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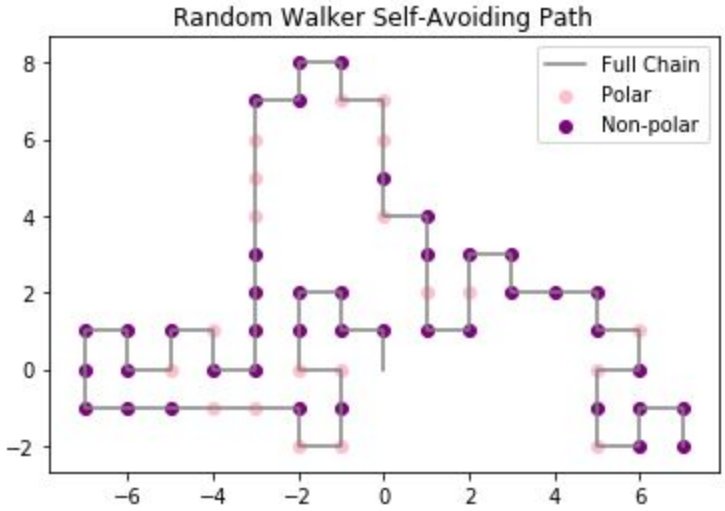
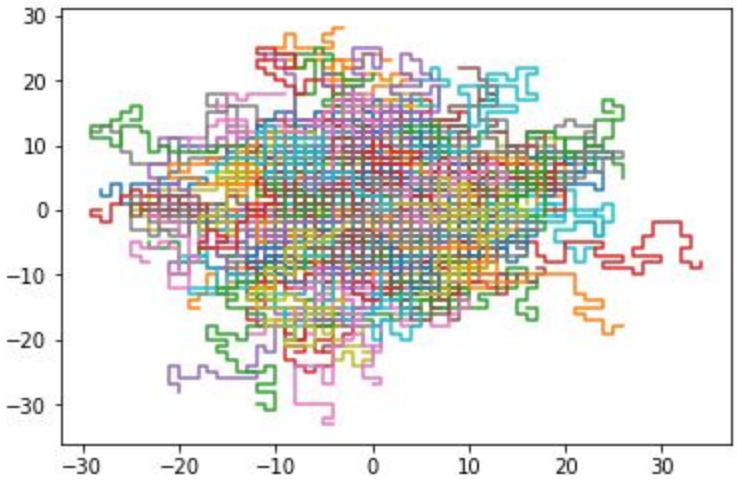
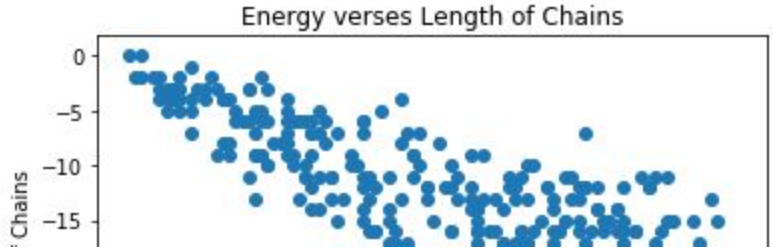
Lab 3
Self-Avoiding Random Walk

The plot below shows one random walker that is self-avoiding in its path. The gray line shows the path and the two colored dots show the polar monomers and non-polar monomers. In a 2-D plot, the succeeds thus far for any number of steps provided. There is no crossover or returning to previous stops/spots. If you view the energy values, it is not quite correct. The value is usually just a few values too high. (i.e. 3 versus 2 or 7 versus 5). This is most likely due to double counting particular paired non-polar monomers that are not connected.



When running multiple simulations, the function still works properly and can handle relatively large values for number of steps. The energy varies with the length. When viewing the trend is it not quite what I expected. There is an overall trend that the energy will increase with the length of the chain, but there is more of a spread in values of the energies of the greater chain lengths.



This could be due to the way I randomize the selection of the polarity of the monomer. How this compares to other professional simulations, it seems too simple in nature. But, in what little I have looked into molecular dynamics, It seems that the trend of a spread in energy is potentially what is expected, according to Toxvaerd, Heilmann, Dyre in their article “Energy conservation in molecular dynamics simulations of classical systems” published in The Journal of Chemical Physics in 2012. It seems energy is conserved but there are variations within the energy proportional to N, the number of steps.

Reference:
https://doi.org/10.1063/1.4726728