Homework 13 Polymer Physics
Due Monday April 21, 2025

LAMMPS is a molecular dynamics package that can be used for coarse grain simulation of spheres. There is a nice webpage that takes you through implementation of LAMMPS on your computer which requires some downloads and compilation. This is marginally easy to do.
https://www2.ph.ed.ac.uk/~cbrackle/lammps_tutorial.html
The first five of these simulations are doable, the sixth is challenging. I'd like you to do the first five simulations on your computer after downloading the package and attempt to do the sixth simulation. Also answer the question at the end of this document. This should give you an idea of what is possible using LAMMPS for soft materials. This webpage was put together by Chris Brackley at Edinburgh University. He published a paper in *Nature* in 2021 that you will find familiar once you complete the fifth example simulation. Brackley C, Gilbert N, Michieletto D, Papantonis A, Pereira MCF, Cook PR, Marenduzzo D *Complex small-world regulatory networks emerge from the 3D organisation of the human genome* Nat. Comm. **12** 5756 (2021).

For this homework, please turn in screen shots of the final structures in each of the simulations using Ovito (a shareware package you can download, open the "dump" files in Ovito).

If you need help you can contact me or you can contact Ugochuckwu Okoli who is my former graduate student now a post doc at the University of Tennessee and who is working with LAMMPS. okoliuo@mail.uc.edu

Question:
Explain what is the "free-energy landscape" for the type of assembly mentioned in Buckley's paper and how does LAMMPS allows you to explore this free-energy landscape.