1 \end{pmatrix}$$

If we use an $O(\Delta x^2)$ forward difference formula at the left end, then $\frac{\partial u}{\partial x}\bigg|_{x=a}$ is approximated by the difference quotient $\frac{-3u_0 + 4u_1 - u_2}{2\Delta x}$, and the boundary condition becomes

$$\frac{-3u_0 + 4u_1 - u_2}{2\Delta x} = 0, \quad \text{so that} \quad u_0 = \frac{4}{3}u_1 - \frac{1}{3}u_2$$

Substituting this into the $j = 1$ expressions gives

$$\begin{aligned} \text{for } \frac{\partial u}{\partial x} : \quad & \frac{1}{2\Delta x}(-u_0 + u_2) = \frac{1}{2\Delta x}\left(-\frac{4}{3}u_1 + \frac{1}{3}u_2 + u_2\right) = \frac{1}{2\Delta x}\left(-\frac{4}{3}u_1 + \frac{4}{3}u_2\right) \\ \text{for } \frac{\partial^2 u}{\partial x^2} : \quad & \frac{1}{\Delta x^2}(u_0 - 2u_1 + u_2) = \frac{1}{\Delta x^2}\left(\frac{4}{3}u_1 - \frac{1}{3}u_2 - 2u_1 + u_2\right) = \frac{1}{\Delta x^2}\left(-\frac{2}{3}u_1 + \frac{2}{3}u_2\right) \end{aligned}$$

Similarly, if we use an $O(\Delta x^2)$ backward difference formula at the right end, then $\frac{\partial u}{\partial x}\bigg|_{x=b}$ is approximated by the difference quotient $\frac{3u_{N+1} - 4u_N + u_{N-1}}{2\Delta x}$, and the boundary condition becomes

$$\frac{3u_{N+1} - 4u_N + u_{N-1}}{2\Delta x} = 0, \quad \text{so that} \quad u_{N+1} = \frac{4}{3}u_N - \frac{1}{3}u_{N-1}$$

Substituting this into the $j = N$ expressions gives

$$\begin{aligned} \text{for } \frac{\partial u}{\partial x} : \quad & \frac{1}{2\Delta x}(-u_{N-1} + u_{N+1}) = \frac{1}{2\Delta x}\left(-u_{N-1} + \frac{4}{3}u_N - \frac{1}{3}u_{N-1}\right) = \frac{1}{2\Delta x}\left(-\frac{4}{3}u_{N-1} + \frac{4}{3}u_N\right) \\ \text{for } \frac{\partial^2 u}{\partial x^2} : \quad & \frac{1}{\Delta x^2}(u_{N-1} - 2u_N + u_{N+1}) = \frac{1}{\Delta x^2}\left(u_{N-1} - 2u_N + \frac{4}{3}u_N - \frac{1}{3}u_{N-1}\right) = \frac{1}{\Delta x^2}\left(\frac{2}{3}u_{N-1} - \frac{2}{3}u_N\right) \end{aligned}$$

In summary, if we use $O(\Delta x^2)$ forward and backward differences for the boundary conditions, then:

$\frac{\partial u}{\partial x}(t, x_j)$ for $j = 1, \dots, N$ becomes an array of expressions $\frac{1}{2\Delta x}A_1\mathbf{u}$ where

$$A_1 = \begin{pmatrix} -\frac{4}{3} & \frac{4}{3} & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ -1 & 0 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & -1 & 0 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & & & \ddots & & & \vdots \\ \vdots & \vdots & & & & \ddots & & \vdots \\ 0 & \cdots & \cdots & \cdots & 0 & -1 & 0 & 1 \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\frac{4}{3} & \frac{4}{3} \end{pmatrix}$$

$\frac{\partial^2 u}{\partial x^2}(t, x_j)$ for $j = 1, \dots, N$ becomes an array of expressions $\frac{1}{\Delta x^2}A_2\mathbf{u}$ where

$$A_2 = \begin{pmatrix} -\frac{2}{3} & \frac{2}{3} & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & & & \ddots & & & \vdots \\ \vdots & \vdots & & & & \ddots & & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 & -2 & 1 \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & \frac{2}{3} & -\frac{2}{3} \end{pmatrix}$$