UNIVERSITY OF SUSSEX

Scientific Computing

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Assignment 3

Deadline: 12pm on Monday, December 5th, 2016.

Penalties will be imposed for submissions beyond this date.

Final submission date: Tuesday, December 6th, 2016

No submissions will be accepted beyond this date.

1. **Conical float** A conical float (see figure) is free to slide on a vertical rod. When the float is disturbed from its equilibrium position, it undergoes oscillating motion described by the differential equation

$$\ddot{y} = g(1 - ay^3)$$

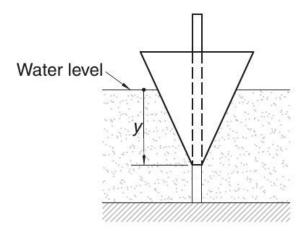
where $a = 1 m^{-3}$ (determined by the density and dimensions of the float) and $g = 9.80665 m/s^2$ is the acceleration of gravity.

- (a) If the float is raised to the position $y_0 = 0.1 \, m$ and released (with zero initial velocity), solve the equation for t = 0 to $2.5 \, s$ and estimate the period and the amplitude of the oscillations. Do the same for initial position $y_0 = 0.9 \, m$. Plot the results. How does the initial displacement affect the results?
- (b) Now consider the linear version of the same problem

$$\ddot{y} = g(1 - ay)$$

with same values of g and a and again estimate the period and amplitude of the oscillations for $y_0 = 0.1$ m and $y_0 = 0.9$ m.

(c) Modify your program so that instead of plotting x against t, it plots dx/dt against x, i.e., the velocity of the oscillators against its position. Such a plot is called a phase space plot. Make sure you say **pylab.axis('equal')** to ensure the plot axes have the same length for the phase space plots. Discuss.



2. **Chemical reaction network:** The *Brusselator* is a theoretical model for an autocatalytic reaction (i.e. one where some of the reactants also serve as catalysts of the reactions) proposed by Ilya Prigogine (Nobel Price in Chemistry

for 1977). The evolution in the concentrations of the catalysts can be described by the (dimensionless) equations:

$$\dot{x} = 1 - (1+b)x + ax^2y \tag{1}$$

$$\dot{y} = bx - ax^2y\tag{2}$$

(for details and derivation see e.g. https://en.wikipedia.org/wiki/Brusselator).

Show how these equations predict x and y to vary for (a) a = 1, b = 1.8 and (b) a = 1, b = 2.02 by plotting in each case (i) x and y as functions of time and (ii) y vs. x (one for the time evolutions and one for x vs. y). Take x(0) = 0 and y(0) = 0 as initial conditions and integrate from t = 0 to t = 100. Discuss the results. This is related to stable points and attractors in dynamical systems and is an example of a chaotic system, where small changes in the initial conditions or parameters could result in large changes in the results.

3. Fourier filtering and smoothing

On Study Direct you'll find a file called dow.txt. It contains the daily closing value for each business day from late 2006 until the end of 2010 of the Dow Jones Industrial Average, which is a measure of average prices of the largest companies of the US stock market.

Write a program to do the following:

- (a) Read in the data from dow.txt and plot them on a graph.
- (b) Calculate the coefficients of the discrete Fourier transform of the data using the function rfft from numpy.fft, which produces an array of $\frac{1}{2}N + 1$ complex numbers.
- (c) Now set all but the first 10% of the elements of this array to zero (i.e., set the last 90% to zero but keep the values of the first 10%).
- (d) Calculate the inverse Fourier transform of the resulting array, zeros and all, using the function irfft, and plot it on the same graph as the original data. You may need to vary the colors of the two curves to make sure they both show up on the graph. Comment on what you see. What is happening when you set the Fourier coefficients to zero?
- (e) Modify your program so that it sets all but the first 2% of the coefficients to zero and run it again. Discuss the results.