Chapter 1
Introduction

1.1 Definition, Notation and Classification

A differential equation involving more than one independent variable and its partial derivatives with respect to those variables is called a *partial differential equation* (PDE).
Consider a simple PDE of the form:

$$\frac{\partial}{\partial x}u(x,y) = 0.$$

This equation implies that the function $u(x,y)$ is independent of x. Hence the general solution of this equation is $u(x,y) = f(y)$, where f is an arbitrary function of y. The analogous ordinary differential equation is

$$\frac{du}{dx} = 0,$$

its general solution is $u(x) = c$, where c is a constant. This example illustrates that general solutions of ODEs involve arbitrary constants, whereas solutions of PDEs involve *arbitrary functions*.

In general, one can classify PDEs with respect to different criterion, e.g.:

- Order;
- Dimension;
- Linearity;
- Initial/Boundary value problem, etc.

By *order* of PDE we will understand the order of the highest derivative that occurs. A PDE is said to be *linear* if it is linear in unknown functions and their derivatives, with coefficients depending on the independent variables. The independent variables typically include one or more *space dimensions* and sometimes time dimension as well.
For example, the wave equation

$$\frac{\partial^2 u(x,t)}{\partial t^2} = a^2 \frac{\partial^2 u(x,t)}{\partial x^2}$$

is a one-dimensional, second-order linear PDE. In contrast, the Fisher Equation of the form

$$\frac{\partial u(\mathbf{r},t)}{\partial t} = \triangle u(\mathbf{r},t) + u(\mathbf{r},t) - u(\mathbf{r},t)^2,$$

where $\mathbf{r} = (x, y)$ is a two-dimensional, second-order nonlinear PDE.

Linear Second-Order PDEs

For linear PDEs in two dimensions there is a simple classification in terms of the general equation

$$au_{xx} + bu_{xy} + cu_{yy} + du_x + eu_y + fu + g = 0,$$

where the coefficients a, b, c, d, e, f and g are real and in general can also be functions of x and y. The PDE's of this type are classified by the value of discriminant $D_\lambda = b^2 - 4ac$ of the eigenvalue problem for the matrix

$$A = \begin{pmatrix} a & b/2 \\ b/2 & c \end{pmatrix},$$

build from the coefficients of the highest derivatives. A simple classification is shown on the following table [11, 7]:

D_λ	Typ	Eigenvalues
$D_\lambda < 0$	*elliptic*	the same sign
$D_\lambda > 0$	*hyperbolic*	different signs
$D_\lambda = 0$	*parabolic*	zero is an eigenvalue

For instance, *the Laplace equation* for the electrostatic potential φ in the space without a charge

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = 0$$

is elliptic, as $a = c = 1$, $b = 0$, $D_\lambda = -4 < 0$. In general, elliptic PDEs describe processes that have already reached steady state, and hence are time-independent.
One-dimensional *wave equation* for some amplitude $A(x,t)$

$$\frac{\partial^2 A}{\partial t^2} - v^2 \frac{\partial^2 A}{\partial x^2} = 0$$

with the positive dispersion velocity v is hyperbolic ($a = 1$, $b = 0$, $c = -v^2$, $D_\lambda = 4v^2 > 0$). Hyperbolic PDEs describe time-dependent, conservative processes, such as convection, that are not evolving toward steady state.
The next example is a *diffusion equation* for the patricle's density $\rho(x,t)$

$$\frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial x^2},$$

where $D > 0$ is a diffusion coefficient. This equation is called to be parabolic ($a = -D$, $b = c = 0$,$D_\lambda = 0$). Parabolic PDEs describe time-dependent, dissipative processes, such as diffusion, that are evolving toward steady state.

Each of these classes should be investigated separately as different methods are required for each class. The next point to emphasize is that as all the coefficients of the PDE can depend on x and y, this classification concept is *local*.

Initial and Boundary-Value Problems

As it was mentioned above the solution of PDEs involve arbitrary functions. That is, in order to solve the system in question completely, additional conditions are needed. These conditions can be given in the form of *initial* and *boundary* conditions. Initial conditions define the values of the dependent variables at the initial stage (e.g. at $t = 0$), whereas the boundary conditions give the information about the value of the dependent valiable or its derivative on the boundary of the area of interest. Typically, one distinguishes

- *Dirichlet conditions* specify the values of the dependent variables of the boundary points.
- *Neumann conditions* specify the values of the normal gradients of the boundary.
- *Robin conditions* defines a linear combination of the Drichlet and Neumann conditions.

Moreover, it is useful to classify the PDE in question in terms of *initial value problem (IVP)* and *boundary value problem (BVP)*.

- *Initial value problem:* PDE in question describes *time evolution*, i.e., the initial space-distribution is given; the goal is to find how the dependent variable propagates in time (e.g., the diffusion equation).
- *Boundary value problem:* A static solution of the problem should be found in some region-and the dependent variable is specified on its boundary (e.g., the Laplace equation).

1.2 Finite difference method

Let us consider a one-dimensional PDE for the unknown function $u(x,t)$. One way to numerically solve the PDE is to approximate all the derivatives by *finite differences*. We partition the domain in space using *a mesh* $x_0, x_1, \ldots, x_N$ and in time using a mesh $t_0, t_1, \ldots, t_T$. Fisrt we assume *a uniform partition* both in space and in time, so that the difference between two consecutive space points will be $\triangle x$ and between two consecutive time points will be $\triangle t$, i.e.,

$$x_i = x_0 + i\triangle x, \qquad i = 0,1,\ldots,M;$$
$$t_j = t_0 + j\triangle t, \qquad j = 0,1,\ldots,T;$$

The Taylor series method

Consider a Taylor expansion of an analytical function $u(x)$.

$$u(x+\triangle x) = u(x) + \sum_{n=1}^{\infty} \frac{\triangle x^n}{n!}\frac{\partial^n u}{\partial x^n} = u(x) + \triangle x\frac{\partial u}{\partial x} + \frac{\triangle x^2}{2!}\frac{\partial^2 u}{\partial x^2} + \frac{\triangle x^3}{3!}\frac{\partial^3 u}{\partial x^3} + \ldots \tag{1.1}$$

Then for the first derivative one obtains:

$$\frac{\partial u}{\partial x} = \frac{u(x+\triangle x) - u(x)}{\triangle x} - \frac{\triangle x}{2!}\frac{\partial^2 u}{\partial x^2} - \frac{\triangle x^2}{3!}\frac{\partial^3 u}{\partial x^3} - \ldots \tag{1.2}$$

If we break the right hand side of the last equation after the first term, for $\triangle x \ll 1$ the last equation becomes

$$\boxed{\frac{\partial u}{\partial x} = \frac{u(x+\triangle x) - u(x)}{\triangle x} + \mathscr{O}(\triangle x) = \frac{\triangle_i u}{\triangle x} + \mathscr{O}(\triangle x)}, \tag{1.3}$$

where

$$\triangle_i u = u(x+\triangle x) - u(x) := u_{i+1} - u_i$$

is called *a forward difference*. The backward expansion of the function u can be written as $\triangle x \ll 1$ the last equation reads

$$u(x+(-\triangle x)) = u(x) - \triangle x\frac{\partial u}{\partial x} + \frac{\triangle x^2}{2!}\frac{\partial^2 u}{\partial x^2} - \frac{\triangle x^3}{3!}\frac{\partial^3 u}{\partial x^3} + \ldots, \tag{1.4}$$

so for the first derivative one obtains

$$\boxed{\frac{\partial u}{\partial x} = \frac{u(x) - u(x-\triangle x)}{\triangle x} + \mathscr{O}(\triangle x) = \frac{\nabla_i u}{\triangle x} + \mathscr{O}(\triangle x)}, \tag{1.5}$$

where

$$\nabla_i u = u(x) - u(x-\triangle x) := u_i - u_{i-1}$$

is called *a backward difference*. One can see that both forward and backward differences are of the order $\mathscr{O}(\triangle x)$. We can combine these two approaches and derive *a central difference*, which yields a more accurate approximation. If we substract Eq. (1.5) from Eq. (1.3) one obtains

$$u(x+\triangle x) - u(x-\triangle x) = 2\triangle x\frac{\partial u}{\partial x} + 2\frac{\triangle x^3}{3!}\frac{\partial^3 u}{\partial x^3} + \ldots, \tag{1.6}$$

what is equivalent to

$$\boxed{\frac{\partial u}{\partial x} = \frac{u(x+\triangle x) - u(x-\triangle x)}{2\triangle x} + \mathscr{O}(\triangle x^2)} \tag{1.7}$$

Note that the central difference (1.7) is of the order of $\mathscr{O}(\triangle^2 x)$.
The second derivative can be found in the same way using the linear combination of different Taylor expansions. For instance, consider

$$u(x+2\triangle x) = u(x) + 2\triangle x \frac{\partial u}{\partial x} + \frac{(2\triangle x)^2}{2!}\frac{\partial^2 u}{\partial x^2} + \frac{(2\triangle x)^3}{3!}\frac{\partial^3 u}{\partial x^3} + \dots \tag{1.8}$$

Substracting from the last equation Eq. (1.1), multiplied by two, one gets the following equation

$$u(x+2\triangle x) - 2u(x+\triangle x) = -u(x) + \triangle x^2 \frac{\partial^2 u}{\partial x^2} + \triangle x^3 \frac{\partial^3 u}{\partial x^3} + \dots \tag{1.9}$$

Hence one can approximate the second derivative as

$$\boxed{\frac{\partial^2 u}{\partial x^2} = \frac{u(x+2\triangle x) - 2u(x+\triangle x) + u(x)}{\triangle x^2} + \mathscr{O}(\triangle x).} \tag{1.10}$$

Similarly one can obtain the expression for the second derivative in terms of backward expansion, i.e.,

$$\boxed{\frac{\partial^2 u}{\partial x^2} = \frac{u(x-2\triangle x) - 2u(x-\triangle x) + u(x)}{\triangle x^2} + \mathscr{O}(\triangle x).} \tag{1.11}$$

Finally, if we add Eqn. (1.3) and (1.5) an expression for the cental second derivative reads

$$\boxed{\frac{\partial^2 u}{\partial x^2} = \frac{u(x+\triangle x) - 2u(x) + u(x-\triangle x)}{\triangle x^2} + \mathscr{O}(\triangle x^2).} \tag{1.12}$$

One can see that approximation (1.12) provides more accurate approximation as (1.10) and (1.11).
In an analogous way one can obtain finite difference approximations to higher order derivatives and differential operators. The coefficients for first three derivatives for the case of forward, backward and central differences are given in Tables 1.1, 1.2, 1.3.

Mixed derivatives

A finite difference approximations for the mixed partial derivatives can be calculated in the same way. For example, let us find the central approximation for the derivative

	u_i	u_{i+1}	u_{i+2}	u_{i+3}	u_{i+4}
$\triangle x\frac{\partial u}{\partial x}$	-1	1			
$\triangle x^2\frac{\partial^2 u}{\partial x^2}$	1	-2	1		
$\triangle x^3\frac{\partial^3 u}{\partial x^3}$	-1	3	-3	1	
$\triangle x^4\frac{\partial^4 u}{\partial x^4}$	1	-4	6	-4	1

Table 1.1 Forward difference quotient, $\mathcal{O}(\triangle x)$

	u_{i-4}	u_{i-3}	u_{i-2}	u_{i-1}	u_i
$\triangle x\frac{\partial u}{\partial x}$				-1	1
$\triangle x^2\frac{\partial^2 u}{\partial x^2}$			1	-2	1
$\triangle x^3\frac{\partial^3 u}{\partial x^3}$		-1	3	-3	1
$\triangle x^4\frac{\partial^4 u}{\partial x^4}$	1	-4	6	-4	1

Table 1.2 Backward difference quotient, $\mathcal{O}(\triangle x)$

	u_{i-2}	u_{i-1}	u_i	u_{i+1}	u_{i+2}
$2\triangle x\frac{\partial u}{\partial x}$		-1	0	1	
$\triangle x^2\frac{\partial^2 u}{\partial x^2}$		1	-2	1	
$2\triangle x^3\frac{\partial^3 u}{\partial x^3}$	-1	2	0	-2	1
$\triangle x^4\frac{\partial^4 u}{\partial x^4}$	1	-4	6	-4	1

Table 1.3 Central difference quotient, $\mathcal{O}(\triangle x^2)$

$$\frac{\partial^2 u}{\partial x\partial y}=\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y}\right)=\frac{\partial}{\partial x}\left(\frac{u(x,y+\triangle y)-u(x,y-\triangle y)}{2\triangle y}+\mathcal{O}(\triangle y^2)\right)=$$
$$=\frac{u(x+\triangle x,y+\triangle y)-u(x-\triangle x,y+\triangle y)-u(x+\triangle x,y-\triangle y)+u(x-\triangle x,y-\triangle y)}{4\triangle x\triangle y}+\mathcal{O}(\triangle x^2\triangle y^2).$$

A nonequidistant mesh

In the section above we have considered different numerical approximations for the derivatives using the equidistant mesh. However, in many applications it is convinient to use a nonequidistant mesh, where the spatial steps fulfill the following rule:

$$\triangle x_i=\alpha\triangle x_{i-1}.$$

If $\alpha=1$ the mesh is said to be equidistant. Let us now calculate the first derivative of the function $u(x)$ of the second-order accurance:

$$u(x+\alpha\triangle x)=u(x)+\alpha\triangle x\frac{\partial u}{\partial x}+\frac{(\alpha\triangle x)^2}{2!}\frac{\partial^2 u}{\partial x^2}+\frac{(\alpha\triangle x)^3}{3!}\frac{\partial^3 u}{\partial x^3}+\ldots \qquad (1.13)$$

Adding the last equation with Eq. (1.4) multiplied by α one obtains the expression for the second derivative

$$\frac{\partial^2 u}{\partial x^2} = \frac{u(x+\alpha\triangle x) - (1+\alpha)u(x) + \alpha u(x-\triangle x)}{\frac{1}{2}\alpha(\alpha+1)\triangle x^2} + \mathscr{O}(\triangle x) \tag{1.14}$$

Substitution of the last equation into Eq. (1.4) yields

$$\boxed{\frac{\partial u}{\partial x} = \frac{u(x+\alpha\triangle x) - (1-\alpha^2)u(x) - \alpha^2 u(x-\triangle x)}{\alpha(\alpha+1)\triangle x} + \mathscr{O}(\triangle x^2)}. \tag{1.15}$$

1.3 von Neumann stability analysis

One of the central questions arising by numerical treatment of the problem in question is stability of the numerical scheme we are interested in [8]. An algorithm for solving an evolutionary partial differential equation is said to be *stable*, if the numerical solution at a fixed time remains bounded as the step size goes to zero, so the perturbations in form of, e.g., rounding error does not increase in time. Unfortunately, there are no general methods to verify the numerical stability for the partial differential equations in general form, so one restrict oneself to the case of linear PDE's. The standard method for linear PDE's with periodic boundary conditions was proposed by John von Neumann [4, 1] and is based on the representation of the rounding error in form of the Fouirer series.

In order to illustrate the procedure, let us introduce the following notation:

$$u^{j+1} = \mathscr{T}[u^j]. \tag{1.16}$$

Here $\mathscr{T}$ is a nonlinear operator, depending on the numerical scheme in question. The successive application of $\mathscr{T}$ results in a sequence of values

$$u^0, u^1, u^2, \ldots,$$

that approximate the exact solution of the problem. However, at each time step we add a small error ε^j, i.e., the sequence above reads

$$u^0 + \varepsilon^0, u^1 + \varepsilon^1, u^2 + \varepsilon^2, \ldots,$$

where ε^j is a cumulative rounding error at time t_j. Thus we obtain

$$u^{j+1} + \varepsilon^{j+1} = \mathscr{T}(u^j + \varepsilon^j). \tag{1.17}$$

After linearization of the last equation (we suppose that Taylor expansion of $\mathscr{T}$ is possible) the linear equation for the perturbation takes the form:

$$\boxed{\varepsilon^{j+1} = \frac{\partial \mathscr{T}(u^j)}{\partial u^j}\varepsilon^j := G\varepsilon^j}. \tag{1.18}$$

This equation is called *the error propagation law*, whereas the linearization matrix G is said to be *an amplification matrix* [5]. Now, the stability of the numerical scheme in question depends on the eigenvalues g_μ of the matrix G. In other words, the scheme is stable if and only if

$$|g_\mu| \leq 1 \quad \forall \mu$$

Now the question is how this information can be used in practice. The first point to emphasize is that in general one deals with the $u(x_i, t_j) := u_i^j$, so one can write

$$\varepsilon_i^{j+1} = \sum_{i'} G_{ii'} \varepsilon_{i'}^j, \tag{1.19}$$

where

$$G_{ii'} = \frac{\partial \mathscr{T}(u^j)_i}{\partial u_{i'}^j}.$$

Futhermore, the spatial variation of ε_i^j (rounding error at the time step t_j in the point x_i) can be expanded in a finite Fourier series in the intreval $[0, L]$:

$$\varepsilon_i^j = \sum_k e^{ikx_i} \tilde{\varepsilon}^j(k), \tag{1.20}$$

where k is the wavenumber and $\tilde{\varepsilon}^j(k)$ are the Fourier coefficients. Since the rounding error tends to grow or decay exponentially with time, it is reasonable to assume that $\tilde{\varepsilon}^j(k)$ varies exponentially with time, i.e.,

$$\varepsilon_i^j = \sum_k e^{\omega t_j} e^{ikx_i},$$

where ω is a constant. The next point to emphasize is that the functions e^{ikx_i} are eigenfunctions of the matrix G, so the last expansion can be interpreted as the expansion in eigenfunctions of G. In addition, the equation for the error is linear, so it is enough to examine the grows of the error of a typical term of the sum. Thus, from the practical point of view one take the error ε_i^j just as

$$\varepsilon_i^j = e^{\omega t_j} e^{ikx_i}.$$

The substitution of this expression into Eq. (1.20) results in the following relation

$$\varepsilon_i^{j+1} = g(k) \varepsilon_i^j. \tag{1.21}$$

That is, one can interpert e^{ikx_j} as an eigenvector corresponding to the eigenvalue $g(k)$. The value $g(k)$ is often called *an amplification factor*. Finally, the stability criterium is then given by

$$\boxed{|g(k)| \leq 1 \quad \forall k}. \tag{1.22}$$

This criterium is called *von Neumann stablity criterium.*

Notice that presented stability analysis can be applied only in certain cases. Namely, the linear PDE in question schould be with constant coefficients and satisfies periodic boundary conditions. In addition, the corresponding difference scheme should possesses no more than two time levels [10]. However, it is often used in more complicated situations as a good estimation for the step sizes used in the approximation.