4 Partial differential equations (PDE).

PDEs arise in physics, engineering, biology, computer sciences, finance, in every problem where the unknown quantity varies in several spatial dimensions or in space and time. The general form of a PDE for a function $u(x_1, x_2, ...x_n)$ is

$$F(x_1, ..., x_n, u, u_{x_1}, u_{x_2}, ..., u_{x_1x_1}, u_{x_2x_2}, u_{x_1x_2}, ...) = 0, \tag{4.1}$$

where

$$u_{x_1} = \frac{\partial u}{\partial x_1}, \qquad u_{x_1x_1} = \frac{\partial^2 u}{\partial x_1^2}, \tag{4.2}$$

and so on, are partial derivatives. The equation (4.1) requires initial and/or boundary conditions.

Often the boundary conditions are clear from the physical formulation behind the PDE. If, for instance, you boil an egg and (4.1) models the temperature distribution inside the egg ('the egg equation') then you need to know the temperature of the water surrounding the egg (boundary condition) and also the initial distribution of temperature inside the egg (is the egg straight from the fridge and therefore uniformly chilled or it spent some time in the kitchen and is cooler on the inside and warmer near the shell). In this example both the initial and boundary conditions are needed to have a unique solution.

Well-posedness.

Even in seemingly natural situations the solution of a PDE may not be well behaved - it may show extreme sensitivity to variations in boundary conditions or changes in control parameters, may not be unique or may not even exist. As an example, return to the boiling egg problem and pose the following question. Suppose boiling begins at $t = 0$min and stops at $t = 10$min when we have a very hard-boiled egg. Suppose at $t = 10$min we know the temperature everywhere inside the egg. Can we go back in time and reconstruct the temperature for earlier times, that is for $t < 10$ min? During boiling, the surface of the egg is subjected to constant fluctuations in temperature (due to rising vapour bubbles in boiling water, flickering flame of the gas oven etc.) In forward time these fluctuations diffuse very quickly and have no noticeable effect on the final product - the boiled egg. But then

in backward time any small perturbations will grow - the problem in reverse time proves to be unstable.

A PDE formulation (inducing the equation, initial and boundary conditions) is said to be well-posed if the solution exists, it is unique and depends continuously on the problem parameters (the parameters may be a part of boundary conditions, for instance). Sometimes the continuous dependence on the parameters is replaced by the condition of stability although many physical problems involving instability phenomena are well-posed in the sense that their solutions can be studied successfully within the PDE framework.

Ill-posed problems are also important and are studied in the theory of inverse problems (re-constructing the cause given an observed effect). Examples include computerized tomography (reconstructing the absorption pattern inside a human body from intensity of X-rays passing through it), inverse heat conduction (to determine the boundary heat flux required for a desired temperature field in continuous steel casting), inverse wave scattering (determine the shape of an obstacle by observing the waves scattered by it in oil exploration). In this course we are concerned with well-posed problems.

Classification of PDEs.

The **order** of a PDE is determined by the order of the highest derivative.

A PDE is linear if F in (4.1) is a linear function of u and all its derivatives. For example,

$$e^{x+y}u + x^{100} \cdot u_x + \sin y \cdot u_y = \tan(xy), \tag{4.3}$$

is a linear first-order PDE. On the other hand,

$$u_{xx}^2 + u_y^2 = 4, \tag{4.4}$$

is a non-linear second-order PDE.

Depending on the severity of non-linearity, subclasses of semi-linear and quasi-linear equations are considered. A second-order semi-linear equation in two independent variables is linear with respect to the second derivatives,

$$a(x,y)u_{xx} + 2b(x,y)u_{xy} + c(x,y)u_{yy} = F(x,y,u,u_x,u_y), \tag{4.5}$$

where the right-hand side could be anything. A quasi-linear equation may have the function and lower-order derivatives in the coefficients to the highest derivatives, for example a first-order quasi-linear PDE in two variables will have the following general form,

$$a(x,y,u)u_x + b(x,y,u)u_y = c(x,y,u). \tag{4.6}$$

As we can see, the highest derivatives in the quasi-linear PDE still appear in a linear combination.

A further classification can be given to linear PDEs, with reference to a forcing term, into homogeneous and non-homogeneous (this is similar to linear ODEs). A homogeneous linear PDE has solutions which satisfy the superposition principle (again in similarity with linear ODEs).

5 First-order PDE.

Hyperbolicity. Characteristics.

To keep things simple, we consider a 1st-order PDE,

$$a(x,y)u_x + b(x,y)u_y = c(x,y), \tag{5.1}$$

with given $a(x,y), b(x,y), c(x,y)$ and unknown $u(x,y)$. The solution is to be found in a certain region in the $(x,y)-$plane. Since this is a first order equation we would expect that knowing the function $u(x,y)$ on some curve Γ in the plane should be enough to find the solution at least in the vicinity of this curve.

[diagram] This, however, is not always the case. Let $x = x(s), y = y(s)$ be

a parametric equation of the curve Γ. Using the chain rule, we can compute the derivative of u along Γ,

$$\frac{du(x(s),y(s))}{ds} = u_x\frac{dx}{ds} + u_y\frac{dy}{ds}. \tag{5.2}$$

But since u_x and u_y are related by (5.1) we have

$$u_x = -\frac{b}{a}u_y + \frac{c}{a}, \tag{5.3}$$

assuming $a \neq 0$ for definiteness. Then for the derivative along Γ we have

$$\frac{du(x(s), y(s))}{ds} = u_y \left(\frac{dy}{ds} - \frac{b}{a}\frac{dx}{ds} \right) + \frac{c}{a}. \tag{5.4}$$

For a general curve Γ, the last formula just establishes a relationship between the derivative along Γ and one of the partial derivatives of u, u_y in this case. However on a curve given by

$$\frac{dy}{ds} = \frac{b}{a}\frac{dx}{ds} \text{ or } \tfrac{dy}{b(x,y)} = \tfrac{dx}{a(x,y)}, \tag{5.5}$$

equation (5.4) reduces to the ODE,

$$\frac{du}{ds} = \frac{c}{a}, \tag{5.6}$$

which we can solve and find u along this curve. Such curves, called characteristic curves or characteristics, have a special significance for the equation (5.1). Firstly, the function u cannot be given an arbitrary distribution along the curve, instead it is sufficient to specify u at one point on the curve and then the equation (5.6) determines u everywhere along the characteristic (in a sense, information propagates along characteristics). Secondly, even if we attempt to specify u along the characteristic, the equation (5.1) does not allow us to compute the solution in the vicinity of the characteristic (the equation degenerates into (5.6)). And the third property used often in analysis of hyperbolic PDEs is that, when written in the characteristic variables, a system of PDEs can be reduced to ODEs and therefore admits explicit solutions.

The conclusion for us from here is that, when setting up initial conditions for the equation (5.1) on a certain curve Γ we need to make sure that $\Gamma$is not a characteristic curve.

A PDE whose solution can be completely described in terms of characteristics are called hyperbolic.

[You may have noticed that the preceding calculation was just a long way of saying that the equation (5.1) rewritten in vector form as,

$$(a, b) \cdot \nabla u = c, \tag{5.7}$$

gives a directional derivative of u along the vector (a, b) in the (x, y)- plane. If the vector (a, b) is everywhere tangent to the curve Γ then the equation (5.1) (or (5.7)) simply tells us how u evolves along Γ and does not say anything about the function u in the vicinity of Γ.]

Finite difference methods.

We shall consider several methods for the simplest PDE with constant coefficients for a function, $u = u(x, t)$, given an initial condition of the form,

$$u_t + au_x = 0, \qquad u(0, x) = u_0(x), \tag{5.8}$$

to be solved for $t > 0$. We assume $a = const > 0$.

There is an exact solution, $u = u_0(x - at)$ which shows that the characteristics of the equation are lines $x - at = const$ in the $(t, x)-$plane.

Numerical solution is considered on the grid $x_n = n\Delta x, t_m = m\Delta t$, with the step sizes Δt and Δx so that $u(x_n, t_m)$ is approximated by $u_{n,m}$.

Explicit method with forward $x-$derivative.

$\uparrow x$

$\bullet(n + 1, m)$

$\bullet(n, m) \qquad \bullet(n, m + 1) \ \rightarrow t$

Approximating the equation in (5.8) at the grid point t_m, x_n we shall attempt forward derivatives in both t and x,

$$\frac{u_{n,m+1} - u_{n,m}}{\Delta t} + a\frac{u_{n+1,m} - u_{n,m}}{\Delta x} = 0, \tag{5.9}$$

hence

$$u_{n,m+1} = (1 + C)u_{n,m} - Cu_{n+1,m}. \tag{5.10}$$

We use here the so-called Courant number,

$$C = a\frac{\Delta t}{\Delta x}. \tag{5.11}$$

Stability.

Let us first consider stability of solutions of the original PDE (5.8). A standard approach is to assume a travelling-wave solution,

$$u = Ae^{i(kx-\omega t)} + c.c. \tag{5.12}$$

where $c.c.$ denotes the complex conjugate, A is a constant amplitude (which in a linear equation is immaterial), k is the wavenumber and ω is the frequency. The wave is assumed periodic in space therefore k is real. The frequency ω should follow from the equation as a function of the wavenumber.

Substitution of (5.12) into (5.8) yields

$$-i\omega + aik = 0. \tag{5.13}$$

This is the dispersion relation for our equation. It follows that $\omega = ak$ which means that waves of given wavenumber neither decay nor grow - they in fact propagate with constant phase speed $c = \omega/k$.

Now we shall try a similar approach to the finite-difference algorithm (5.10). In the numerical stability theory this is known as the von Neumann stability analysis. We take

$$u_{n,m} = \lambda^m e^{ink} \tag{5.14}$$

with real k. The aim is to compute λ. Using $u_{n,m+1} = \lambda^{m+1}e^{ink}, u_{n+1,m} = \lambda^m e^{i(n+1)k}$, the equation (5.10) gives us

$$\lambda = 1 + C - Ce^{ik}. \tag{5.15}$$

It is almost obvious that $|\lambda| > 1$ therefore the method is unstable.

Note: the equation (5.8) is a first-order advection equation, a is the advection speed (e.g. the speed of wind carrying particles). When $a > 0$ the advection is in the positive $x-$direction. In such interpretation the forward $x-$derivative is called a downwind approximation (downwind scheme, downwind derivative etc). So our approximation can be called a forward in time downwind scheme.

Discussion: where does instability come from? Sketch the location of the approximation nodes and draw a characteristic through the node $(n, m + 1)$ to see what happens. Region of dependence and influence for a hyperbolic PDE.

Explicit method with backward $x-$derivative.

$$\begin{array}{cc} \uparrow x & \\ \bullet(n,m) & \bullet(n,m+1) \\ \bullet(n-1,m) & \\ & \rightarrow t \end{array}$$

This is a forward-time backward-space approximation or an upwind scheme,

$$\frac{u_{n,m+1}-u_{n,m}}{\Delta t}+a\frac{u_{n,m}-u_{n-1,m}}{\Delta x}=0, \tag{5.16}$$

giving

$$u_{n,m+1}=(1-C)u_{n,m}+Cu_{n-1,m}. \tag{5.17}$$

The Courant number is the same, $C=a\Delta t/\Delta x$. Now using the von Neumann substitution (5.14) we get

$$\lambda=1-C+Ce^{-ik}. \tag{5.18}$$

By sketching λ in the complex plane, for example, we can see that the scheme is unstable if $C>1$and stable in the case $C<1$.Hence the method is stable if

$$a\Delta t/\Delta x<1 \text{ or } \Delta t<\Delta x/a. \tag{5.19}$$

The stability condition (5.19) is known as the Courant-Friedrichs-Lewy condition.

Discussion: derive the CFL condition graphically considering the characteristic line relative to the nodes of the computational grid.

Lax-Friedrichs method.

Second-order central derivative in x and forward in t, only for the time derivative calculation $u_{n,m}$ is replaced by the average of the neighbouring points.

$$\begin{array}{cc} \uparrow x & \\ \bullet\ (n+1,m) & \\ \bullet(n,m) & \bullet(n,m+1) \\ \bullet(n-1,m) & \rightarrow t \end{array}$$

We have (5.8) discretized as follows,

$$\frac{u_{n,m+1} - \frac{1}{2}\left(u_{n+1,m} + u_{n-1,m}\right)}{\Delta t} + a\frac{u_{n+1,m} - u_{n-1,m}}{2\Delta x} = 0, \tag{5.20}$$

or

$$u_{n,m+1} = \frac{1}{2}\left(u_{n+1,m} + u_{n-1,m}\right) - \frac{C}{2}\left(u_{n+1,m} - u_{n-1,m}\right). \tag{5.21}$$

The Courant number is the same, $C = a\Delta t/\Delta x$. Testing for stability,

$$u_{n,m} = \lambda^m e^{iknx}, \tag{5.22}$$

we obtain

$$\lambda = \frac{1}{2}\left(e^{ikx} + e^{-ikx}\right) - \frac{C}{2}\left(e^{ikx} - e^{-ikx}\right), \tag{5.23}$$

$$\lambda = \cos kx - iC\sin kx. \tag{5.24}$$

The magnitude of λ is given by

$$|\lambda|^2 = \cos^2 kx + C^2\sin^2 kx = 1 - \sin^2 kx + C^2\sin^2 kx \tag{5.25}$$

$$= 1 + (C^2 - 1)\sin^2 kx. \tag{5.26}$$

For stability, $0 < |\lambda| < 1$, we find $0 < C^2 < 1$, hence Lax-Friedrichs algorithm is conditionally stable.

The Lax-Friedrichs scheme tends to give smoothed-out solutions - any initial discontinuities in u become leveled out over time. This is due to an interesting and important phenomenon of numerical dissipation which we can illustrate as follows. Re-write (5.20) as

$$\frac{u_{n,m+1} - u_{n,m}}{\Delta t} + a\frac{u_{n+1,m} - u_{n-1,m}}{2\Delta x} = \frac{u_{n+1,m} - 2u_{n,m} + u_{n-1,m}}{2\Delta t}. \tag{5.27}$$

The last equation we can interpret as a finite-difference approximation of the diffusion-type equation,

$$u_t + au_x = \frac{1}{2}\frac{(\Delta x)^2}{\Delta t}u_{xx}, \tag{5.28}$$

where the diffusion coefficient (viscosity) in front of u_{xx} denoted often as D depends on the grid size,

$$D = \frac{1}{2}\frac{(\Delta x)^2}{\Delta t}. \tag{5.29}$$

For any finite values of the step sizes the diffusion coefficient is finite hence giving the effect of dissipation in the numerical solution.