

## Problem set 1

**Due: January 16**

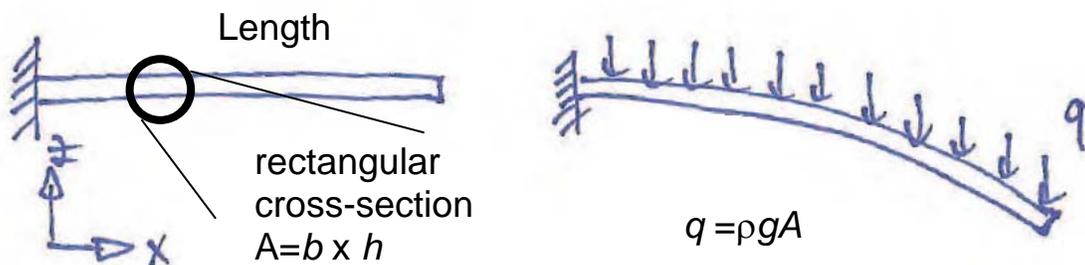
This week's lectures contained an introduction into continuum mechanical concepts. In addition to more traditional engineering applications, continuum theory is also extremely valuable in analyzing the mechanics of small-scale materials such as individual molecules, thin films. It is also an essential part of fracture many fracture theories.

As pointed out in the lecture notes, the significance of elasticity problems goes far beyond simply studying reversible deformation. For example, a beam bending problem similar as the one studied in the lecture can be used to carry out coupling from atomistic to mesoscopic scales within a hierarchical multi-scale modeling framework.

This first assignment is focused around basic continuum mechanics and introductory material on molecular dynamics simulation.

### PART A

In the first and second lecture, we have discussed a beam bending problem with the following geometry:



In class, we have obtained the section force and moment distribution ( $F_z$  and  $M_y$ ), as well as the distribution of curvatures. The purpose of this first problem set is to determine the distribution of displacements along the  $x$ -direction using the differential beam equilibrium equations (see Section 2.5.5 in the lecture notes).

- 1) Write out the equilibrium equations for this case.
- 2) Write out all boundary conditions (displacements, moments, forces, rotations etc.).
- 3) Solve the differential equilibrium equations so that you obtain the displacement distribution  $u_z$  and the rotation distribution  $\omega_y$ , all as a function of  $x$ .

Compare the results for  $F_z$  and  $M_y$  with those obtained earlier.

### PART B – Basic molecular dynamics

1. Many materials failure processes occur at extremely short time scales. Molecular modeling can provide important information about how a crystal undergoes deformation, including all atomic details and their temporal resolution, often beyond the capabilities of current experimental techniques.

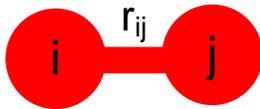
Is Monte Carlo (MC) or Molecular Dynamics (MD) advantageous for such instability problems? Describe why; give keywords only.

2. Write the differential equation you solve in molecular dynamics and explain how it relates to Newton's laws explained in the first lecture.

### PART C – Interatomic potentials

1. A popular potential to describe the interaction between atoms is the Morse function (named after physicist Philip M. Morse), a pair potential that describes the energy stored in the bond between pairs of atoms (here  $i$  and  $j$ ) as:

$$\varphi(r_{ij}) = D \left\{ 1 - \exp(-B(r_{ij} - r_m)) \right\}^2. \quad (1)$$



The Morse potential has three parameters,  $r_m$ ,  $D$  and  $B$ .

What are the units of these three potential parameters (e.g. length, energy, ...)?

Write the total energy of a system of  $N$  particles, assuming only pair wise interactions between atoms, without any cutoff radius, as summations over particles and energy expressions, in terms of  $\varphi(r_{ij})$ .

2. By taking the first derivative of  $\varphi(r_{ij})$  (denoted by  $\varphi'(r_{ij})$ ) with respect to  $r_{ij}$  (proportional to the force between particles  $i$  and  $j$ ) and setting it to zero, calculate the equilibrium position between pairs of atoms, denoted by  $r_0$ .

Discuss all possible solutions that yield  $\varphi'(r_{ij}) = 0$ , and which specific terms are required to be zero for each case. Express the corresponding atomic separation as a function of the potential parameters, for each solution.

Calculate the limiting value of  $\varphi(r_{ij})$  for  $r_{ij} \rightarrow \infty$  and for  $r_{ij} \rightarrow 0$ .

From these results, calculate the energy stored in each bond, as a function of potential parameters.

Discuss the dependence of these properties on the parameter  $B$ . What influence does the parameter  $B$  have?

**Hint:** Consider that the second derivative of  $\varphi(r_{ij})$  corresponds to the force constant  $k = \varphi''(r_{ij} = r_0)$ ; without considering the actual derivatives you can see that the second partial is proportional to  $B$  with some exponent. This force constant approximates the potential behavior in the vicinity of the equilibrium position  $r_0$ , *i.e.* if the bonds are soft or stiff, within a harmonic approximation  $\varphi(r_{ij}) \sim k(r - r_0)^2$ .

- Using the above results, sketch the potential shape, drawing  $\varphi(r_{ij})$  as a function of the distance between two particles  $r_{ij}$ , indicating the value of specific potential parameters  $r_m$  and  $D$  in the plot.