School of Physics & Astronomy

THE UNIVERSITY of EDINBURGH

Modelling and Visualisation in Physics

PHYS10035 (SCQF Level 10)

Tuesday 1st May, 2018 09:30 - 12:30
(May Diet)

Please read full instructions before commencing writing.

Examination Paper Information

Answer all questions overleaf.
Completed codes should be uploaded via Learn as a single zip file immediately after the examination has finished. If technical problems arise with the submission process, you can email the zip file to dmarendu@ph.ed.ac.uk.
Figures should be submitted electronically, they should also be described in the script book.
You may use any resources available on the internet at the beginning of the examination, or present in your CPlab home directory but you may not communicate with any other person electronically or otherwise.

Special Instructions

- Only authorised Electronic Calculators may be used during this examination.
- A sheet of physical constants is supplied for use in this examination.
- Attach supplied anonymous bar codes to *each* script book.

Special Items

- School supplied Constant Sheets
- School supplied barcodes

Chairman of Examiners: Prof A Trew
External Examiner: Prof S Clark

Let us consider the following partial differential equation in 2 spatial dimensions,

$$\frac{\partial \varphi}{\partial t} = D\nabla^2\varphi + \alpha\varphi\left(1-\varphi\right),$$

where φ indicates the concentration of some chemical, α denotes a reaction rate, and D is the diffusion coefficient of the chemical. This equation is known as the *Fisher equation*.

a. Using an appropriate finite difference scheme, with periodic boundary conditions in space, write a Python code to solve the Fisher equation on an $N \times N$ grid, subject to the initial condition that $\varphi = 1$ for $|\mathbf{r}| < R$ (where $\mathbf{r}$ is the position vector linking any point of the grid to the grid centre, and R is the "radius" of the initial droplet), and $\varphi = 0$ elsewhere. Your code should display the density field, φ, in real time as it is running. It should also be possible to set the values of N and R when the code is run. Here and in what follows you can set $D = \alpha = 1$; you can further set the spatial discretisation $\Delta x = 1$ (you need to find a small enough time step Δt for the algorithm to remain stable). **[25]**

b. Use your code to study qualitatively the behaviour of a system with $N = 50$, where $R = 10$ initially. Show/sketch a few snapshots of the system over time, discussing the behaviour you see. **[3]**

c. Now consider an effectively 1D system with size N (so that points are labelled by x, with $0 \leq x \leq N-1$), in which initially φ is 1 for $x \leq x_0$, and 0 otherwise. Consider a lattice of 1000 sites and $x_0 = N/10$. You can use your previous code on an $N \times 1$ lattice to avoid modification of the array structure. Instead of periodic boundary conditions, in this 1D case you should set $\varphi(0) = 1$, and a "no-flux" boundary at $x = N-1$, which consists of imposing $\varphi(N-1) = \varphi(N-2)$ at $x = N-1$ (the rightmost boundary).

   Using this code, calculate the integral over space of φ, and plot its value over time. Fit the linear regime of this plot to compute the speed with which the integral increases – this is the velocity of the "Fisher waves" with which the high density region invades the rest. **[6]**

d. Repeat the calculation using a different initial condition, which starts from $\varphi(0) = 1$ and decays to zero exponentially, $\varphi(x) = \exp(-kx)$, with $k > 0$. Plot the wave velocity as a function of the decay rate of the exponential k, for $0.1 \leq k \leq 1$, using a resolution of 0.1 for the values of k. **[8]**

e. Modify the 2D code written for point a. to solve the following, related, Cahn-Hilliard equation with reaction,

$$\frac{\partial \varphi}{\partial t} = M\nabla^2\mu + \alpha\varphi\left(1-\varphi\right),$$

   where M is a mobility, and the chemical potential μ is defined as

$$\mu = a\varphi\left(\varphi-1\right)\left(\varphi-2\right) - k\nabla^2\varphi,$$

   with a and k two positive constants. Solve the equation numerically for $M = a = k = 0.1$, $\alpha = 0.0003$, $N = 30$; for the initial condition you should set $\varphi = 1$ and add some noise. You can take $\Delta x = 1$, and you should set an appropriate value of Δt for your finite difference algorithm to remain stable. Sketch or show the contour plot of φ in steady state. You should also include a data file with the values of φ at steady state. **[8]**