



BIOINFORMATICS II - SS 16

7. EXERCISE SHEET

TO BE DELIVERED NOT LATER THAN 12-06-2016

	Exercise	Points
Theoretical	1	10
Practical	2	30

Exercise 1: Calculation of the work (10 Points)

Calculate the work made by a point moving in a force field:

$$\mathbf{F} = (3x + y)\mathbf{i} + (x + 2y)\mathbf{j}$$

along the paths:

$$\gamma_1(t) = \begin{cases} t\mathbf{i}, & t \in [0, 3) \\ 3\mathbf{i} + (t - 3)\mathbf{j} & t \in [3, 6] \end{cases}$$

$$\gamma_2(t) = \begin{cases} t\mathbf{i} + t\mathbf{j}, & t \in [0, 3] \end{cases}$$

Represent the two curves. Does the work depend on the choice of the path?

Exercise 2: Generating a grid for Katchalski-Katzir (30 Points)

Generate a 3d grid for the Katchalski-Katzir method, for coefficients:

$$\alpha_1 = \alpha_2 = 1$$

$$\gamma_1 = \gamma_2 = 0$$

$$\beta_1 = \beta_2 = 2$$

In order to save computational time, generate a hash grid. The grid for Katchalski-Katzir needs to be more much more fine-grained than the hash grid (you may want to read `HashGrid3_test.C` for the hash grid implementation). In order to determine if a point belongs to the inside, outside or to the boundary of the protein in a Katchalski-Katzir grid, consider the following definition:

- outside: the distance of the center point of the cell from every atom of the protein is greater than the Van der Waals radius plus 10%
- inside: the distance of the center point of the cell from any atom of the protein is less than the the Van der Waals minus 10%,
- boundary: otherwise.

Van der Waals radii can be found through `BALL (PTE_test.C)`. Test your implementation using as protein the first model of `1L2Y.pdb`. Produce three contour plots considering the Katchalski-Katzir grid values for cells along the x, y, z planes crossing the center of the grid.