UNIVERSITY OF SUSSEX
Scientific Computing
Tutor: Dr. Ilian Iliev, Office: Pev 3 4C5

Problem Sheet 8 (Problem 2 will be assessed)
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. Consider the differential equation (called van der Pol oscillator):

$$x''(t) = -x - \epsilon(x^2 - 1)x'(t), \qquad x(0) = 0.5, x'(0) = 0,$$

where ϵ is a positive constant. As the value of ϵ increases, this equation becomes increasingly stiff.

   (a) Convert this equation to two first-order equations.

   (b) Run the Euler method code (which you made during the last workshop) with $\epsilon = 10$, and $[a, b] = [0, 10\pi]$ and different choices of step-size: $h = 0.02, 0.005, 0.001$. Calculate also an 'exact' solution by using `scipy.integrate.odeint` (**Note that the in-build method has a different interface to the function defining the equation(s) compared to the previously used Runge-Kutta solver - the arguments are reversed! Result is also formatted differently, check the help and the examples in the Jupyter notebook on SD.**) Plot all solutions, including the 'exact' one in one figure using linear axes, and the absolute errors of all solutions with respect to the 'exact' solution in another figure using semi-log axes. What do you observe?

   (c) Solve the same equation using the Runge-Kutta method of 4th order provided in class and $h = 0.02$. What do you observe?

What do you conclude based on your results from (b) and (c)?

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.