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Sheet 7
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Scientific Computing

Ordinary Differential Equations: Numerical Methods

Exercise 15: Particle Simulation

Consider a spherical particle which carries a constant electric charge $q > 0$ and is suspended in water. The particle shall move at a velocity $v(t) \in \mathbb{R}^3$. The force $F \in \mathbb{R}^3$ acting on the particle due to an external electric field $E(t) \in \mathbb{R}^3$ and a magnetic field $B(t) \in \mathbb{R}^3$ is given by the *Lorentz force*:

$$F_{lorentz}(t) := q(E(t) + v(t) \times B(t)) \tag{1}$$

with the operator $\times$ defined as the cross-product

$$a \times b := \begin{pmatrix} a_2 b_3 - a_3 b_2 \\ a_3 b_1 - a_1 b_3 \\ a_1 b_2 - a_2 b_1 \end{pmatrix} \tag{2}$$

for vectors $a, b \in \mathbb{R}^3$. Due to the viscous resistance of the fluid, the drag force acts onto the particle as well:

$$F_{drag}(t) := -6\pi\eta r v(t) \tag{3}$$

where $\eta > 0$ is the fluid viscosity and $r > 0$ the radius of the particle. A system of ordinary differential equations evolves for the particle velocity $v(t)$ as follows:

$$\frac{dv}{dt} = \frac{1}{m}\left(F_{lorentz} + F_{drag}\right) \tag{4}$$

where m denotes the mass of the particle.

(a) Write down the specific differential equation for a magnetic field $B(t) := (0, 0, 2t)^\top$, an electric field $E(t) := (1, 0, 0)^\top$, a mass, viscosity and electric charge $q = m = \eta = 1$ as well as a radius $r = \frac{1}{6\pi}$. You may further assume that the particle is initially at rest, i.e. $v(t = 0) = \vec{0}$.

(b) Formulate the explicit Euler method for the equations derived in (a) and solve the first three time steps "by hand" using a time step $\tau = \frac{1}{2}$.

(c) Write a maple sheet to study the influence of the time step τ on your solution. Simplify the magnetic field to $B(t) := (0, 0, 1)^\top$, solve the ODE system from (a) analytically and compute the error

$$e(t) := \sqrt{(v_x^{analytic}(t) - v_x^{euler}(t))^2 + (v_y^{analytic}(t) - v_y^{euler}(t))^2}$$

for $\tau = 2^{-n}$, $n \geq 1$; here $v_x^{euler}(t), v_y^{euler}(t)$ denote your explicit Euler solutions. Consider the time interval $t \in [0, 10]$ in your studies. What do you observe?

(d) Formulate the second-order Adams-Moulton method for the equations derived in (a) and solve the first time step for $\tau = \frac{1}{2}$.

Solution:

(a) We can first write down the differential equation for the particle velocity for every velocity component:

$$\begin{aligned}
\frac{dv_x(t)}{dt} &= \frac{1}{m}\Big(q(E_x(t) + v_y(t)B_z(t) - v_z(t)B_y(t)) - 6\pi\eta r v_x(t)\Big) \\
\frac{dv_y(t)}{dt} &= \frac{1}{m}\Big(q(E_y(t) + v_z(t)B_x(t) - v_x(t)B_z(t)) - 6\pi\eta r v_y(t)\Big) \\
\frac{dv_z(t)}{dt} &= \frac{1}{m}\Big(q(E_z(t) + v_x(t)B_y(t) - v_y(t)B_x(t)) - 6\pi\eta r v_z(t)\Big)
\end{aligned} \tag{5}$$

Inserting all quantities according to the description of this exercise, the system reduces to:

$$\begin{aligned}
\frac{dv_x(t)}{dt} &= -v_x(t) + 2t \cdot v_y(t) + 1 \\
\frac{dv_y(t)}{dt} &= -2t \cdot v_x(t) - v_y(t) \\
\frac{dv_z(t)}{dt} &= -v_z(t)
\end{aligned} \tag{6}$$

Since the particle has zero velocity at the beginning, the third velocity component will always remain zero. Hence, it is enough to consider the two-dimensional system

$$\begin{aligned}
\frac{dv_x(t)}{dt} &= -v_x(t) + 2t \cdot v_y(t) + 1 \\
\frac{dv_y(t)}{dt} &= -2t \cdot v_x(t) - v_y(t)
\end{aligned} \tag{7}$$

from now.

(b) The explicit Euler method for the equations (7) is given by:

$$\begin{aligned}
\frac{v_x(t+\tau) - v_x(t)}{\tau} &= -v_x(t) + 2t \cdot v_y(t) + 1 \\
\frac{v_y(t+\tau) - v_y(t)}{\tau} &= -2t \cdot v_x(t) - v_y(t)
\end{aligned} \tag{8}$$

This results in the update rule:

$$\begin{aligned}
v_x(t+\tau) &= (1-\tau)v_x(t) + 2\tau t v_y(t) + \tau \\
v_y(t+\tau) &= (1-\tau)v_y(t) - 2\tau t v_x(t)
\end{aligned} \tag{9}$$

For $\tau = \frac{1}{2}$, we obtain:

$$\begin{aligned} v_x(t+\tfrac{1}{2}) &= \tfrac{1}{2}v_x(t) + tv_y(t) + \tfrac{1}{2} \\ v_y(t+\tfrac{1}{2}) &= \tfrac{1}{2}v_y(t) - tv_x(t) \end{aligned} \tag{10}$$

Starting with $v_x(t=0) = 0, v_y(t=0) = 0$, we finally obtain:

$$\begin{aligned} v_x(\tfrac{1}{2}) &= \tfrac{1}{2}, & v_y(\tfrac{1}{2}) &= 0 \\ v_x(1) &= \tfrac{3}{4}, & v_y(1) &= -\tfrac{1}{4} \\ v_x(\tfrac{3}{2}) &= \tfrac{5}{8}, & v_y(\tfrac{3}{2}) &= -\tfrac{7}{8} \end{aligned} \tag{11}$$

(c) See ws7_15c.mw. Halvening the time step yields a reduction of the error by a factor of two. For our problem, the explicit Euler method hence shows an error of order $O(\tau)$.

(d) The Adams-Moulton method is given by the following update rule:

$$y(t+\tau) = y(t) + \frac{\tau}{2}(f(t, y(t)), f(t+\tau, y(t+\tau))) \tag{12}$$

Applying this discretisation scheme to Eq. (7) results in

$$\begin{aligned} v_x(t+\tau) &= v_x(t) + \frac{\tau}{2}\left(-v_x(t) + 2tv_y(t) + 1 - v_x(t+\tau) + 2(t+\tau)v_y(t+\tau) + 1\right) \\ v_y(t+\tau) &= v_y(t) + \frac{\tau}{2}\left(-2tv_x(t) - v_y(t) - 2(t+\tau)v_x(t+\tau) - v_y(t+\tau)\right) \end{aligned} \tag{13}$$

or in matrix-vector form:

$$\begin{pmatrix} 1+\frac{\tau}{2} & -\tau(t+\tau) \\ \tau(t+\tau) & 1+\frac{\tau}{2} \end{pmatrix} \begin{pmatrix} v_x(t+\tau) \\ v_y(t+\tau) \end{pmatrix} = \begin{pmatrix} \left(1-\frac{\tau}{2}\right)v_x(t) + \tau t v_y(t) + \tau \\ -\tau t v_x(t) + \left(1-\frac{\tau}{2}\right)v_y(t) \end{pmatrix} \tag{14}$$

Due to the implicit nature of the Adams-Moulton method, we need to solve this linear system of equations in each time step. For the first time step, we can insert $\tau = \frac{1}{2}$, $t = 0$ and $v_x(t=0) = v_y(t=0) = 0$ into Eq. (14):

$$\begin{pmatrix} \frac{5}{4} & -\frac{1}{4} \\ \frac{1}{4} & \frac{5}{4} \end{pmatrix} \begin{pmatrix} v_x(\frac{1}{2}) \\ v_y(\frac{1}{2}) \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix} \tag{15}$$

Solving this system of equations yields $v_x(\frac{1}{2}) = \frac{5}{13}$, $v_y(\frac{1}{2}) = -\frac{1}{13}$.
Remark: The second-order Adams-Moulton method is just the trapezoidal rule from the last exercise. In terms of solving partial differential equations, the arising time stepping method is also known as *Crank-Nicolson scheme*.

Exercise 16: Runge-Kutta Methods and Direction Fields

Consider the direction field of a one-dimensional ODE $\frac{dp}{dt} = f(t, p(t))$ as given in Fig. 1. To compute approximate solutions $p_n \approx p(t_n)$ at times $t_n = n \cdot \tau$, the following second-order Runge-Kutta scheme is given to compute the population size p_{n+1} of the next time step:

$$\begin{aligned} \widehat{p}_{n+1} &= p_n + \tau f(t_n, p_n) \\ p_{n+1} &= \frac{1}{2}\left(p_n + \tau f(t_{n+1}, \widehat{p}_{n+1}) + \widehat{p}_{n+1}\right) \end{aligned} \tag{16}$$

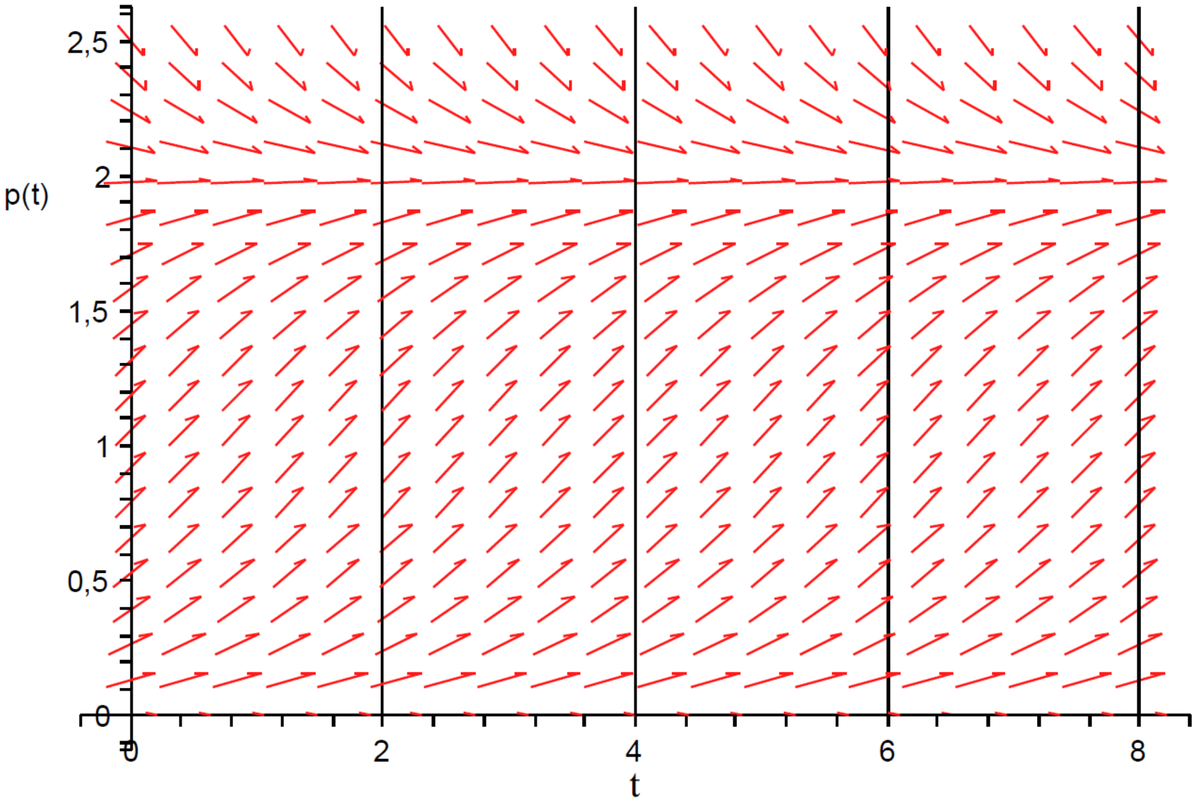

Figure 1: Direction field for exercise 16a.

(a) With initial condition $p_0 = p(0) = 0.125$, perform the first four steps of this scheme (to compute p_1, p_2, p_3, p_4) by drawing the approximate solutions into the direction field in Fig. 1 (graphical solution only).
The stepsize shall be $\tau = 2$, as illustrated by the four intervals drawn into the direction field. Mark from which arrows you obtain the directions of the numerical steps—you are allowed to add an arrow to the direction field, if no arrow is plotted at the precise required position.

(b) Consider the direction field in Fig. 2. Perform the first three steps of the explicit Euler scheme by drawing the approximate solution in this direction field. Start at $y(t = 0) = -1$ and use a time step $\tau = 3$. What do you observe? What happens for $\tau = 2$ and $\tau = 1.5$?

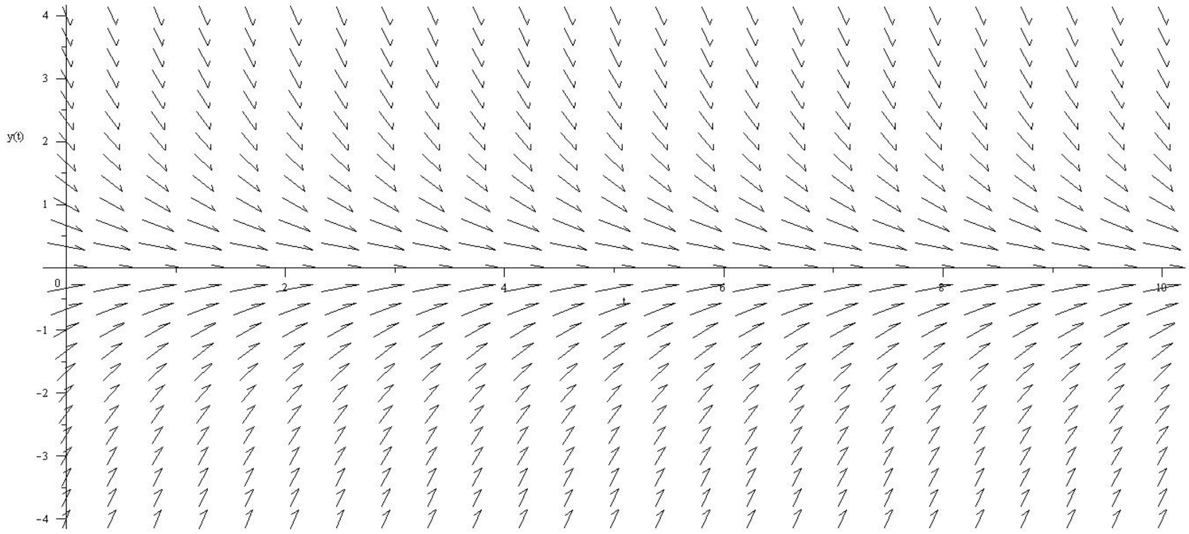

Figure 2: Direction field for exercise 16b.

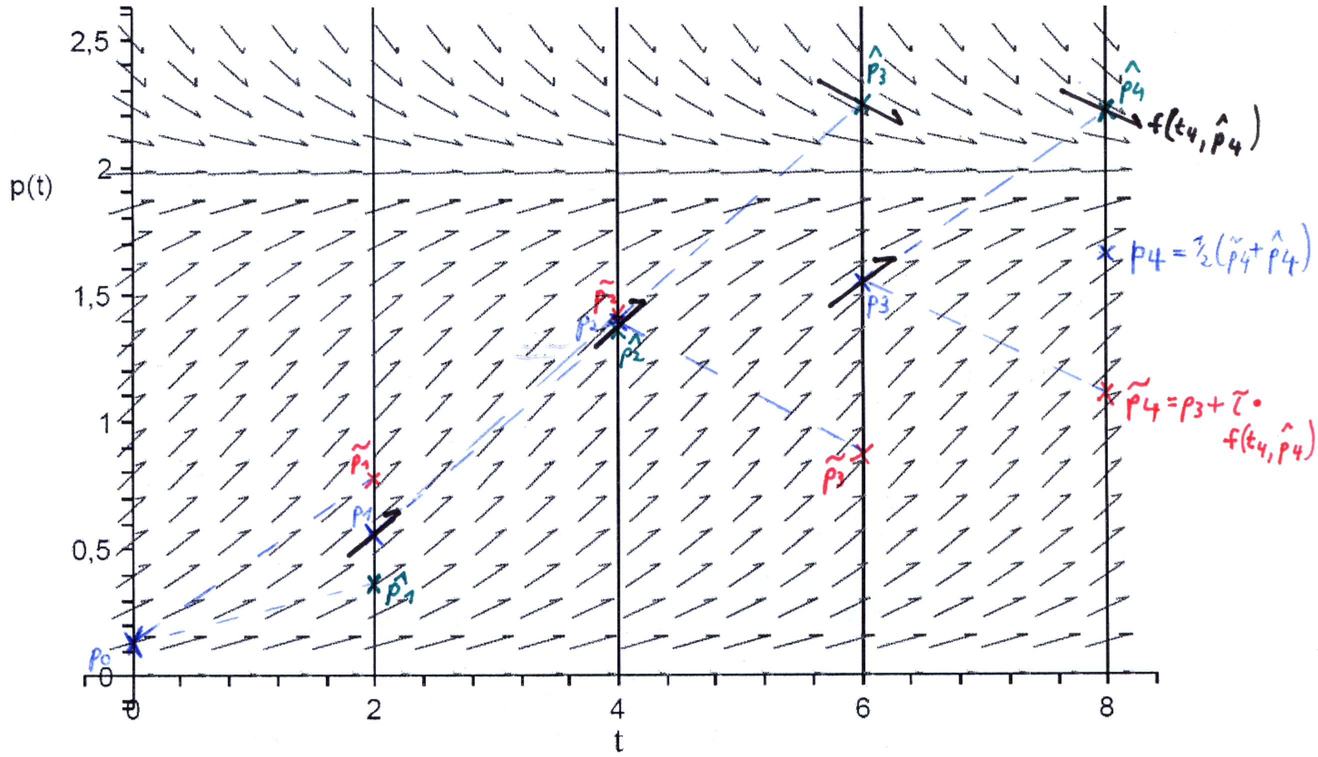

Figure 3: Solution to exercise 16a.

Solution:

(a) The drawing is shown in Fig. 3. We further introduce a point $\tilde{p}_{n+1} := p_n + \tau f(t_{n+1}, \widehat{p}_{n+1})$.

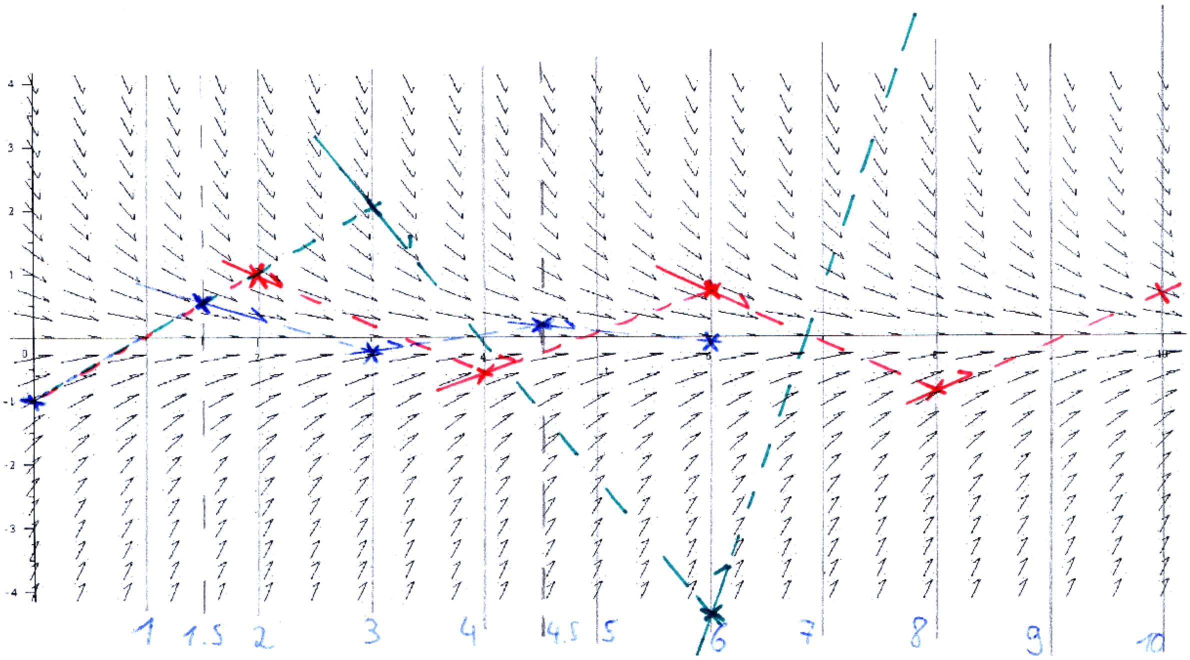

Figure 4: Solution to exercise 16b.

Using this new point, we can write the update rule as:

$$\begin{aligned} \widehat{p}_{n+1} &= p_n + \tau f(t_n, p_n) \\ \tilde{p}_{n+1} &= p_n + \tau f(t_{n+1}, \widehat{p}_{n+1}) \\ p_{n+1} &= \tfrac{1}{2}\left(\tilde{p}_{n+1} + \widehat{p}_{n+1}\right) \end{aligned} \tag{17}$$

From this, we can understand how the drawing works:

1. Determine the gradient at the point $(t_n, p_n(t_n))$; for $t_0 = 0$, this point is given by $(0, 0.125)$. The gradient is given by the respective vector in the plot. If there's no arrow, you need to draw it yourself considering the neighbourhood of the respective point.
2. Walk along this vector until you reach the time $t_{n+1} = t_n + \tau$. The point at this position corresponds to $(t_{n+1}, \widehat{p}_{n+1} = p_n + \tau f(t_n, p_n))$.
3. In order to determine $\tilde{p}_{n+1}$, we need the gradient at $(t_{n+1}, \widehat{p}_{n+1})$. This gradient corresponds to the vector of the direction field at the position $(t_{n+1}, \widehat{p}_{n+1})$. We draw a straight line parallel to this vector through p_n. The point of this straight line at $t_{n+1} = t_n + \tau$ corresponds to $\tilde{p}_{n+1}$.
4. Finally, we obtain p_{n+1} from averaging the values $\tilde{p}_{n+1}$ and $\widehat{p}_{n+1}$.

(b) The explicit Euler method corresponds to the very first step of the Runge-Kutta method from (a), i.e. $\widehat{p}_{n+1}$ corresponds to the explicit Euler solution. You can hence just carry out steps 1 and 2 from (a) and use $p_{n+1} = \widehat{p}_{n+1}$. The solutions are sketched in Fig. 4. The blue crosses correspond to the time step $\tau = 1.5$, the red crosses represent the explicit

Euler method for $\tau = 2$ and the green crosses illustrate the behaviour of the explicit Euler method for $\tau = 3$. We can observe that

- the method is unstable for $\tau = 3$. In this case, we diverge from the critical point with each time step in an oscillatory manner.
- the method is close to the stability regime for $\tau = 2$. The solution oscillates around the critical point. It neither converges nor diverges further away from the solution.
- the method is stable and converges towards the critical point for $\tau = 1.5$. The numerical solution oscillates around the critical point. However, the amplitude of the oscillations is reduced with each time step.

Remark: The vector field that was used corresponds to the ODE $\frac{dy}{dt} = -y$. The explicit Euler method reads $y_{n+1} = y_n + \tau(-y_n) = (1-\tau)y_n$ in this case. Since $1-\tau$ represents the eigenvalue of this iterative scheme, we observe for $\tau > 0$:

$$\begin{array}{lll} y_n \stackrel{n\to\infty}{\longrightarrow} 0 & \text{for} & \|1-\tau\| < 1 \Leftrightarrow \tau \in (0,2) \\ y_n \stackrel{n\to\infty}{\longrightarrow} \pm\infty & \text{for} & \|1-\tau\| > 1 \Leftrightarrow \tau \in (2,\infty) \\ y_n \stackrel{n\to\infty}{\longrightarrow} \pm y_0 & \text{for} & \|1-\tau\| = 1 \Leftrightarrow \tau = 2 \end{array} \tag{18}$$