Scientific Computing for D. Phil. Students II
Homework 3

Due at the start of lecture at 3pm on Monday 25 February 2013. The answers you submit should be attractive, brief, complete, and should include program listings and plots where appropriate. If using MATLAB, *the use of "publish" is strongly recommended.*

Problem 1 (Event detection in ODE solvers.) Suppose we want to model a bouncing ball using

$$y'' + 0.1y' = -1, \qquad y(0) = 1, y'(0) = 2,$$

where $y(t)$ is height about the ground and $y'(t)$ is the velocity. Here "-1" is our gravity constant and the $0.1y'$ represents damping (e.g., due to air resistance). Suppose that each time the ball hits the ground (i.e., $y(t) = 0$), we want to reverse the sign of its velocity and multiple the magnitude by 0.9 (that is, send it bouncing back upwards with 90% of its velocity).

In MATLAB, read `help ode45` regarding event detection.[1] Use this feature to implement the above. Plot the solution using a different (maybe random) colour between events. Solve until approximately $t = 24$.

Now additionally assume that each time the ball reaches apex, we instantaneously decrease its height by 10% and give it a *downward* velocity of magnitude 0.6 (maybe this is a crude model of dribbling a basketball). Stop the calculation when you find the first peak below 0.5. Return the value of the height at this peak and that time at which it occurs. Make sure these are accurate to six digits, a claim you should justify.

You can read more about event location in the "Dense output" Chapter of [1, Ch II.6].

Problem 2 (Chaos.) Write a program that calls a MATLAB or Python ODE solver to solve the system of three ODEs

$$\dot{x} = -y - z, \quad \dot{y} = x + \frac{1}{5}y, \quad \dot{z} = \frac{1}{5} + z(x - c),$$

where c is a parameter, on the time interval $0 \le t \le 500$. Take $c = 2$ and initial condition $x = y = z = 0$ and use `plot3` with `tspan = 0:.1:500` and line type "." to produce a plot of the trajectory in the x-y-z phase space. As $t \to \infty$, does the system appear periodic or chaotic? Modify your program so that it also computes results corresponding to initial conditions $x = 10^{-12}$, $y = z = 0$, and make a semilog plot of the size of the difference between the new result and the old one as a function of t.

Now repeat these runs for $c = 3$, $c = 4$, and $c = 5$; which cases seem chaotic?

Problem 3 (Gray–Scott pattern formation in 1D.) The Gray–Scott equations are a pair of coupled reaction-diffusion equations that lead to remarkable patterns (See Pearson, *Science* 1993, and search online for "xmorphia".) The PDEs are:

$$u_t = \varepsilon_u \Delta u - uv^2 + F(1 - u), \qquad v_t = \varepsilon_v \Delta v + uv^2 - (c + F)v,$$

where u and v are functions of space and time. For this question, try $c = .065$ and $F = .06$.

[1] I expect you can do this with Python too although I haven't tried...

First, set the diffusion constants to zero. Solve the resulting ODEs numerically with the forward Euler method and determine (experimentally or otherwise) the time-step restriction on k. Try various initial conditions, what steady state solutions do you observe? This is known as the *zero-diffusion steady state*.

Usually we think of diffusion as a process that smooths and stabilizes: not so here. Alan Turing in 1952 [2] proposed what is now known as the *Turing Instability* (he also proposed it as a possible mechanism for animal coat pattern formation: still a topic of current research). To investigate this phenomenon on the G–S equations, take these values for the diffusion constants: $\varepsilon_u = 6 \times 10^{-5}$ and $\varepsilon_v = 2 \times 10^{-5}$. Now write a code to solve the G–S equations on $-1 \le x < 1$ with periodic boundary conditions. Use an initial condition like:

```
>> v = abs(x-0.1)<.1  +  0.05*randn(size(x));
>> u = 1 - v;
```

Based on your answer for the ODEs and what you know about the heat equation, can you guess a reasonable time-step restriction?

Problem 4 (Gray–Scott in 2D.) Reconsider the above equations but this time u and v are functions of x, y, t. We will consider two sets of parameter values:

$$\text{(I) } c = .065, F = .06, \qquad \text{(II) } c = .065, F = .03,$$

(and use ε as above). Write a program to solve the G–S equations on a $M \times M$ regular grid in the square $0 \le x, y \le 1$ with periodic boundary conditions. For initial conditions take

$$u(x,y) = \min\{1, 10\sqrt{(x-.2)^2 + (y-.2)^2}\}, \quad v(x,y) = \max\{0, 1 - 10\sqrt{(x-.3)^2 + 2(y-.3)^2}\};$$

u and v are plotted above. It is up to you whether your code is implicit or explicit.

Produce four plots of $u(x,y)$ corresponding to parameters (I) and (II) and times $t = 500$ and $t = 3000$. Use `contourf` or `pcolor` to make the plots.

Next compute four numbers: the values $u(0.75, 0.75)$ for the four cases above. By experimenting with various grid resolutions and time steps, can you obtain numbers that are correct to several digits of accuracy? What numerical evidence can you offer of this accuracy?

References

[1] E. Hairer, S. P. Nørsett, and G. Wanner. *Solving ordinary differential equations I: Nonstiff problems.* Springer-Verlag, second edition, 1993.

[2] A. M. Turing. The chemical basis of morphogenesis. *Phil. Trans. Roy. Soc. Lond.*, B237:37–72, 1952.