

## Mini Project 1: Self-avoided random walk

Selenium (Se) is known to form linear chain polymers in which the bond angles about any Se centre is close to 90 degrees and all Se-Se bonds have the same length  $a$ . Assuming that all dihedral angles can only be one of 0, 90, 180 or 270 degrees, build a Se polymer chain with  $N$  atoms by using a self-avoided random walk (SARW) on a 3-dimensional grid of  $M \times M \times M$  points, with  $M = 50$ . Assume that each grid point has a cubic volume  $a^3$  so that the grid point separation in each direction is  $a$ . The grid thus represents a cubic box extending from 0 to  $Ma$  in any of the three cartesian directions.

A) Consider the following values for  $N$  : 10, 20, 40, 60, and 80. For each value

1. Generate 20 polymers SARW procedure ensuring that in each polymer no atom falls outside the box.
2. Plot a histogram of the end-to-end distances  $R_N$  (in units of  $a$ ) obtained from the 20 polymers.
3. Calculate the average end-to-end distance  $\langle R_N \rangle$  and its variance in the distribution,  $\langle R_N^2 \rangle$ .
4. Compute the average time taken to add a new atom to the polymer ( $t_N$ ).

B) Obtain plots of  $\langle R_N \rangle$ ,  $\langle R_N^2 \rangle$  and  $t_N$  as a function of  $N$ .

C) Write a short paragraph (maximum of 500 words) on what you understood from this project.

**SARW:** To perform a self-avoided random walk, start from the origin (0,0,0) and add an atom there ( $r_0$ ). Next, using a (pseudo-)random generator, generate a triplet of integers (i,j,k) where i,j,k could be either +1 or -1. Adding this to the previous coordinate gives the guess for the location of the next atom in the chain. If this new position is not on top of an existing atom and if its not outside the box then accept the position ( $r_1$ ). Repeat the site generation step from the newly created site until  $N$  atoms have been added. For end-to-end distance calculate  $|r_{N-1} - r_0|$ .

**Note:** It is important to check the performance of your random-number generator. Provide a test for the same along with the rest of the answers.