

Solutions – problem set 1

PART A

A1)

$$\begin{aligned}\frac{d^2 M_x}{dx^2} &= 0, \\ \frac{d^2 M_y}{dx^2} + q_z &= 0, \\ \frac{d^2 M_z}{dx^2} - q_y &= 0.\end{aligned}$$

Load only in z direction, therefore only consider the equation for M_y . With

$$M_y = EI_{zz}\theta_{y,0}$$

and

$$\theta_{y,0} = -\frac{\partial^2 u_{z,0}}{\partial x^2}$$

we arrive at the equilibrium equation:

$$-EI_{zz}\frac{\partial^4 u_{z,0}}{\partial x^4} + q_z = 0$$

$$A2) \quad u_z(x=0) = 0$$

$$M_x = M_z = 0$$

$$M_y(x=L) = 0$$

$$\omega_y(x=0) = 0$$

$$\Theta_y(x=0) = 0$$

$$Q_z(x=L) = 0$$

$$u_z(x=0) = 0$$

A3) Solution after integration:

$$Q_z(x) = \rho g A(x - L)$$

$$M_y(x) = \frac{1}{2}\rho g A(x - L)^2.$$

$$\omega_y(x) = \frac{\rho g A}{EI_{zz}} \left(\frac{x^3}{6} - \frac{Lx^2}{2} + \frac{L^2x}{2} \right),$$

$$u_z(x) = -\frac{\rho g A}{EI_{zz}} \left(\frac{x^4}{24} - \frac{L}{6}x^3 + \frac{L^2x^2}{4} \right)$$

Results for Q_z and M_y match those obtained in class.

PART B

B1) MD is better suited since it can describe nonequilibrium processes; and provides full information about the dynamics. MC is suited for equilibrium processes.

$$B2) \quad m \frac{d^2 r_j}{dt^2} = -\nabla_{r_j} U(r_j), \quad \text{for } j=1..N,$$

which is a system of coupled 2nd order nonlinear differential equations that can be solved by discretizing the equations in time.

PART C – Interatomic potentials

C1) Units: $[r_m] = \text{Angstrom}$, $[B] = 1/\text{Angstrom}$, and $[D] = \text{Energy}$.

These units can easily be derived based on the following arguments: The potential itself expresses the energy as a function of distance; the argument of the exponential needs to be unit less.

The total energy of the system is given by the sum over the energetic contributions over all pairs of atoms in the system.

This can be written using two summations, with a prefactor of 1/2 to account for the fact that bonds are double counted (e.g. one accounts for bond 2-3 and the energy of this bond is counted again when the bond 3-2 is considered):

$$U_{total} = \frac{1}{2} \sum_{i=1}^N \sum_{j=1, i \neq j}^N \varphi(r_{ij})$$

This expression sums the energy contributions of the pair-wise interactions of all atoms, without considering the interaction of atoms with itself ($i \neq j$).

C2) The force between pairs of atoms goes to zero either at the equilibrium distance between pairs of atoms - given by $r_{ij} = r_0 = r_m(\exp(-B(r_{ij} - r_m)) = 1)$, or for $r_{ij} \rightarrow \infty$

($\exp(-B(r_{ij} - r_m)) = 0$). If no potential cutoff is introduced, two atoms will always assume the equilibrium position r_0 . Note that r_0 only depends on r_m , and on no other potential parameters.

For $r_{ij} \rightarrow \infty$, $\varphi(r_{ij}) \rightarrow D$, and for $r_{ij} \rightarrow 0$, $\varphi(r_{ij}) \rightarrow D \cdot (1 - \exp(B \cdot r_m))^2$ (repulsion).

For $r_{ij} \rightarrow r_0$, $\varphi(r_{ij}) \rightarrow 0$. Thus, the potential energy stored in each bond is given by D (also denoted as “Morse potential [energy]”).

The potential parameter B changes the shape of the potential (wider or more narrow) around the equilibrium separation.

Not required: The parameter B controls the width of the potential and is equal to the square root of half the force constant $k = \varphi''(r_{ij} = r_0)$ divided by the Morse potential,

$$B = \sqrt{\frac{k}{2D}}.$$

C3) Sketch of the Morse potential, indication the parameters r_m and D :

