# In-Class Work: Molecular Dynamics Simulation

**Outline:**

- We will start class today with discussing the results for the tasks 3. & 4. of last class (here first page).
  - You find solution programs for inclass MD-work in
    `~kvollmay/share.dir/inclass2021.dir/md3.py`
    and similarly `md4.py`
    and resulting data are in
    `~kvollmay/share.dir/inclass2021.dir/out3sim100.dat`
    `~kvollmay/share.dir/inclass2021.dir/out3theory.dat`
    and similarly other files.
  - I will teach you a few figure making tools (using xmgrace) as we look at the results. We look at the results.
  - I will explain the surprising results and how to fix the problem
- We will work on the driven damped pendulum. (here second page)
  - I will give you intro to driven damped pendulum.
  - You program it.

## 3. Harmonic Oscillator & Surprise

**3a.** Numerically integrate this time for the harmonic oscillator, so $F_x^{\mathrm{net}} = -kx$. We can also analytically solve this equation. Let's choose $t_0 = 0.0, x_0 = 5.0, v_0 = 0.0$, then the theoretical solution is

$$x(t) = 5.0\cos(\omega_0 t) \qquad v_x(t) = -5.0\omega_0 \sin(\omega_0 t)$$

where $\omega_0 = \sqrt{(k/m)}$. So we know the period $T = 2\pi/\omega_0$. Let's choose $\Delta t = T/n_{\mathrm{div}}$. Integrate $F_x^{\mathrm{net}} = -kx$ for $k = m = 1$ and for $n_{\mathrm{div}} = 100$ and do $n_{\max} = 10 n_{\mathrm{div}}$ MD steps. Print also the analytical solution and compare. **Note: Before you update $x(t)$, you need to copy the value of $x(t)$ into a temporary variable for example `xold=x` only then you can update $x$ and then $v$. For $v$ you need to use `xold`.** Try also with $n_{\mathrm{div}} = 1000$. What happens?

**3b.** Also determine the theoretical and numerical total energy

$$E_{\mathrm{tot}} = \frac{1}{2}kx^2 + \frac{1}{2}mv_x^2$$

as function of time, so $E_{\mathrm{tot}}(t)$. If you print for example into `out3sim100.dat` $t, x, v_x, E_{\mathrm{tot}}$ and similarly into the other files, you can compare the $E(t)$ results with

```
xmgrace -block out3theory.dat -bxy 1:4 -block out3sim100.dat -bxy 1:4 -block out3sim1000.dat  -bxy 1:4
```

### 4. Euler-Cromer

In the Gould et al. book the first page of chapter 3 describes the Euler-Cromer step instead of the Euler step. Repeat the integration and compare again with the theoretical solution.

### 5. Integration Methods

In case you would like to learn about further integration techniques, you may like to read the Appendix 3A which is near the end (page 30 out of 41 pages) of Chapter 3 of the Gould et al. book.

### 6. Driven Damped Pendulum Intro & Trajectory

**6a.** I will give you an introduction to the equation of motion for the driven damped pendulum. We just derived the essential equation for the simulation of the driven, damped pendulum to be

$$\frac{d^2\theta}{dt^2} = \tilde{A}\cos(\tilde{\omega}_{\mathrm{D}}\, t) - \sin(\theta) - \tilde{\gamma}\,\frac{d\theta}{dt} \qquad (3)$$

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

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

You may use the just presented solution to the MD-inclass step 4.
`~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 -legend load`

**6b** 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 (if time) I will show you a few tools with `xmgrace`.