In-Class Work: Molecular Dynamics Simulations

6. Driven Damped Pendulum Intro & Trajectory

6b. At the end of last class we ended up with the essential equation for the simulation of the driven, damped pendulum to be

$$\frac{d^2\theta}{dt^2} = \tilde{A}\cos(\tilde{\omega}_D t) - \sin(\theta) - \tilde{\gamma}\frac{d\theta}{dt} \tag{3}$$

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

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

Please note that these parameters are different than the inclass-handout from last class. Use the parameters given here.

You may use the solution to our March 9 classwork `~kvollmay/share.dir/inclass.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 `out6.dat` you can do this with

`xmgrace -block out6.dat -bxy 1:2 -bxy 1:3`

6c What is the energy of the driven damped pendulum? Since we chose as time unit $1/\omega_0^2$ 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

$$\Delta t = \frac{2\pi}{\tilde{\omega}_D N_{dt}}$$

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

8. Poincaré Plot (if time)

8a. Incorporate periodic boundary conditions for θ, i.e. ensure that `thetanew` satisfies

$$-\pi < \theta \leq \pi$$

8b. To get $\omega(\theta)$ measured in phase with T_{D} determine Δt as $\Delta t = (2\pi/\tilde{\omega}_{\mathrm{D}})/n_{\mathrm{print}}$. Use $n_{\mathrm{print}} = 200$ and do 100000 MD-steps. (So set $n_{\mathrm{print}} = N_{\mathrm{dt}}$. To ensure to not plot the transient plot only after 20000 MD-steps. Look at the Poincaré plot $\omega(\theta)$ for the $\tilde{A}$ values of the above 7a-7d. Get me, when you have the results.