School of Physics & Astronomy

THE UNIVERSITY *of* EDINBURGH

Modelling and Visualisation in Physics

PHYS10035 (SCQF Level 10)

Tuesday 3rd May, 2022 13:00 – 16:00
(May Diet)

Please read full instructions before commencing writing.

Examination Paper Information

Answer all questions overleaf.

Special Instructions

- A sheet of physical constants is supplied for use in this examination.
- This is an open book examination.
- You may use books, notes, approved electronic calculators, and passive internet resources.
- Your answers must be entirely your own work.
- You **must not** seek the assistance of any other person, organisation, or service.
- You **must not** use responsive internet tools or software resources such as programmable calculators or computer algebra packages.

Special Items

- School supplied Constant Sheets

Chairman of Examiners: Prof J Dunlop
External Examiner: Prof I Ford

Anonymity of the candidate will be maintained during the marking of this examination.

A solution of 3 reactive chemical species, with concentrations a, b, and c respectively, is described by the following coupled partial differential equations in 2 spatial dimensions,

$$\begin{aligned} \frac{\partial a}{\partial t} &= D\nabla^2 a + qa(1-a-b-c) - pac, \qquad (1) \\ \frac{\partial b}{\partial t} &= D\nabla^2 b + qb(1-a-b-c) - pab, \\ \frac{\partial c}{\partial t} &= D\nabla^2 c + qc(1-a-b-c) - pbc. \end{aligned}$$

In Eqs. (1) D is a diffusion coefficient (equal for all species), whereas q and p are positive reaction parameters, whose value will be specified later on.

a. Using an appropriate finite difference scheme, with periodic boundary conditions in space, write a Python code to solve Eqs. (1) on a 50×50 grid, subject to the initial condition that a, b and c are all equal to a different random number, between 0 and 1/3, at each grid point. For the visualisation, define a type field τ for each point in the grid, which is equal to 1 (e.g., shown in red), 2 (e.g., shown in green), 3 (e.g., shown in blue) or 0 (e.g., shown in gray), if the maximum field at that point is a, b, c, or $(1-a-b-c)$ respectively. Your code should allow you to display the type field τ in real time as it is running. **[20]**

b. Throughout these questions you can set the spatial step $\Delta x = 1$, while you need to find a small enough time step Δt for the algorithm to converge. Set parameters as $D = 1$, $q = 1$, and $p = 0.5$. Compute the fraction of grid points for which the type field equals 1, 2 and 3 respectively, and plot these as a function of time. Discuss the behaviour you see and record a snapshot for the type field defined in Part a. **[5]**

c. For the same parameters as in Part b., compute the time to absorption, which is the time needed for one of the three fractions computed to reach 1, and then stop the simulation. Repeat this computation for 10 independent simulations, and find the average time to adsorption with its error. There is a (very small) probability that the time to adsorption is large: to avoid these computationally more costly cases you should disregard simulations which have not reached adsorption by a time $T = n\Delta t = 1000$, where n is the number of update steps. **[5]**

d. Now set $D = 0.5$, $q = 1$, $p = 2.5$. Discuss the behaviour you see and record a snapshot for the type field defined in Part a. **[5]**

e. Record the value of the a field in any two points in the grid. Show with a suitable plot that these values oscillate in time, and find the period, for instance by counting the peaks in your plots over a long time, or by fitting to a sinusoidal function. Show that the analysis of the behaviour of the two points in the grid leads to the same period. **[5]**

f. For the same parameter values as in Parts d. and e., find the probability that two cells have the same type field as a function of their distance r. You need to get data up to $r = N/2$ only (with $N = 50$, i.e. the system size), but can record more. For simplicity, you can compare cells along the same row, so that the distance is the distance along the horizontal direction x. Plot the correlation and comment on the behaviour. Repeat this calculation for $D = 0.3$ and $D = 0.4$ (with other parameters as in Part d.), commenting on the resulting plots and their differences. **[10]**