

## Chapter 2

# Finite difference schemes

The definition of a derivative given in (1.10),

$$\frac{d}{dx}f(x_0) = \lim_{\Delta x \rightarrow 0} \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}, \quad (2.1)$$

could also have been given as

$$\frac{d}{dx}f(x_0) = \lim_{\Delta x \rightarrow 0} \frac{f(x_0) - f(x_0 - \Delta x)}{\Delta x}, \quad (2.2)$$

or as

$$\frac{d}{dx}f(x_0) = \lim_{\Delta x \rightarrow 0} \frac{f(x_0 + \Delta x) - f(x_0 - \Delta x)}{2\Delta x}. \quad (2.3)$$

Actually, all three definitions are equivalent for a continuously derivable function  $f$ . These definitions are the basis for so-called finite-difference schemes. For the case that the function  $f$  is given on a discrete grid with the finite spatial increment  $\Delta x$ , its derivative may be approximated by one of the methods (2.1) - (2.3) by omitting the lim. These approximations will of course not be equivalent. In the next sections, methods will be discussed with the aid of which the quality of the different differencing schemes will be quantified.

### 2.1 Accuracy and consistency

In order to test the accuracy of a scheme, the finite-difference approximation has to be compared to the approximated differential. In the case of the first-order derivative from (2.1) - (2.3), we obtain by means of a Taylor expansion:

$$f(x_0 \pm \Delta x) = f(x_0) \pm \Delta x \partial_x f(x_0) + \frac{\Delta x^2}{2} \partial_{xx} f(x_0) \pm \frac{\Delta x^3}{6} \partial_{xxx} f(x_0) + \dots \quad (2.4)$$

By means of this, the approximation order of the approximation (2.1) may be found:

$$\frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x} - \partial_x f(x_0) = \frac{\Delta x}{2} \partial_{xx} f(x_0) + \frac{\Delta x^2}{6} \partial_{xxx} f(x_0) + \dots \quad (2.5)$$

The right hand side of (2.5) is the so-called truncation error, and the lowest power of  $\Delta x$  in the truncation error is the order of accuracy of the finite-difference approximation. Thus, the finite-difference approximation (2.1) is of first order in  $\Delta x$  which may also be denoted saying that the scheme is  $\mathcal{O}(\Delta x)$ . The same is found for method (2.2). For the central differencing we find however:

$$\frac{f(x_0 + \Delta x) - f(x_0 - \Delta x)}{2\Delta x} - \partial_x f(x_0) = \frac{\Delta x^2}{6} \partial_{xxx} f(x_0) + \frac{\Delta x^4}{120} \partial_{xxxxx} f(x_0) + \dots \quad (2.6)$$

such that this scheme is  $\mathcal{O}(\Delta x^2)$ .

Of course, a higher order of approximation does not guarantee a better approximation in general, since (i) the higher derivatives in the leading truncation terms (e.g.  $\partial_{xxx} f(x_0)$  in (2.5)) may be large and (ii) the overall numerical scheme might be numerically instable, as we have demonstrated in chapter 1.

Approximations of higher than second order may be constructed as well.

After having examined the accuracy of individual derivatives, we will now analyse the accuracy of approximation for partial differential equations. As a basic test case we use the linear advection equation with constant velocity,

$$\partial_t \psi + c \partial_x \psi = 0 \quad (2.7)$$

with  $c > 0$ , which is discretised on a grid equivalent to that described in assignment 1. The advection equation is discretised by means of the so-called upwind scheme

$$\frac{\phi_i^{j+1} - \phi_i^j}{\Delta t} + c \frac{\phi_i^j - \phi_{i-1}^j}{\Delta x} = 0. \quad (2.8)$$

The *modified equation* for this scheme is now formulated in the point  $(x_0, t_0)$ :

$$\frac{\psi(x_0, t_0 + \Delta t) - \psi(x_0, t_0)}{\Delta t} + c \frac{\psi(x_0, t_0) - \psi(x_0 - \Delta x, t_0)}{\Delta x} = 0. \quad (2.9)$$

The difference between the modified equation and the differential equation is then built for checking the consistency of the scheme determining its order of approximation:

$$\begin{aligned} & \frac{\psi(x_0, t_0 + \Delta t) - \psi(x_0, t_0)}{\Delta t} + c \frac{\psi(x_0, t_0) - \psi(x_0 - \Delta x, t_0)}{\Delta x} \\ & - (\partial_t \psi(x_0, t_0) + c \partial_x \psi(x_0, t_0)) \\ & = \frac{\Delta t}{2} \partial_{tt} \psi(x_0, t_0) - \frac{c}{2} \Delta x \partial_{xx} \psi(x_0, t_0) \\ & \quad + \frac{\Delta t^2}{6} \partial_{ttt} \psi(x_0, t_0) + \frac{c}{6} \Delta x^2 \partial_{xxx} \psi(x_0, t_0) + \dots \\ & = \mathcal{O}(\Delta t) + \mathcal{O}(\Delta x). \end{aligned} \quad (2.10)$$

Thus, the finite-difference scheme (2.8) is consistent with the linear advection equation (2.7) to first order in time and first order in space.

As shown in equations (1.25) and (1.26), a wave equation can be derived from the advection equation, with the aid of which the modified equation (2.10) may be reformulated:

$$\begin{aligned} & \frac{\psi(x_0, t_0 + \Delta t) - \psi(x_0, t_0)}{\Delta t} + c \frac{\psi(x_0, t_0) - \psi(x_0 - \Delta x, t_0)}{\Delta x} \\ & - \left( \partial_t \psi(x_0, t_0) + c \partial_x \psi(x_0, t_0) - \frac{c}{2} \Delta x \left( 1 - \frac{\Delta t}{\Delta x} c \right) \partial_{xx} \psi \right) \\ & = \frac{\Delta t^2}{6} \partial_{ttt} \psi(x_0, t_0) + \frac{c}{6} \Delta x^2 \partial_{xxx} \psi(x_0, t_0) + \dots, \end{aligned} \quad (2.11)$$

such that the finite difference approximation (2.8) is a second-order in time and space approximation to the advection-diffusion equation with the diffusivity

$$\nu_{num} = \frac{c}{2} \Delta x (1 - \mu). \quad (2.12)$$

with the so-called Courant number

$$\mu = \frac{\Delta t}{\Delta x} c. \quad (2.13)$$

This diffusivity caused by the numerical scheme is referred to as *numerical diffusion*. Obviously, for  $\mu > 1$ , this advection-diffusion is mathematically ill-posed, since the viscosity becomes negative, a clear sign that the scheme will be unstable for  $\mu > 1$ . Interestingly, the numerical diffusivity vanishes for  $\mu = 1$ , in which case the advection velocity equals the so-called grid velocity  $\Delta x / \Delta t$ , such that all discrete values are simply shifted by one grid index per time step.

## 2.2 Stability and convergence

We have shown in the previous paragraphs how the order of consistency of an approximation methods to a differential equation can be proven. However, as the short numerical calculation in equation (1.6) (where a consistent central difference approximation to the advection equation failed) has shown, consistency is not sufficient for convergence. Before we start to introduce methods for checking the convergence of numerical schemes, it is necessary to introduce quality measures for the numerical approximation. For calculating the absolute size of a vector  $\vec{\phi}$ , two norms are typically used, the maximum norm, defined as

$$\|\vec{\phi}\|_{\infty} = \max_{1 \leq i \leq M} |\phi_i|, \quad (2.14)$$

and the Euclidean norm, defined as

$$\|\vec{\phi}\|_2 = \left( \sum_{i=1}^M \phi_i^2 \right)^{1/2}. \quad (2.15)$$

It should be noted that (2.14) and (2.16) are generalisations of the  $n$ -norm

$$\|\vec{\phi}\|_n = \left( \sum_{i=1}^M |\phi_i|^n \right)^{1/n}. \quad (2.16)$$

A finite-difference scheme  $\phi_i^j$  is said to be convergent of order  $(p, q)$  towards the solution  $\psi$  if in the limit of  $\Delta t, \Delta x \rightarrow 0$ ,

$$\|\psi(j\Delta t, i\Delta x) - \phi_i^j\| = \mathcal{O}[(\Delta t)^p] + \mathcal{O}[(\Delta x)^q]. \quad (2.17)$$

The Lax equivalence theorem (*Lax and Richtmyer* [1956]) proves that

*if a finite-difference scheme is linear, stable, and accurate (i.e. consistent) of order  $(p, q)$ , then it is convergent of order  $(p, q)$ .*

Thus, in addition to consistency, stability of the scheme is required. An numerical scheme will be classified as unstable, when the numerical solution grows more rapidly than the physical solution. A stability criterium which satisfies the Lax equivalence theorem is that for any time  $T$  there exists a constant  $C_T$  such that

$$\|\phi^j\| \leq C_T \|\phi^0\| \quad \text{for all } j\Delta t \leq T, \quad (2.18)$$

and all sufficiently small values of  $\Delta t$  and  $\Delta x$ . The constant  $C_T$  may depend on  $T$ , but not on  $\Delta t$  or  $\Delta x$ . However, this relatively weak constraint (2.18) may in practical applications still fail, since it allows for quite some oscillations of the numerical solution.

For many conservation laws for example, the norm of the physical solution is constant with time, such that numerical solutions with this property will also be stable:

$$\|\phi^j\| \leq \|\phi^0\| \quad \text{for all } j. \quad (2.19)$$

The condition (2.19) is much stronger than (2.18) and is thus not necessary for stability.

### 2.2.1 The energy method

One simple but not general method for estimating the stability of a numerical scheme is the energy method. Here, the sum of all squares of the numerical solution,

$$\sum_i \left( \phi_i^j \right)^2, \quad (2.20)$$

will be calculated and its tendency in time will be evaluated. It should be noted that for this stability method, periodic boundary conditions are required.

Let us again consider the first-order upwind method for the linear advection equation. With the Courant number  $\mu$  from (2.13), this scheme may be formulated as

$$\phi_i^{j+1} = (1 - \mu)\phi_i^j + \mu\phi_{i-1}^j. \quad (2.21)$$

Squaring on both sides and summing over the spatial index  $i$  leads to

$$\sum_i \left(\phi_i^{j+1}\right)^2 = \sum_i \left\{ (1-\mu)^2 \left(\phi_i^j\right)^2 + 2(1-\mu)\mu\phi_i^j\phi_{i-1}^j + \mu^2 \left(\phi_{i-1}^j\right)^2 \right\}. \quad (2.22)$$

With

$$\sum_i \left(\phi_i^j\right)^2 = \sum_i \left(\phi_{i-1}^j\right)^2 \quad (2.23)$$

(shifting by one index in a periodic domain) and

$$\sum_i \phi_i^j \phi_{i-1}^j \leq \left(\sum_i \phi_i^j\right)^{1/2} \left(\sum_i \phi_{i-1}^j\right)^{1/2} = \sum_i \left(\phi_i^j\right)^2, \quad (2.24)$$

(Schwartz inequality) we obtain

$$\sum_i \left(\phi_i^{j+1}\right)^2 \leq \sum_i \left( (1-\mu)^2 + 2(1-\mu)\mu + \mu^2 \right) \left(\phi_i^j\right)^2 = \sum_i \left(\phi_i^j\right)^2, \quad (2.25)$$

such that the *total energy* of the numerical solution does not increase. The condition for obtaining (2.25) is that

$$\mu(1-\mu) \geq 0. \quad (2.26)$$

For  $\mu \geq 0$ , (2.26) is equivalent to  $0 \leq \mu \leq 1$ , which means that the first-order upwind scheme is stable for this range. For negative  $\mu$ , we obtain a contradiction to (2.26), such that stability for the downwind scheme cannot be proven (implying the well-known fact that the downwind scheme is unstable). Therefore, also the instability of the central difference scheme is shown, which is exactly the average of the upwind and the downwind scheme. Thus the stability criterium for the upwind scheme is

$$0 \leq c \frac{\Delta t}{\Delta x} \leq 1, \quad (2.27)$$

meaning that the physical velocity  $c$  must not exceed the grid velocity  $\Delta x/\Delta t$ . The upwind scheme is thus called *conditionally stable*, whereas the downwind and the central scheme are *unconditionally unstable*.

### 2.2.2 Von Neumann's method

One drawback of the energy method is that for each scheme to be considered, a new strategy has to be found how to calculate the energy of the numerical solution.

A more generic method for testing the stability of numerical approximation schemes is the Von Neumann method, which is however also straight-forward only for periodic boundary conditions. Furthermore it can only be applied to

linear schemes with constant coefficients. For each time step, the numerical solution is represented by a finite Fourier series of the form

$$\phi_j^n = \sum_{k=-N}^N a_k^n e^{ikj\Delta x}. \quad (2.28)$$

Note that in comparison to this, each periodic function  $f(x, t)$  may be represented by an infinite Fourier series of the form

$$f(x, t) = \sum_{k=-\infty}^{\infty} a_k(t) e^{ikx}. \quad (2.29)$$

A key property of each Fourier mode in (2.29) is an eigenfunction of the derivative operator:

$$d_x e^{ikx} = ik e^{ikx} \quad (2.30)$$

This property is used in the discrete space for studying the stability of numerical schemes. After one iteration, the solution for a specific discrete Fourier mode  $\phi_j^n = e^{ikj\Delta x}$  will be of the form:

$$\phi_j^{n+1} = A_k e^{ikj\Delta x} \quad (2.31)$$

with the complex so-called amplification factor  $A_k$ . For linear schemes with constant coefficients, the amplification factor will be constant for each time step, such we can write:

$$a_k^n = A_k a_k^{n-1} = (A_k)^n a_k^0. \quad (2.32)$$

For the stability of a numerical scheme, it will be required that each Fourier component of (2.28) is bounded. The Von Neumann stability criterium is therefore formulated as

$$|A_k| \leq 1 + \gamma \Delta t \quad (2.33)$$

with  $\gamma$  being independent of  $k$ ,  $\Delta t$  and  $\Delta x$ . (2.33) guarantees that a consistent scheme converges for  $\Delta x, \Delta t \rightarrow 0$ . For problems with bounded solutions, (2.33) may be limited to

$$|A_k| \leq 1. \quad (2.34)$$

As an illustration, the linear advection problem with the first-order upwind scheme will be tested again. Expressing the solution at each point as a specific Fourier component,  $\phi_j^n = e^{ikj\Delta x}$ , and inserting into (2.21), we obtain

$$A_k e^{ikj\Delta x} = (1 - \mu) e^{ikj\Delta x} + \mu e^{ik(j-1)\Delta x}, \quad (2.35)$$

which gives after division by  $e^{ikj\Delta x}$

$$A_k = (1 - \mu) + \mu e^{-ik\Delta x}, \quad (2.36)$$

and with the absolute value of  $A_k$  being the square root of the product of  $A_k$  with its complex conjugate,

$$\begin{aligned} |A_k|^2 &= ((1 - \mu) + \mu e^{-ik\Delta x}) ((1 - \mu) + \mu e^{ik\Delta x}) \\ &= 1 - 2\mu(1 - \mu)(1 - \cos(k\Delta x)). \end{aligned} \quad (2.37)$$

Thus, condition (2.34) is fulfilled and thus the numerical scheme is stable for

$$1 - 2\mu(1 - \mu)(1 - \cos(k\Delta x)) \leq 1. \quad (2.38)$$

Since  $1 - \cos(k\Delta x) \geq 0$ , this reduces to

$$\mu(1 - \mu) \geq 0, \quad (2.39)$$

which is identical to (2.26), such that we have proven the same stability criterium by means of the Von Neumann method.

### 2.2.3 Courant-Friedrichs-Lewy condition

In temporal-spatial numerical grid, for each point a domain of influence and a domain of dependence for a certain numerical scheme may be drawn. The Courant-Friedrichs-Lewy (CFL) condition says that the discrete solution must not be independent of data that determine the solution of the associated partial differential equation. Thus the physical domain of dependence as defined by the partial differential equation must be inside the numerical domain of dependence, figure 2.1. With  $1/c$  denoting the slope of the physical velocity in the  $x - t$  domain, this means

$$\frac{1}{c} \geq \frac{\Delta t}{\Delta x} \Rightarrow \mu = c \frac{\Delta t}{\Delta x} \leq 1 \quad (2.40)$$

which is the CFL condition for the first-order upwind scheme. It should be noted that the CFL criterium is a necessary, but not a sufficient stability condition.

## 2.3 Time differencing

There is a big variety of possible discretisations of the time derivative in partial differential equations. Thus, the temporal discretisation is here dealt with separately. For practical applications, there are of course a number of constraints to be obeyed.

- Higher order scheme are desirable, but they often require big storage (which may be a problem in three-dimensional models) or require a high number evaluation of complicated functions. Furthermore, spatial resolution is usually the reason for low accuracy of complex models (doubling the spatial resolution usually means the increase of grid points by a factor of 8 and the reduction of time step by a factor of 2, such that the extra costs are a factor of 16 !).

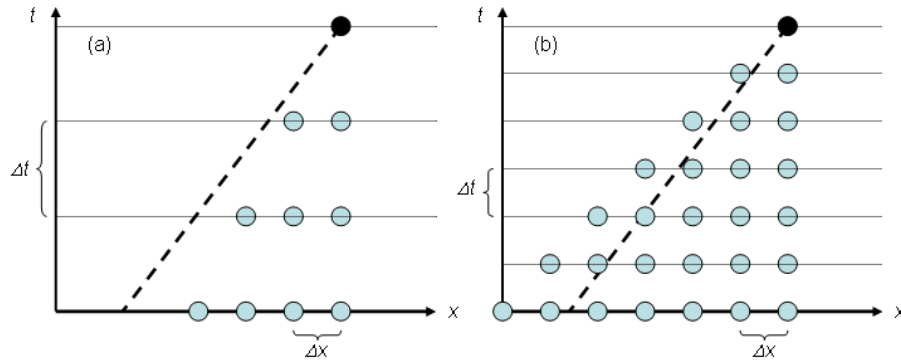


Figure 2.1: Graph showing the physical and numerical domains of dependence for the solution of an advection equation. In panel a, the physical domain of dependence is not covered by the numerical domain of dependence, and thus the numerical solution is unstable. In panel b, the time step is reduced such that now the physical domain of dependence fully lies within the numerical domain of dependence, such that the numerical solution is stable. The figure has been adapted from *Durran* [1999].

- Low order schemes are often known for strong damping or amplifying a numerical solution, which may be a significant problem in situations with low physical damping.
- Implicit time stepping schemes for three-dimensional models have the problem that huge systems of linear equations have to be solved.

It is thus a matter of compromise between accuracy and computational costs, which time stepping scheme to use.

Let us again consider the linear advection equation

$$\partial_t \psi + c \partial_x \psi = 0. \quad (2.41)$$

The representation of the function  $\psi$  as a Fourier series would be of the following form:

$$\psi(x, t) = \sum_{k=-\infty}^{\infty} b_k(t) \exp(ikx), \quad (2.42)$$

such that (2.41) is represented as

$$d_t b_k = -ikc b_k. \quad (2.43)$$

This equation will be used for examining amplitude and phase errors of temporal discretisation methods.

(2.43) represents an oscillation equation of which the most general form is

$$d_t\psi = i\kappa\psi, \quad (2.44)$$

the analytical solution of which is

$$\psi(t) = \psi_0 \exp(i\kappa t). \quad (2.45)$$

Integration of (2.44) over one time step yields thus

$$\psi(t_0 + \Delta t) = \psi(t_0) \exp(i\kappa\Delta t) = A_e\psi(t_0), \quad (2.46)$$

where  $A_e$  is an *exact amplification factor* which is a complex number with the absolute value 1. Thus, the solution  $\psi$  moves per time step a distance of  $\kappa\Delta t$  radians on a circle with constant amplitude.

Now, it is desirable that numerical solutions to (2.44) reproduce this behaviour of the solution to sufficient accuracy. Let us define a numerical complex amplification factor  $A$  as

$$\phi^{n+1} = A\phi^n. \quad (2.47)$$

When rewriting  $A$  as

$$A = |A| \exp(i\theta) \quad (2.48)$$

with

$$|A| = (\mathcal{R}(A)^2 + \mathcal{I}(A)^2)^{1/2}, \quad \theta = \arctan\left(\frac{\mathcal{I}(A)}{\mathcal{R}(A)}\right) \quad (2.49)$$

then it is clear that  $|A|$  is the amplitude error and  $R = \theta/(\kappa\Delta t)$  is the phase error of the numerical scheme.

For  $|A| > 1$ , the scheme would be amplifying, for  $|A| < 1$  damping and for  $|A| = 1$  neutral. For  $R > 1$ , the scheme would be accelerating, and for  $R < 1$ , it would be decelerating.

In the following, we will investigate several schemes for their amplitude and phase error.

### 2.3.1 One-stage two level schemes

A general ordinary differential equation may be written as

$$d_t\psi = F(\psi), \quad (2.50)$$

where  $\psi$  and  $F$  may be vectors. The general form of one-stage two level schemes is

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = (1 - \alpha)F(\phi^n) + \alpha F(\phi^{n+1}), \quad (2.51)$$

or, alternatively,

$$\phi^{n+1} = \phi^n + (1 - \alpha)\Delta t F(\phi^n) + \alpha\Delta t F(\phi^{n+1}), \quad (2.52)$$

For  $\alpha = 0$ , we obtain the Euler forward scheme, for  $\alpha = 1$  the Euler backward scheme and for  $\alpha = 0.5$  the trapezoidal scheme.

For  $F(\psi) = i\kappa\psi$ , the order of approximation of (2.51) is estimated as usual:

$$\begin{aligned} & \frac{\psi(t_0 + \Delta t) - \psi(t_0)}{\Delta t} - (1 - \alpha)i\kappa\psi(t_0) - \alpha i\kappa\psi(t_0 + \Delta t) \\ & - \psi'(t_0) + i\kappa\psi(t_0) \\ & = \frac{\Delta t}{2}i\kappa\psi'(1 - 2\alpha) + \mathcal{O}(\Delta t^2), \end{aligned} \quad (2.53)$$

where  $\psi'' = ik\psi'$  has been used. Thus, the scheme is of second order for  $\alpha = 0.5$  and of first order else.

Application of (2.52) to (2.44) results in

$$\phi^{n+1}(1 - \Delta t i \kappa \alpha) = \phi^n(1 + \Delta t i \kappa(1 - \alpha)), \quad (2.54)$$

such that the amplification factor is expressed as

$$A = \frac{\phi^{n+1}}{\phi^n} = \frac{1 + \Delta t i \kappa(1 - \alpha)}{1 - \Delta t i \kappa \alpha}, \quad (2.55)$$

which results in

$$\begin{aligned} |A|^2 &= \frac{1 + \Delta t^2 \kappa^2(1 - \alpha)^2}{1 + \Delta t^2 \kappa^2 \alpha^2} \\ &= 1 + (1 - 2\alpha) \frac{\Delta t^2 \kappa^2}{1 + \Delta t^2 \kappa^2 \alpha^2}. \end{aligned} \quad (2.56)$$

Thus, the Euler forward scheme is amplifying, the Euler backward scheme is damping and the trapezoidal method is neutral. Although the Euler forward scheme is amplifying, we have for  $\Delta t \leq 1$

$$|A|_{\alpha=0} = (1 + \kappa^2 \Delta t^2)^{1/2} \leq 1 + \kappa^2 \Delta t^2 \leq 1 + \kappa^2 \Delta t, \quad (2.57)$$

such that the von Neumann stability criterium is fulfilled and the scheme is stable.

With (2.48), the phase error may be estimated. When  $\bar{A}$  denotes the conjugate complex of  $A$ , then  $\mathcal{R}(A) = 0.5(A + \bar{A})$  and  $\mathcal{I}(A) = -0.5i(A - \bar{A})$ . With this, the phase error of (2.51) is

$$R = \frac{1}{\kappa \Delta t} \arctan \left( \frac{\kappa \Delta t}{1 - \alpha(1 - \alpha)\kappa^2 \Delta t^2} \right), \quad (2.58)$$

such that for the Euler forward and the Euler backward we have

$$R_{forward} = R_{backward} = \frac{\arctan \kappa \Delta t}{\kappa \Delta t}. \quad (2.59)$$

By expressing the arctan-function with its Taylor series,

$$\arctan x = x - \frac{x^3}{3} + \frac{x^5}{5} + \dots, \quad (2.60)$$

it is clear that  $0 < R_{forward} = R_{backward} < 1$ , such that the schemes are both decelerating. With (2.60), the approximate error is

$$R_{forward} = R_{backward} \approx 1 - \frac{(\Delta t \kappa)^2}{3}, \quad (2.61)$$

such that the phase error is  $\mathcal{O}(\Delta t^2)$ .

For the trapezoidal scheme, the exact phase error is

$$R_{\alpha=0.5} = \frac{1}{\kappa \Delta t} \arctan \left( \frac{\kappa \Delta t}{1 - 0.25 \kappa^2 \Delta t^2} \right), \quad (2.62)$$

which is approximated for small  $\kappa \Delta t$  by mean of the Taylor series (2.60) and

$$1/(1-x) = (1+x)/(1-x^2) \approx 1+x \quad (2.63)$$

as

$$R_{\alpha=0.5} \approx \frac{1}{\kappa \Delta t} \arctan \left( \kappa \Delta t \left( 1 + \frac{\kappa^2 \Delta t^2}{4} \right) \right) \approx 1 - \frac{\kappa^2 \Delta t^2}{12}. \quad (2.64)$$

### 2.3.2 Multi-stage two level schemes

In contrast to the one-stage schemes, the multi-stage schemes compute one or more intermediate results which are used for increasing the order of approximation. As an example, two-stages two level schemes are generally of the following form:

$$\begin{aligned} \tilde{\phi}^{n+\alpha} &= \phi^n + \alpha \Delta t F(\phi^n), \\ \phi^{n+1} &= \phi^n + \beta \Delta t F(\tilde{\phi}^{n+\alpha}) + (1-\beta) \Delta t F(\phi^n), \end{aligned} \quad (2.65)$$

with the free parameters  $\alpha$  and  $\beta$ , and the intermediate solution  $\tilde{\phi}^{n+\alpha}$ .

Application of (2.65) to the oscillation equation (2.44) results in

$$\phi^{i+1} = \phi \{1 - \alpha \beta \kappa^2 \Delta t^2 + i \kappa \Delta t\}, \quad (2.66)$$

such that the amplification factor is

$$1 - \alpha \beta (\kappa \Delta t)^2 + i \kappa \Delta t, \quad (2.67)$$

which results into

$$|A|^2 = 1 + (1 - 2\alpha\beta)(\kappa\Delta t)^2 + \alpha^2\beta^2(\kappa\Delta t)^4. \quad (2.68)$$

With this it is clear, that high-order two-stage two level schemes are obtained by setting

$$\alpha\beta = \frac{1}{2}. \quad (2.69)$$

The class of schemes fulfilling (2.69) is called the class of Runge-Kutta schemes, examples of which are the Heun scheme ( $\alpha = 1, \beta = \frac{1}{2}$ ) and the midpoint method ( $\alpha = \frac{1}{2}, \beta = 1$ ).

It is clear from (2.68) that all Runge-Kutta schemes are unstable ( $|A|^2 > 1$ ), but since the order is high, this is often acceptable for simulations of short duration.

To cure this problem, often a non-Runge-Kutta is used with  $\alpha = 1$  and  $\beta = 1$  (Matsuno scheme), for which the stability criterium may be derived from (2.68) as

$$|A|^2 = 1 - (\kappa\Delta t)^2 + (\kappa\Delta t)^4. \quad (2.70)$$

Thus, the Matsuno scheme is stable for  $0 \leq \kappa\Delta t \leq 1$ .

The relative phase change for the two-stage two level schemes is

$$R = \frac{1}{\kappa\Delta t} \arctan \left( \frac{\kappa\Delta t}{1 - \alpha\beta(\kappa\Delta t)^2} \right), \quad (2.71)$$

such that for the Runge-Kutta schemes we obtain

$$R_{RK2} \approx 1 + \frac{1}{6}(\kappa\Delta t)^2, \quad (2.72)$$

and for the Matsuno scheme

$$R_{Mat} \approx 1 + \frac{2}{3}(\kappa\Delta t)^2. \quad (2.73)$$

### 2.3.3 Three level schemes

A further increase in temporal resolution may be obtained by three-level schemes, for which numerical solutions on three time levels have to be stored. The explicit form of such schemes is given as:

$$\phi^{n+1} = \alpha_1\phi^n + \alpha_2\phi^{n-1} + \beta_1\Delta t F(\phi^n) + \beta_2\Delta t F(\phi^{n-1}), \quad (2.74)$$

with constant coefficients  $\alpha_1, \alpha_2, \beta_1$  and  $\beta_2$ . A check for conditions for second-order accuracy results in

$$\alpha_1 = 1 - \alpha_2, \quad \beta_1 = \frac{1}{2}(\alpha_2 + 3), \quad \beta_2 = \frac{1}{2}(\alpha_2 - 1), \quad (2.75)$$

with a free choice for  $\alpha_2$ . Significant simplifications of (2.74) are obtained by the following two choices: Leap-frog scheme for  $\alpha_2 = 1$ , such that  $\alpha_1 = 0, \beta_1 = 2$  and  $\beta_2 = 0$ ,

$$\frac{\phi^{n+1} - \phi^{n-1}}{2\Delta t} = F(\phi^n), \quad (2.76)$$

and the Adams-Bashforth scheme for  $\alpha_2 = 0$ , such that  $\alpha_1 = 1, \beta_1 = 1.5$  and  $\beta_2 = -0.5$ ,

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \frac{3}{2}F(\phi^n) - \frac{1}{2}F(\phi^{n-1}). \quad (2.77)$$

Application of the leap-frog scheme into the oscillation equation (2.44) leads to

$$\phi^{n+1} = \phi^{n-1} + 2i\kappa\Delta t\phi^n. \quad (2.78)$$

Considering the constant amplification factor  $A$  with  $\phi^n = A\phi^{n-1}$  and  $\phi^{n+1} = A^2\phi^{n-1}$ , we obtain the following quadratic equation for  $A$ :

$$A^2 - 2i\kappa\Delta t A - 1 = 0, \quad (2.79)$$

with the solutions

$$A_{\pm} = i\kappa\Delta t \pm \sqrt{1 - \kappa^2\Delta t^2}. \quad (2.80)$$

For well-resolved wave numbers with  $\kappa\Delta t \rightarrow 0$ , we obtain  $A_+ \rightarrow 1$  and  $A_- \rightarrow -1$ , with  $A_+$  denoting the *physical mode* and  $A_-$  denoting the *computational mode*, representing an artificial numerical oscillation. For  $|\kappa\Delta t| \leq 1$ , we obtain  $|A_+| = |A_-| = 1$ , such that both modes are stable. However, for  $\kappa\Delta t > 1$ , we obtain

$$|A_+^2| = \left| i \left( \kappa\Delta t + \sqrt{\kappa^2\Delta t^2 - 1} \right) \right| = \kappa\Delta t + \sqrt{\kappa^2\Delta t^2 - 1} > \kappa\Delta t > 1, \quad (2.81)$$

such that the physical mode is unstable. For high resolution, the relative phase error of the physical mode can be approximated by

$$R_+ \approx 1 + \frac{(\kappa\Delta t)^2}{6}, \quad (2.82)$$

which means that the leapfrog scheme is accelerating. The disadvantage of the leapfrog scheme is the undamped computational mode, which is typically avoided by some filtering techniques. Another method is to use the Adams-Bashforth scheme (2.77) instead, for which the amplification factor can be approximated by

$$|A_+| \approx 1 + \frac{1}{4}(\kappa\Delta t)^4, \quad |A_-| \approx \frac{1}{2}\kappa\Delta t, \quad (2.83)$$

i.e., the physical mode is amplifying and the computational mode is strongly damped and the relative phase error of the physical mode as

$$R_+ \approx 1 + \frac{5}{12}(\kappa\Delta t). \quad (2.84)$$