



BIOINFORMATICS II - SS 16

5. EXERCISE SHEET

TO BE DELIVERED NOT LATER THAN 29-05-2016

	Exercise	Points
Practical+Theoretical	1	10+10
Practical	1	10

Exercise 1: Simple coarse grained model (10+10 Points)

Write a program that, given a PDB file (for example, the first model of 1l2y) simulate the dynamics of a protein with a model such that the C_α atoms are bounded by a spring. The elastic constant and the equilibrium distance between C_α atoms needs to be estimated with some theoretical/empirical considerations.

Save the PDB after the optimization (all the atoms needs to be save, not only C_α).

Exercise 2: Nosè-Hoover (10 Points)

Consider a system composed by an harmonic oscillator, with mass and elastic constant put equal to one. Assume that that the initial condition is:

$$\begin{cases} x(0) = 1.0 \\ \dot{x}(0) = 1.0 \end{cases}$$

Implement a C++ program that simulate the system with a system fixing the velocity to a value of 0.8 or to 1.2. Make a plot of the evolution in time of the variables x and v . You may want to consider <http://tinyurl.com/j445jks>.

Exercise 3: Molecular dynamics – BALL (10 Points)

Write a program that, receiving a PDB file as input argument, perform molecular dynamics for an amount of time specified as input argument. Plot the energy and the temperature as functions of time. You may want to read the documentation at <http://tinyurl.com/gp4fdbf>.