07 – Partial Differential Equations

Almaz Khabibrakhmanov, Mario Galante, Alexandre Tkatchenko

AA 2021/2022 Computational Methods for MSc in Physics

Basic Definitions



$$\frac{\partial f}{\partial x}(x_0, y_0) \stackrel{\text{def}}{=} \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x, y_0) - f(x_0, y_0)}{\Delta x}$$

The shorthand notation:
$$f = f(t, x)$$
 $f_t = \frac{\partial f}{\partial t}(t, x)$ $f_x = \frac{\partial f}{\partial x}(t, x)$

$$f = f(t, x)$$

$$f_t = \frac{\partial f}{\partial t}(t, x)$$

$$f_{x} = \frac{\partial f}{\partial x}(t, x)$$

$$f_{xx} = \frac{\partial^2 f}{\partial x^2}(t, x)$$

$$f_{xt} = \frac{\partial^2 f}{\partial t \, \partial x}(t, x)$$
 $f_{tt} = \frac{\partial^2 f}{\partial t^2}(t, x)$

$$f_{tt} = \frac{\partial^2 f}{\partial t^2}(t, x)$$

The physical examples

The example calculation:

$$f(t,x) = t^2 \sin x$$

$$f_t = 2t \sin x$$

$$f_{tt} = 2 \sin x$$

$$f_{xt} = 2t \cos x$$

$$f_{xt} = 2t \cos x$$

$$f_{xx} = -t^2 \sin x$$

Maxwell equations:

$$\operatorname{div} \mathbf{D} = 4\pi\rho$$

$$\operatorname{div} \boldsymbol{B} = 0$$

$$\operatorname{rot} \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} \\
4\pi \qquad 1 \ \delta$$

$$\cot \mathbf{H} = \frac{4\pi}{c}\mathbf{j} + \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t}$$

Wave equation:

$$u_{tt} = c^2 \Delta u$$

Heat equation:

$$u_t = \kappa \Delta u$$

Poisson equation:

$$\Delta \phi = -4\pi \rho$$

2nd Order PDE: General Classification



The general linear second-order PDE in two independent variables has the form:

$$A(x,y)u_{xx} + 2B(x,y)u_{xy} + C(x,y)u_{yy} + \cdots$$
 (lower order terms) = 0

1. $B^2 - AC < 0$ – elliptic PDE. The example: Laplace equation:

$$u_{xx} + u_{yy} = 0 \ (A = C = 1, B = 0)$$

2. $B^2 - AC = 0$ – parabolic PDE. The example: heat (or diffusion) equation:

$$u_t = u_{xx} (A = 1, B = C = 0)$$

3. $B^2 - AC > 0$ – hyperbolic PDE. The example: wave equation:

$$\frac{1}{c^2}u_{tt} = u_{xx} (A = 1, B = 0, C = -1/c^2)$$

Understanding the Problem



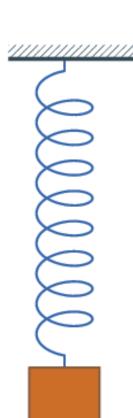
We will consider the 1D wave equation as the example:

$$u_{tt} = c^2 u_{xx}$$
, $0 \le x \le a$; $0 \le t \le t_{max}$

Possible physical problem: vibrations of the string

To solve this, we need the initial and boundary conditions

Harmonic oscillator



The equation to solve:

$$m\ddot{x} = -kx$$

The initial conditions:

$$\begin{cases} x(0) = x_0 \\ \dot{x}(0) = v_0 \end{cases}$$

String vibrations



The equation to solve:

$$u_{tt} = c^2 u_{xx}$$

The initial conditions:

$$\begin{cases} u(0,x) = f(x) \\ u_t(0,x) = g(x) \end{cases}$$

$$g(x)$$
 – the analogue of the initial velocity

The boundary conditions:

$$\begin{cases} u(t,0) = \phi(t) = 0 \\ u(t,a) = \psi(t) = 0 \end{cases}$$

The string is fixed at its ends

Types of Initial & Boundary Conditions



Boundary conditions put constraints on the values of u(t, x) at x = 0 and x = a.

They can be specified in different ways:

1. Dirichlet boundary conditions:

$$\begin{cases} u(t,0) = \phi(t) \\ u(t,a) = \psi(t) \end{cases}$$

Put on the solved function itself

2. Neumann boundary conditions:

$$\begin{cases} u_{\chi}(t,0) = \phi(t) \\ u_{\chi}(t,a) = \psi(t) \end{cases}$$

Put on the derivative of the solved function

3. Mixed boundary conditions:

$$\begin{cases} u(t,0) = \phi(t) \\ u_{\chi}(t,a) = \psi(t) \end{cases}$$

Just a combination of the two above

The Formulation and the Solution

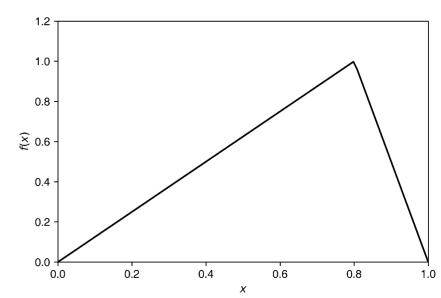


$$u_{tt} = c^2 u_{xx}, \qquad 0 \le x \le a; \ 0 \le t \le t_{max}$$
 (1)

The initial conditions:

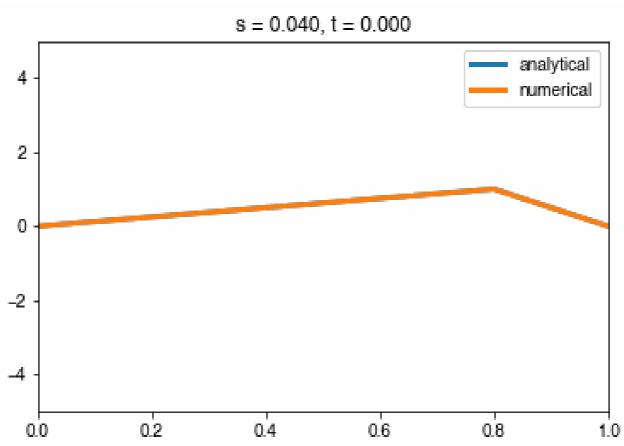
$$\begin{cases} u(0,x) = f(x) \\ u_t(0,x) = g(x) = 0 \end{cases}$$

$$f(x) = \begin{cases} 1.25 \frac{x}{a} &, x \le 0.8a \\ 5\left(1 - \frac{x}{a}\right), x > 0.8a \end{cases}$$



The boundary conditions:

$$\begin{cases} u(t,0) = \phi(t) = 0 \\ u(t,a) = \psi(t) = 0 \end{cases}$$

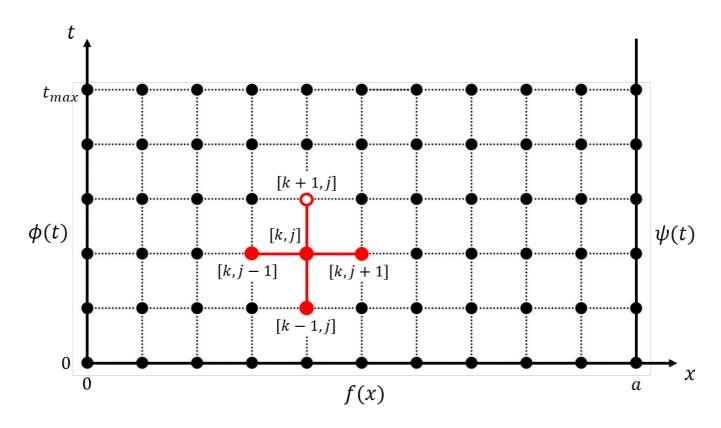


Explicit Forward (Euler) Method



We are going to discretize our equation on the 2D grid in space and time:

Also known as the "cross" scheme



We approximate the second derivatives using central differences:

$$u_{tt} = \frac{u_j^{k+1} - 2u_j^k + u_j^{k-1}}{\Delta t^2}, \qquad u_{xx} = \frac{u_{j+1}^k - 2u_j^k + u_{j-1}^k}{\Delta x^2}$$

Using Eq. (1) and $s = \frac{c\Delta t}{\Delta x}$, we solve for u_j^{k+1} at time step k+1:

$$u_j^{k+1} = -u_j^{k-1} + 2u_j^k(1 - s^2) + s^2(u_{j+1}^k + u_{j-1}^k)$$
 (2)

Dealing with Initial / Boundary Conditions



For Dirichlet-type conditions, everything is straightforward:

$$u(0,x) = f(x) \rightarrow u_j^0 = f(x_j), \forall j = 1, ..., n_x$$

However, Neumann-type conditions (which are put on the derivatives) require additional numerical approximation. Imagine we have the following initial condition:

$$u_t(0,x) = g(x)$$

To maintain this condition, we have to discretize it:

$$u_t(0,x) \approx \frac{u_j^1 - u_j^{-1}}{2\Delta t} = g_j \equiv g(x_j)$$
 (3)

In other words, we introduce a 'ghost', fictitious layer with k = -1. This layer is required **only** to evaluate **the first timestep**. The only purpose of it is to simulate the correct value of the derivative at the beginning. Afterwards we can forget about this 'ghost' layer.

Dealing with Initial / Boundary Conditions



Solving the Eq. (3) we obtain:

$$u_j^{-1} = u_j^1 + 2\Delta t g(x_j)$$

In the special case when g(x) = 0, this means $u_j^{-1} = u_j^1$. Then, our finite difference expression will change a bit at the first timestep:

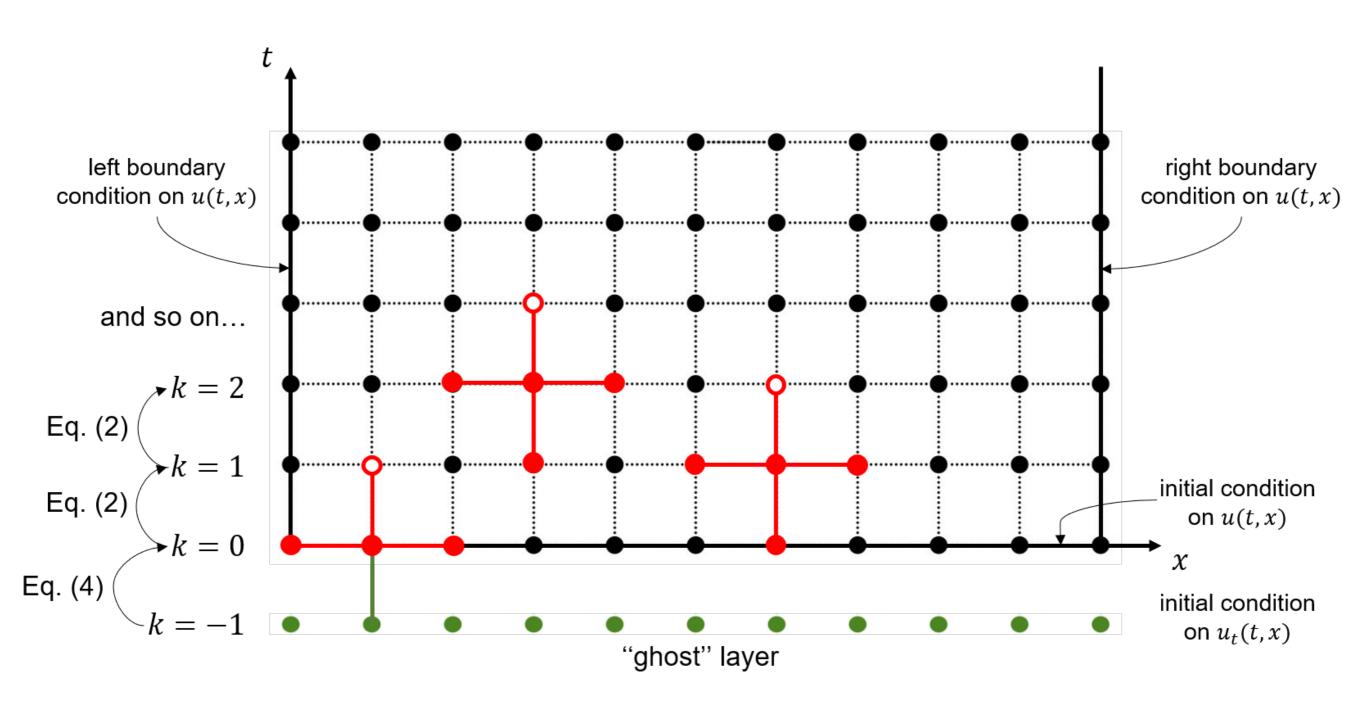
$$u_{j}^{1} = -u_{j}^{-1} + 2u_{j}^{0}(1 - s^{2}) + s^{2}(u_{j+1}^{0} + u_{j-1}^{0})$$

$$u_{j}^{-1} = u_{j}^{1}$$

$$u_{j}^{1} = u_{j}^{0}(1 - s^{2}) + \frac{1}{2}s^{2}(u_{j+1}^{0} + u_{j-1}^{0})$$
(4)

Scheme of the Solution Algorithm





Stability of the Explicit Forward Method



There is a single dimensionless parameters in our problem which defines its scale:

$$s = \frac{c\Delta t}{\Delta x}$$

It appears that this parameter called **Courant number** plays the key role in determining the stability of numerical schemes for <u>hyperbolic equations</u>.

If the errors made at one timestep of the calculation do not cause the errors to be magnified as the computations are continued, then the scheme is **stable**.

If, on the contrary, the errors grow with time the numerical scheme is said to be unstable.

It can be shown that Explicit Forward Method considered here is stable, if the following condition is fulfilled:

$$s = \frac{c\Delta t}{\Delta x} \le 1$$

The Analytical Solution



$$u_{tt} = c^2 u_{xx}$$
, $0 \le x \le a$; $0 \le t \le t_{max}$

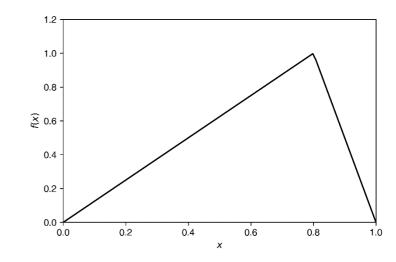
The initial conditions:

$$\begin{cases} u(0,x) = f(x) & \{u(t,0) = \phi(t) = 0 \\ u_t(0,x) = g(x) = 0 & \{u(t,a) = \psi(t) = 0 \end{cases}$$

The boundary conditions:

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

$$u(t,a) = \psi(t) = 0$$



The general solution of this equation:

$$u(t,x) = \frac{f(x-ct) + f(x+ct)}{2}$$

(5)

We should define f(x) for arbitrary x. To satisfy boundary conditions, we can do:

$$f(-x) = -f(x), \quad f(x+2a) = f(x)$$

This extended function f(x) should be used to calculate the analytical solution according to the Eq. (5).

