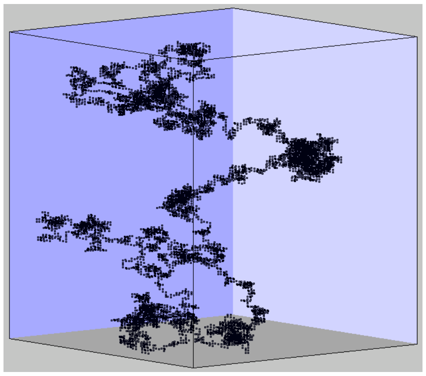
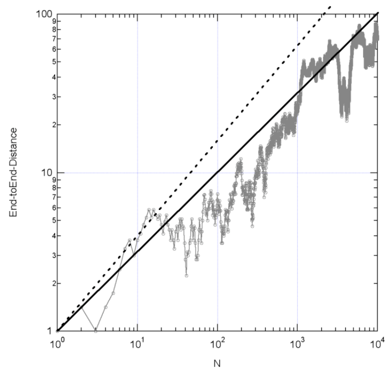
# 070402  Quiz 1 Polymer Properties

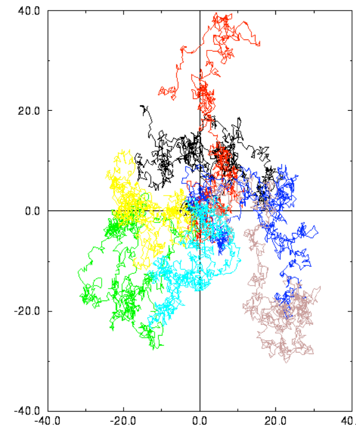
The polymer chain is modeled as a random structure as if the atoms of an ideal gas were tied together in a string. The following picture (a) shows an attempt at simulating a random walk on a cubic lattice. (b) shows the distance from the start of the chain as a function of chain index. (c) shows 7 such walks.



(a)




(b)




(c)

1) Do you agree or disagree with the following statements (explain your position):

   a) The walk in (a) is not random because there are several locations where clustering can be seen and clustering is not random.

   b) The walk in (a) is not random because it crosses itself in several locations.

   c) Figure 1 (b) shows the end to end distance as a function of chain index but because the walk does not follow the lower line it is not random. (Explain the lower line.)

   d) The walks in (c) are not random because they vary in length and direction.

2) A series of simulations of the type shown above could be used to generate a probability distribution for the end-to-end distance of random walks of length N steps. (Figure 1 (c) above shows 7 2D-simulations for example.)

   a) What function, P(R) would describe the probability of finding a walk of length R as a function of N and the step length $l_K$?

   b) Give this function.

   c) Is this a symmetric function about 0? Explain.

3) Using the function you wrote in question 2 it is possible to calculate moments of the distribution, for example the mean, $\langle R \rangle$, is given by $\langle R \rangle = \int R\, P(R)\, dR$.

   a) Give the value of $\langle R \rangle$. In words explain this value.

   b) Give the value of $\langle R^2 \rangle$. In words explain this value.

   c) Give the value of $\langle R^3 \rangle$. In words explain this value.

4) Explain how the value for $\langle R^2 \rangle$ you gave in question 3 can be obtained by considering the double sum of dot products of paired vectors in the chain.

5) Random walks are often constructed using a cubic lattice. How do you think this lattice effects the walk, that is how would a walk on a square lattice differ from a walk on a cubic lattice or a random walk in 3D space that is freely jointed?

Answers : **070402 Quiz 1 Polymer Properties**

1a) In a random spatial distribution you expect to see clustering that is randomly arranged. This is similar to the distribution of darts in a poorly thrown game of darts. The absence of clustering indicates that there is a mechanism at play that leads to the repulsion of chain elements such as excluded volume.
b) Random walks generally cross themselves since there is no excluded volume in a random walk.
c) The lower line follows 1 decade or R for 2 decades of N so 2 log(R) = log(N) or $\log(R^2) = \log(N)$ for the expression $R^2 = Nl_K^2$. The walk doesn't exactly follow this law but it is fairly close at large N. The law is followed for the average of a collection of walks not for an individual walk.
d) Random walks are expected to vary randomly in direction and length about an RMS value.

2a) The Gaussian distribution function describes such as walk with $\sigma^2 = Nl_K^2$.
b) $P(R) = \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^3 \exp\left(\frac{-3R^2}{2\sigma^2}\right)$
c) The function is symmetric about 0 since only $R^2$ occurs in the function.

3a) $\langle R \rangle = 0$ since the function is symmetric
b) $\langle R^2 \rangle = Nl_K^2$ The value is the classic result for a random walk.
c) All odd moments are 0 for a symmetric distribution function, $\langle R^3 \rangle = 0$.

4) $\langle R^2 \rangle = \sum_{j=1}^{n} \sum_{i=1}^{n} \langle r_i \bullet r_j \rangle = \sum_{j=1}^{n} \sum_{i \neq j}^{n} \langle r_i \bullet r_j \rangle + \sum_{i}^{n} \langle r_i \bullet r_i \rangle = nl_K^2$
The double sum is split in to two parts where i ≠ j and i = j. For i ≠ j there is no memory between two steps so no correlation and the average is 0 so the first sum is a sum of 0's. The second sum is the square of the same length which is summed n times.

5) The lattice effects $l_K$ but not the scaling behavior of the walk.