FB 08 Informatik
Lehrstuhl f. Software-Technik und Bioinformatik

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BIOINFORMATICS II - SS 16

2. EXERCISE SHEET

TO BE DELIVERED NOT LATER THAN 08-05-2016

	Exercise	Points
Practical	1	10
Practical	2	10
Practical	3	20

Exercise 1: Handling a PDB file – `Ball` (10 Points)
Create a `C++` (*using* `Ball`) code that, given as input a filename, read the pdb and translate all the atoms (i.e., add to all the coordinates) the vector **d**:

$$\mathbf{d} = (1, 1, 1)$$

For example, given the vector **x**

$$\mathbf{x} = (1, 2, 3)$$

the translation will be:

$$\mathbf{x} + \mathbf{d} = (2, 3, 4).$$

The result expected is the PDB with the other lines unchanged, and only the positions modified in order to get a valid PDB.

Exercise 2: Extracting C_α from a PDB file – `Ball` (20 Points)
Create a `C++` (*using* `Ball`) code that, given as input a filename, read the pdb and print the positions of the C_α atoms. You may want to read how to use `Vector3` (for example in `ball/source/TEST/Vector3_test.C`), `AtomIterator` (for example in `ball/source/TEST/AtomIterator_test.C`) and the `getName` method of `Atom` (for example in `ball/source/TEST/Atom_test.C`). Pay attention to difference from an iterator and an object (`AtomIterator` is not the same as `Atom`). The C_α atoms in the PDB are named `CA`. The output of your program, once that the input file is `1l2y_simplified.pdb`, should be:

```
(-8.608, 3.135, -1.618)
(-4.923, 4.002, -2.452)
...
(0.852, 10.027, 1.285)
```

Exercise 3: Differential equation – Second order (20 Points)
Using as reference:
`http://tinyurl.com/oz9qd7r`,
find the solution of the differential equations:

(a) $y''(x) + y(x) = \sin(2x)$

(b) $y''(x) + y(x) = \sin(x)$

(c) $y''(x) - y(x) = 0$

Hint: You should focus on
`http://tinyurl.com/ctuky5g`
in order to solve the not homogenous equations.