Exercise Sheet Velocity Verlet MD

1. A C-program `velocityVerletSho.c` is provided which integrates the equation of motion for the simple harmonic oscillator according to the Velocity-Verlet algorithm. For simplicity, the mass and force constant are defined as `MASS=1` and `K=1`, respectively. The initial conditions are defined as `X0=1` (coordinate) and `V0=0` (velocity). The number of integration steps is `NSTEPS` and the time step size is given by `deltat = Tper / TFAC`, where `Tper` is the period of oscillation and `TFAC` is the number of time steps per period of oscillation. The program can be compiled with

   `gcc -o velocityVerletSho program/velocityVerletSho.c`

   and run with

   `./velocityVerletSho`

   For each time step, it prints the time in units of period, coordinate, momentum, total energy

$$E_{tot} = \frac{1}{2}mv^2 + \frac{1}{2}kx^2 \tag{1}$$

   The output can be written to a file `out.dat` with

   `./velocityVerletSho > out.dat`

   That is, in this file, there are five columns which report the time in units of period, coordinate, momentum, total energy and the energy of the shadow Hamiltonian, respectively.

   - Look at the program and verify the equation of motion of the simple harmonic oscillator, as well as the equations of the Velocity-Verlet algorithm.

   - Edit, compile and run the program for variables `TFAC=10, 50` and `100` and write corresponding output data to files `out10.dat`, `out50.dat` and `out100.dat`, respectively.

   - Make phase space plots for the three above runs, *i.e.* plot the momentum *vs.* the coordinate. Interpret.

   - Plot the energy *vs.* time. Interpret.