MATH0086 Exercise 1

The deadline: 5pm on the last Friday before the reading week. Hand-in instructions will be posted on Moodle.
Typesetting: LaTeX is preferred (useful for future); MS Word is acceptable; handwritten answers will incur a penalty of 15 marks.
Size: 15 pages maximum in a single pdf file.

The Brusselator

The Brusselator is a model of certain autocatalytic 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. Denote $x(0) = x_0$, $y(0) = y_0$.

Part A (60 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 $n = 0, 1, 2, \ldots$. You do not need to derive the RK4 algorithm, refer to literature instead. Write a MATLAB code to solve the finite-difference equations. The use of built-in MATLAB solvers such as ode45 or similar is not allowed. Remember to include one sample of the working code in the write-up.

Run the MATLAB commands $A = 1 + \text{rand}$, $B = 6 + 3 * \text{rand}$ once and record the computed values of A, B to four decimal places. This will be your individual choice of the parameters in this part.

Compute the solution of the difference equations with A,B as above and with the initial conditions $x_0 = 0$, $y_0 = 1$. In order to show the overall trend in the solution, you need to choose a suitable time interval and 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 trajectory in the phase plane will approach a limit cycle as time increases (the limit cycle is a closed orbit corresponding to a time-periodic process).

2. The next task is to investigate whether the limit cycle is a global attractor. The global attractor 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). Consider only the starting points in the first quadrant, $x_0 > 0$, $y_0 > 0$. Present all solutions on a single graph in the phase plane. On the basis of your computations, is the limit cycle likely to be a global attractor?

The following two questions address the computational side of your investigation.

3. Stability. According to your computations, would you describe the method as stable (conditionally or unconditionally) or unstable, and why?

4. Accuracy of the solution. Nominally the RK4 is 4th-order accurate - can you design a procedure to verify this computationally? Note that there is no exact solution to the initial-value problem.

Part B (40 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 of the phase plane.