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# Worksheet 7
# Problems

## Ordinary Differential Equations: Numerical Methods

### (H) Exercise 1: Charged 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 $\times$ is defined as the cross-product

$$a \times b := \begin{pmatrix} a_2b_3 - a_3b_2 \\ a_3b_1 - a_1b_3 \\ a_1b_2 - a_2b_1 \end{pmatrix} \tag{2}$$

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 python script to study the influence of the time step $\tau$ 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 $\tau = \frac{1}{2}$.

## (I) Exercise 2: 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 Figure 1.

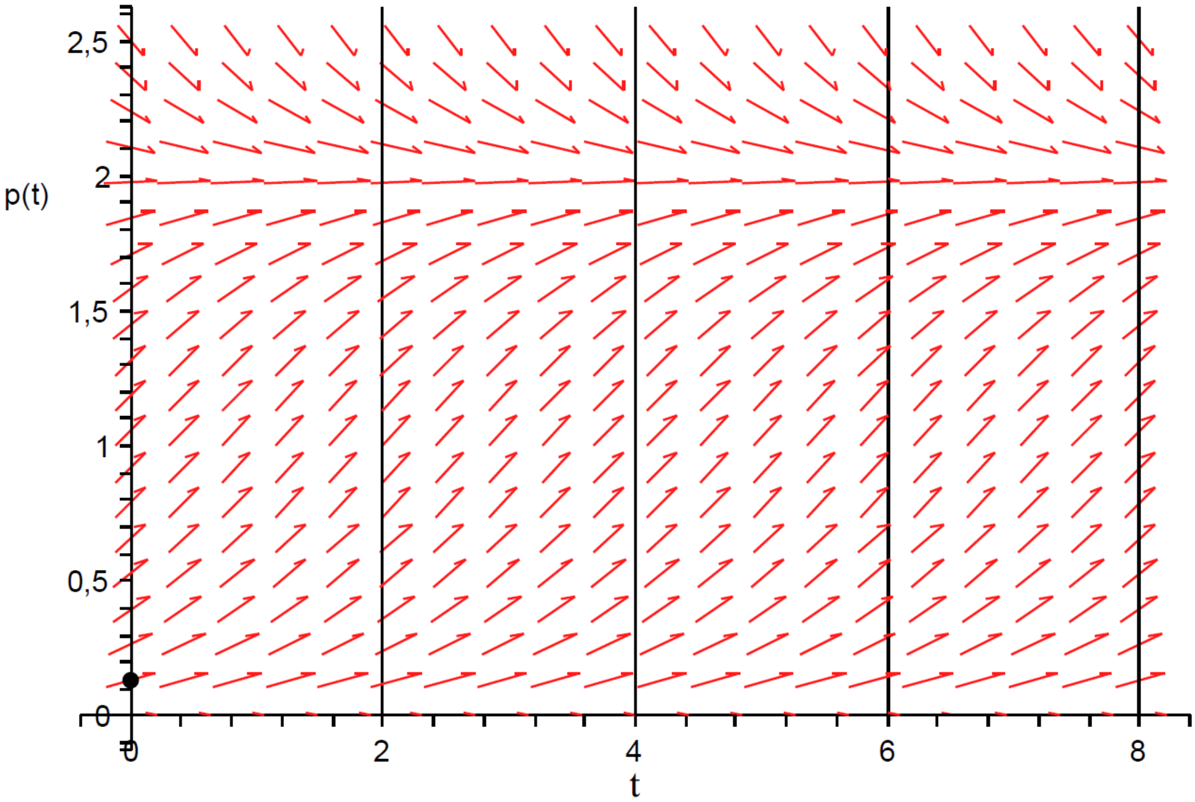


Figure 1: Direction field for Exercise 2 task (a), the initial value $p_0 = 0.125$ is marked by a point.

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:

$$\begin{aligned} \widehat{p}_{n+1} &= p_n + \tau f(t_n, p_n) \\ p_{n+1} &= \tfrac{1}{2}\left(p_n + \tau f(t_{n+1}, \widehat{p}_{n+1}) + \widehat{p}_{n+1}\right) \end{aligned} \tag{5}$$

(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 Figure 1 (graphical solution only).

The step size 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 Figure 2. Perform the first three steps of the explicit Euler

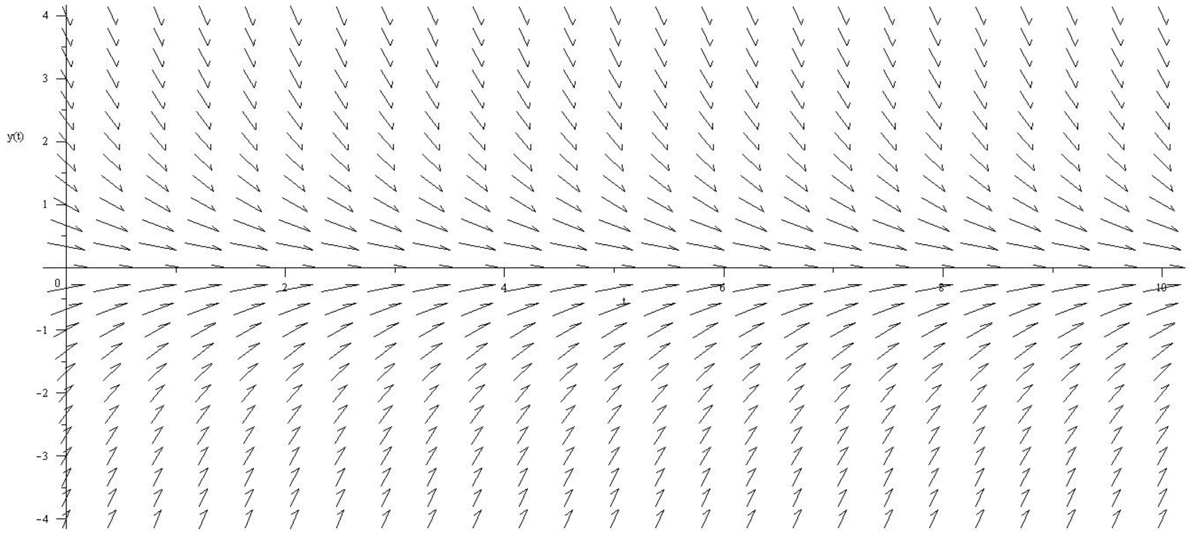


Figure 2: Direction field for Exercise 2 task (b).

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 $\tau = 1.5$?

## (I) Exercise 3: One-step and Multistep Numerical Methods

Consider the direction field of a one-dimensional differential equation $\mathrm{d}p/\,\mathrm{d}t = f(t, p)$, where $f(t, p) = (1 - p(t))/2$ (Verhust model - saturation), as given in Figure 3.

(a) To compute approximate solutions $p_n \approx p(t_n)$ at times $t_n = n\tau$, the following multistep numerical scheme is given:

$$p_0 = p(0) = 1/2 \qquad \text{(initial condition)} \tag{6}$$

$$p_1 = p_0 + \tau f(t_0, p_0) \tag{7}$$

$$p_{n+2} = 5p_n - 4p_{n+1} + \tau(2f(t_n, p_n) + 4f(t_{n+1}, p_{n+1})) \tag{8}$$

Compute the first four steps of this scheme ($p_1, p_2, p_3, p_4$) with time step size $\tau = 1$, and draw the numerical solution (points connected by lines) on Figure 3. If a point is outside the plot domain, you do not have to visualize it.

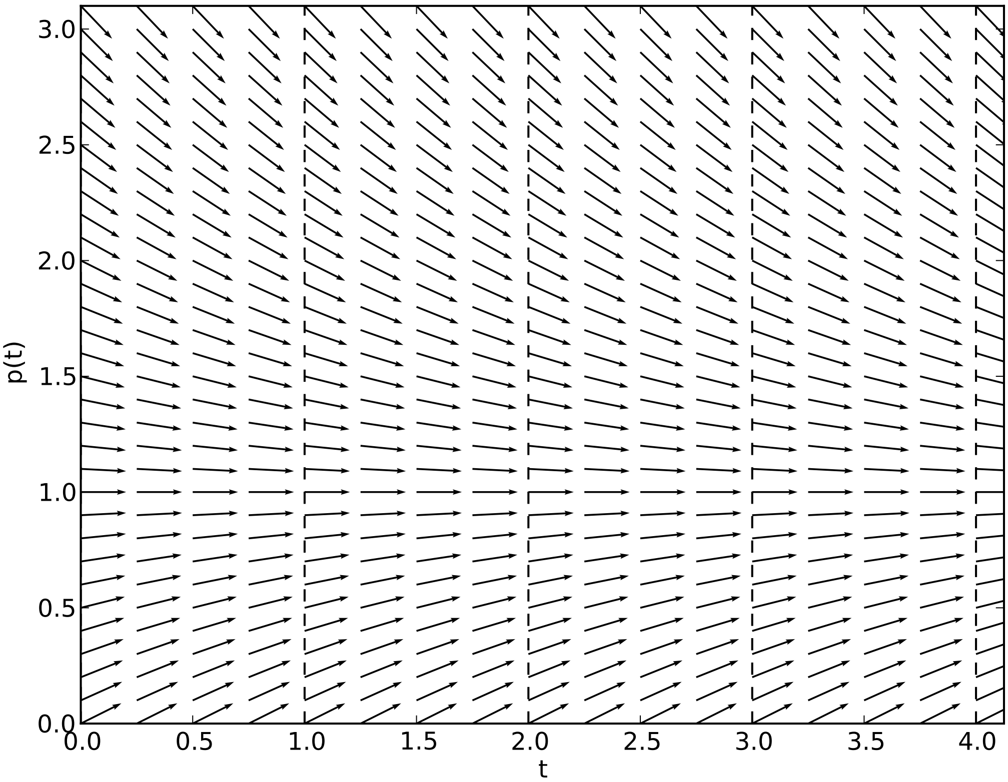


Figure 3: Direction field for $\mathrm{d}p/\,\mathrm{d}t = (1 - p(t))/2$.

(b) Consider the one-step Midpoint method:

$$p_0 = p(0) = 3.0 \qquad \text{(initial condition)} \tag{9}$$

$$p_{n+1} = p_n + \tau f\left(t_n + \frac{1}{2}\tau, p_n + \frac{\tau}{2} f(t_n, p_n)\right). \tag{10}$$

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 Figure 3 (graphical solution only). The step size shall be $\tau = 1$, 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.

(c) What can you conclude about the numerical stability of the methods from a) and b) for $\tau = 1$?

(d) List two advantages and two disadvantages of multistep methods in comparison to one-step methods.

### (H*) Exercise 4: Particle in Rotating Tube

A small spherical particle is located in a very long rotating tube full of liquid, which does not move relative to the tubes walls.

We are interested in the particle motion along the tube axis $x$, see Figure 4. Therefore, the

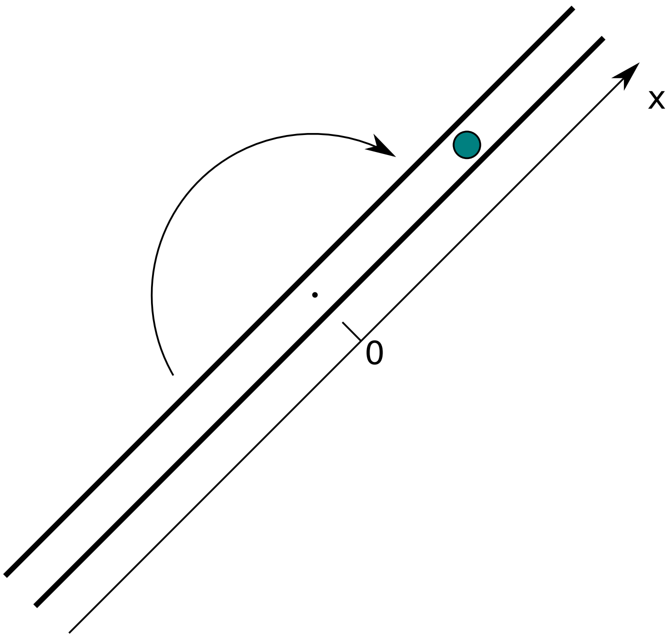


Figure 4: A rotating tube with liquid and particle inside.

rotating reference frame is used to derive the equation of the particle motion. In this reference frame, we consider two dominating forces acting on the particle along $x$ axis: the Stokes drag force and the buoyancy type force.

The model is approximated by the following ODE

$$\frac{d^2x}{dt^2} = (1-\gamma)\,x - \lambda\frac{dx}{dt}, \tag{11}$$

where $\gamma = \rho_l/\rho_p > 0$ is the ratio of densities ($\rho_l$, $\rho_p$ – liquid and particle densities) and $\lambda \geq 0$ is the friction coefficient.

(a) Transform the second order ODE (11) into a system of first-order ODEs.

(b) The matrix-vector form of the linear system of ODEs is given by

$$\frac{d\mathbf{y}}{dt} = \begin{pmatrix} 0 & 1 \\ 1-\gamma & -\lambda \end{pmatrix} \mathbf{y}. \tag{12}$$

Find the critical point of the system.

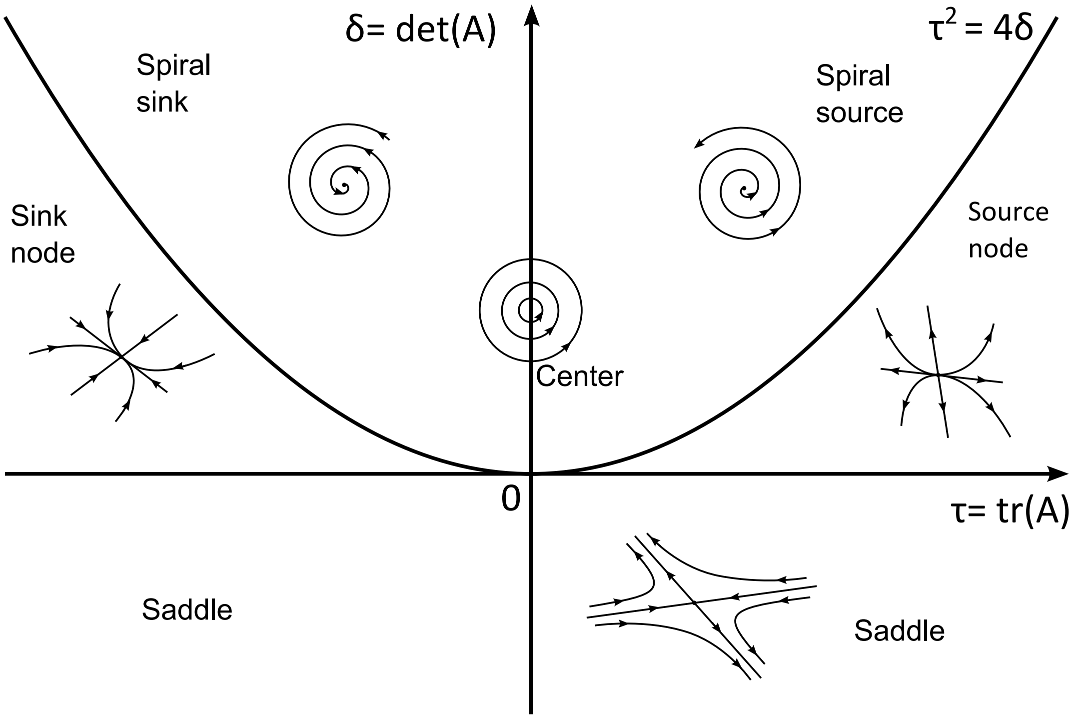


Figure 5: Type and stability of a critical point in two dimensions.

(c) Study how the type of the fixed point depends on $\gamma$, when $\lambda = 1$. Name all possible types of critical points and $\gamma$ ranges at which these types occur. For the critical point classification you may use Figure 5.

(d) Sketch the direction field of the system of ODEs with fixed $\gamma = 1/4$ and $\lambda = 1$. Use eigenvalues and eigenvectors to determine the direction field.

## (H*) Exercise 5: Indoor Air Quality Modeling

The quality of indoor air can be characterized by the concentration of volatile organic compounds (VOCs). The sources of VOCs may be located outdoors or within a building.

In the simplest indoor air quality model, the concentration of VOC is described by two differential equations:

$$\begin{aligned} V\frac{\partial x}{\partial t} &= Qc_{in} - Qx - k_a A x + k_d A y + q, \\ \frac{\partial y}{\partial t} &= k_a x - k_d y, \end{aligned} \tag{13}$$

where the following notations are used:

| | |
|---|---|
| $x$ | VOC concentration within the room, |
| $c_{in} = 1$ | VOC inflow concentration, |
| $V = 64$ | volume of the room, |
| $Q = 192$ | air inflow and outflow, |
| $q = 192$ | rate of VOC sources inside the room, |
| $A = 32$ | area of reacting surface, |
| $k_a = 4, k_d = 2$ | ad- and desorption coefficients, |
| $y$ | adsorbed concentration of VOC on area $A$. |

(a) Use the parameter values from the table above and write the final set of equations for unknowns $x$ and $y$ in the matrix-vector form $\partial \mathbf{c}/\partial t = A \cdot \mathbf{c} + \mathbf{b}$, where $\mathbf{c} = [x, \quad y]^T$.

(b) Compute the critical points, and the eigenvalues and eigenvectors of the matrix $A \in \mathbb{R}^{2\times 2}$ of the system $\partial \mathbf{c}/\partial t = A \cdot \mathbf{c} + \mathbf{b}$. Use the eigenvectors and eigenvalues of matrix $A$ to sketch the $x, y$ direction field.

(c) In case the inflow air is clean from VOCs ($c_{in} = 0$) and there are no VOC sources inside the room ($q = 0$), formulate the Implicit Euler method for the corresponding ODE from task (a) using a time step size $\tau$. Compute the explicit form of the resulting update scheme for $x(t + \tau), y(t + \tau)$.

Hint: you may use the following formula to invert $2 \times 2$ matrices:

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} \tag{14}$$