Heinrich-Heine-Universität Düsseldorf Institut für Theoretische Physik II Computational Physics Wintersemester 2018/2019 Prof. Dr. J. Horbach Dr. S. Ganguly (saswati@thphy.uni-duesseldorf.de.de) M. Golkia (mehrdad.golkia@hhu.de) Blatt 3 vom 30.10.2018 Abgabe bis 12:30 Uhr am 6.11.2018

<u>Problem 3.1</u>: Runge-Kutta

Consider the ODE

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{y}(t) = \mathbf{f}(\mathbf{y}(t), t) \tag{1}$$

with initial condition $\mathbf{y}(0) = \mathbf{y}_0$. The 4th order Runge-Kutta (RK4) algorithm for Eq. (1) is:

$$\mathbf{k}_{1} = \mathbf{f} (t_{n}, \mathbf{y}_{n})$$

$$\mathbf{k}_{2} = \mathbf{f} (t_{n} + \delta t/2, \mathbf{y}_{n} + \delta t \mathbf{k}_{1}/2)$$

$$\mathbf{k}_{3} = \mathbf{f} (t_{n} + \delta t/2, \mathbf{y}_{n} + \delta t \mathbf{k}_{2}/2)$$

$$\mathbf{k}_{4} = \mathbf{f} (t_{n} + \delta t, \mathbf{y}_{n} + \delta t \mathbf{k}_{3})$$

$$\mathbf{y}_{n+1} = \mathbf{y}_{n} + \frac{\delta t}{6} (\mathbf{k}_{1} + 2\mathbf{k}_{2} + 2\mathbf{k}_{3} + \mathbf{k}_{4}) .$$
(2)

a) Consider the harmonic oscillator described by the equations

$$\frac{dv}{dt} = -x$$
$$\frac{dx}{dt} = v,$$

with x the displacement from the rest position and v the velocity of the oscillator. Show that in this case, Eqs. (2) can be written as follows

$$x_{n+1} = x_n + v_n \delta t - \frac{1}{2} x_n \delta t^2 - \frac{1}{6} v_n \delta t^3 + \frac{1}{24} x_n \delta t^4$$

$$v_{n+1} = v_n - x_n \delta t - \frac{1}{2} v_n \delta t^2 + \frac{1}{6} x_n \delta t^3 + \frac{1}{24} v_n \delta t^4 .$$
(3)

b) Solve Eqs. (3) numerically for the initial conditions $v_0 = 0$ and $x_0 = 1$ using the RK4 algorithm and compare the time evolution of the total energy as well as the trajectory x(t) with those obtained in problem 2.2 (Euler and Euler-Cromer algorithms).

Problem 3.2: Time Reversibility

Consider a mathematical pendulum Fig. 1 as described by the equations

$$\dot{\theta} = \omega,
\dot{\omega} = -\frac{g}{L}\sin(\theta).$$
(4)

with θ , ω and $\alpha = \dot{\omega}$ the angular displacement, angular velocity and torque, respectively.

a) With initial conditions $\omega(0) = \omega_0$ and $\theta(0) = \theta_0$ show analytically that

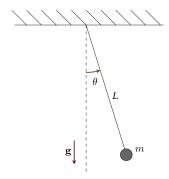


Figure 1:

i) the 2nd order Runge-Kutta algorithm

$$\theta_{n+1} = \theta_n + \omega_n \delta t - \frac{1}{2} \sin(\theta_n) \delta t^2$$

$$\omega_{n+1} = \omega_n - \sin\left(\theta_n + \frac{1}{2}\omega_n \delta t\right) \delta t$$
(5)

is not time reversible.

ii) the velocity-Verlet algorithm

$$\theta_{n+1} = \theta_n + \omega_n \delta t - \frac{1}{2} \sin(\theta_n) \delta t^2$$

$$\omega_{n+1} = \omega_n - \frac{1}{2} \left(\sin(\theta_n) + \sin(\theta_{n+1}) \right) \delta t$$
(6)

is time reversible.

- b) Using Euler and Euler-Cromer algorithms solve Eqs. (4) for g=10 and L=10. Use the time step $\delta t=0.5$ and the initial conditions $\omega_0=0$ and $\theta_0=7^{\circ}$.
- c) Plot the results for θ, ω and also energy E and compare them to the analytical solution. (For the analytical solution consider the small angle approximation $\sin(\theta) \approx \theta$.)
- d) Redo the previous steps for the different time steps $\delta t = 0.1, 0.05, 0.01, 0.005$ and explain your observation.
- e) The behavior of a mathematical pendulum generally can be described as linear, oscillatory and rotational corresponding to small (where the harmonic approximation holds), intermediate and large values of θ_0 . Plot the phase portrait for these three different regimes, considering proper θ_0 .
- f) The choice of $\theta_0 = \pi$ is a very interesting case (the so called Separatrix angle). How long will it take for the pendulum to reach $\theta = \pi$?