



Assignment Sheet Nr. 3

Paul Monderkamp, Matr.Nr. 2321677

monderkamp@thphy.uni-duesseldorf.de

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1 Exercise 1

1.1 Exercise 1 (a)

3.1 a)

For harm. osc.
 $f(t_n, Y_n) = f(Y_n)$

$$Y_{n+1} = \begin{pmatrix} x_{n+1} \\ v_{n+1} \end{pmatrix}$$

$$= Y_n + \frac{\delta t}{6} (k_1 + 2k_2 + 2k_3 + k_4)$$

$$= Y_n + \frac{\delta t}{6} \left(f(Y_n) + 2f\left(Y_n + \frac{\delta t}{2} f(Y_n)\right) + 2f\left(Y_n + \frac{\delta t}{2} f\left(Y_n + \frac{\delta t}{2} f(Y_n)\right)\right) + f\left(Y_n + \delta t f\left(Y_n + \frac{\delta t}{2} f\left(Y_n + \frac{\delta t}{2} f(Y_n)\right)\right)\right) \right)$$

$$\left\{ f(Y_n) = \dot{v}(t_n) = \begin{pmatrix} v \\ -x \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}}_A Y_n \right\}$$

$$= Y_n + \frac{\delta t}{6} \left(A Y_n + 2A\left(Y_n + \frac{\delta t}{2} A Y_n\right) + 2A\left(Y_n + \frac{\delta t}{2} A\left(Y_n + \frac{\delta t}{2} A Y_n\right)\right) + A\left(Y_n + \delta t A\left(Y_n + \frac{\delta t}{2} A\left(Y_n + \frac{\delta t}{2} A Y_n\right)\right)\right) \right)$$

$$= Y_n + \frac{\delta t}{6} \left(A Y_n + 2A Y_n + \delta t A^2 Y_n + 2A Y_n + \delta t A^2 \left(Y_n + \frac{\delta t}{2} A Y_n\right) + A Y_n + \delta t A^2 \left(Y_n + \frac{\delta t}{2} A \left(Y_n + \frac{\delta t}{2} A Y_n\right)\right) \right)$$

(1)

Figure 1.1: first part of the derivation of the formula

$$= Y_n + \frac{\delta t}{6} (3A Y_n + \delta t A^2 Y_n + 2A Y_n + \delta t A^2 Y_n + \frac{\delta t^2}{2} A^3 Y_n + A Y_n + \delta t A^2 Y_n + \frac{\delta t^2}{2} A^3 (Y_n + \frac{\delta t}{2} A Y_n))$$

$$= Y_n + \frac{\delta t}{6} (6A Y_n + 3\delta t A^2 Y_n + \delta t^2 A^3 Y_n + \frac{1}{4} \delta t^3 A^4 Y_n)$$

$$A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

$$A^2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$A^3 = -\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = -A = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

$$A^4 = -A^2 = \mathbb{I}$$

$$= \left(1 + \frac{\delta t^4}{24}\right) Y_n + \delta t A Y_n + \frac{1}{2} \delta t^2 A^2 Y_n + \frac{1}{6} \delta t^3 A^3 Y_n$$

$$= \left(1 + \frac{\delta t^4}{24}\right) \begin{pmatrix} x_n \\ y_n \end{pmatrix} + \delta t \begin{pmatrix} y_n \\ -x_n \end{pmatrix} - \frac{\delta t^2}{2} \begin{pmatrix} x_n \\ y_n \end{pmatrix} + \frac{1}{6} \delta t^3 \begin{pmatrix} -y_n \\ x_n \end{pmatrix}$$

which is equiv to
the formula in 2.1 a

(2)

Figure 1.2: second part of the derivation of the formula

1.2 Exercise 1 (b)

1.2.1 Code

```
#include <iostream>
#include <cmath>
#include <fstream>
using namespace std;

int main()
{
    double tmin      = 0.0;
    double tmax      = 50.0;
    const int N      = 500;
    double dt        = (double)(tmax - tmin)/(N-1);

    double y[N][4];
    y[0][0] = 1.0;
    y[0][1] = 0.0;
    y[0][2] = 0.5*(y[0][0]*y[0][0]+y[0][1]*y[0][1]);
    y[0][3] = 0.0;

    for (int i=0;i<N-1;i++)
    {
        y[i+1][0] = y[i][0] + y[i][1]*dt - 0.5*y[i][0]*dt*dt -
            (1.0/6.0)*y[i][1]*pow(dt,3.0)+
            (1.0/24.0)*y[i][0]*pow(dt,4.0);
        y[i+1][1] = y[i][1] - y[i][0]*dt - 0.5*y[i][1]*dt*dt +
            (1.0/6.0)*y[i][0]*pow(dt,3.0)+
            (1.0/24.0)*y[i][1]*pow(dt,4.0);
        y[i+1][2] = 0.5*(y[i+1][0]*y[i+1][0]+y[i+1][1]*y[i+1][1]);
        y[i+1][3] = dt*i;
    }
    ofstream outputfile;
    outputfile.open("3_1_b_results.txt");

    for (int i=0; i<N;i++)
    {
        outputfile << y[i][0] << " " << y[i][1]
            << " " << y[i][2] << " " << y[i][3] << endl;
    }
    outputfile.close();
    return 0;
}
```

1.2.2 Results

The following results are achieved via the code in the previous subsection.

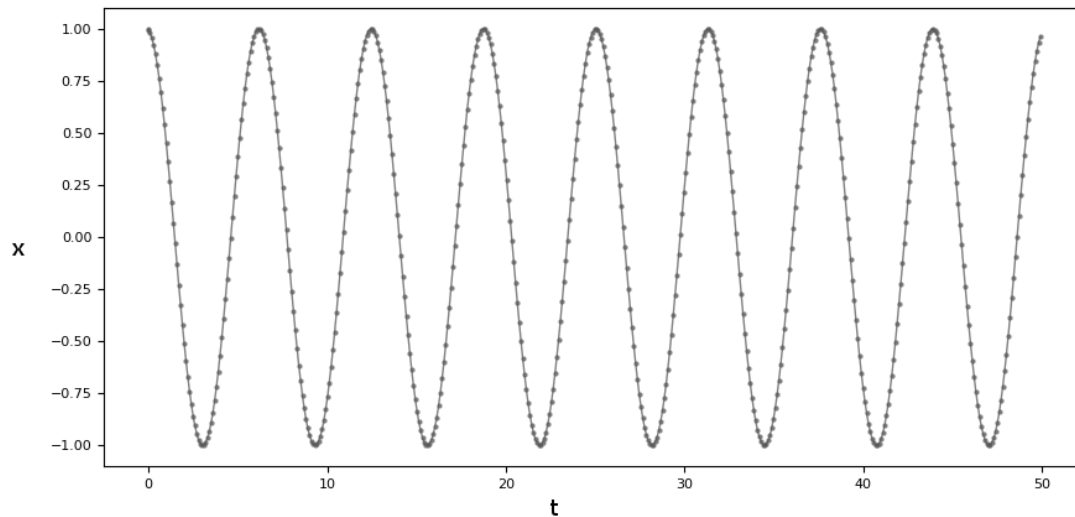


Figure 1.3: time evolution of the x coordinate of the harmonic oscillator

Figure 3.3 shows the time evolution of the x coordinate of a one dimensional harmonic oscillator solved with the Runge-Kutta 4 scheme. There is no apparent divergence from the analytical solution visible in the timeframe of the simulation.

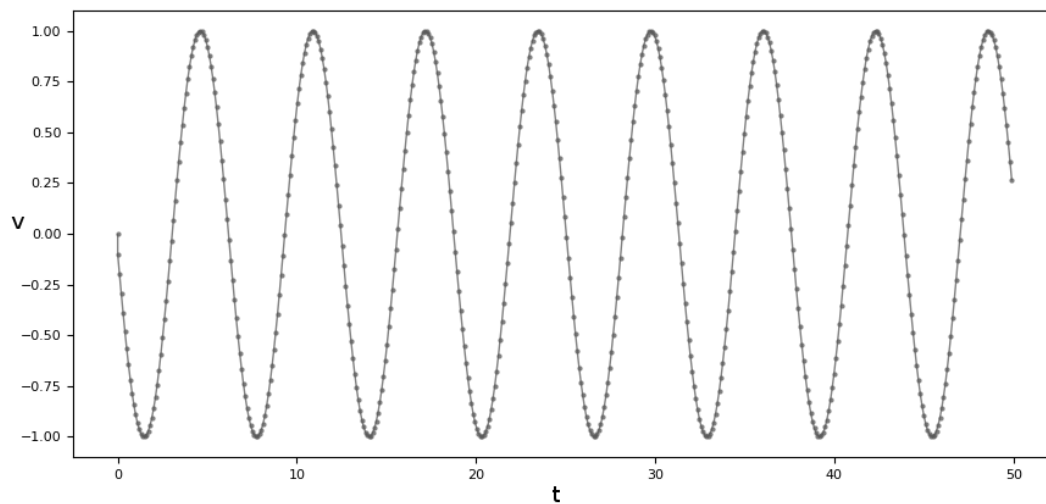


Figure 1.4: time evolution of the velocity of the harmonic oscillator

Figure 3.4 shows the time evolution of the velocity of a one dimensional harmonic oscillator solved with the Runge-Kutta 4 scheme. Similarly to the x coordinate, there is no visible instability in the timeframe of the simulation period.

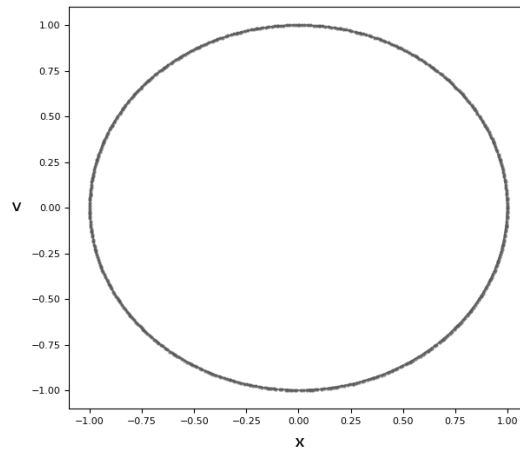


Figure 1.5: phase space trajectory of the harmonic oscillator

Figure 3.5 shows the phase space profile for the simulation results above. The trajectory seems reasonably spherical.

2 Exercise 2

2.1 Exercise 2 (a)

$$\begin{aligned} i) \quad \theta(t+\delta t) &= \theta(t) + \omega(t)\delta t - \frac{1}{2} \sin(\theta(t)) \delta t^2 \\ \omega(t+\delta t) &= \omega(t) - \sin(\theta(t) + \frac{1}{2} \omega(t) \delta t) \delta t \end{aligned}$$

to check time reversibility :

$$t \leftrightarrow t + \delta t$$

$$\delta t \leftrightarrow -\delta t$$

$$\theta(t + \delta t) = \theta_{n+1}$$

$$\theta(t) = \theta_n$$

ω analogously

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

it is impossible to
solve either one of these
eq. ~~of~~ for θ_{n+1} or ω_{n+1}
and thus old eq.
cannot be obtained from them

Figure 2.1: time reversibility for Runge-Kutta 2 scheme

$$\theta_{n+1} \leftrightarrow \theta_n \quad ; \quad \delta t \rightarrow -\delta t$$

(i)

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

$$\omega_n = \omega_{n+1} + \frac{1}{2} \delta t [\sin \theta_{n+1} + \sin \theta_n]$$

$$\rightarrow \cancel{\theta_{n+1} = \theta_n + \omega_{n+1} \delta t +}$$

$$\omega_{n+1} = \omega_n - \frac{1}{2} \delta t [\sin \theta_{n+1} + \sin \theta_n] \quad \checkmark$$

in first eq.:

$$\begin{aligned} \theta_{n+1} &= \theta_n + \delta t \left(\omega_n - \frac{1}{2} \delta t [\sin \theta_{n+1} + \sin \theta_n] \right) \\ &\quad + \frac{1}{2} \sin \theta_{n+1} \delta t^2 \end{aligned}$$

$$= \theta_n + \delta t \omega_n - \frac{1}{2} \delta t^2 \sin \theta_n \quad \checkmark$$

\Rightarrow time reversible

Figure 2.2: time reversibility for velocity Verlet algorithm