MXB261 - Modelling and Simulation Science

Assignment 2 - A Simulation Project - 80 marks, contributing 40% of final grade

Due Date: end of Monday 24 October 2016

This is a Group Project: 4 students per group.

The theme of this project is how spatial aspects can affect system dynamics.

You are to submit your m-files, movie files (.avi), a pdf of the report, and a Statement of Contribution showing who has worked on which item(s).

The Report

The Report should have the following structure:

- an **Introduction**, setting the scene for the content;
- a **Methods** section, where you describe the approaches you took to find answers to Parts 1, 2 and 3;
- a **Results** section, to describe the answers to your investigations for each of Parts 1, 2 and 3; include here plots that justify your answers;
- a **Discussion and Conclusions** section, where you synthesise the research and investigations you carried out, and communicate your views on how spatial aspects can affect system dynamics.

Part 1: Random Walk Distributions (20 marks in total)

(a) (7 marks) Simulate a random walk in 1D (so the walker moves either left or right in a straight line). Store the final position of the walker after $M = 500$ steps. Also calculate the mean-square distance (MSD) from the start position. Repeat for $N = 500$ walkers. Your investigation should address the following:

   i. What should the expected MSD be, and what numerical MSD did you get?

   ii. What distribution do you observe, when plotting a histogram of the final positions of the walkers?

   iii. Create a movie of the histograms (for $N = 500$) after $M = 10, 20, 30$, and so on up to $M = 500$ steps.

(b) (10 marks) Simulate a random walk in 2D, with a choice of 4 directions North, South, East and West, for each step. Store the final position of the walker, and calculate the MSD, for $M = 4000$ steps. Repeat for 1000 walkers. For this part, your investigation should address the following:

i. What do you expect the MSD to be, in this two-dimensional setting? And what value do you get numerically?
ii. What do you think the probability distribution is here, looking at a scatterplot of the final positions of the walkers?
iii. Plot a histogram of the x-coordinates of the final positions, and a histogram of the y-coordinates of the final positions. Does this match the distribution you expected?
iv. Plot a histogram of the MSD values. What is the distribution of this data? (Note - this may actually be difficult to answer.)

(c) (3 marks) The code should be well-commented, well-structured, and with the algorithms implemented correctly.

Part 2: Random Walks in a spatially-crowded environment (20 marks in total)

Construct a grid of size 200 x 200. Populate the grid with obstacles, according to the patterns described below. Simulate a random walk of 750 steps: the walker will start at a central position, and will move North, South, East or West unless the proposed move would hit an obstacle (in which case the walker does not move, but the 'step' is still counted) or unless the move takes the walker off the grid (in which case the walker is abandoned and not counted in the calculations). Your investigation requires you to simulate 1000 such walks, and explore the distributions of the end-positions and the MSD, in each of the following situations (where the obstacle configuration remains constant for all 1000 walks):

- the obstacles are placed on the grid randomly, with the number of obstacles at a density of 10%, 20%, 30%, and 40% of the total grid cells;
- obstacles are placed to form compartments via fences, where there are 8 fences along the lines given by $x = 80$, $x = 90$, $x = 110$, $x = 120$, $y = 80$, $y = 90$, $y = 110$, $y = 120$. The fence lines have a certain porosity according to the number of obstacles along each fence - the density of the obstacles in each fence line will be 10%, 20%, 30% and 40%.

(a) (4 marks) Provide a quantitative analysis of MSD versus density of obstacles/fences.

(b) (4 marks) Provide a quantitative analysis of the distribution of end-positions versus density. Include histograms to demonstrate your results.

(c) (4 marks) Provide an interpretation of these results, commenting on the effects of spatial crowding on diffusion as simulated via a random walk.

(d) (4 marks) Provide plots of the walkers' final positions for the four different densities, for the obstacle case and the fences case.

(e) (4 marks) The code
  - should be well-commented and well-structured;

- should have the correct allocation of obstacles, according to density;
- should have the correct allocation of compartments, according to density;
- should be correctly implemented, taking into account 'no move' if the walker were to collide with an obstacle or part of the fence line.

Part 3: Population growth of a parasite (40 marks in total)

(a) (10 marks) The deterministic model is described by the following differential equation system

$$\begin{aligned}\frac{dX_1}{dt} &= k_1X_1X_2 - k_2X_1\\ \frac{dX_2}{dt} &= k_3 - k_4X_2 - k_5X_1\end{aligned}$$

where X_1 represents a population of parasites that feeds off a population X_2. Your investigation here requires you to

- Determine the equilibrium solutions for this system.
- Solve this system numerically using ODE45, over a suitable time span. Choose parameter values (say between 0 and 1); for appropriate initial values $[X_1(0), X_2(0)]'$, plot X_1 and X_2 versus time as well as plotting the phase plot X_1 vs X_2, in order to demonstrate the equilibrium solution.
- Choose alternative parameter values so that $X_1 \to 0$. Solve numerically via ODE45, and plot X_1 and X_2 versus time as well as plotting the phase plot X_1 vs X_2.
- Investigate alternative initial values that may cause the food supply X_2 to drop rapidly. What do you observe? Plot X_1 and X_2 versus time as well as plotting the phase plot X_1 vs X_2.
- In the report, you should explain the interdependencies you observe between X_1 and X_2 with relation to the chosen parameter and initial values, and include a comment on whether the ODE model captures realistic dynamics.

(b) (15 marks) A spatial stochastic model is to be constructed to explore whether this approach captures the system dynamics realistically. This will be an agent-based model, where you construct a grid of cells (200 x 200) and populate that grid with F agents for food and P agents for parasites, according to various densities (see below). There is to be one agent only per cell. The rules for the simulation are as follows:

- Each parasite in turn will attempt to move to a neighbouring cell that is N, S, E or W of its current position; if the new cell is empty, the parasite moves; if the new cell is already occupied by a P, the move doesn't take place; if the new cell is occupied by F, the food is consumed (the F is replaced by the P), and a birth event takes place with the new P being placed in the original cell.

- A parasite dies after f_1 steps and is removed from the grid.
- For each food agent, the agent dies if a uniform random sample $u < f_2$, and it is removed from the grid.
- Food creation - explore the effects of **each** of the following two options, for a selection of parameter values:
  - Create f_3 new F-agents and position them randomly in empty cells.
  - For each F-agent, if a uniform random sample $u < f_4$ then create a new F-agent and place it in an empty neighbouring cell (if one exists).

You are to investigate the following two scenarios:

- the random placement of F and P agents;
- the random placement of P but localised distributions of F.

For each of these scenarios, you should

- Initialise F and P populations at densities 10%, 20%, 30% and 40% of the grid;
- simulate the evolution of this system;
- keep a record of population counts over time;
- choose appropriate parameter values that demonstrate each of the following dynamics
  - parasites dying out
  - food dying out
  - parasites and food reaching equilibrium

In the report, you should describe the relationship between the population density levels, the food-placement strategy, and the observed system dynamics. You should also comment on the advantages and disadvantages of such a spatial model compared to the ODE model. Include plots (parasites and food versus time, and parasites versus food) to illustrate your results.

(c) (10 marks) Create a movie of the spatial stochastic model above, capturing the output at regular time points as the simulation evolves.

(d) (5 marks) The code:

- well-commented and well-structured
- correct implementation of ODE45
- correct placement of the initial population within the spatial grid (both scenarios)
- correct implementation of the population densities (both scenarios)
- 'birth' and 'death' rules for parasites correctly coded
- food 'death', and food creation (both options), correctly coded
- parasite movement rules correctly coded