3. Exercise for the lecture "numerical fluid dynamics" SoSe 18

We noticed that the pace of the exercise sheets is a bit too high especially for programming beginners. If needed we will leave out a few sheets along the way. It is important that you work on the exercises carefully especially recurring ones like the harmonic oscillator. You do not have to solve every sheet in the week it is released! Please tell the Professor or the Tutor if you feel left behind!

Task 1

On the last exercise sheet there was a task about the harmonic oscillator

$$\begin{aligned} M\frac{\mathrm{d}^2x}{\mathrm{d}t^2} &= -kx \text{ with the energy} \\ E_{\mathrm{tot}} &= \frac{1}{2}Mv^2 + \frac{1}{2}kx^2 \text{ and the initial conditions} \\ x(0) &= 1 \text{ and } v(0) = 0. \end{aligned}$$

This equation is now going to be solved with the Verlet-Algorithm and checked for energy conservation.

Differential equations of the form $x'' = f(x)$ occur often in physics and therefore a special method should be derived. A canonical way would be to use finite differences of second order

$$\frac{x_{i-1} - 2x_i + x_{i+1}}{\mathrm{d}t^2} + \mathcal{O}(\mathrm{d}t^3) = f(x_i).$$

Here the equation for x_1 has to be solved separately

$$x_1 = x_0 + \mathrm{d}t(v_0 + \frac{1}{2}\mathrm{d}t f(x_0)) + \mathcal{O}(\mathrm{d}t^3).$$

This equation can be derived by Taylor expansion. The terms x_0 and v_0 are the initial conditions. For running a simulation the calculation of the velocity is not needed, but for calculating the energy and resuming the simulation after a halt, it is. Therefore an expression for the velocity can also be found by Taylor expansion

$$v_i = \frac{x_i - x_{i-1}}{\mathrm{d}t} + \frac{1}{2}\mathrm{d}t f(x_i).$$

How does the time evolution of the energy behave and what does the trajectory in the phase space look like? Compare the time evolution to the theoretical prediction.

Task 2

Solve the harmonic oscillator as in the last task but this time with a Crank-Nicolson scheme

$$\frac{x^{n+1} - x^n}{\Delta t} = \tfrac{1}{2}\left(f^{n+1}(x) + f^n(x)\right).$$

Here $f(x)$ is the right hand side of the differential equation and n the time step index. This scheme only solves differential equations of first order. Therefore you will have to write the equation of the harmonic oscillator in a system of first order equations as done on the last sheet. Analyse the time evolution of the coordinates and the energy as done before.

Task 3

The stability of numerical methods for integrating the equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \lambda x$$

depends on the product $h\lambda$, with the step size h. Plot in the complex $h\lambda$-plane the boundaries of stability for these methods:

a) Euler

b) Adams-Bashforth 2. order

c) Adams-Bashforth 3. order.

This task is easier in a language that supports complex arithmetic (C++, Fortran, Python or Julia).