260069-1 PHF Computational Physics Exercises 3

We are going to study the following chemical reaction

$$A \xrightarrow{k_1} B$$

$$B \xrightarrow{k_2} C$$

where A, B and C are the concentrations of three substances and  $k_1$ ,  $k_2$  are the reaction rates.

The initial concentrations  $A(t_0)$ ,  $B(t_0)$ ,  $C(t_0)$  should be 1.0, 0.0, 0.0, respectively. In the following we will investigate four different cases  $k_2 = 1, 10, 100, 1000$ , with  $k_1 = 1$  in all cases. The first 10s of the reaction dynamics should be calculated using different numerical methods. The following questions should be answered:

- the corresponding (linear) system of first order ODEs needs to be determined:  $\dot{x} = f(x, t)$
- implement the following numerical methods and compare the performance and stability: explicit Euler, Heun, (implicit Euler)
- compare with the analytical solution (or with the timeintegrators provided by scipy.integrate)

- What are the maximum step-sizes that lead to stable results? Calculate the eigenvalues of the Jacobian matrix  $J = \frac{\partial f}{\partial x}$  and compare the stability behaviour with the theoretical predictions (optional)
- visualize the stable solution



