

Homework 3 solutions:

1. This problem is about the number of degrees of freedom needed for each transformation and because you can perform each transformation sequentially you can take the max degree of freedom needed. The solution is:

- a. 2 points;
- b. 2 points;
- c. 2 points;
- d. 3 points.

2. Simply compute:

rms initial = 1.4448

translation vector = (0.5639 0.3646 -0.1409)

rms final = 1.2715

3. a. the approximate number is when we try all possible free positions of a link. All possible conformations are 4^8 but each link has only 3 free positions so eliminating the conformation with returning links we get 3^8 approximate conformations.

b. see the code for this example the answer is :4076 conformations

c. using the code to find all conformations compute the energy of the sequence for each conformation. Min energy = -2, conformations with this energy 116

d. nrConformations (-2) = 116

nrConformations (-1) = 764

nrConformations (0) = 3187

P(-2) = 0.0285

P(-1) = 0.1879

P(0) = 0.7836