FB 08 Informatik
Lehrstuhl f. Software-Technik und Bioinformatik

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BIOINFORMATICS II - SS 16

8. EXERCISE SHEET

TO BE DELIVERED NOT LATER THAN 19-06-2016

	Exercise	Points
Theoretical	1	10
Practical	2	30

Exercise 1: Minimize RMSD (10 Points)
Consider for the RMSD for two structures A, B the definition (R being a 3x3 matrix representing rotation, and T a 3D vector representing the translation):

$$\texttt{RMSD}(A,B) = \min_{R,T} \sqrt{\frac{1}{N}\sum_{1} N\|A_i - R(B_i - T)\|}$$

proof that finding the translation that optimizes RMSD when no rotation is involved is the one that move the center of mass of A into the center of mass of B.

Exercise 2: Molecular Dynamics – `BALL` (30 Points)
Using `BALL` (and other `C++` libraries), write a program that:

- Accept a PDB id as input argument, and download the corresponding PDB file (you can use `wget`)
- Select the first model, and the first chain of the model
- Get the list of aminoacids of the obtained chain as a string
- Using peptide builder, create a long chain of aminoacids (sequence as the previous point)
- Save the PDB with the the chain
- Equilibrate (minimizing energy) the system
- Perform Molecular Dynamics on the system (vacuum or in water)

The last two points shall be achieved via `GROMACS`. After the molecular dynamics simulation, compare the result calculating the RMSD and the CMO, that is the number of contacts present in the reference and in the predicted structure divided by the sum of contacts in the reference plus the contacts in the predicted.