27-534/734 Methods of Computational Materials Science

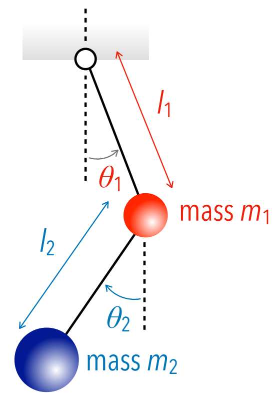
Laboratory 1 | Classical Models

Due date

This assignment is due on **Monday, February 16**. Submit your work online through CANVAS by midnight of the due date.

Laboratory Part 1 (40 points)

[Lecture 6, Hamilton's equations]



(1) We consider a pendulum of mass m = 2 kg and length l = 1.5 m in a gravitation field g. Write the Hamiltonian of the system. (2 points) Derive the equations of motion. (3 points) Solve these equations using Matlab or Python. (3 points) Determine the period τ of the pendulum. (2 points)

(2) We now consider a double pendulum consisting of two masses $m_1 = 1.5$ kg and $m_2 = 2$ kg in a gravitation field g. The lengths of the double pendulum are $l_1 = 3$ m and $l_2 = 2$ m. The angles θ_1 and θ_2 define the directions of the two pendulums with respect to the vertical axis, as shown in the figure. The corresponding angular velocities are denoted $\omega_1 = \dot{\theta}_1$ and $\omega_2 = \dot{\theta}_2$. The coordinates of the masses along the cartesian axes are denoted (x_1, z_1) and (x_2, z_2).

(Optional for 27-534) Derive equations of motion of the double pendulum. (10 points)

$$\begin{pmatrix} \dot{\theta}_1 \\ \dot{\theta}_2 \end{pmatrix} = \begin{pmatrix} \omega_1 \\ \omega_2 \end{pmatrix}$$

$$\begin{pmatrix} \dot{\omega}_1 \\ \dot{\omega}_2 \end{pmatrix} = \begin{pmatrix} (m_1 + m_2) l_1 & m_2 l_2 \cos(\theta_1 - \theta_2) \\ m_2 l_1 \cos(\theta_1 - \theta_2) & m_2 l_2 \end{pmatrix}^{-1} \begin{pmatrix} -m_2 l_2 \omega_2^2 \sin(\theta_1 - \theta_2) - (m_1 + m_2) g \sin(\theta_1) \\ m_2 l_1 \omega_1^2 \sin(\theta_1 - \theta_2) - m_2 g \sin(\theta_2) \end{pmatrix}$$

Download the code `double_pendulum.m` and complete it. Show your code. (5 points)

Using the initial conditions $\theta_1 = \pi/2$ rad, $\theta_2 = \pi/6$ rad, $\dot{\theta}_1 = 0$ rad/s, $\dot{\theta}_2 = -3\pi/2$ rad/s, solve the equation of motion from t = 0 s to t = 20 s with a time discretization of 10^5 time points and plot the trajectory of the two masses. (10 points)

Hint. To plot the trajectories, you may modify the code as follows

```
x1 = l1 * sin(theta_1(n));
z1 = - l1 * cos(theta_1(n));
x2 = x1 + l2 * sin(theta_2(n));
z2 = z1 - l2 * cos(theta_2(n));
plot(x1,z1,'.','MarkerSize',1,'Color','red')
plot(x2,z2,'.','MarkerSize',1,'Color','blue')
drawnow
```

Discuss why the double pendulum is said to exhibit a chaotic motion, looking for the definition of this term. (5 points)

Laboratory Part 2 (60 points)

[Lecture 4, velocity Verlet integration]

We simulate the motion of Li ions in a $LiMn_2O_4$ electrode. Upload the notebook laboratory1.ipynb on **Google Colab**, together with the LAMMPS input files limn2o4.A.in and limn2o4.A.data.

(1) Read the file limn2o4.A.in and explain each command line. (5 points)

Hint. LAMMPS commands are explained at docs.lammps.org/Commands_all.html)

In which ensemble is the simulation run? (3 points)

Which time integration algorithm is used for this simulation? (2 points)

(2) By approximating the time derivative of the force as $\mathbf{H}_{i,n} = \dot{\mathbf{F}}_{i,n} \approx (\mathbf{F}_{i,n+1} - \mathbf{F}_{i,n})/\Delta t$ and by writing the Taylor expansions of $\mathbf{r}_{i,n+1}$ and $\mathbf{v}_{i,n+1}$ in terms of $\mathbf{r}_{i,n}$, $\mathbf{v}_{i,n}$, $\mathbf{F}_{i,n}$, and $\mathbf{H}_{i,n}$, derive the discretized equations discussed in lecture:

$$\mathbf{r}_{i,n+1} = \mathbf{r}_{i,n} + \Delta t\, \mathbf{v}_{i,n} + \Delta t^2/m\, (\mathbf{F}_{i,n+1}+2\mathbf{F}_{i,n})/6$$
$$\mathbf{v}_{i,n+1} = \mathbf{v}_{i,n} + \Delta t/m\, (\mathbf{F}_{i,n+1}+\mathbf{F}_{i,n})/2.$$

(10 points)

(3) Modify limn2o4.in to simulate the time evolution of $LiMn_2O_4$ over 5 ps with a time step of 0.1, 0.5, 1.0, 1.5, and 2 fs. Plot the evolution of the total energy in each case. (5 points)

Which time step would you select for the fluctuations of the total energy to be lower than 0.1 eV over 5 ps? (5 points)

(4) Now upload and read the input `limn2o4.B.in` and `limn2o4.B.data`. In which ensemble is the simulation run and which thermostat is used? (2 × 2 points)

What is the unit of the relaxation parameter T_{damp}? (1 point)

Compute the mass of the thermostat $M_\mathsf{T} = (3N+1)k_\mathrm{B}T\,\mathsf{T}^2_{\text{damp}}$ in eV·ps² where N is the number of atoms. (5 points)

(5) The Hamiltonian of a molecular system coupled to a Nosé-Hoover thermostat is

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m_i s^2} + \frac{P_s^2}{2M} + U(\mathbf{r}_1, \cdots, \mathbf{r}_N) + Ndk_\mathrm{B}T\ \ln(s)$$

Derive the resulting equations of motion. Show all your derivation. (5 points)

Rewrite the equations under rescaled variables

$$dt \to s dt,\ \mathbf{p}_i \to s\,\mathbf{p}_i \text{ with } \zeta = \mathrm{d}(\ln s)/\mathrm{d}t = s^{-1}\mathrm{d}s/\mathrm{d}t.$$

(5 points)

(6) Using `limn2o4.B.in`, perform simulation with a time step of 0.5 fs over a time window of 10 ps at 5,000 K using a Nosé-Hoover thermostat with a time scale of 5 fs, 50 fs, and 500 fs. Plot the evolution of the temperature in these three cases. (3 points)

Discuss the influence of the time scale of the thermostat T_{damp}. (2 points)

Note. The temperature is set to an unphysical large value to accelerate the simulation.

(7) (Optional for 27-534) By performing simulations with a time step of 0.5 fs over a time window of 10 ps, plot the mean square displacement of Li atoms as a function of time for select temperature between 1,000 K and 10,000 K:

$$\mathrm{MSD}_n = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{r}_{i,n} - \mathbf{r}_{i,1})^2$$

where N is the number of lithium atoms, n is the time iteration, and $\mathbf{r}_{i,n}$ is the position of atom i at iteration n. (5 points)

Extra Credit

Part 1. Derive the equations of motion for a triple pendulum. (5 points)

Part 2. Using the relation $\mathrm{MSD} \approx 6Dt$, estimate the diffusion coefficient D of Li in $LiMn_2O_4$ for each temperature of Question 7. Express the diffusion coefficient in SI units. Discuss your result. (5 points)