Problem set 4

Due November 17, 2026

1. Demonstrate that the radius of gyration of a linear polymer chain with n bonds [and, consequently, $(n+1)$ beads numbered from 0 through n]

$$s^2 = \frac{1}{n+1}\sum_{i=0}^{n} \|\mathbf{r}_i - \mathbf{r}_C\|^2$$

where $\mathbf{r}_i = [x_i, y_i, z_i]^T$ is the vector of the Cartesian coordinates of the ith bead and $\mathbf{r}_C$ is that of the chain center, respectively,

$$\mathbf{r}_C = \frac{1}{n+1}\sum_{i=0}^{n} \mathbf{r}_i$$

can be expressed in terms of site distances

$$s^2 = \frac{1}{(n+1)^2}\sum_{i=0}^{n-1}\sum_{j=i+1}^{n} r_{ij}^2$$

where

$$r_{ij} = \|\mathbf{r}_j - \mathbf{r}_i\| = \sqrt{(x_j - x_i)^2 + (y_j - y_i)^2 + (z_j - z_i)^2}$$

2. Using the UNRES server (`https://unres-server.chem.ug.edu.pl`), run Langevin dynamics simulations for polyglycine chains with 10, 20, and 40 residues (run 200,000 MD steps as per standard settings), starting from random-generated structures at $T = 350$ K. Compute the average end-to-end distance from each run. Make a plot of the square of the end-to-end distance in chain length and determine its slope to calculate the characteristic ratio (C_∞)) defined as

$$C_\infty = \lim_{n\to\infty} \frac{\langle r_n^2 \rangle}{nb^2}$$

where r_n is the end-to-end distance for an n-bead chain and b is the bond length; for the UNRES model, $b = 3.8$ Å.

Use the data of the second half of each trajectory.

To access the data, click the "Download as zip" button and unpack the zip file. The end-to-end distance can be calculated either exactly by extracting the coordinates stored in `file_GB000.pdb` and computing the distance between the first and the last 'CA' atom of each conformation or, in a simpler manner, by extracting the radius of gyration from `file_GB000.stat`, in which it is stored in column #9, and taking advantage of the fact that the square of the radius of gyration is equal to 1/6 of the square of the end-to-end distance in the long-chain limit (`9.012` in a sample line of a `file_GB000.stat` file quoted below.

```
 600 120.00 44.068 86.450 130.518 0.559 369.822 350.000 9.012
0 0.03294 232.347 0
```

Compare the obtained value with that calculated by Tanaka and Nakajima (*Polymer J.*, **1971**, 2, 717-724) who obtained a value of 2.17. Comment on the difference.