HW2

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1 Answers

1. the binary representation of the decimal integer 121 is 1111001.

L in my case is defined as total number of atoms instead of number of atom for each side.

2. Madelung constant for NaCl with L =10000000: -1.752935294 using for loop, it takes 9.706836938sec, Madelung constant for NaCl with L =10000000: -1.752935294 without using for loop, it takes 0.319865226 sec. From this result, we can see that both methods gives similar Madelung constant, but it is a lot faster for the method without using for loop.

3. See figure 1 below.

4. (a) the two solutions for this equation is (-9.999894245993346e-07, -999999.999999)

   (b) Derivation: $x = \frac{-b\pm\sqrt{b^2-4ac}}{2a} = \frac{-b\pm\sqrt{b^2-4ac}}{2a}\frac{-b\mp\sqrt{b^2-4ac}}{-b\mp\sqrt{b^2-4ac}} = \frac{4ac}{2a(-b\mp\sqrt{b^2-4ac})} = \frac{2c}{-b\mp\sqrt{b^2-4ac}}$

   the two solutions for this equation is (-1.000000000001e-06, -1000010.5755125057). Those two answers computed by computer is not the same, which may due to the limitations of floating-point arithmetic in representing such numbers during computation. That is, since b squared is very large compare to 4ac, when they perform subtraction there may be round-off error occurs.

   (c) by increasing the precision of each number, the result I got is (-0.0000010000000000010000,-999999.999998999999999999000). In the code I wrote, I assume there will be two roots for the entered quadratic.

2 Figure

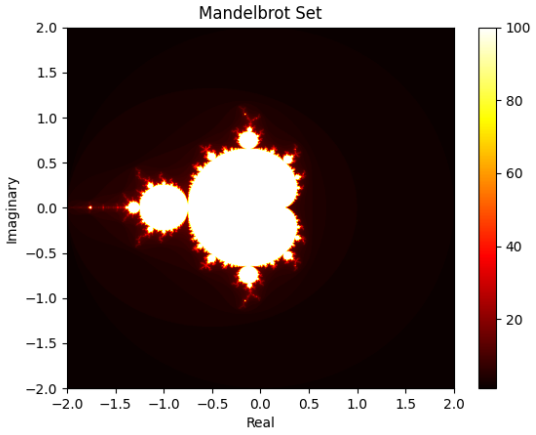

Figure 1: The Mandelbrot Set, plot using hot scheme