GM04/MM04 Exercise 1

The deadline: hand in your work before the reading week.

Format: preferably LaTeX (useful); MS Word is acceptable; handwritten - penalty 10 marks. No binding, use a stapler or a paper clip.

Size: 20 pages maximum.

The Brusselator

The Brusselator is a model of certain autocatalitic reactions described in terms of chemical concentrations $x(t)$ and $y(t)$ where t is time. The governing equations are

$$\frac{dx}{dt} = A - Bx + x^2y - x, \tag{1}$$

$$\frac{dy}{dt} = Bx - x^2y, \tag{2}$$

with positive constants A and B. The system has one equilibrium (i.e. time-independent) state, $x_{eq} = A$, $y_{eq} = B/A$.

The task is to investigate the behaviour of the system for various choices of the parameters A and B.

Part A (worth 70 per cent)

1. Write down a finite-difference fourth-order accurate Runge-Kutta (RK4) approximation of the Brusselator equations on a uniform grid, $t_n = nh$, with the time step h for $n = 0, 1, 2, ...$. No need to derive the RK4 algorithm from scratch, refer to literature.

2. Write down a Matlab code to solve the finite-difference equations subject to initial conditions $x(0) = x_0$, $y(0) = y_0$ for some constants x_0, y_0. You are not allowed to use built-in Matlab solvers such as ode45 or similar.

3. Compute the solution for $A = 2$, $B = 6$, $x_0 = 0$, $y_0 = 1$. You need to decide on a suitable time interval to show the overall trend in the solution and on the value of the time step. Give the reasoning behind your choices. Show the solution as time-dependent graphs $x(t)$, $y(t)$ and also in the phase plane (x, y). It is expected that the solution path in the phase plane will approach a limit cycle as time increases (the limit cycle is a closed orbit corresponding to a time-periodic evolution).

4. Keeping $A = 2$, $B = 6$, the next task is to investigate whether the limit cycle is a global attractor. This means that every trajectory (perhaps except one) becomes asymptotically close to the limit cycle as $t \to \infty$. To check this, make a few more computations, taking x_0, y_0 at several points in different parts of the phase plane (the trajectories can start inside or outside the limit cycle, obviously). Consider only starting points in the first quadrant, $x_0 > 0$, $y_0 > 0$. What is your conclusion with regard to the global 'attractiveness' of the limit cycle?

The next two questions refer to the purely computational side of your investigation.

5. Stability; according to your computations, is the method stable for every choice of the time step?

6. Accuracy of the solution; nominally the RK4 is 4th-order accurate - can you design a procedure to verify this computationally?

Part B. For an extra 30 per cent, investigate as far as you can the behaviour of the Brusselator system for other choices of the parameters A and B keeping these parameters positive (and the initial conditions in the first quadrant).