In-Class Work: Molecular Dynamics Simulation (Driven Damped Pendulum

You find the solutions to the previous classes on molecular simulations for example in

`~kvollmay/share.dir/inclass2023.dir/md3.py`

At the beginning of class I will introduce the equations of motion for the driven damped pendulum.

6. Driven Damped Pendulum Intro & Trajectory

6a. We just derived the essential equation for the simulation of the driven, damped pendulum to be

$$\frac{d^2\theta}{dt^2} = \tilde{A}\cos(\tilde{\omega}_{\rm D}\, t) - \sin(\theta) - \tilde{\gamma}\,\frac{d\theta}{dt} \tag{4}$$

where we replaced $\tilde{t}$ by t simply for the convenience of notation. In the computer simulation we solve this equation numerically, i.e. our goal is to determine $\theta(t)$ and $\dot{\theta}(t)$.

Using the Euler method as written on the white board, program this driven damped pendulum. Use

$$\theta_0 = -2.5 \quad \omega_0 = 0.0 \quad \tilde{A} = 0.95 \quad \tilde{\omega}_{\rm D} = 2.0/3.0 \quad \tilde{\gamma} = 0.5 \quad \Delta t = 0.01 \quad n_{\rm max} = 10000$$

Print only every 10th MD-step $t, \theta(t), \omega(t)$. (In the following I will call this `nprint=10`.) Look at $\theta(t)$ and $\omega(t)$. If your data are in the file `out6sim.dat` you can do this with
`xmgrace -block out6sim.dat -bxy 1:2 -bxy 1:3 -legend load`

6b What is the energy of the driven damped pendulum? Since we chose as time unit $1/\omega_{\sf SHO}$ and as moment of inertia unit I our energy unit is $I\omega_{\sf SHO}^2$ and this means that in the program you want to determine $\tilde{E} = \frac{E}{I\omega_{\sf SHO}^2}$. Please get me when you have your expression for $\tilde{E}$. Then add the determination of $\tilde{E}$ to your program and print $\tilde{E}(\tilde{t})$ and look at your results with `xmgrace`. Get me also when you have your result. We will discuss the interpretation of your result.

7. Period Doubling (if time)

Next we will vary $\tilde{A}$ and will observe how $\tilde{A}$ influences $\theta(t)$ and $\omega(t)$. For this task and also for next class, we will use a special time step Δt. We will use

$$\Delta t = \frac{2\pi}{\tilde{\omega}_{\rm D} N_{\rm dt}}$$

Please ask when you get to this, I will briefly explain why we choose Δt this way. Use $N_{\rm dt} = 200$ and increase `nmax` to 100000.

7a. Look at $\theta(t), \omega(t)$ and $E(t)$ for $\tilde{A} = 1.049$.

7b. Look at $\theta(t), \omega(t)$ and $E(t)$ for $\tilde{A} = 1.053$.

7c. Look at $\theta(t), \omega(t)$ and $E(t)$ for $\tilde{A} = 1.054$.

7d. Look at $\theta(t), \omega(t)$ and $E(t)$ for $\tilde{A} = 1.07$.

7e. Get me when you got all results for 7a-7d. (Get them all on the screen, so that your class members can see them also.)