PHYS 2425: Lab 2
Statistical Mechanics for Optimization

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PHYS 2425: Computational physics

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Abstract

The main objective of this lab is to solve complex optimization problems by using the principle that nature finds the lowest energy by cooling down slowly. By comparing gradient descent to simulated annealing we will be able to write a simulation that arranges atoms into perfect crystal structures automatically. This process shows the geometric structure of atoms in a crystal that minimizes the total energy.

Introduction

In this lab we learned how to solve physics problems while using simulated annealing. Annealing is a heat treatment process that involves heating a metal or material to a specific high temperature for an amount of time and then cooling it slowly. We did this by implementing the Metropolis Criterion which uses thermal noise to escape local minima. Then to apply real physics we simulate Lennard-Jones Clusters which are small groups of particles interacting through LJ pair potential, which balances short-range electron repulsion and long-range van der Waals attraction.

Methods

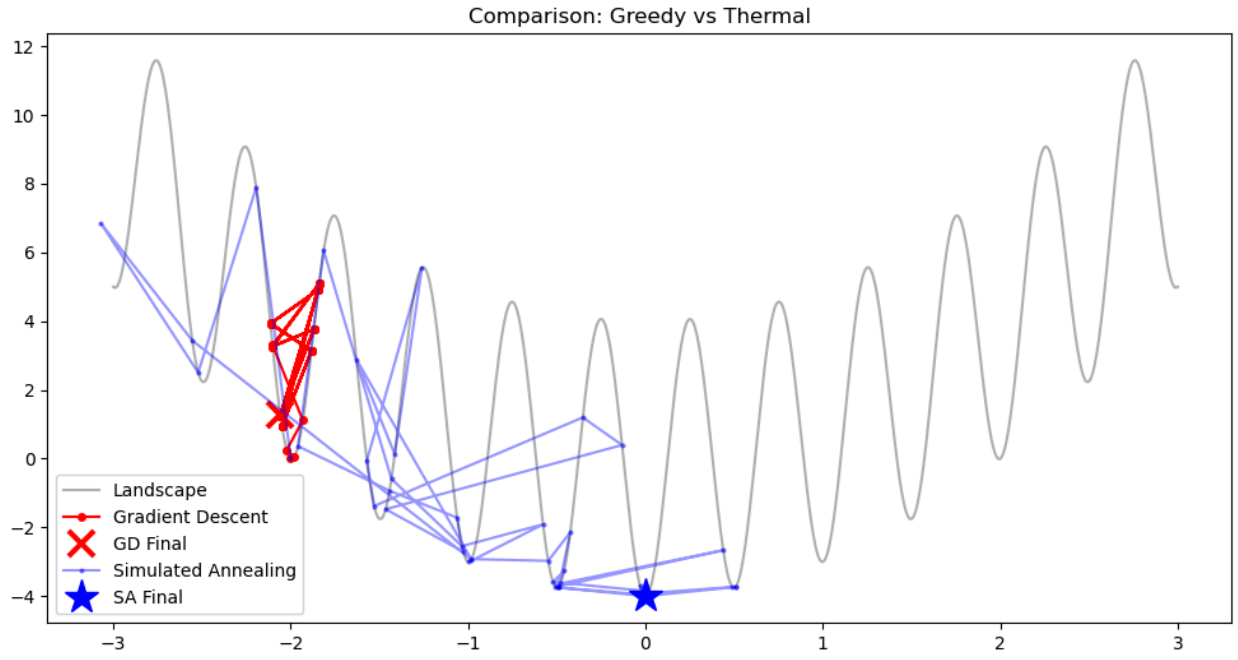
We started with a one dimensional function that represents a difficult energy landscape, but has a general parabolic shape and is covered in local ripples to show the differences between simulated annealing and gradient descent when solving for a minimum. This effect was created by a cos function. Next we calculated slope by using the gradient descent, which was done with a simple for loop. We then went to make a “physical solver” to find the local lows. The algorithm works by randomly moving the x to a new spot, calculate the energy difference, then move to a new location where the energy could be even lower. The graph will be included in the appendix, figure 1.

Now, for the real world application, and part 2 of the lab, we simulate actual crystal growth, argon specifically. We redefine the energy again that allows us to calculate the way the molecules will bind, and allow us to find the connection that is the most structurally stable, with the least energy to bind. The system cooling and the graph of what the structure will look like are also attached in the appendix, figure 2.

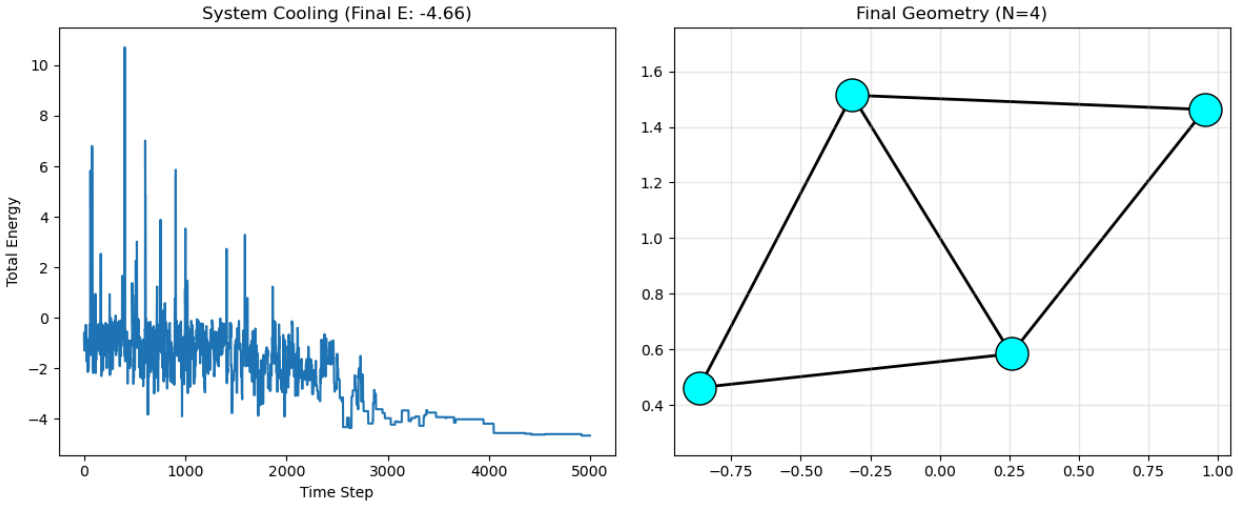
Discussion

All the questions are answered in the code.

Appendix



(Figure 1)



(Figure 2)