In-Class Work: Molecular Dynamics Simulations

Note: For the following in-class work you may use the solution to last class

`~kvollmay/share.dir/inclass.dir/md4.py`

6. Driven Damped Pendulum Intro & Trajectory

6a. I will give you in class first an introduction to the driven damped pendulum and how to rescale time to get the fewest number of independent parameters.
6b. So we ended up with the essential equation for the simulation of the driven, damped pendulum to be

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

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

$$\theta_0 = 0.0 \quad \omega_0 = 1.9 \quad \tilde{A} = 0.9 \quad \tilde{\omega}_{\mathrm{D}} = 2.0/3.0 \quad \tilde{\gamma} = 0.5 \quad \Delta t = 0.005 \quad n_{\max} = 5000$$

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 Think about what the energy of the driven damped pendulum is, and print and look at $E(t)$.