Computational Projects

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The Observer II, Jeffrey Smart (1983-84).

Introduction

This course involves complex systems of interacting “particles". However, the particles might not be particles in the usual physics sense, but can be other objects - cars on a road, people in a crowd, stock-market prices, flocking birds, or trees in a bushfire. The methods of statistical physics can be applied to all these systems and many more.

Physics is a human creation, and as such it is subject to fashions. They become trendy for a short time. The tide washes in and washes out again, leaving stuff on the shore. Much of this stuff is detritus, but in rare cases it is valuable and worth keeping. The 20th century had its societal tides of fascism, communism, feminism, environmentalism etc. . Statistical mechanics has had its own recent tides. Determining what is worth keeping from them is very difficult in part because the work is so recent. Are the ideas of a fractal or “self organised criticality" or cellular automata, worth teaching students - or are they fads, to be consigned to the dustbin of history?

The computation part of this course has several motivations. One is that we can expose the student to many systems which it is impossible (or at least crazily difficult) to study in any other way. Another is that it gives students exposure to modern statistical systems, and the methods used to study them. The ideal gas is a wonderful system - but surely something has been achieved since the 19th century? A third, and crucial point is that many (by far the vast majority) students will not become professional physicists. They will become teachers, scientific consultants, public servants, defence force personnel, financial analysts, and a whole host of other jobs. The skills used here are much more likely to of use to them than solutions of Maxwell’s equations.

Many of the models used here are lattice-based, i.e. each particle can sit at a point on a lattice, but not in between. The lattice is usually square (in 2D) , but does not have to be - triangular lattices are also common. The reason for using a lattice is usually one of simplicity. Computers work best if a model is discrete. Moreover lattices allow collisions between particles to be easily ascertained - continuum models make this difficult.

Lastly, this document is a work in progress. Different projects will be added as time goes on.

What Is Expected.

For these projects you will need to do two things:

(a) Write some code. Those of you who have less experience or need help, do not despair. We will have a tutor dedicated to helping you code.

(b) Output some data and draw some figures or graphs - perhaps with some limited description.

Each project is only worth 2% of the total mark, so two marks. 1 % of this is for writing a program and the other 1 % is for the actual output. For the output you are **not** expected to write a coherent report. If the output is clearly wrong it will be sent back to you for improvement. This part of the course is thus iterative.

You have a choice of projects. You must do at least 5. There is a range of difficulty. Some are trivial, others more challenging. Of course you will get more out of the more challenging projects. For some of you this will be the most interesting part of the course.

You are of course expected to write your own code. There are are many online codes available for many of these projects and the ANU has very strict rules about plagiarism. Most of you seem to have experience with Python, so this should be your language of choice. If you choose to write in another language, that is OK, but the amount of help you can receive from the lecturers and tutors might diminish.

In many cases there are already online simulations for the systems discussed here. These can sometimes to useful to use as comparisons with your work, but beware, some of them use slightly different models, or are wrong.

Sometimes we mention “extensions" to these projects. These are optional and are not needed to get your 1%. In many cases we do not know what the outcome of these is, but they look interesting. Feel free to invent your own extensions and tell us about them in your answer - once you have a code, it is often easy to extend.

1 A Simple Metropolis Problem

The Metropolis Monte Carlo method can be used to simulate vastly complex systems with many million particles. Here we start with the simplest possible system. We have one “spin" which has two states. State 0 has energy 0, state 1 has energy 1. Write a Metropolis simulation for this system.

You should:

(1) Plot of spin versus Monte Carlo steps, for 100 steps, and on the same graph plot the running average of the spin. Do this for two different values of kT, near 1.

2 Size of a Random Walk

The simplest model of a polymer involves a sequence of bonds of fixed length λ, where each bond can make any angle with the previous bond. This is called the freely-jointed chain model. Here will will study it in 3D. We start at the origin. Then we choose an angle θ randomly between 0 and 2π. We make a step of length λ at an angle of θ top the $+x$ direction. We then repeat, making N steps in total.

We can measure the size of the polymer by finding the end to-end-vector **R** and squaring it. We then take the square root of this to get the root-mean-square size. We will set $\lambda = 1$ Note that this model is “off-lattice" or continuum, we are not using any lattice.

You should:

(1) Plot an example walk of say 100 steps.

(2) Generate walks between say 10 and 10^6 steps and make a log-log plot of the root mean square size versus total number of steps. You may need to average over several walks for each length to get good data.

Extensions:

(1) For a given length, say 10^4 steps, plot the probability distribution of the root mean square size. You will need to average over many realisations to get reasonable data.

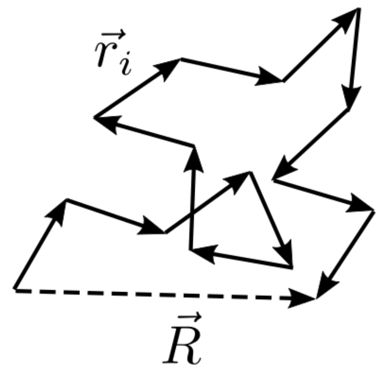


Figure 1: The freely-jointed chain.

3 Squashing a Polymer

Take the model of a polymer given in the last section, starting at the origin in two dimensions. Now imagine two plates situated at $y = \pm\frac{D}{2}$, i.e., two parallel planes separated by a distance D. Imagine starting D very large and then slowly decreasing it. If $D > 2N\lambda = 2N$, no configuration of the polymer chain can intersect the plates, and the polymer does not know the plates are there. However, as D decreases this is not the case. Suppose for each distance D you generate $Q = 10^5$ random walks. In lectures you will have learned that the partition function , Z for a system with zero Hamiltonian is just the number of states. For this system for a given D and a given number of trials Q, we calculate the number of trials $n(D)$ which actually stay between the plates. The partition function is then $Z \propto n(D)$. This gives us the free energy $F = -kT\ln(Z) =\propto -kT\ln(n(D))$, and hence the force keeping the plates apart $f = -dF/dD$.

You should:

(1) Plot some typical states which lie between plates and different plate distances for say $N = 10000$.

(2) Plot log-log graphs of the free energy and force (with $kT = 1$) for various plate distances. For plate distances of order 1 or less the results look somewhat different because it such cases we are going down to the size of one link or less.

4 Inertialess Langevin Simulation

Consider a particle in a 1D W potential $U(x) = -x^2 + \alpha x^4$, where α is a positive number. Take $kT = 1$ and the friction constant $\xi = 1$. For a given α start the particle at the bottom of the left well. There is a barrier height E which is the energy between the bottom of the wells and the barrier between them.

You should:

(1). Plot some typical trajectories $x(t)$ for different barrier heights, some less than kT and some of several kT.

(2) Measure the average time τ needed to go from the left well to the right well as a function of barrier height. Plot $\ln(\tau)$ versus E.

5 1D Traffic Flow: Rule 184

One fairly recent application of statistical physics has been to models of traffic flow. These models range from the very primitive through to those which are much more complicated. Here we present perhaps the most primitive model, but even this one shows non-trivial behaviour. This model also has the advantage that it can be applied to many systems which have nothing to do with traffic. It is as follows. We take a 1D array where each element in the array (or lattice site) can be either “spin" 0 (no car) or “spin" 1 (a car). We then proceed forward in one time step. Each lattice site is updated simultaneously (i.e. we make a new lattice). The rule for updating site i depends on the the spins at sites $i-1$, i and $i+1$ i.e. $s(i-1)s(i)s(i+1)$. It is $111 \to 1$, $101 \to 1$, $100 \to 1$, $011 \to 1$. All other combinations give 0. This models traffic flow to the right because a car only moves right if there is a space to move to.

We assume periodic boundary conditions, so that if we have a lattice of length n with the sites labelled $0,1,2,....n-1$, then if we try and address lattice site i what we mean is $i mod n$.

The way to plot this data is to print a row of squares for the lattice and then keep printing another row underneath it as it is updated. A random initial configuration will quickly stabilise into a pattern.

You should:

(1) Show the pattern you get for different density (2) Plot a graph of average speed versus linear car density for the density varying from near 0 (empty) to near 1 (full).

6 2D Traffic Flow: The Biham-Middleton-Levine Model

We now put the traffic on a 2D lattice. There are red cars (which can only move right) and blue cars (which can only move down). We out the cars on the lattice randomly and assume periodic boundary conditions. The rules for motion are alarmingly simple. At one time step we try and move all the red cars simultaneously - if a car can move (i.e. nothing is blocking it) , we move it one step to the right. We then do the same with the blue cars. The model is simple, but the behaviour is rich.

You should:

(1) Show some time sequences of the whole lattice , where you go from random to organised free flow, as well as jamming.

(2) Plot the mobility versus time for different values of the density.

Extensions:

(1) Put in some Volvos - i.e. slow. cars which move only each nth step. What effect does this have, apart from road rage.

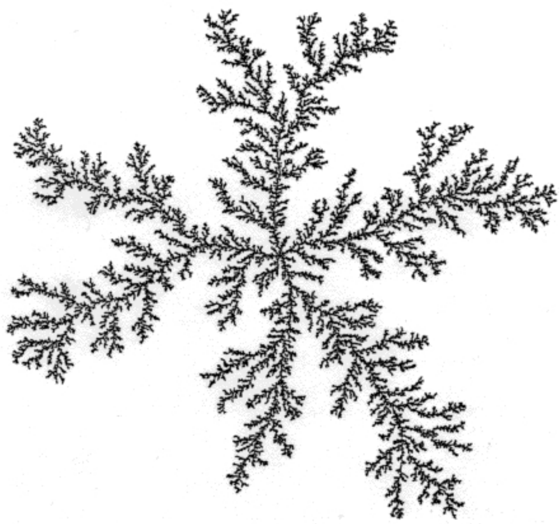
(2) Similarly declare a square area to be subjected to road works, so everyone must slow down. What do you see?

7 Diffusion Limited Aggregation

The problem of the growth of objects by accretion of smaller objects is of great importance in many areas of science. An obvious example is in the formation of planets. Another is the formation os salt crystals from solution. In 1981 Tom Witten and Len Sander at the University of Michigan came up for a model of cluster formation that was limited by diffusion. In the extreme limit there is only one mobile particle on the lattice at once. As usual the model is crazily simple and the output is complex and unexpected. Witten and Sander start with a seed particle in the middle of the lattice. This is fixed. Another particle, starts to diffuse in from a distance. By “diffuse" we mean perform a random walk. At each time step it can move up, down left or right. It keeps doing this till it leaves the system, or till it sticks side on with the seed (i.e. the seed becomes one of its nearest neighbours). Another particle then is launched. It can stick to either two of the original particles.

In practice we can speed things up a bit. At any time the cluster will have a radius R given by the smallest circle that can be drawn with the origin at centre which still encloses the whole cluster. Launch the particles from $R+3$ where 1 is the lattice spacing. When doing this make sure you are not biasing your launch, because of the int() function on the computer - if you do this you will get very anisotropic clusters which grow mainly in two of the quadrants. Also, once a diffuser moves to say $3R$ you can kill it and start again from another location. Initially you should set $R = 4$ and only increase it when the cluster grows bigger than this.

You should get something like this:



You should: (1) Show a picture of one DLA you made, with at least 1000 particles. (2) Draw a log-log graph of $lR(N)$, i.e. the size of the cluster as a function of the number of particles. You will find that $R \sim N^{\omega}$, where ω is not 2, giving you a hint that the object is a fractal.

8 The Schelling Model: Ethnic Segregation in Cities

This project is here for a number of reasons. First it is an interesting stat. mech. system, but one outside of the bounds of traditional physics. It also shows many of the things which physical systems show such as phase separation, disordered phases, surfactants separating phases, and frustration. It is an example of an "agent-based" model and falls into the loose category of game theory. This project allows you to examine one aspect of identity politics in an *objective* fashion, by calculation. When Schelling proposed his model, it was not a trendy topic at all, and his work was initially ignored, and rarely cited.

In most cities one finds ethnic/racial clustering. New York is the classic example, with well-defined enclaves of Indians, Chinese, Russians, Hispanics, Blacks, Whites, and just about every other category. These clusters, which change gradually over time, are natural, and generally make a city more interesting both to live in and visit. Closer to home Sydney has its Hurstville, Cabramatta, Lakemba and The Shire. Chicago is a third (somewhat less positive) example.

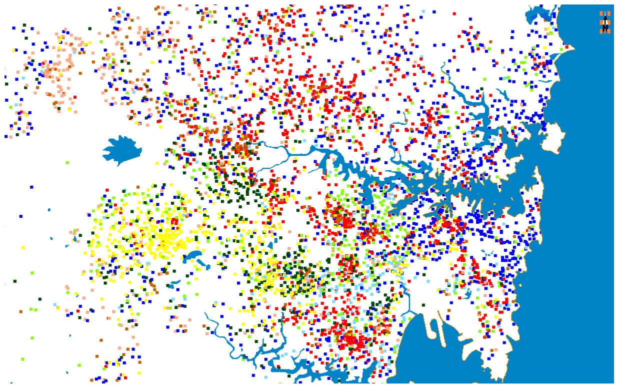


Figure 2: Map of Sydney (2006), The Shire not shown. Each dot indicates 100 persons born in Britain (dark blue), Greece (light blue), China (red), India (brown), Vietnam (yellow), Philippines (pink), Italy (light green) and Lebanon (dark green).

In 1969 the economist Thomas Schelling (Nobel Prize, 2005) set out to try and model this. He pointed out that sometimes there is segregation in housing due to government policy, sometimes due to historical accident, and sometimes due to discrimination by landlords. Schelling however was more interested in a different and overwhelmingly more dominant explanation: people segregate not because they have a passionate dislike for other groups but because they have some (usually practical) preference for their own group. For example, many cities have Jewish clusters, in part because the residents can be close to a Kosher butcher and a Synagogue and can set up an Eruv. It would be seem to be crazy to suggest that Jews are living in the East-

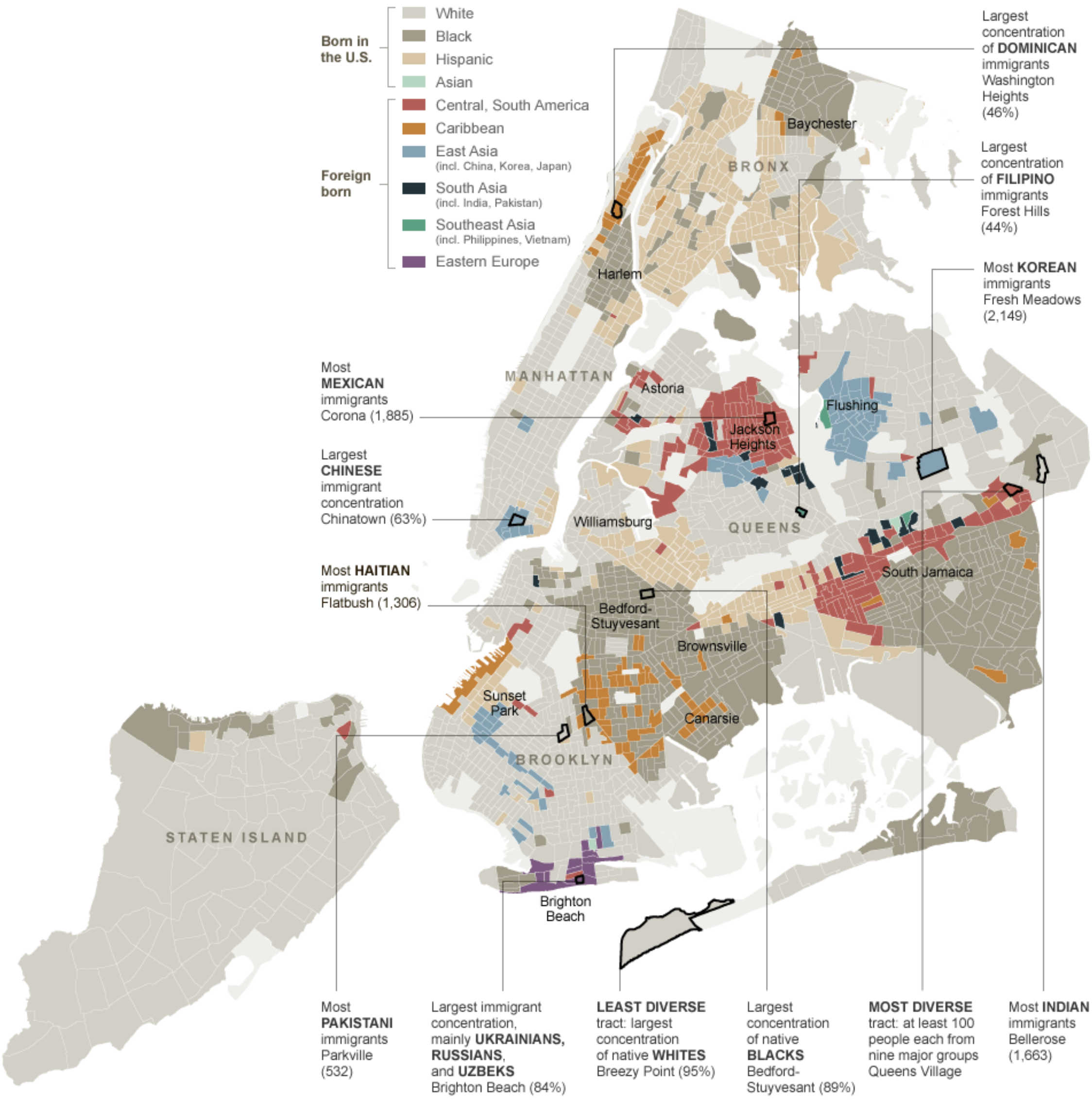


Figure 3: From the *New York Times* Jan 22, 2011.

ern suburbs of Sydney rather than Hurstville because of discrimination by Hurstville landlords and real-estate agents.

What Schelling's model shows is that even a slight preference for your own group leads to very substantial segregation - individual preferences lead inevitably to clustering of whole groups, way beyond what any person desires for themselves as an individual. His model is extremely simple. It ignores many details (for example some people do not care who their neighbours are, as long as they don't play Led Zeppelin at full volume at 3 in the morning)- but the results are interesting and not what the average person would expect. As one paper put it “Elegantly simple and easy to simulate, it provided a persuasive explanation of an unintuitive result: that local behaviour can cause global effects that are undesired by all."

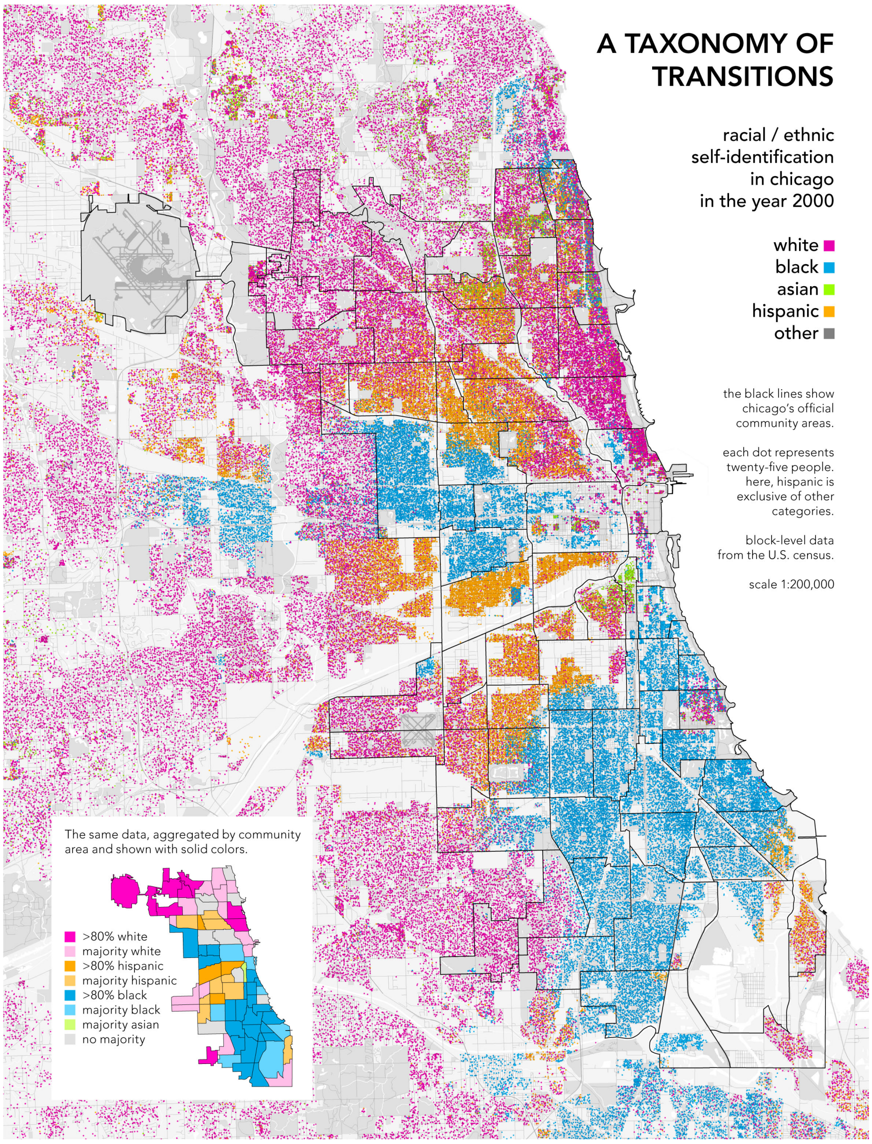


Figure 4: Chicago, from: http://www.radicalcartography.net/index.html?chicagodots, where you can view it in much more detail.

The model is as follows. We have an n by n square lattice of n^2 sites. Each site represents a house. These are of three kinds. White is a vacant house, and red and blue are houses of different ethnicities. In the program white is 0, blue is 1 and red is 2. Each house has 8 neighbours. The blue houses prefer to have blue neighbours and the red houses red neighbours. We introduce a *similarity, s* . We also introduce the neighbour fraction f which specifies what the fraction of the neighbours of a given house are of the same colour as it . When counting the fraction, f we ignore vacant houses. For example if a blue house has 4 blue neighbours, 3 red neighbours and 1 white neighbour the fraction of neighbours it has which are blue is $f = 4/(4+3)$. If the fraction of similarly-coloured neighbours is greater than or equal to the similarity i.e. $f \geq s$ then the house is satisfied and it will not move. However, if this is not true, $f < s$ the house then moves to a random vacant house, i.e. a blue-white or a red-white swap is done.

The model proceeds as follows. A site is chosen at random. If this site is white then choose another site. If the site is coloured, check the fraction of neighbours. Move if this is unsatisfactory. Repeat for another random site. Finish if all sites are satisfied.

Periodic boundary conditions are used. This means that if we try and address a location with row=i and column =j, the actual location is just i mode n and j mode n. This means that the sites are labelled as $i = 0, \ldots n-1$ and $j = 0, \ldots n-1$.

We first set up the system with sites randomly filled with blue red or white. We then iterate. There are three fundamental parameters. B the fraction or blues. R the fraction of reds. s the similarity. It is suggested you start with $B = R = 0.4$ and $s = 0.3$ and see what develops.

In order to complete this project you need to do the following. Choose a convenient lattice size, 10 by 10 at minimum, 100 by 100 looks good.

(1) Set the fraction of reds and blues to be equal (say 0.45) and run it for different values of the similarity, producing some maps of the city. Note that for high values of the similarity the system never reaches a steady solution.

(2) Plot a graph of the fraction os coloured sites that have at least one neighbour of a different colour, versus similarity.

(3) Again versus similarity, plot the fraction of neighbouring houses for say blue that are red, i.e. in this case we count vacant houses, so that the fraction of red neighbours is equal to the number of red neighbours divided by 8.

Some extensions:

(0) Look at what happens for unequal similarities i.e. red or blue have different s.

(1) Suppose the blues like the blues, but the reds also like the blues. What happens?

(2) Put some major roads or green spaces or waterways into the system. These can be coloured green. They do not change i.e. you cannot move into a lake or park or onto a road. Suppose you put two roads as a cross in your city - presumably these roads split the colours.

(3) Put another colour in - what happens?

(4) Do it in 3D.

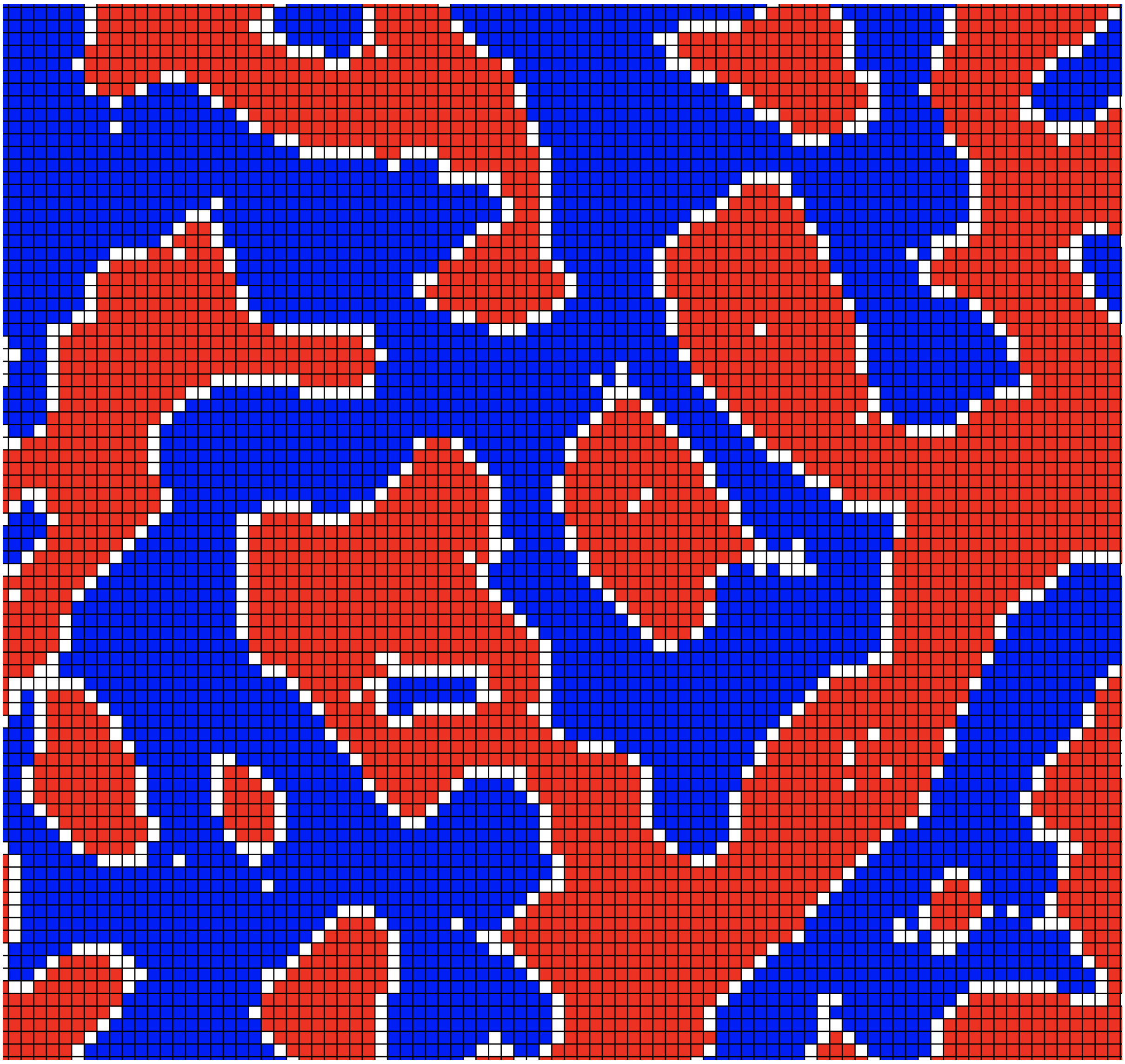


Figure 5: A screen shot of part of the simulation. Note that although the system starts off with reds and blues randomly distributed, it rapidly achieves almost complete segregation for high enough values of the similarity, s. Note also that is this case the vacant houses (white) act as a surfactant between the two phases, just as detergent lies between oil and water.

9 The Schelling Mode in 1D

There has been much less work done on the Schelling model in one dimension (i.e. on a line, or with periodic boundary conditions - a ring). Try and simulate this. In this case there are of course only 2 neighbours, but the best thing to do is to look at a neighbourhood radius of R sites.

You should look at how R and the similarity s, as well as the fraction of each colour affect the outcome.

10 The Sznajd Model: Groupthink and Social Acceptance

“All mass movements, as one might expect, slip with the greatest ease down an inclined plane represented by large numbers. Where the many are, there is security; what the many believe must of course be true; what the many want must be worth striving for, and necessary, and therefore good."

Carl G. Jung, The Undiscovered Self (1958), p. 33

In the Schelling model we saw how individual choices lead to group outcomes which most people do not want. The Sznajd model studies the opposite effect - the effect of the group environment on the individual. It is a model of how individuals can accept as true, statements which are false, but which are held by the “group" as being true. It is thus a model (in part) of “social validation" - people are often reluctant to give an answer in public which deviates from the accepted social norm, even though in private they will give their true opinion. People often mouth the politically correct view while thinking the opposite, so they fit in. Universities, which purport to be bastions of freedom of speech, sometimes become the opposite due to this effect - they encourage every superficial diversity but not diversity of opinion. This in part also explains why opinion polls can be a very poor indicator of what happens in a secret ballot: "Oh no, I would never vote for that nasty Trump person ...."

The model is one of social influence. It is in 1D and each site on the lattice is assigned a spin $S = \pm 1$. At each step a site i is chosen at random, the spins at i and $i+1$ are examined, and the spins either side of these (i.e. at $i-1$ and $i+2$) are updated. The rules are as follows:

(A) If $S_i = S_{i+1}$ then $S_{i-1} = S_{i+2} = S_i$. i.e. if the two middle spins have the same opinion, then the two outer spins copy their opinion - groupthink.

(B) If $S_i \neq S_{i+1}$ then $S_{i-1} = S_{i+1}$ and $S_{i+2} = S_i$. i.e. if the two middle spins disagree then the outer spins take the opinion of their other neighbour - disagreement leads to further disagreement.

Like the Schelling model this model is vastly over-simplified. For example, in a large organisation such a university, a religious order, a sporting group or even a country it is often easier to publicly agree with the person at the top rather than actually express your own divergent opinion.

Start the system off in a random configuration with a certain fraction f of $S = +1$.

You should:

(1) Draw some state diagrams, of the initial state, the intermediate states, and the final state. You should find three separate behaviours (all up, all down, alternating) i.e. two dictatorships and one stalemate. These are like two ferromagnetic phases and one antiferromagnetic.

(2) Plot graphs of the magnetisation $M \equiv \frac{1}{N}\sum_{i=1}^{N} S_i$ versus time.

Extensions:

(1) This model shows the effect of neighbour interactions. However, in practice the leadership of the whole society often attempts to impose views. There might be different ways of modelling this, but one would be that sometimes, with a small probability p the rules get overridden and the spin becomes $+1$.

11 Other Topics to be Included Later

Ising model (both in 1D and 2D)
Lattice Gas
Sandpile Models
Other cellular automata.
Models of swarms.
Percolation.
Epitaxial Growth