PH 235 FALL 2015

ASSIGNMENT 2

Assigned Date: February 6, 2017

Due Date: 11:50pm, February 16, 2017 only via moodle (See syllabus for late policy)

Total Points: 100

All problems in this assignment are from the optional textbook for the course *Computational Physics* authored by Mark Newman.

Instructions:

1. Create a folder titled YourLastName-HW2.
2. In this parent folder, create subfolders, one for each of the problems below and name each subfolder as YourLastName-ExerciseNumber for easier tracking.
3. Populate the folders with (a) the solution code for each problem, (b) screen shots of results when possible and (c) a text document with a short description of your approach, whether you successfully solved the problem. If you did not solve the problem, explain solution status (partial credit will be given for reasonable attempts).
4. Submit a zipped version of the parent folder to the moodle assignment link.

Problem 1: Ex 3.The Mandelbrot set(20 points)

The Mandelbrot set, named after its discoverer, the French mathematician Benoît Mandelbrot, is a *fractal*, an infinitely ramified mathematical object that contains structure within structure within structure, as deep as we care to look. The definition of the Mandelbrot set is in terms of complex numbers as follows.

Consider the equation

$$z' = z^2 + c,$$

where z is a complex number and c is a complex constant. For any given value of c this equation turns an input number z into an output number z'. The definition of the Mandelbrot set involves the repeated iteration of this equation: we take an initial starting value of z and feed it into the equation to get a new value z'. Then we take that value and feed it in again to get another value, and so forth. The Mandelbrot set is the set of points in the complex plane that satisfies the following definition:

> *For a given complex value of c, start with $z = 0$ and iterate repeatedly. If the magnitude $|z|$ of the resulting value is ever greater than 2, then the point in the complex plane at position c is* not *in the Mandelbrot set, otherwise it is in the set.*

In order to use this definition one would, in principle, have to iterate infinitely many times to prove that a point is in the Mandelbrot set, since a point is in the set only if the iteration never passes $|z| = 2$ ever. In practice, however, one usually just performs some large number of iterations, say 100, and if $|z|$ hasn't exceeded 2 by that point then we call that good enough.

Write a program to make an image of the Mandelbrot set by performing the iteration for all values of $c = x + iy$ on an $N \times N$ grid spanning the region where $-2 \leq x \leq 2$ and $-2 \leq y \leq 2$. Make a density plot in which grid points inside the Mandelbrot set are colored black and those outside are colored white. The Mandelbrot set has a very distinctive shape that looks something like a beetle with a long snout—you'll know it when you see it.

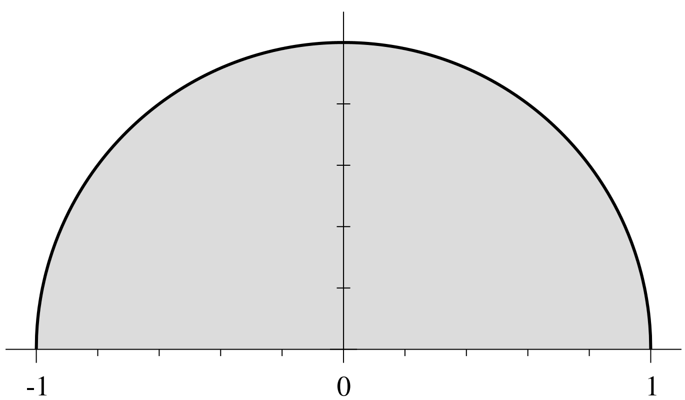
Hint: You will probably find it useful to start off with quite a coarse grid, i.e., with a small value of N—perhaps $N = 100$—so that your program runs quickly while you are testing it. Once you are sure it is working correctly, increase the value of N to produce a final high-quality image of the shape of the set.

Problem 2: Ex 4.4: Calculating integrals (10 points)

Suppose we want to calculate the value of the integral

$$I = \int_{-1}^{1} \sqrt{1 - x^2}\, dx.$$

The integrand looks like a semicircle of radius 1:



and hence the value of the integral—the area under the curve—must be $\frac{1}{2}\pi = 1.57079632679\ldots$

Alternatively, we can evaluate the integral on the computer by dividing the domain of integration into a large number N of slices of width $h = 2/N$ each and then using the Riemann definition of the integral:

$$I = \lim_{N \to \infty} \sum_{k=1}^{N} h y_k \,,$$

where

$$y_k = \sqrt{1 - x_k^2} \qquad \text{and} \qquad x_k = -1 + hk.$$

We cannot in practice take the limit $N \to \infty$, but we can make a reasonable approximation by just making N large.

1. Write a program to evaluate the integral above with $N = 100$ and compare the result with the exact value. The two will not agree very well, because $N = 100$ is not a sufficiently large number of slices.

2. Increase the value of N to get a more accurate value for the integral. If we require that the program runs in about one second or less, how accurate a value can you get?

Problem 3: Ex 5.7 Trapezoidal and Romberg (20 points)

Consider the integral

$$I = \int_0^1 \sin^2 \sqrt{100x}\, \mathrm{d}x$$

1. Write a program that uses the adaptive trapezoidal rule method of Section 5.3 and Eq. (5.34) to calculate the value of this integral to an approximate accuracy of $\epsilon = 10^{-6}$ (i.e., correct to six digits after the decimal point). Start with one single integration slice and work up from there to two, four, eight, and so forth. Have your program print out the number of slices, its estimate of the integral, and its estimate of the error on the integral, for each value of the number of slices N, until the target accuracy is reached. (Hint: You should find the result is around $I = 0.45$.)

2. Now modify your program to evaluate the same integral using the Romberg integration technique. Have your program print out a triangular table of values, as on page 161, of all the Romberg estimates of the integral. Calculate the error on your estimates using Eq. (5.49) and again continue the calculation until you reach an accuracy of $\epsilon = 10^{-6}$. You should find that the Romberg method reaches the required accuracy considerably faster than the trapezoidal rule alone.

Problem 4: Ex 5.21 Electric field of a charge distribution(25 points)

Suppose we have a distribution of charges and we want to calculate the resulting electric field. One way to do this is to first calculate the electric potential ϕ and then take its gradient. For a point charge q at the origin, the electric potential at a distance r from the origin is $\phi = q/4\pi\epsilon_0 r$ and the electric field is $\mathbf{E} = -\nabla\phi$.

1. You have two charges, of $\pm 1\,\mathrm{C}$, 10 cm apart. Calculate the resulting electric potential on a $1\,\mathrm{m} \times 1\,\mathrm{m}$ square plane surrounding the charges and passing through them. Calculate the potential at 1 cm spaced points in a grid and make a visualization on the screen of the potential using a density plot.

2. Now calculate the partial derivatives of the potential with respect to x and y and hence find the electric field in the xy plane. Make a visualization of the field also. This is a little trickier than visualizing the potential, because the electric field has both magnitude and direction. One way to do it might be to make two density plots, one for the magnitude, and one for the direction, the latter using the "`hsv`" color scheme in `pylab`, which is a rainbow scheme that passes through all the colors but starts and ends with the same shade of red, which makes it suitable for representing things like directions or angles that go around the full circle and end up where they started. A more sophisticated visualization might use the arrow object from the `visual` package, drawing a grid of arrows with direction and length chosen to represent the field.

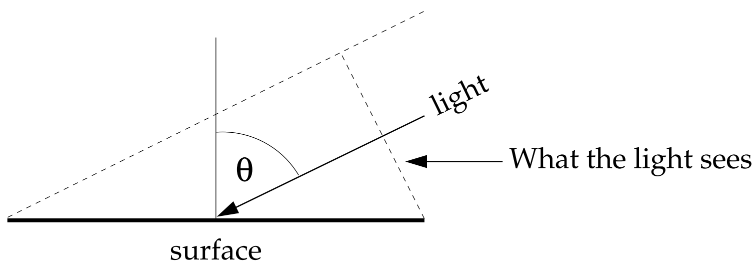
3. Now suppose you have a continuous distribution of charge over an $L \times L$ square. The charge density in Cm^{-2} is

$$\sigma(x,y) = q_0 \sin\frac{2\pi x}{L} \sin\frac{2\pi y}{L}.$$

Calculate and visualize the resulting electric field at 1 cm-spaced points in 1 square meter of the xy plane for the case where $L = 10\,\mathrm{cm}$, the charge distribution is centered in the middle of the visualized area, and $q_0 = 100\,\mathrm{Cm}^{-2}$. You will have to perform a double integral over x and y, then differentiate the potential with respect to position to get the electric field. Choose whatever integration method seems appropriate for the integrals.

Problem 5: Ex 5.23 Image Processing and the STM(25 points)

When light strikes a surface, the amount falling per unit area depends not only on the intensity of the light, but also on the angle of incidence. If the light makes an angle θ to the normal, it only "sees" $\cos\theta$ of area per unit of actual area on the surface:



So the intensity of illumination is $a\cos\theta$, if a is the raw intensity of the light. This simple physical law is a central element of 3D computer graphics. It allows us to calculate how light falls on three-dimensional objects and hence how they will look when illuminated from various angles.

Suppose, for instance, that we are looking down on the Earth from above and we see mountains. We know the height of the mountains $w(x,y)$ as a function of position in the plane, so the equation for the Earth's surface is simply $z = w(x,y)$, or equivalently $w(x,y) - z = 0$, and the normal vector $\mathbf{v}$ to the surface is given by the gradient of $w(x,y) - z$ thus:

$$\mathbf{v} = \nabla[w(x,y) - z] = \begin{pmatrix} \partial/\partial x \\ \partial/\partial y \\ \partial/\partial z \end{pmatrix} [w(x,y) - z] = \begin{pmatrix} \partial w/\partial x \\ \partial w/\partial y \\ -1 \end{pmatrix}.$$

Now suppose we have light coming in represented by a vector $\mathbf{a}$ with magnitude equal to the intensity of the light. Then the dot product of the vectors $\mathbf{a}$ and $\mathbf{v}$ is

$$\mathbf{a} \cdot \mathbf{v} = |\mathbf{a}|\,|\mathbf{v}| \cos\theta,$$

where θ is the angle between the vectors. Thus the intensity of illumination of the surface of the mountains is

$$I = |\mathbf{a}|\cos\theta = \frac{\mathbf{a}\cdot\mathbf{v}}{|\mathbf{v}|} = \frac{a_x(\partial w/\partial x) + a_y(\partial w/\partial y) - a_z}{\sqrt{(\partial w/\partial x)^2 + (\partial w/\partial y)^2 + 1}}.$$

Let's take a simple case where the light is shining horizontally with unit intensity, along a line an angle ϕ counter-clockwise from the east-west axis, so that $\mathbf{a} = (\cos\phi, \sin\phi, 0)$. Then our intensity of illumination simplifies to

$$I = \frac{\cos\phi\,(\partial w/\partial x) + \sin\phi\,(\partial w/\partial y)}{\sqrt{(\partial w/\partial x)^2 + (\partial w/\partial y)^2 + 1}}.$$

If we can calculate the derivatives of the height $w(x, y)$ and we know ϕ we can calculate the intensity at any point.

1. In the on-line resources you'll find a file called `altitude.txt`, which contains the altitude $w(x, y)$ in meters above sea level (or depth below sea level) of the surface of the Earth, measured on a grid of points (x, y). Write a program that reads this file and stores the data in an array. Then calculate the derivatives $\partial w/\partial x$ and $\partial w/\partial y$ at each grid point. Explain what method you used to calculate them and why. (Hint: You'll probably have to use more than one method to get every grid point, because awkward things happen at the edges of the grid.) To calculate the derivatives you'll need to know the value of h, the distance in meters between grid points, which is about 30 000 m in this case. (It's actually not precisely constant because we are representing the spherical Earth on a flat map, but $h = 30\,000$ m will give reasonable results.)
2. Now, using your values for the derivatives, calculate the intensity for each grid point, with $\phi = 45°$, and make a density plot of the resulting values in which the brightness of each dot depends on the corresponding intensity value. If you get it working right, the plot should look like a relief map of the world—you should be able to see the continents and mountain ranges in 3D. (Common problems include a map that is upside-down or sideways, or a relief map that is "inside-out," meaning the high regions look low and *vice versa*. Work with the details of your program until you get a map that looks right to you.)
3. There is another file in the on-line resources called `stm.txt`, which contains a grid of values from scanning tunneling microscope measurements of the (111) surface of silicon. A scanning tunneling microscope (STM) is a device that measures the shape of surfaces at the atomic level by tracking a sharp tip over the surface and measuring quantum tunneling current as a function of position. The end result is a grid of values that represent the height of the surface as a function of position and the data in the file `stm.txt` contain just such a grid of values. Modify the program you just wrote to visualize the STM data and hence create a 3D picture of what the silicon surface looks like. The value of h for the derivatives in this case is around $h = 2.5$ (in arbitrary units).