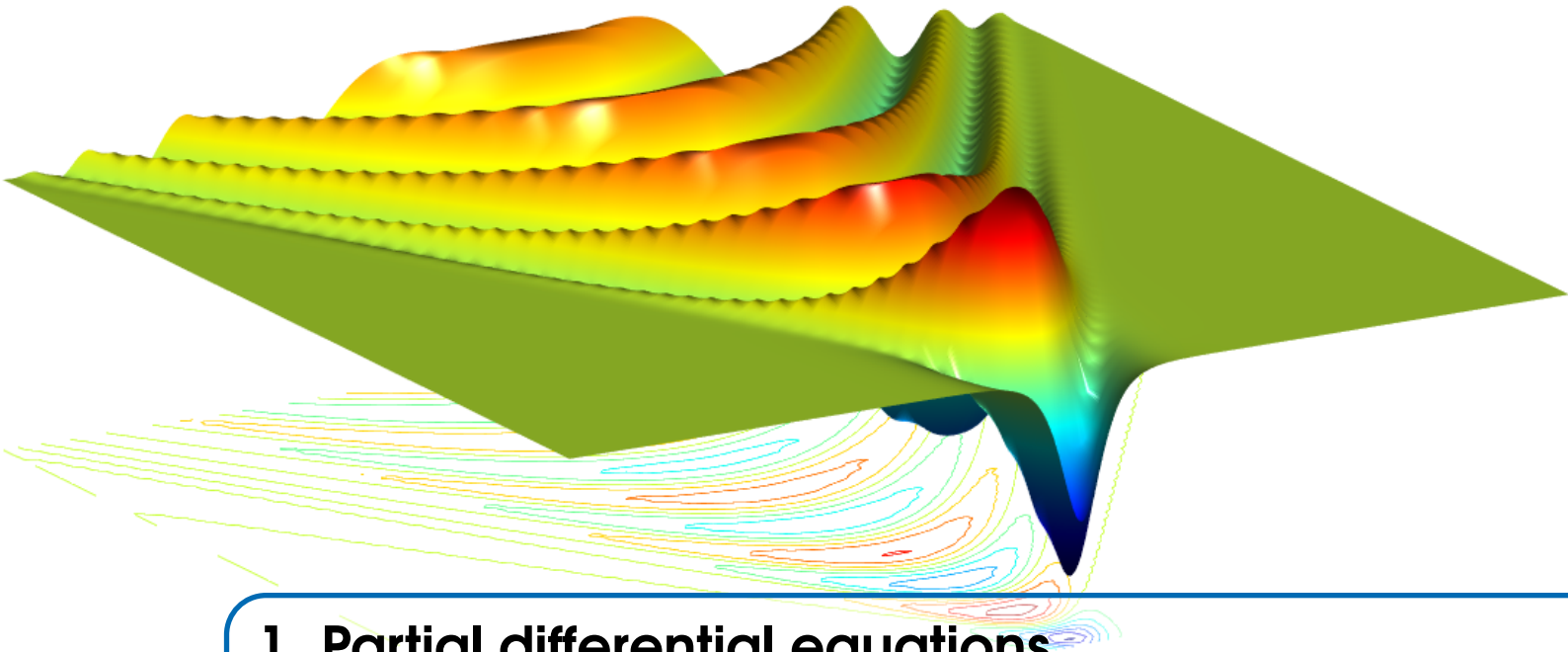


1. Partial differential equations

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 $\sin(k\Delta x)/k\Delta x$.

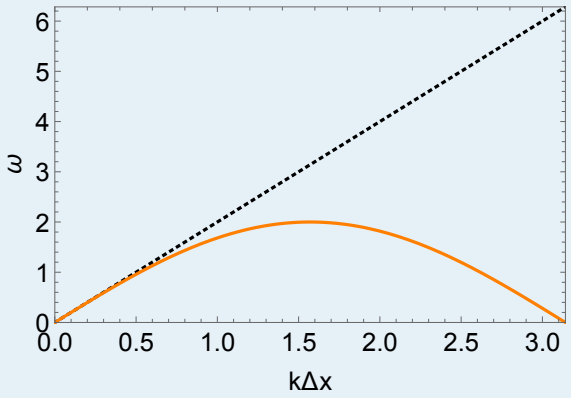


Figure 1.1: Real frequency ω of a plane wave as a function of the wave-number k. The black-dashed line corresponds to the dispersion relation of the original PDE (1.1), the solid orange line to the solution (1.13) for the semi-discretized equation (1.10). For the latter, the phase velocity $v_{ph} =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

1.1.2 The Courant-Friedrichs-Lewy criterion

The Courant-Friedrichs-Lax criterion (short CFL criterion) gives us a first idea how we have to choose Δt, once we chose Δx.

Suppose we integrate the evolution of the initial condition $u^0(x)$, and we are at time $t_n = n\Delta t$, at position $x_j = j\Delta x$. From the analytic solution we know, that the value is $u_j^n = u^0(x_j - Vt_n)$. At time t_0 this value was a distance Vt_n away (to the left) from our position x_j. Our numerical scheme of course does not know about this. But we have to make sure, that it is possible for the scheme to propagate the information from $(x_j - Vt_n, 0)$ to (x_j, t_n). If our scheme transports information in positive x direction, but at a velocity that is too small, we can not expect to get the correct value for u_j^n. On the other hand, if information is transported to fast, the correct value has already passed our position.

Obviously, the ideal case is that the algorithm transports all information with the correct velocity V. We can achieve this by choosing $C = 1$, i.e. $\Delta t = \Delta x/V$, because then (1.18) becomes

$$u_i^{n+1} = u_{i-1}^n , \tag{1.20}$$

from which we deduce

$$u_i^n = u_{i-n}^0 , \tag{1.21}$$

which means that we get the analytically correct value, even though we use discrete values of u.

Why should we now even think about other algorithms to solve Problem (1.1) if we just found a way to get analytically correct values from a discretized distribution? The answer is simple: As soon as V is not spatially constant any more, it will not be possible to choose Δt such that $C = 1$ is fulfilled everywhere. Hence, we have to understand what happens when $C \neq 1$ and whether there is some indication that we should aim for $C < 1$ or $C > 1$ if we are not able to meet $C = 1$.

1.1.3 Von Neumann stability

A Von Neumann analysis is a method to determine the stability of algorithms for linear PDEs. A stable algorithm guarantees that we get finite values from finite input values. To investigate this, we make use of the linearity of the equation itself and the method we employ to solve it. Since everything is linear, we might think of u as being composed out of Fourier modes. Once we know what our algorithm does to each Fourier mode, we know what it does to our initial values.

To do a Neumann stability analysis, we assume that $u_j^0 = \exp(\mathrm{i}k\Delta x j)$, i.e. that our initial value is a Fourier mode with wave-number k. That there are only discrete wave-numbers available for k can go unattended here, we can specify this later, for now k is completely free.

When we insert u^0 into the upwind scheme, we will obtain ξu^0 as a result (due to linearity). The (in general complex) factor ξ is the amplification factor. After n steps, we will have $\xi^n u^0$. If $|\xi| > 1$ we get exponential growth, so the method is be unstable. The case in which no amplitude growth occurs is $|\xi| = 1$, and for $|\xi| < 1$ we have a damping of the Fourier mode.

We insert $u_j^n = \xi^n \exp(\mathrm{i}k\Delta x j)$ into (1.18) and obtain

$$\xi(k) = 1 - C + C\exp(-\mathrm{i}k\Delta x)\,. \tag{1.22}$$

For $C = 1$ we have $|\xi| = 1$ for all k. This is again the ideal case, as we already found out in the section above. If $C > 1$, i.e. $V\Delta t/\Delta x > 1$, we have $|\xi| > 1$ for some k. The Fourier-modes for these k numbers will grow exponentially. We will investigate later which modes these are exactly. For $C < 1$, we have $|\xi| < 1$ for all modes, except the constant mode $k = 0$. This means we expect a damping of the solution. Note that $\xi(k)$ is a complex number. The magnitude of ξ decides about the growth of the mode, the phase of ξ describes phase-errors that the Fourier-mode will experience.

1.1.4 Forward time centered space

Can the upwind method be improved by using better approximations to the derivatives? The FTCS (forward time centered space) algorithm is the first try to improve the upwind scheme by using second order, centered differences in x. The approximation of the time-derivative still is a first order forward Euler.

The FCTS scheme for Eq. (1.1) is

$$u_i^{n+1} = -\frac{C}{2}\left(u_{i+1}^n - u_{i-1}^n\right) + u_i^n\,. \tag{1.23}$$

The Neumann analysis yields the amplification factor

$$\xi(k) = 1 - \mathrm{i}C\sin(k\Delta x)\,. \tag{1.24}$$

Obviously, this scheme is unstable for all values of C, since $|\xi| > 1$ for all $k \neq 0$.

Lax stabilization of FTCS

Lax found, that it is possible to stabilize FTCS by replacing $u_i^n \to \frac{1}{2}(u_{i+1}^n + u_{i-1}^n)$ in the approximation of the time-derivative. This modifies (1.23) to

$$u_i^{n+1} = -\frac{C}{2}\left(u_{i+1}^n - u_{i-1}^n\right) + \frac{1}{2}(u_{i+1}^n + u_{i-1}^n)\,. \tag{1.25}$$

The amplification factor for this method is

$$\xi(k) = \cos(k\Delta x) - \mathrm{i}C\sin(k\Delta x)\,, \tag{1.26}$$

which implies $|\xi| \leq 1$ for $C \leq 1$. Here we find, that the method is stable, provided we choose the correct value for C. For $C = 1$, the u_{i+1}^n part cancels out, and we recover the upwind method.

It is interesting to re-engineer Eq. (1.25) and find the equation of which (1.25) is a discretization. We find

$$\frac{\partial u}{\partial t} = -V\frac{\partial u}{\partial x} + \frac{\Delta x^2}{2\Delta t}\frac{\partial^2 u}{\partial x^2}\,, \tag{1.27}$$

which is the original equation plus an additional diffusive term with the coefficient $\Delta x^2/(2\Delta t)$. Thus, Lax stabilization introduces artificial diffusion to prevent instability. The amount of diffusion depends on the prefactor.

1.1.5 Staggered Leap Frog

The leap frog method uses second order derivatives in time and in space. The spatial derivative is approximated at the central time over which the temporal step leaps (like a frog). The leap frog scheme for (1.1) is

$$\frac{u_i^{n+1} - u_i^{n-1}}{2\Delta t} = -V\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x}\,. \tag{1.28}$$

Now, u^{n+1} is a function of u^n and u^{n-1},

$$u_i^{n+1} = -C\left(u_{i+1}^n - u_{i-1}^n\right) + u^{n-1}\,. \tag{1.29}$$

The second order approximation of the time-derivative introduced a new problem. The original problem (1.1) is a first order initial value problem in t, i.e. we have to specify one initial condition in time. From Eq. (1.29) we see, that now, we need two initial conditions in time! Of course they can not be independent of each other, otherwise we would start with inconsistent initial conditions.

To solve the problem with the second initial conditions, we can use to following idea. The time integration is accurate up to second order in Δt. This means, we only have to get the second initial conditions correct up to second order in t. Assume we know u^0 and we additionally need u^{-1} to start the integration. For u^{-1} we can write a Taylor's series

$$u^{-1} = u(x,-\Delta t) = u(x,0) - \Delta t\frac{\partial u}{\partial t}|_{t=0} + \frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial t^2}|_{t=0} + \mathscr{O}(\Delta t^3)\,. \tag{1.30}$$

In general we only know $u^0 = u(x,0)$. We can make use of the PDE (1.1) itself to replace all temporal derivatives with spatial derivatives. From (1.1) it follows, that

$$\frac{\partial u}{\partial t}|_{t=0} = -V\frac{\partial u}{\partial x}|_{t=0}\,, \tag{1.31}$$

$$\frac{\partial^2 u}{\partial t^2}|_{t=0} = V^2\frac{\partial^2 u}{\partial x^2}|_{t=0}\,. \tag{1.32}$$

Replacing these terms in (1.30) allows us to obtain the second initial condition, consistent up to second order in Δt.

The Neumann stability analysis for (1.29) yields the amplification factor

$$\xi(k) = -\mathrm{i}C\sin(k\Delta x) \pm \sqrt{1 - C^2\sin^2(k\Delta x)}\,. \tag{1.33}$$

The magnitude of $\xi(k)$ is 1 for all values of $C \leq 1$, which means that the leap frog method is stable and has no damping of the amplitude.

Unfortunately, there is again a potential spoiler. Since both derivatives are approximated by central differences, the temporal evolution of all values at grid nodes with even index is purely determined by values at other nodes with even index. The even grid points decouple completely from the uneven points and vice versa. This problem is known as mesh-drifting instability.

1.1.6 Lax-Wendroff method

A second order scheme which avoids mesh-drifting is the Lax-Wendroff method. This scheme first advances the solution from u^n to $u^{n+1/2}$ via

$$u_{i+1/2}^{n+1/2} = \frac{1}{2}\left(u_{i+1}^n + u_i^n\right) - \frac{V\Delta t}{2\Delta x}(u_{i+1}^n - u_i^n)\,. \tag{1.34}$$

We note that these intermediate values in time are defined at intermediate points in space. Using these values, we may step from u^n to u^{n+1},

$$u_i^{n+1} = u_i^n - C\left(u_{i+1/2}^{n+1/2} - u_{i-1/2}^{n+1/2}\right)\,. \tag{1.35}$$

Substituting (1.34) into (1.35), we get

$$u_i^{n+1} = u_i^n - C\left[\frac{1}{2}\left(u_{i+1}^n + u_i^n\right) - \frac{C}{2}\left(u_{i+1}^n - u_i^n\right) - \frac{1}{2}\left(u_i^n + u_{i-1}^n\right) + \frac{C}{2}\left(u_i^n - u_{i-1}^n\right)\right]\,. \tag{1.36}$$

From here we can see the reason, why mesh-drifting should not occur anymore. The temporal evolution of the value u_i^n depends on u_{i-1}^n, u_{i+1}^n and u_i^n itself. Odd and even positions do not decouple any longer.

The Neumann stability analysis for (1.36) gives

$$\xi(k) = 1 - \mathrm{i}C\sin(k\Delta x) - C^2(1-\cos(k\Delta x))\,, \tag{1.37}$$

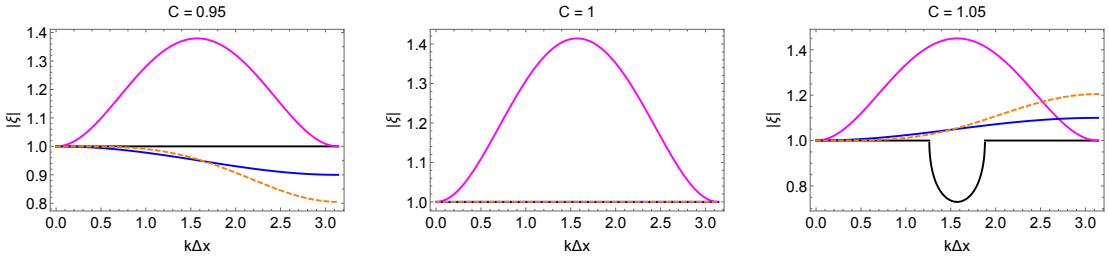
or

$$|\xi(k)|^2 = 1 - C^2(1-C^2)(1-\cos(k\Delta x))^2\,. \tag{1.38}$$

We find again, that the method is stable for $C \leq 1$. In case of $C < 1$ we have $|\xi| < 1$ and some damping, which mainly affects long wave-length oscillations.

1.1.7 Conclusions for the advection equation

In conclusion, we discussed several methods to solve the advection equation (1.1) and found none of them free of problems. For this particular equation it turns out, that the CFL number C is closely related to stability. However, this has not to be true for other equations. We observed, that the discretizations in time and space should not be treated independently.



(a) (b) (c)

Figure 1.2: Comparison of amplification factors for Upwind (blue), FTCS (magenta), Leap Frog (black) and Lax-Wendroff (orange, dashed). The three graphs show $|\xi(k\Delta x)|$ for different values of C. Values of $|\xi|$ larger than 1 correspond to instability. Note that only one of the roots of $|\xi|$ is plotted for Leap Frog.

We will close this section with Fig. 1.2 which summarizes some of our findings. The plots show the amplification magnitudes $|\xi|$ versus $k\Delta x$ for different choices of C. By plotting $|\xi|$ versus

$k\Delta x$ and not only versus k, we are independent of the spatial discretization, thus, the results are valid in a general context. For $C = 1$ we find all but the FTCS algorithms to be stable. If $C < 1$, all again all methods except FTCS are stable, but now only Leap frog provides undamped solutions. Upwind and Lax-Wendroff suffer from damping. Lax-Wendroff shows substantial damping only for larger values of $k\Delta x$: Thus it dampens shorter wave-lengths modes more than upwind, but at the same time has better accuracy for longer wave-length modes than upwind. And of course second order precision in time, which means reduced computational effort.

In case of $C > 1$ all our algorithms are unstable. Note that ξ has two roots with different magnitudes for Leap frog. Only one of the roots is plotted here. The result for the other root looks like the red line, but is mirrored along the $k\Delta x = 0$ line.

1.2 The diffusion equation

The diffusion (or heat) equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}, \quad D = \text{const.}, \tag{1.39}$$

is the prototypical parabolic partial differential equation. The fundamental solution to this equation is

$$u(x,t) = \frac{1}{\sqrt{4\pi D t}} e^{-x^2/4Dt}. \tag{1.40}$$

Figure 1.3 shows the graph of this solution at different times. As a characteristic time-scale we may choose the time it takes to double the full width at half maximum (FWHM). From (1.40) we see that if the FWHM is d at time t_1, the FWHM has been increased to Nd at $t_2 = N^2 t_1$. Figure 1.3 exemplifies this time scale.

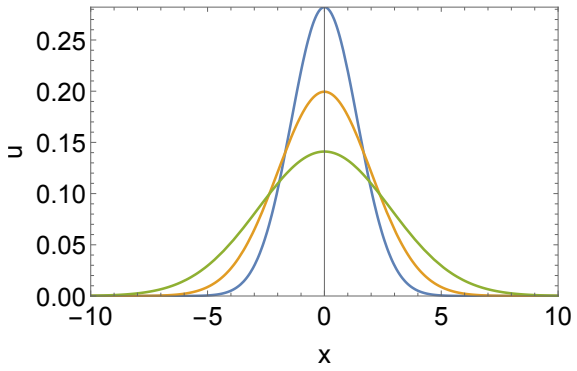


Figure 1.3: Fundamental solution (1.40) for $D = 1$ at times $t = 1$ (blue), $t = 2$ (orange) and $t = 4$ (green).

Like for the advection equation, the analytic solution is known and there is for now no direct need for a numerical solution to this equation. This is, however, only true if the initial distribution $u(x,t = 0)$ is analytically known and as long as the process by which u changes is purely diffusive. If D is not constant, we should start from the more general equation

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right). \tag{1.41}$$

1.2.1 Euler forward method

The Euler forward discretization to (1.39) is

$$\frac{u_i^{n+1}-u_i^n}{\Delta t} = D\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}, \tag{1.42}$$

to which we can also refer as forward-time centered-space discretization. Rearranging gives,

$$u_i^{n+1} = u_i^n + \frac{D\Delta t}{\Delta x^2}\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right), \tag{1.43}$$

from which we find the amplification factor for a mode with wavenumber k to be

$$\xi = 1 - 4\frac{D\Delta t}{\Delta x^2}\sin^2(k\Delta x/2). \tag{1.44}$$

For stability we require $|\xi| < 1$, hence, the von Neumann stability criterion is

$$\Delta t \leq \frac{1}{2}\frac{\Delta x^2}{D}. \tag{1.45}$$

Contrary to the advection equation, the explicit discretization is stable for the diffusion equation. Explicit schemes always have the benefit, compared to implicit schemes, that they are simple to implement. However, we shall see that the required time steps Δt are very small compared to the characteristic time-scales. Hence, every step is conceptually and computationally simple, but the number of time steps can be large. What may not be a problem in one-dimensional situations can become severe in higher dimensions.

1.2.2 Euler backward method

The Euler backward discretization to (1.39) is

$$\frac{u_i^{n+1}-u_i^n}{\Delta t} = D\frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{\Delta x^2}, \tag{1.46}$$

which results in the implicit equations

$$-\alpha u_{i+1}^{n+1} + (1+2\alpha)u_i^{n+1} - \alpha u_{i-1}^{n+1} = u_i^n, \quad \alpha = \frac{D\Delta t}{\Delta x^2}. \tag{1.47}$$

Thus, every time step becomes equivalent to solving the system of linear equations

$$\begin{pmatrix} 1+2\alpha & -\alpha & 0 & 0 & 0 & \dots & 0 \\ -\alpha & 1+2\alpha & -\alpha & 0 & 0 & \dots & 0 \\ 0 & -\alpha & 1+2\alpha & -\alpha & 0 & \dots & 0 \\ \vdots & & & & & & \vdots \\ 0 & \dots & & 0 & -\alpha & 1+2\alpha & -\alpha \\ 0 & \dots & & & 0 & -\alpha & 1+2\alpha \end{pmatrix} \cdot \mathbf{u}^{n+1} = \mathbf{u}^n. \tag{1.48}$$

In the fomulation of (1.48) we have used Dirichlet boundary conditions $u_0 = u_{N+1} = 0$. As the system is tri-diagonal (and even Toeplitz) it is most effectively solved by using the Thomas algorithm, which scales as $\mathcal{O}(N)$. Remember, that an inversion of the coefficient matrix is to be avoided, as the inverse of a sparse matrix is in general dense and thus every time step would be an $\mathcal{O}(N^2)$ matrix-vector product.

The stability analysis of (1.47) gives

$$\xi = \frac{1}{1+4\alpha\sin^2(k\Delta x/2)}, \tag{1.49}$$

from which we find that $|\xi| \leq 1$ for all α. The implicit backward Euler method is unconditionally stable.

1.2.3 The Crank-Nicolson method

Even though the Euler backward method is stable, it is still only first order in time. A second-order method is obtained by

$$\frac{u_i^{n+1}-u_i^n}{\Delta t} = D\frac{\partial^2 u}{\partial x^2}\bigg|_{t=t_{n+1/2}}, \tag{1.50}$$

which is the trapezoidal rule for ODEs (see Sec. **??**). In the context of PDEs, in particular the heat equation, this method is known as the *Crank-Nicolson* method. The spatial derivative at time $t_{n+1/2}$ is approximated by the average of the second-oder approximations at times t_n and t_{n+1},

$$\frac{u_i^{n+1}-u_i^n}{\Delta t} = \frac{D}{2}\left[\frac{u_{i+1}^n-2u_i^n+u_{i-1}^n}{\Delta x^2}+\frac{u_{i+1}^{n+1}-2u_i^{n+1}+u_{i-1}^{n+1}}{\Delta x^2}\right], \tag{1.51}$$

thus, it is an implicit method. We obtain

$$-\alpha u_{i+1}^{n+1}+(2+2\alpha)u_i^{n+1}-\alpha u_{i-1}^{n+1} = \alpha u_{i+1}^n+(2-2\alpha)u_i^n+\alpha u_{i-1}^n, \quad \alpha=\frac{D\Delta t}{\Delta x^2}, \tag{1.52}$$

which corresponds to a system of linear equations of the form $\mathsf{M}_1\cdot\mathbf{u}^{n+1}=\mathsf{M}_2\cdot\mathbf{u}^n$, where the matrices $\mathsf{M}_{1,2}$ are tri-diagonal. The stability analysis determines the amplification factor to be

$$\xi = \frac{1-2\alpha\sin^2(k\Delta x/2)}{1+2\alpha\sin^2(k\Delta x/2)}, \tag{1.53}$$

the Crank-Nicolson method is therefore stable for any value of α.

1.2.4 Discussion of the amplification factors

By calculation of the amplification factors, we found that the explicit Euler method is conditionally stable, and that the implicit Euler and Crank-Nicolson methods are unconditionally stable. But how do the methods compare when we operate them in their stable regime? To answer this question, we have to remember that the amplification factor $\xi(k)$ is the values by which the Fourier coefficient of u for the wavenumber k is multiplied per time-step Δt.

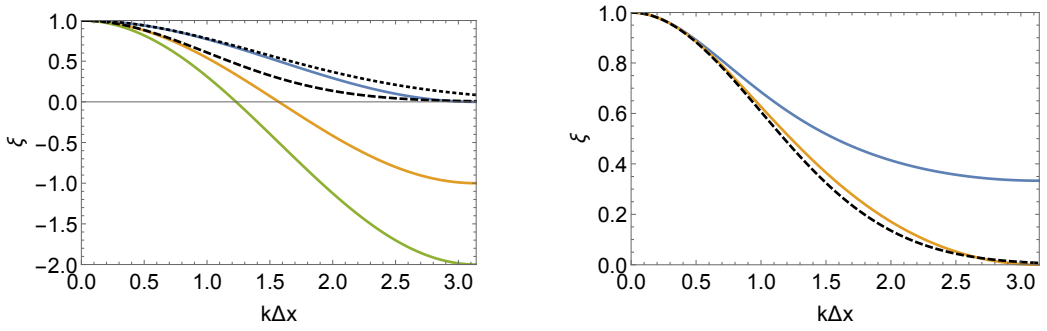
After Fourier transformation in x, the diffusion equation (1.39) becomes

$$\frac{\partial}{\partial t}\hat{u}(k,t) = -k^2 D\hat{u}(k,t), \tag{1.54}$$

hence, $\hat{u}(k,t)=\tilde{u}_0(k)\exp(-k^2Dt)$ is the solution in Fourier space. Per time step Δt, every Fourier coefficient $\hat{u}(k)$ is thus multiplied by the factor $\xi_{ana}=\exp(-k^2D\Delta t)$.

Let us first investigate the Euler forward method. Figure 1.4a shows ξ for three different values of $\alpha=D\Delta t/\Delta x^2$ as a function of $k\Delta x$. The marignal case is $\alpha=1/2$ (orange line), for larger values of α the algorithm is unstable (e.g. $\alpha=3/4$, green line). For the two stable cases, $\alpha=1/2$ and $\alpha=1/4$, respectively, the analytical factors $\xi_{ana}=\exp(-(k\Delta x)^2\alpha)$ are shown as black broken lines. We see that for smaller values of α, the numerical amplification factors match the analytic factors better, but in general agreement is only good for small k, i.e. long wavelenghts.

In Fig. 1.4b we compare Euler backward to Crank-Nicolson for $\alpha=0.5$ to ξ_{ana}. Here we can see the benefit of Crank-Nicolson compared to the Euler backward methods. Both are stable, but the Crank-Nicolson ξ is much closer to ξ_{ana} than the Euler backward method.



(a) (b)

Figure 1.4: (a) Amplification factor ξ for the Euler forward method when applied to the diffusion equation. The lines correspond to $\alpha = 1/4$ (blue line), $\alpha = 1/2$ (orange line) and $\alpha = 3/4$ (green line), where $\alpha = D\Delta t/\Delta x^2$. The black lines show the analytic factors ξ_{ana} for $\alpha = 1/2$ (dashed line) and $\alpha = 1/4$ (dotted line). (b) Amplification factor $|\xi|$ for the Euler backward (blue line) and the Crank-Nicolson (orange line) method, respectively. The black dashed line shows ξ_{ana}, all lines are for $\alpha = 1/2$.

1.3 Schrödinger Equation

Schödinger's equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial t^2}\psi - V(x,t)\psi = 0 \tag{1.55}$$

for the complex wave function ψ is one of the central equations in quantum mechanics, but as we will see this type of equation may also appear in other contexts. Here, we will restrict the discussion to time-independent potentials, i.e. $V(x,t) = V(x)$. In order to simplify the notation, we set $\hbar = 1, m = 1/2$.

The free Schrödinger equation, $V = 0$, resembles the diffusion equation, only that now we deal with a complex function. Our first approach may thus be an implicit treatment,

$$\mathrm{i}\frac{\psi_i^{n+1} - \psi_i^n}{\Delta t} = -\frac{\psi_{i+1}^{n+1} - 2\psi_i^{n+1} + \psi_{i-1}^{n+1}}{\Delta x^2} + V_i\psi_i^{n+1}\,. \tag{1.56}$$

The von Neumann analysis gives the amplification factor

$$\xi_i = \left(1 + \mathrm{i}\left[\frac{4\Delta t}{\Delta x^2}\sin^2\left(\frac{k\Delta x}{2}\right) + V_i\Delta t\right]\right)^{-1}, \tag{1.57}$$

which depends on the spatial position x_i due to the possible spatial dependence of V. We see, that $|\xi| < 1$ for all $\Delta t/\Delta x^2$ ratios, as V can be always chosen such that $V(x) > 0$ for all x, thus, the implicit treatment is unconditionally stable. The implicit treatment. however, has a drawback, it is not unitary, i.e.

$$\int_{-\infty}^{\infty} |\psi|^2 dx = \text{const.} \tag{1.58}$$

is not conserved.

...

With

$$H = -\frac{\partial^2}{\partial t^2} + V(x,t) \tag{1.59}$$

the formal solution of (1.55) becomes $\psi(x,t) = \exp(-\mathrm{i}Ht)\psi(x,0)$. A second order unitary approximation is

$$\exp(\mathrm{i}H\Delta t) = \frac{1-\frac{1}{2}\mathrm{i}H\Delta t}{1+\frac{1}{2}\mathrm{i}H\Delta t} + \mathscr{O}(\Delta t^2)\,. \tag{1.60}$$

Using this expansion we find

$$(1+\tfrac{1}{2}H\Delta t)\psi_i^{n+1} = (1-\tfrac{1}{2}H\Delta t)\psi_i^n\,, \tag{1.61}$$

which is nothing else than the Crank-Nicolson method when we replace the derivative in H by a finite difference. Eventually, we have to solve a system of linear equations.