Computational Physics: Problem Set 2

Zifeng Li

September 20, 2023

1 Questions

1.1 What is the binary representation of the decimal integer 121?

1111001

1.2 Exercise 2.9 of Newman.

The chosen number of L is 150. The calculated Madelung constant for nacl is: 1.743728380221397 (using for loop method). For loop method elapsed time in seconds: 33.252091902000004. The calculated Madelung constant for nacl is: 1.743728380220058 (using arrays). Array method elapsed time in seconds: 1.556169262.

1.3 Exercise 3.7 of Newman.

The resulted figure is shown below in Figure 1.

1.4 Exercise 4.2 of Newman.

For part a, the resulted roots are -9.999894245993346e-07 and -999999.999999. For part b, the resulted roots are -1000010.5755125057 and -1.000000000001e-06. There are clearly some errors in the results. In fact, the error stems from discriminant term because when b is positive and much larger than a and c, the discriminant term will be very close to b. When the computer calculate -b+discriminant, the two terms nearly cancel each other out due to the inaccuracy in float numbers in python. So we need to use the -b+discriminant part of the formula in part a and the -b-discriminant part of the formula in part b to minimize the errors for positive b value. For part c, the resulted roots are -9.999894245993346e-07, -1.0000000000001e-06.

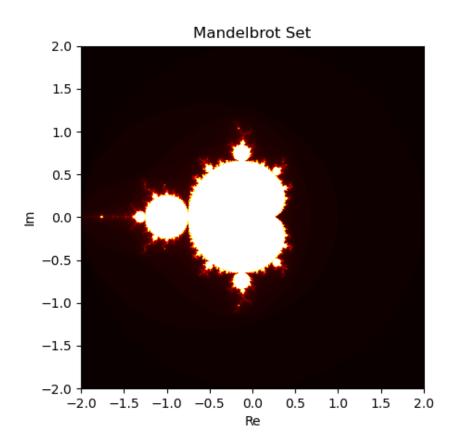


Figure 1: This is just an example. Notice that both axes of the figure are labeled, and the units are given.