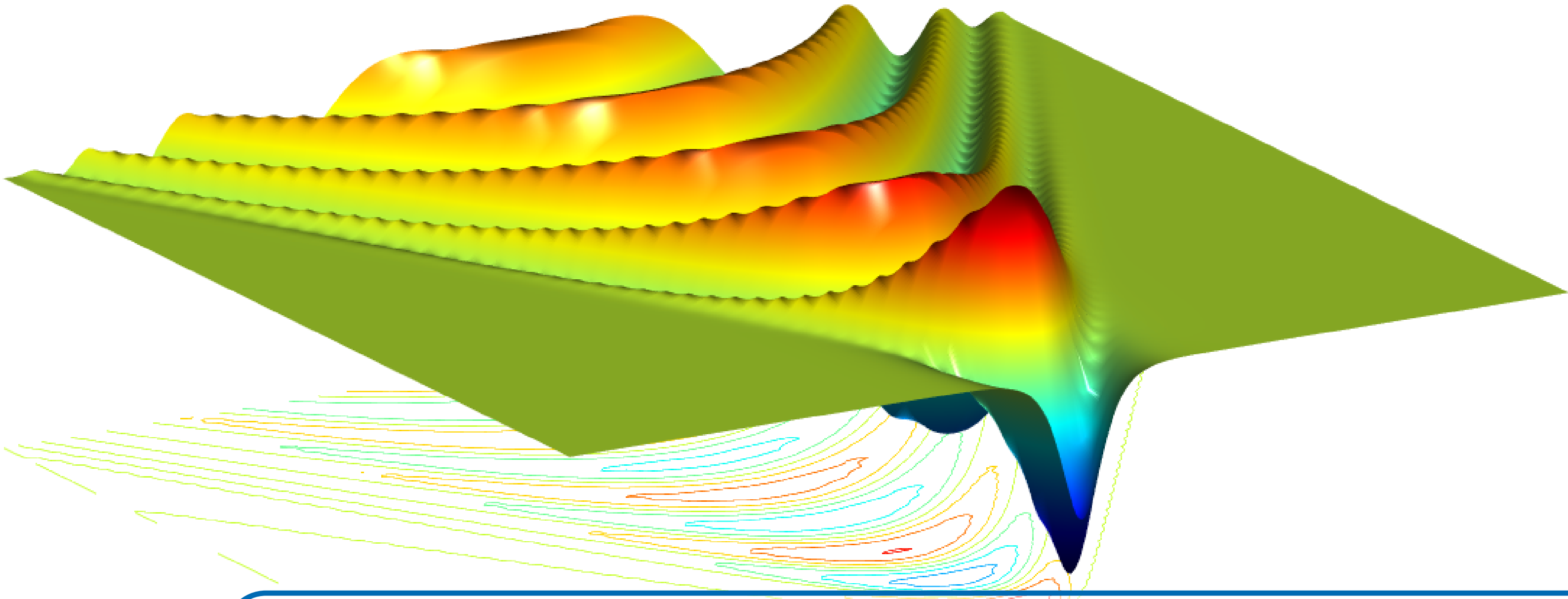

1. Partial differential equations

In this chapter we discuss initial value problems for partial differential equations. We begin by considering the most simple partial differential equation, the advection equation,

$$\frac{\partial u}{\partial t} + V\frac{\partial u}{\partial x} = 0\,, \quad V = \text{const.}\,. \tag{1.1}$$

Afterwards, we will consider the diffusion equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}\,, \quad D = \text{const.}\,, \tag{1.2}$$

and we shall see that algorithms that work for Eq. (1.1) do not necessarily perform well for Eq. (1.2). All problems in this chapter will be initial value problems in time, i.e. we assume that $u(x,t=0) = u^0(x)$ is known and that solutions $u(x,T)$ are sought.

Equations (1.1) and (1.2) are not only prototypical examples for hyperbolic and parabolic partial differential equations, respectively, but are, in combination, relevant to many continuum models. The general advection-diffusion equation,

$$\frac{\partial u}{\partial t} = \nabla\cdot(D\nabla u) - \nabla\cdot(\mathbf{v}u) + R\,, \tag{1.3}$$

describes the rate of change of a quantity u (e.g. concentration, mass density or temperature) due to diffusion ($\nabla\cdot(D\nabla u)$), advection ($\nabla\cdot(\mathbf{v}u)$) and sources (or sinks) R. Under the assumption that $u(x,y,z,t) = u(x,t)$ (one-dimensional geometry) and that $D =$const.,$\mathbf{v} = V\hat{\mathbf{e}}_x$ and $R = 0$, we have

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} - V\frac{\partial u}{\partial x}. \tag{1.4}$$

1.1 The advection equation

Before we start to develop numerical schemes to treat Eq. 1.1, let us shortly summarize the analytic properties of the solutions. In fact, this equation can be solved analytically, hence, it will play the role of a reference case.

The general solutions of this PDE are of the form $u(x,t) = u(x - Vt)$. Thus, this PDE couples temporal to spatial phenomena, but space and time may only appear in the combination $x - Vt$ in the solution (This allows for example to rewrite the equation as an ODE in terms of a new variable $\xi = x - Vt$). Once we know the initial condition $u^0(x)$, we immediately find $u(x,t) = u^0(x - Vt)$. All that Eq. (1.1) does, is to translate the initial distribution $u^0(x)$ in time by the distance Vt. The shape of u is completely preserved. For $V = c$, we might think of Eq. (1.1) as a wave equation for right-traveling electromagnetic waves in vacuum. In fact, the second order wave-equation

$$\frac{\partial^2 E}{\partial t^2} - c^2 \frac{\partial^2 E}{\partial x^2} = 0 \tag{1.5}$$

we know from electrodynamics is closely related to Eq. (1.1), since the operator in (1.5) can also be written in the form

$$\frac{\partial^2}{\partial t^2} - c^2 \frac{\partial^2}{\partial x^2} = \left(\frac{\partial}{\partial t} - c\frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right), \tag{1.6}$$

which leads to the conclusion, that Eq. (1.5) supports right- and left-traveling waves.

Let us now start to develop numerical methods to solve Eq. (1.1). When we discussed ODEs, we found that we have to introduce approximations to the differential operators in order to develop numerical schemes. It is the same here, but now we have to approximate the operators $\partial/\partial x$ and $\partial/\partial t$.

Let us start with a general observation. Assume we decided on a way how to approximate the spatial derivative in Eq. (1.1). By this semi-discretization, we made the step from a continuous function $u(x,t)$ to a set of discrete values $u(x_i,t)$. We arrive at a system of ODEs,

$$\frac{\partial u_i}{\partial t} = -V\left(\frac{\partial u}{\partial x}\right)_i, \quad i = 1,\ldots,N. \tag{1.7}$$

Note, that since the approximation of $(\partial u/\partial x)_i$ involves neighboring positions $\ldots, i-1, i+1, \ldots$, this is a system of coupled ODEs. In principle we already know how to proceed from here. We might think of applying the methods we discussed earlier to solve the system ODEs. Maybe use our standard work-horse Runge-Kutta algorithm? Well, there might be a few surprises for us. Let us start with a very simple scheme to see to which points we will have to pay attention.

■ **Example 1.1** Let us consider three semi-discretizations of Eq. (1.1) and compare them to the original equation by studying the dispersion relations $\omega(k)$. First, we note that Eq. (1.1) is a linear PDE and thus supports plane-wave solutions of the form $u(x,t) = \exp(\mathrm{i}(\omega t - kx))$. When inserting this into (1.1), we obtain the analytic dispersion relation $\omega = kV$.

We now discretize the spatial derivative in (1.1) in three different ways:

$$\frac{\partial u}{\partial t} = -V\frac{u(x,t) - u(x-\Delta x,t)}{\Delta x}, \tag{1.8}$$

$$\frac{\partial u}{\partial t} = -V\frac{u(x+\Delta x,t) - u(x,t)}{\Delta x}, \tag{1.9}$$

$$\frac{\partial u}{\partial t} = -V\frac{u(x+\Delta x,t) - u(x-\Delta x,t)}{2\Delta x}. \tag{1.10}$$

Equations (1.8) and (1.9) are first-order approximations and (1.10) is a second-order approximation. Inserting the plane-wave ansatz for $u(x,t)$ into all three equations (1.8)-(1.10) leads to the three dispersion relations,

$$\omega_1 = \frac{V}{\Delta x}\left[\sin(k\Delta x) + \mathrm{i}(1-\cos(k\Delta x))\right], \tag{1.11}$$

$$\omega_2 = \frac{V}{\Delta x}\left[\sin(k\Delta x) - \mathrm{i}(1-\cos(k\Delta x))\right], \tag{1.12}$$

$$\omega_3 = \frac{V}{\Delta x}\sin(k\Delta x). \tag{1.13}$$

From all three dispersion relations we recover the analytic dispersion relation $\omega = kV$ in the limit $k\Delta x \to 0$. For finite $k\Delta x$ however, the first two cases, (1.11) and (1.12), give complex frequencies ω for real k. Assuming that $\omega = \omega_r + \mathrm{i}\omega_i$ and hence

$$u(x,t) = e^{\mathrm{i}(\omega t - kx)} = e^{-\omega_i t} e^{\mathrm{i}(\omega_r t - kx)}, \tag{1.14}$$

we see that the complex part of ω is responsible for exponential damping ($\omega_i > 0$) or growth ($\omega_i < 0$). The two first-order semi-discretizations (1.8),(1.9), thus, lead to systems in which plane waves become damped (1.8) or amplified (1.9). Only for the discretization (1.10) ω is purely real, however, different from the analytic expression.

From

$$u(x,t) = e^{\mathrm{i}(\omega_r t - kx)} = e^{\mathrm{i}k((\omega_r/k)t - x)} = e^{\mathrm{i}\phi}, \tag{1.15}$$

we see that $v_{ph} = \omega_r/k$ is the velocity with which the phase ϕ of the wave propagates, it is the *phase velocity*. The phase velocity that we obtain from (1.13) is

$$v_{ph} = \frac{V}{k\Delta x}\sin(k\Delta x). \tag{1.16}$$

The semi-discretized system (1.10) thus describes undamped propagation of plane waves, but with a phase velocity that depends on the wave number k and that is smaller than the phase-velocity V of plane waves in Eq. (1.1) by a factor $\sin(k\Delta x)/k\Delta x$.

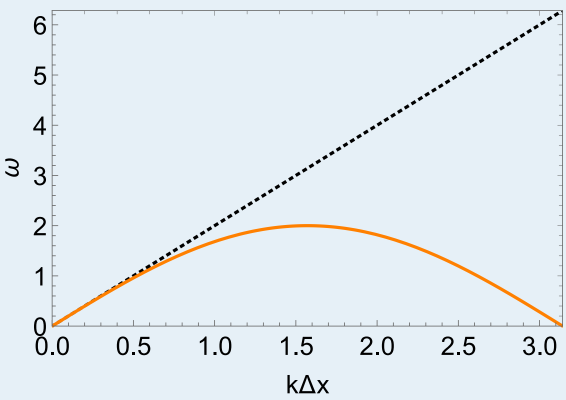

Figure 1.1: Real frequency ω of a plane wave as a function of the wave-number k. The black-dashed line corresponds to the dispersion relation of the original PDE (1.1), the solid orange line to the solution (1.13) for the semi-discretized equation (1.10). For the latter, the phase velocity $v_{ph} = \omega/k$ is a function of k and we have only good agreement with the original dispersion relation for small values of $k\Delta x$.

■

1.1.1 Upwind differencing

The most simple way to approximate the differential operators in Eq. (1.1) is using first-order approximations. Using the notation $u_i^n = u(x_i, t_n) = u(i\Delta x, n\Delta t)$, we get

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -V \frac{u_i^n - u_{i-1}^n}{\Delta x} \,. \tag{1.17}$$

On the left side, we recognize a forward Euler step in time. The spatial derivative is a left-sided difference. We might also use a right-sided difference here. Both are of order Δx. However, we choose the left-sided difference, since we know from the analytical discussion, that the solution will strictly propagate from left to right. This means, that if we update the value at a position i, we should only take into account the prior value at i and to the left of it.

We rearrange terms and arrive at the *upwind* scheme,

$$u_i^{n+1} = -\frac{V\Delta t}{\Delta x}\left(u_i^n - u_{i-1}^n\right) + u_i^n \,. \tag{1.18}$$

The fraction on the right side is also known as Courant-Friedrichs-Lax number, we abbreviate it as

$$C = \frac{V\Delta t}{\Delta x} \,. \tag{1.19}$$

In Eq. (1.18) appear the spatial and the temporal step sizes Δx and Δt, respectively. Usually, we first choose Δx (by choosing the number of nodes N), such that we sample our function good enough in space. How do we choose Δt? From where do we know what is a sufficiently small, but still as large as possible, choice? How can we infer, that we made a bad choice?