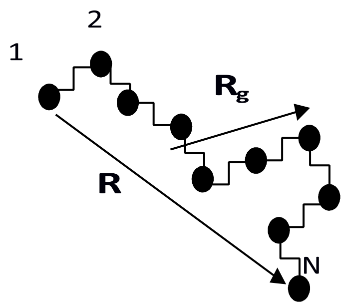
1. ***Ergodicity - Size of a single polymer molecule in an ideal solution***

The size of a single, linear polymer molecule in an ideal solution ($\Delta H_{mix} = 0$) can be described by a random walk. The random walk picture describes the size of a polymer. To illustrate this concept, we can imagine the polymer molecule as a series of *N* beads connected by (*N* - 1) springs (also known as the *bead-spring model*). Then, the backbone of the polymer molecule follows a random walk, and the mean square end-to-end distance is described by the equation,



$$\boxed{\langle \boldsymbol{R} \cdot \boldsymbol{R} \rangle = (N-1)b^2 \approx Nb^2}$$

which is essentially a random walk result. Here, *b* is the equilibrium spring (bond) length. Similarly, the radius of gyration of the polymer is given by

$$\boxed{\langle R_g^2 \rangle \approx \frac{1}{6} N b^2}$$

You are provided with a LAMMPS script (**`in.polymer`**) with which you can run a molecular dynamics simulation of a polymer bead spring model. The LAMMPS script produces two output files, (1) a dump file with position coordinates, and (2) a "**`polymer.out`**" file which has the radius of gyration of the polymer as a function of time.

You can run this file in a loop to run replica systems which are part of an ensemble, and can calculate ensemble averages at the end. There are parts of the input LAMMPS script marked as **`*MODIFY*`** which you can modify. To run the LAMMPS program, use the following command at the prompt,

```
> ./lmp_g++ < in.polymer
```

The input file is a data file called **`data.polymer.`*****N*** where *N* corresponds to the number of beads in the polymer chain.

Run the program and answer the following,

a. For $N = 20$ and an ensemble size of 10, calculate the ensemble-average value of the radius of gyration of the polymer.

b. For any one system from the ensemble in part (a), calculate the time-averaged value of the radius of gyration for the polymer with $N = 20$.

c. Show that the values in parts (a) and (b) satisfy the ergodic hypothesis.

d. Calculate the ensemble-average and time-average values for $N = 20$, 30, 40, 50 and 100. Prepare a table to list the values and show that ergodicity is satisfied.

e. Plot $\langle R^2_g \rangle^{1/2}$ *vs.* N from the table in part (d) on a log-log plot and calculate the slope of the plot. What is the value of the slope? What is the value you expect from Eq. (2)?

NOTE: You can visualize the trajectories in the dump file using the visualization tool VMD.