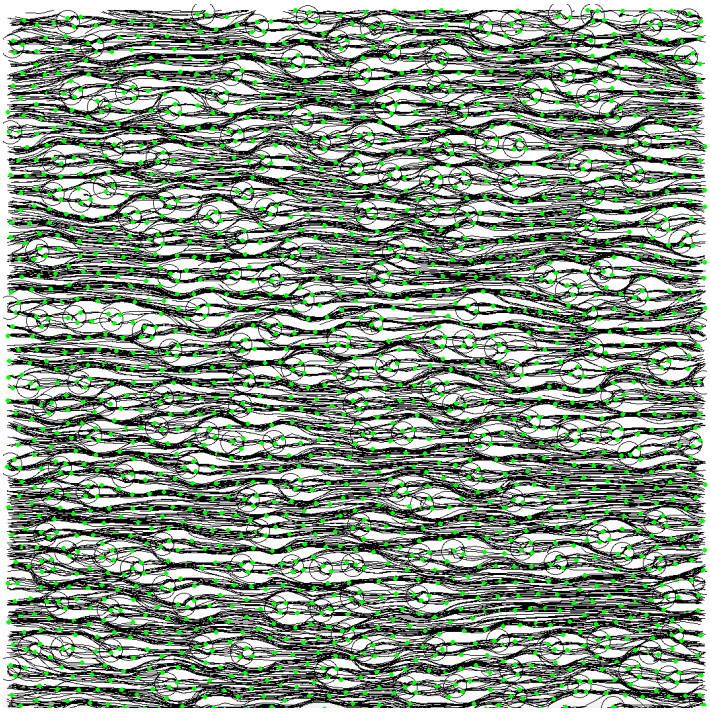
Assignment #2: Molecular Dynamics Simulation, Pinning Sites



Moving through quenched disorder

Simulation Methods course

Fall 2019

Writing the Simulation

On the webpage I give you a code for the version that includes the pinning sites. You can use this version to generate the IV curves.

If you want to rewrite the whole simulation, you should write the simulation in C/C++ or something low level (a language that compiles) so that you can control it better (what happens with the cpu and memory usage). High level languages are not used in simulation because of the performance is more important than the ease of coding. Do not use Java or some high level language, or Matlab to write the simulation itself. You can use these tools or whichever tool you like to plot the results of the simulation. I give you a plot tool that uses X11 libraries and works in Linux + macOS (with some X11 library for macOS like Quartz).

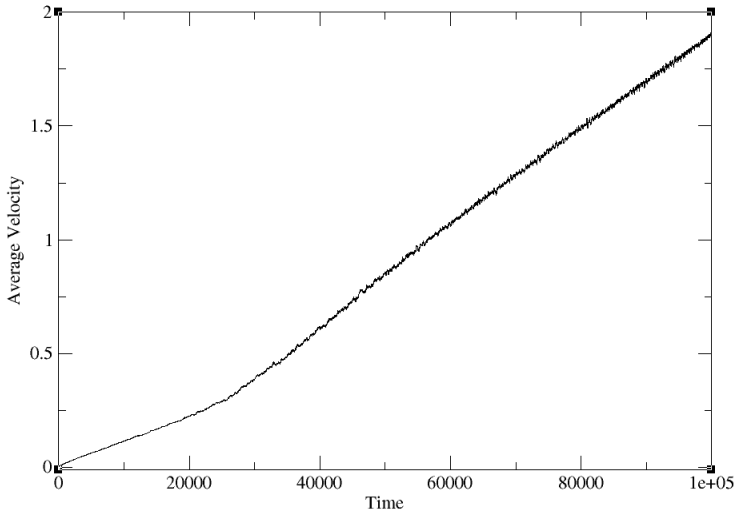
In this molecular dynamics simulation you will simulate a system made of one kind of particles that are being pulled through the system. You can see in the **calculate_external_force**() routine that **the force is increased slowly** and gradually in time. You can also see in the write_statistics() routine that we write out the average velocity vs time (you can change that to write average velocity vs driving force).

You can make the change in the code you are using for plotting to show where the pinning sites are (as large circles).

You have the code that does the simulation and the plot program. The code includes the force calculation for the pinning sites. You need to show that by making the pinning sites stronger or more numerous, the IV curves change

What you need to present:

- you ran the code for different number of pinning sites and you see a change in the IV curve, with more pinning sites the deviation from the straight line (ohmic regime) is larger (like in picture this is for 400 pinning sites:)

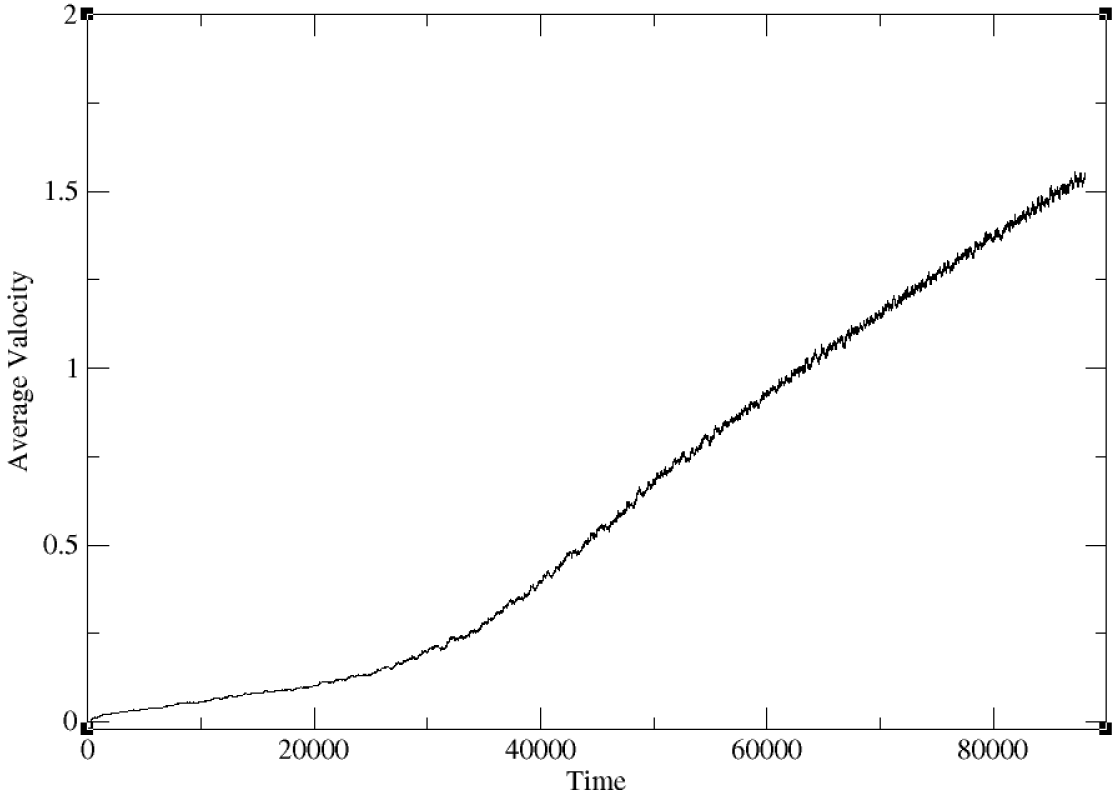


can

this

- you ran the code for different strengths of pinning sites
this is where we store how strong the pinning sites are:
pinningsites[i].f_max if you change this and run again the de-pinning (the dip in the IV curve) should happen later in time (at higher force) right now it's 2.0 you can try 1.0, 1.5, 2.0, 2.5, 3.0 etc

- I will want to see some videos with high number of pinning sites
- I will ask about aspects of the code to see if you understood it


2
1.5
1
0.5
0
Average Valocity
0
20000
40000
60000
80000
Time