Computational Physics HW2

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P1: Numpy.float32 represents a real number with 32-digit of binary numbers. It approximates the number to be the form of $\pm(1 + \sum_{i=0}^{22} m_i 2^{-(i-23)})2^{e-127}$ then represents it with the nearest mantissa m_i and exponent e from the format. In the 32-digit of binary numbers, the first digit on the left represents the positive or negative sign; the following 8 digit is the binary form of the exponent e; the last 23 digit are the mantissa ms. In this method, 100.98763 is represented by 01000010110010011111100110101011. The round-off error of such representation is about $2.7514648479609605 \times 10^{-6}$.

P2: From the equation given in Exercise 2.9, we can cancel the physical constants on both sides and get $M = \sum_{i,j,k=-L}^{L} (-1)^{i+j+k} \frac{1}{\sqrt{i^2+j^2+k^2}}$, not i=j=k=0. In the first method, we write a for loop to add the potentials from atoms at different positions on the grid. In the second method, we write coordinates of the grid and calculate potentials as an array-like object. Notice here we have to use floating point data type to record coordinates such that certain calculations could be allowed. For L = 100, the time to execute for loop is about 40s whereas for grid method, it's only 0.25s. Both methods agree the Madelung constant for sodium in sodium chloride to be -1.7418.

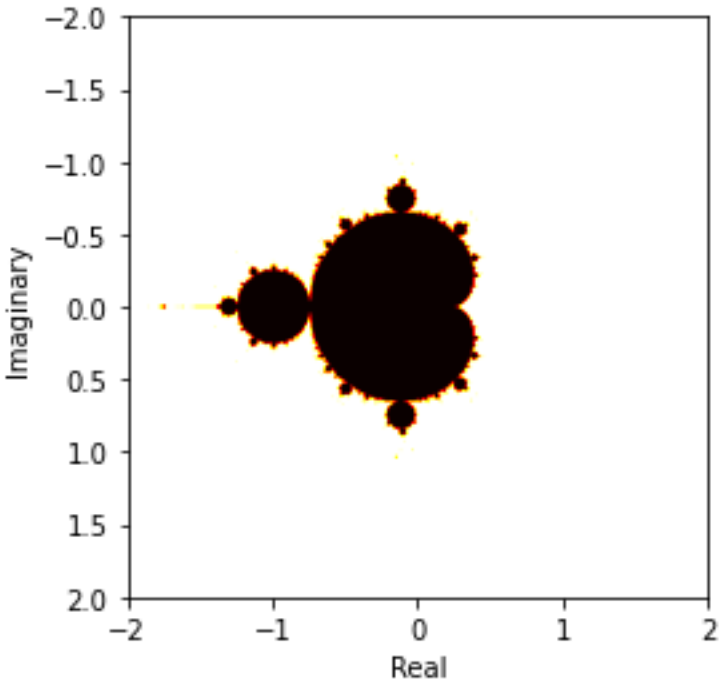

Figure 1: **Mandelbrot**

P3: