In-Class Work: Molecular Dynamics Simulations

6. Driven Damped Pendulum Intro & Trajectory

6b. In the last class we were deriving the differential equation for the driven damped harmonic oscillator in terms of unitless variables. We showed that the essential equation for the simulation of the driven, damped pendulum is

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

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

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

You may use the solution to our task 4. of the MD-inclass work.
`~kvollmay/share.dir/inclass2021.dir/md4.py`
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`

6c What is the energy of the driven damped pendulum? Since we chose as time unit $1/\omega_0$ and as torque unit $I\omega_0^2$ our energy unit is also $I\omega_0^2$ and this means that in the program you want to determine $\tilde{E} = \frac{E}{I\omega_0^2}$. 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 and I will show you a few tools with `xmgrace`.

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

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

Please ask when you get to this, I will briefly explain why we choose Δt this way. Use $N_\mathrm{dt} = 200$ 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.)