

Ps 2 Problem 2

Adam Guerin

September 18, 2023

Abstract

This document has an outline of a program that calculates the madelung constant in two ways

1 Introduction

Madelung constant is a constant that depends on your material in condensed matter physics and an ions distance between different charges in the material.

2 Methods

I calculated it in two different ways. A naive triple for loops and using the `numpy.where()` function. I tried to be all clever and turn a 3d array into a 1d and just using `np.sum` after weighting correctly but i couldn't get it to work. `numpy.where()` was about 5 times faster than the triple for loops.

3 Results

Both gave the same value 1.75 but in different times 2.4 seconds and .5 seconds for the for loops and the where function respectively.

4 Discussion

Only needed about a 50x50x50 lattice to solve this correctly. If you needed a much bigger one the naive approach would probably be much worse than it is.