Forming and performing agent based modelling techniques using stochastic methods

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Abstract

A core observation to the study of this paper is the micro random behavioural dynamics of multiple seemingly independent agents. What is commonly observed in systems made up of such agents is emergence of overall deterministic rectified behaviours. In realistically large systems of agents, there will exist an alarmingly large number of different configurations of states. In such a large system, there is a large difference in likeliness between different possible states. This marries the concept of agent based modelling with statistical physics. Systems tending towards these likely states are analogous to a thermodynamic system tending towards equilibrium. For this reason, statistical physics techniques are essential for developing agent based models. Examples of this are shown by firstly simulating an initially equal wealth distributed market economy. The distribution of wealth after a short amount of time steps of random exchange represents the Boltzmann-Gibbs distribution. The second application of agent based modelling was used to describe the quantum mechanical causality of Ferromagnetism using an Ising type model. Here the net alignment of dipoles in a Ferromagnetic lattice at equilibrium is dependant of the net temperature of the lattice.

Contents

1 Introduction

Statistical physics is a well known agreed upon science that often describes the dynamics of systems comprising of particles with interactions and general behaviour occurring on different time scales. It is therefore great at modelling the stochastic behaviour of ensembles of these particles. It is found that systems that may appear random on the small scale, tend towards some likely equilibrium state. Agent based modelling describes models that are made up of various interacting components whose behaviour is a result of their characteristics and or their environment. The aim of this project is to develop the approach of combining known computational architectures of agent based models - and results of statistical physics which could allow us to examine various forms of systems comprised of independent interacting components, in a stochastic manner.

To do this, a considerable set of mathematical tools need to be established to be successful in this type of modelling. There is significant aim at understanding the principles of some of the modelling techniques that can be used to solve complex systems with interaction properties we can define. To perform a subset of these techniques it is sometimes convenient to use various agent based modelling packages imported in a programming language. For the experiments that are being performed, the simulations are done in Python. Demonstrating agent based modelling, two simulations were performed. The first involves the exchange of currency in a simplified market economy. For this, the Mesa package designed for agent based modelling on a spacial domain was used.

The second agent based model simulated is the Ising model of a Ferromagnetic material/ lattice. Mesa could be used to do this simulation. It is not. The algorithm used to sample random states for the lattice requires a large order of magnitude of iterations. Therefore the algorithm and storage structure is coded from first principles in Python using the LLVM compiler Numba[16].

The literature and results of this study form a majority of foundation of modern agent based modelling. The further applications are vast and potentially much more advanced.

2 Brownian motion to active motion

2.1 Passive Brownian motion

Coined in 1827[1], Brownian motion was named the phenomenon of pollen particles possessing unbiased erratic motion when immersed in a liquid[1]. Due to the motion being erratic and unbiased, the Brownian particle will on average stay in the same place. This means that if a Brownian particle in N dimensions is first observed at $\vec{0}^N$, the mean position of the particle over a long enough time measurement - will be where it started[2].

$$\langle \vec{x}^N \rangle = \vec{0}^N \tag{1}$$

To begin speaking about the quantitative behaviour, we refer to Einstein's theoretical findings of this motion in 1905[1]. Einstein showed that for a Brownian particle (A particle exhibiting Brownian motion) - the mean square displacement (MSD) at time t is related to the diffusion constant D[1].

$$\langle [\vec{x}(t) - \vec{x}(0)]^2 \rangle = \langle \Delta \vec{x}^2(t) \rangle = 2Dt \tag{2}$$

Diffusion is generally thought of as the tendency (average motion) is to spread from a region of high concentration to that of a low concentration. In this way, a state of equilibrium may be achieved[3]. Already this is interesting, the motion of a single particle has been related to a supposed constant belonging to an ensemble of particles. Furthermore, noting the conservation of the particle number in a given system, the density of Brownian particles $\rho(\vec{x}, t)$ in a system obeys a continuity equation[2].

$$\partial_t \rho(\vec{x}, t) + \nabla \cdot \vec{j} = \alpha(\vec{x}, t) \tag{3}$$

Here α is the in and out flux of particles of the system, I.e. the difference in the number of particles that are entering or exiting the system[1]. At this point, this

quantity is set to zero.

$\vec{j}$ is the Brownian particle flux in the volume. This quantity is given by Frick's Law: $\vec{j} = -D\nabla^2\rho(\vec{x}, t)$. This is inserted into the continuity equation to give:

$$\partial_t \rho(\vec{x}, t) = D\nabla^2 \rho(\vec{x}, t) \tag{4}$$

The idea that should be understood so far is that it is the same to observe statistical properties of a Brownian particle versus an ensemble of them[1].

Considering Newton's second law, the equation of motion of a particle due to forces $\vec{F}(t)$ acting on the particle with mass m is given by $\vec{F}(t) = m\ddot{\vec{x}}$. It is bought forward the findings of Langevin, where the following forces are considered:

$$\vec{F}(t) = -\gamma_0 \dot{\vec{x}} + \vec{f}(t) - \nabla_{\vec{x}} U \tag{5}$$

The first term here is easily identified as the frictional force on the particle which is related to it's velocity by it's frictional constant given by γ_0. The second term is the stochastic force f acting on the Brownian particle resulting its random behaviour over time. It is important here to emphasise the word random in the last sentence. $\vec{f}(t \neq t')$ is unrelated to $\vec{f}(t')$. Hence the stochastic force is always compensating for previous (and future random behaviour [1].) The last term U represents an external potential, provided if one is exists[2].

2.2 Active Brownian motion

Active Brownian motion adds the characteristic of the Brownian particle being able to store energy from its environment. This gives this particle potential energy in which it can convert it to kinetic energy - thus giving itself propulsion[1]. It is helpful to see an i^{th} particle's internal energy depot $e_i(t)$ as an additional degree of freedom belonging to the particle. A further property of this degree of freedom is that the energy depot is assumed to have a constant dissipation over time[1].

2.3 Active motion

Active motion is now broader / less strict than active Brownian motion. This term is now not restricted to physically microscopic particles, but rather independent self propelled movements within the system[1]. The purpose of this nomenclature is to carry on from where we started with the stochastic behaviour of objects (so small that they can be considered particles.) Only now, the "particle" is anything with its own energy supply belonging to a system where the behaviour can be considered statistical. A simple example of this extension can be seen as the movement of a flock of birds[1].

3 Modelling systems of agents

3.1 Macro and micro components

Most observed behaviour in general life situations / systems is made up of large amounts of interacting components. The most extreme indication of this is we have from Avogadro's number that the number of individual atoms that make up a unit mole ($O(10^{23})$). Conveniently most observed behaviour can be seen as the result of interacting small scale behaviour which is of much larger size scale than an atom. A larger "small" scale behaviour would be an individual bird in a flock. In this study, large scale behaviour being controlled by independent smaller components is deemed complex behaviour[1]. Naturally analysing large scale systems in this manner by simulating the interactions of what we call agents by looking at all individual interactions is a recipe for success. The flaw obviously is that this would be far too much computing.

The computational demand can be reduced using observations from statistical physics - such as was seen with the Langevin equations. In this way we can begin planning strategies of modeling. Something supporting this argument would be that when we have multiple interacting entities in a complex system, behaviour is observed that would not be present in a system composing of just one such example entity. A classic example of this is the composition and properties of different periodic elements composing of only protons, neutrons and electrons. Any interaction between these entities is consequently non-linear. Via this, in our observation of

the whole system may present structures that would not be there independently[1].

There is then of interest of how once these new structures are established - the behaviour of each of our smaller scale components collectively may be influenced. This phenomenon has been called "self-organisation"[1]. Further mathematical components of this behaviour would be external potentials, in or out flux of components of the system, and boundary conditions belonging to various parameters[1].

As was discussed with active Brownian motion, this behaviour produces out of equilibrium states. Typically the behaviour is analysed using non-linear relationships in the form of differential equations and computer simulations[1]. As modern computing power continues to increase, the effectiveness of large scale models made up of smaller scale entities increases alongside.

This class of system may be where the result of individual interactions consist of known quantities and the forces at play are known physical forces made up of the established fundamental forces such as electro-dynamic. Key focus in this study is using these methods where the systems are made up not of tiny particles interacting in a potential but systems made up of entities such as birds in a flock or boldly humans in a socioeconomic system. A very bold example of this would be an election within a population where the 'force' between the entities is analogous to influence between people. There are two ways of verifying such a computational model. Firstly we can compare results with collected behavioural data of a system we are trying to emulate[1]. Second we can compare the computed results via this approach with the predictions of an analytical model[1].

In both of these situations over-fitting may be observed. This is generally when the experimental model has too many parameters. There are similar but different consequences in both cases. When we are comparing to an analytical model, overfitting may be where the total global behaviour has high correlation to the compared analytical model, but when looking at the evolution of smaller groups or individual entities, there is no physical resemblance. In the case of comparing to empirical data, it is slightly different. Say we are using machine learning and are using such data as input data to train parameters in a neural network. If say instance a neural network contains too many parameters, the model may be overfitted to the data it is being trained on and is of poor value when using the model on a different set of input data.

For this reason, the prescription we follow in this study is to only to include as much detail as necessary when describing this entities which shall be called agents. This allows easier formation of a true analytical model. Secondly in the prescription, only the simplest set of axioms are defined which will govern interactions between agents. Upon comparative success of the model, further detail can be added and assessed[1].

3.2 Multi agent systems

Previously, the concept of artificial intelligence focussed on characteristics and rationality inspired by psychology[1]. The current state of this research community now reasons that interaction and distribution compose the basic concept of intelligence and thus must be considered when trying to imitate it. To say this in famous computer scientist's words of Marvin Minsky, "intelligence is the result of numerous interacting modules, each solving primitive tasks"[1].

This is analogous to a macro micro link in "complex" systems. Here macro would refer to the system and micro being various individual components of the system. In practice, individual "micro" dynamics of the system cannot be easily be used to predict a systems macro behaviour. For this type of study, statistical physics is acknowledged for being able to predict behaviour in large systems made up of essentially individual variables. In this way, macroscopic properties can observed by looking at statistical expected states of the micro components of the system, rather than each individual configuration[1].

The notion of *agents* is one belonging to informatics. There is not necessarily a strict definition for an agent, but a "notion of agency" can be seen as a self executing behaviour[1]. A stronger notion of this so called agency involves individual agents possessing their own internal model of the system / environment they belong to, I.e. knowledge of a human[1]. The sophistication of this stronger notion of will naturally vary from system to system. The wealth of this concept is being able to explore cooperative behaviour / interaction of a many agent system[1]. The so called strength of agency splits agents into two sets. First *reflexive agents* there is a strong notion of agency and each agent can responds to the environment as a result of its own internal algorithms on the assessment of the situation. *Reactive agents* however have immediate/ axiomatic response to stimulus[1].

Multi agent systems can consist of a large number of not necessarily identical agents, with potentially varying degrees of internal complexity / intelligence[1]. This intelligence may include reinforcement learning[4]. A relevant application of this school of thought would be autonomous traffic systems, where each agent or car would have its own purpose / destination but as well to interact safely / not crash with other cars / agents. This is a research and development example here but many proposed agent based systems exist in physical, biological, social, economic and financial areas of research[1].

In terms of the reflexive agents, we will need to develop computational techniques where we store the relevant information regarding the surrounding system which will be available to a given agent to process internally. In most cases we will need to look at information regarding parameters such as phase space and time. Another thing that will often be paramount to consider is that often the only relevant information is the more recent events and dynamics[1]. For this reason, the relevant information could mostly be that of short term memory. This is important to grasp as it means that in terms of computational storage, as we will in this case be able to use less of the memory hardware available.

Figure 1: Photo of a multi-agent system, where an individual agent is a bird, the multi-agent system is the flock. This is the result of the non-linear feedback between the birds in the flock thus rectifying their motion to their uniformed observed motion. A key physical potential in such a system is air resistance, if a bird can fly in a slipstream of other birds, it has to do less work[6]. This is just one example of something that affects the behaviour and contributes to the feedback resulting in a flock. This photograph was taken by James Crombie in March 2021. Image source can be seen at[7]

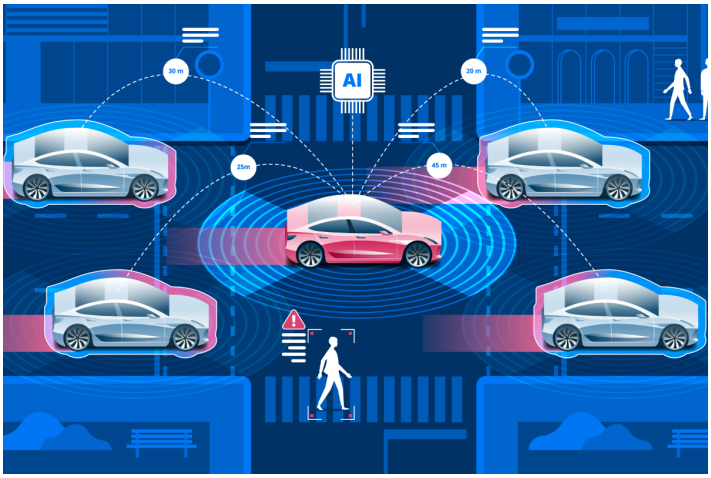

Figure 2: Plot showing the multi agent system of autonomous cars. Reactive components of such an agent would need to be able to respond to the relative speeds of neighbouring agents/ cars, obey traffic laws and above to have no collision with another car or pedestrian. The reactivity of such an agent would therefore also be some form of prioritisation in terms of safety over time spent travelling. The source of this sketch is given in [8]

3.3 Basic computing techniques for advanced systems

It is clear from some of the bolder examples of multi agent based systems that there may in many cases be no available analytical model of entirely known parameters to compare simulation results[1]. We thus need to develop some computational architecture for describing such systems. It has been continually implied that the particle dynamics courtesy of statistical physics will serve as paradigm to the agent based models created. The problem that is arrived at is that these paradigms allow at most so far to describe a system of multi reactive agents. An example of such reactive agents can actually be found in the realm of particle dynamics if we consider active Brownian particles located in an asymmetrical potential. If the active particles have enough self propulsion, we may see rectified motion and limit cycles in the dynamics of the particles[1]. This means that we must extend this approach to incorporate *reflexive* properties.

John von Neumann came up with the method of *cellular automation* which defines a cell as a square on a discrete grid or some high dimensional volume if necessary[1]. von Neumann proposed each cell or block is allowed to take on two possible states. This discrete system is then evolved iterativly in finite time steps. An example

of the causality in such a system would is how the states of neighbouring cells in certain proximities affect the evolution of individual cells. With this, different behaviours can be defined for certain cases and neighbourhoods (both spacial and the types of states in the given neighbourhood.) With such a format, boundary and initial conditions corresponding to the system we are modelling may be imposed[1]. This method has had many applications in statistical physics, population biology, sociology and economics[1].

Let's give two example of where this is relied on. The Ising model model in statistical physics arranges atoms of the same kind in some discrete lattice characteristic of the material it attempts to model. Each atom at it's location can be in one of two states, the spin of the magnetic dipole moment may have spin of 1 or -1. This model describes ferromagnetism[9]. Another example of where this has been used to great extent is in game theory which was too pioneered by von Neumann. This is mostly applicable to sociology, psychology and economics. It involves the interaction of rational decision makers[10].

Cellular automation is a useful tool but it is far from a silver bullet for modelling all types of reflexive agent properties. Firstly we must sacrifice working in a continuous environment. Each state variable is fixed in space and can only take on one of two states.

Another architecture that may be used to describe multi agent systems is that called *blackboard architecture*. The blackboard can be considered as a data repository for given agents[1]. This is useful in systems where every agent need not have have access to all the information or historical data in the system. It is useful too that we may have many different blackboards which may be accessed independently by the agents in the system[1]. To permit many distributed blackboards in this study, we incorporate *Flip-Tick Architecture* (FTA.) FTA is based off of the combination of several different defined quantities. Agents which are individual units responsible for processing data in a periodic fashion[1]. These agents are grouped into different ensembles of agents. The agents in an ensemble behave in a synchronous way. As with all numerical simulations, time is discretised in order to process it. After a cycle for an ensemble is complete, we advance time by one increment (tick of a clock.) After the tick, a new cycle begins[1]. The agents interact over the cycles by accessing input data (which are called tags) from the backboards they may have access to. This reflexive agent may then process the data embedded in the tags and further write tags to a blackboard. A *tag* is considered to be data created

by an agent which is used to communicate to other agents. These tags may be only presented on the blackboards for some finite amount of time in cases where only a short term memory of events is necessary[1]. To introduce where the flip occurs, the tags are displayed on the blackboards for some finite time where the agents in the ensembles may "read" this information. If all the ensembles that are accessing a particular blackboard have all completed one cycle, the blackboard is *flipped*. Once this blackboard is flipped (to the other side,) the previous information is still available. The agents can then write new tags (to communicate with other agents) to this side of the blackboard. After this writing of new and important old information is written to the blackboard, the global time of the system is advanced by a single increment and we may begin the reading cycles[1].

3.4 Brownian agents

It follows that the study being approached here is that combining the tools available in the statistical interaction of particles and the application of agent based modelling using the simplifications and similarities available. With this we begin to define the Brownian agent.

Suppose we have such a system of $N \in \mathbb{N}$ agents. Let's then define an index naming each agent $i \in N$. Next we represent given variables in the system which affect the behaviour of an individual agent i with the index k. The notation that will be used to identify each single variable of each agent is u_i^k. These variables may be the result of internal degrees of freedom - affecting actions or external stimulus[1]. Some examples of such variables will be spacial, I.e. $u_i^1 = \mathbf{r}$, $k = 2$ may extend to the corresponding velocity field. There may be classes of variables that are responsible for the response of an agent that are not continuous variables. In other words variables may in certain cases have only a binary (or some finite) input and output[1].

A simplified example of such an variable and output/ response would be a car being driven safely by a person or artificial intelligence stopping if a traffic light is red or continuing at a safe speed if the light is green. Examples of continuous variables would be the response to such a driver/agent may be the response to other drivers dependant on their relative speed.

Similar to the mathematics of Brownian motion, these state variables are described by[1]:

$$\frac{du_i^k}{dt} = f_i^k + F_i^{\text{stoch}} \tag{6}$$

This behaviour of the state variable is therefore related to *causality* of the right hand side. We need to underline for the process of defining Brownian agents that the causes of the response's of the state variable is due to the superposition of deterministic and stochastic *forces* at play[1]. This characterises the idea of the Brownian agent. We can analyse overall global behaviour over a long period of time by essentially summing up and averaging all of these smaller scale interactions that occur in smaller (finite) timescales[1]. This allows the use of Langevin like techniques. We can represent these summed and averaged 'stimuli' on an individual agent that only occur on a smaller time scale as a stochastic term F^{stoch}. The stimuli which will be observable on a global level at the viewed lager time scale are summed up as the deterministic term as we had too with the Brownian motion f_i^k[1]. This approach reduces the amount of processing on the so called smaller scale or 'microscopic' level of interactions. The stochastic and deterministic forces acting on an agent variable may be functions of various - to all state variables u_i^k which is denoted $\vec{u}$. Realistically we must also consider interactions and observations which result from factors external to our agents. This may be the in and out flux of resources or a potential of some sort[1]. These types of factors will be summarised as $\vec{\sigma} = \{\sigma_1, \sigma_2, \ldots, \sigma_L\}$[1]. Thus a deterministic component f_i^k may be a function of $\vec{u}, \vec{\sigma}, t$.

A generalised approach to describing the summed up deterministic force is to consider a so called global potential $V(\vec{u}, \vec{\sigma}, t)$ being some high dimensional quantity which is a function of all variables at play. With this concept we assume the way in which we are modelling our system is conservative (for example total energy is conserved in a system, number of agents is kept constant etc) we can then apply what is known from gradient systems in classical mechanics to describe each deterministic component of a particular agent i[5]. Hence the deterministic forces may in this context be given by[1]:

$$f_i = -\frac{\partial V}{\partial u_i} \tag{7}$$

An example of this sort of landscape is visualised in figure 3. The problem arising

has already been mentioned, in such a gradient system, we demand global conservative properties[5]. Because of this, we modify this idea of the potential landscape to an *adaptive potential landscape*. For this situation, we attempt to adjust the potential landscape due to the actions of our individual agents. This is an example of non-linear feedback in a system, where one agent may affect the potential governing the entire system, which then the altered potential landscape may/ will affect the responses of other agents in the system[1].

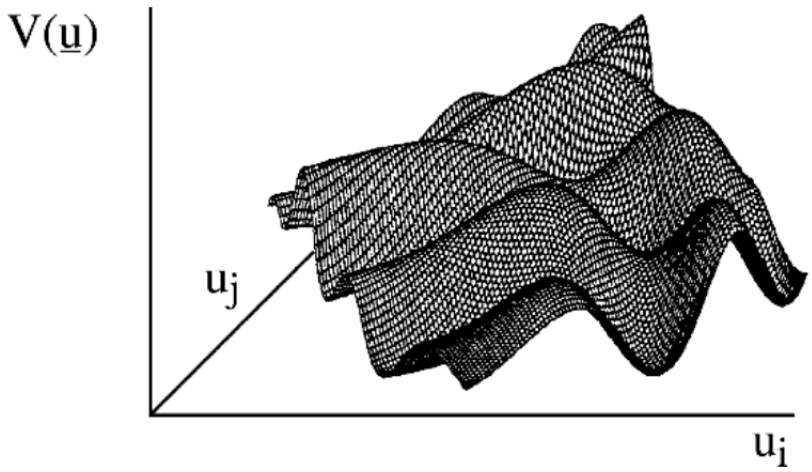

Figure 3: A low dimensional example of such a landscape where $\vec{u} = \{u_i, u_j\}$. The source of this sketch is [1] page 27.

With the creation of this adaptive potential landscape concept, we can just as easily include coupling of agents that are "far" away in the space $\vec{u}$ as those in local areas as which was mostly considered when looking at the explanation and examples of CA. Further advantageous is that this structure allows for global coupling of agents with regards to certain behaviours. The way in which these interactions/ coupling may occur using this concept can be those that behave differently as time moves forward. The various time scales in which an interaction may occur may now too be accounted for[1].

The adaptive landscape is thus a medium in which the various agents interact. This is reminiscent of an electric field where the charged particles behave as the agents[1]. In our case, the adaptive landscape which the agents are somewhat contained in, provides "information" which the agents via their design/ properties are reactive or reflexive to. What has been proposed here in many regards is a rather

more robust version of the blackboard / tag-board architecture which incorporates FTA. In more complex multi agent systems, the agents (especially reflexive ones) will make decisions based on processing via different internal degrees of freedom θ. Supposing that our agents exist in an (time) evolving system of physical space, it is proposed that an adaptive landscape may be given by the multi component scalar field $h_\theta(\boldsymbol{r}, t)$, where each component represents what we had as blackboards before[1].

Let's consider the quantity α that previously denoted the difference between the influx and out-flux of Brownian particles in a system. At this point in the study we are dealing with a broad notion of "information" available to N agents in the system via the adaptive landscape. This can then be given by[1]:

$$\alpha(\boldsymbol{r}, t) = \sum_{i=1}^{N} \delta_{\theta_i,\theta}\{s_i\delta(\boldsymbol{r} - \boldsymbol{r}_i) - k_{\theta_i}h_\theta(\boldsymbol{r}_i, t)\} \tag{8}$$

We already have a tool for quantifying the rate at which field varies over time via the diffusion equation[1]. Combining this with equations 3,4, the diffusion of information is given as[1]:

$$\frac{\partial h_\theta(\boldsymbol{r}, t)}{\partial t} = \sum_{i=1}^{N} \delta_{\theta_i,\theta}\{s_i\delta(\boldsymbol{r} - \boldsymbol{r}_i) - k_{\theta_i}h_\theta(\boldsymbol{r}_i, t) + D_{\theta_i}\nabla^2 h_\theta(\boldsymbol{r}_i, t)\} \tag{9}$$

Now to unpack this. s_i indicates the magnitude of the influence of the information being added to the system via agent i, the lifetime of this information in the system given by agent i is $\frac{1}{k_{\theta_i}}$ and naturally the diffusion (how much it spreads) constant for the information given by i is D_{θ_i}. The Kronecker delta function is used to choose the component of the scalar field that corresponds to the internal degrees of freedom of agent i[1].

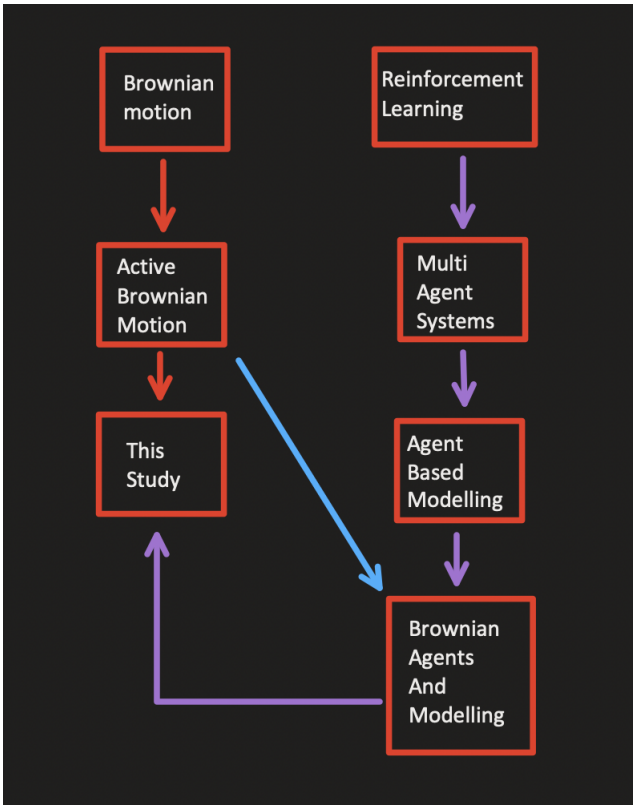

Figure 4: Flowchart of the what has been describes and how the various sciences here relate to each other.

4 Boltzmann-Gibbs distribution of wealth

To begin we need to re-establish the concept of thermal equilibrium. Take an isolated system with no in or out-flux of energy. Such a system will always be at thermal equilibrium. For the internal thermal interactions, all interactions and exchanges must be conservative. In a closed homogeneous system of particles, Clausius' equality states all processes in this system are reversible[9], I.e. where δQ is the incremental transfer of heat in the system and T the total constant temperature of the system:

$$\oint \frac{\delta Q}{T} = 0 \tag{10}$$

This allows the definition of thermodynamic entropy S. Which is defined by measuring the quantity $ds = \frac{\delta Q}{T}$. Thus in a reversible system, S is constant. If the

system had non reversible processes, for instance the random transfer of energy between particles within a neighbourhood in the system, the second law of thermodynamics states that entropy of this system must increase[9]. This comes from the fact that despite this behaviour, the system always stays at thermal equilibrium. This increase in entropy may be observed in rectified motion developing in a system or canonical distributions of the total energy of the system amongst the particles.

The distribution that describes the system described here is the Boltzmann-Gibbs probability density function[9]. For the total energy of the system given by T, given enough time, the system's total energy will be distributed amongst all the particles i via[9]:

$$P(\epsilon) = Ce^{-\frac{\epsilon}{T}} \tag{11}$$

This once normalised (constant C,) gives the density of particles with a given energy.

Suppose we consider an economy is a closed system. Consider for simulation sake, the system is constructed on a spacial grid. To do the simulation this structure is a two dimensional array. Using the Mesa package, this grid is given topological properties of a torus[11]. This means that the space we create has no physical boundaries but wraps around in a continuous manner whilst still being finite. Next, suppose this grid is filled with a finite - set number of agents (N.) To start from a state of unbias, initial location of these agents on the grid is chosen at random and there can be multiple agents occupying the same cell as well as no agents occupying a single cell. Initially, each agent begins with one unit of currency at random location in an unbounded grid. The total wealth (also N units) of the system is thus evenly distributed amongst the N agents. The format of this model uses cellular automation which the first principles have already been discussed. We then introduce "steps"[11] of the model which would be analogous to time discretisation. At each time step, each agent in a random order for every step makes two actions in the system. For each step, a new random order in which the agent perform their two action is created, via sampling without replacement.

The first action every agent does when it comes to its turn in a step is: Of the agent's location, the agent moves to one of its neighbouring cells again via a random choice. Since this is a grid, the agent would move up, down, right, left or in the four diagonal directions one unit via a random choice. The second action that takes place is the

exchange / motion of the economy. If the agent has non zero currency and the cell has multiple occupants, of the other occupants, one other agent is chosen randomly to exchange in this scenario. The other agent then receives one unit of currency c and the acting agent looses one unit of currency c, thus conserving the total wealth of the system N. This could be interpreted as a type of active motion as was discussed. Only here the stochastic motion occurs on a discrete grid of cells and the internal depot of an agent is currency not energy.

It is then only natural to pose that after enough steps in a system with a large enough ensemble of agents that the net constant wealth of the system be distributed amongst the identical agents via the Boltzmann-Gibbs distribution. We can therefore deduce the probability distribution of the total wealth amongst all the agents be of the form:

$$\rho(c) = \frac{1}{N} e^{-\frac{c}{N}} \tag{12}$$

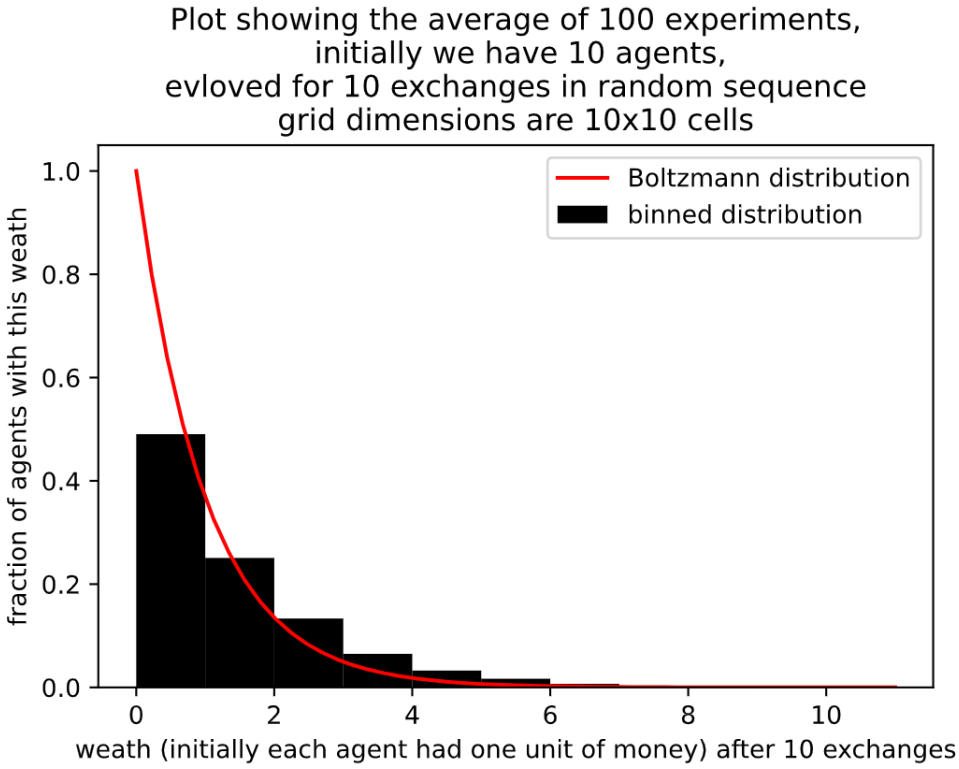

Figure 5: Here are the results from the simulation that has been described up to this point.

In this model, this dominant distribution forms by under twenty steps. It is very notable at how short a time scale is required for this rectification of sorts to happen.

At a glance, the design for such the movement in the landscape and simple trading seems to at best describe a very primitive economy. For one, the total wealth is constant and there is no inflation. This may make it seem like this model does not account for enough information then. However it is simple to argue that; the rate at which the total wealth of the system - beginning with all agents being equal, become distributed in this way, practically happens on a much shorter time scale than any net in/out flux of currency to the system. As for inflation, this in reality is part of the response in a system to becoming distributed in this way - thus occurring on a longer time scale.

But still, then this may resemble a community of gamblers betting on rolls of dice in the perspective so far. In an intelligent economy, the exchange of money is not random but a result of deterministic strategies. Conveniently, this simple model's relevance is redeemed when considering a large population of a country trading in one currency. Since the people (which are represented by agents in the model) making up the population are heterogeneous, which trade deterministically in vastly varying amounts of currency. From this perspective, trade between people in a population of millions whilst conserving the net wealth available in the economy would very much be observed as random - non related processes[12].

Something neglected in this model is debt, if the agent has zero wealth, it is not forced to trade and go into negative wealth. The model does describe how with trade occurring stochastically, even if all agents begin equal, the unequal Boltzmann distribution of the wealth begins to form. But practically when a person goes into debt, they can escape primarily in a few ways. If they declare bankruptcy and liquidate their assets, they are technically still trading in the same currency in the economy. This implies that in the model, currency c of an agent includes all personal assets. This practical method of getting out of debt is therefore not necessary to include in the model. Loaning money could be considered included in various deterministic trade mentioned too resulting in the overall observed random process.

As an experiment, a bail out method is added to the model. If an agent had zero wealth and it was its turn to act, if there are other agents sharing the cell that have currency, one of these such agents is chosen at random to donate one unit of

currency to the agent that is currently acting. This idea is reminiscent of bad debt in a real world economy. The effect of this bail out had no impact on the underlying distribution presented in figure 5. From a perspective of statistical physics, this distribution of wealth is seemingly irreversible in the population.

In the age of telecommunications, trade partners are not restricted to living in the same area, but the argument of net random movement is still valid. All of this is arguing that this model despite having very simple rules of interactions, is still meaningful in a real economy.

Another interesting outcome is the resulting occupation of the cells in the grid once the distribution has been established. A small number of cells develop very high occupancy whilst there exist some cells with medium level occupancy. Mostly though the grid is filled cells mostly having negligible occupancy

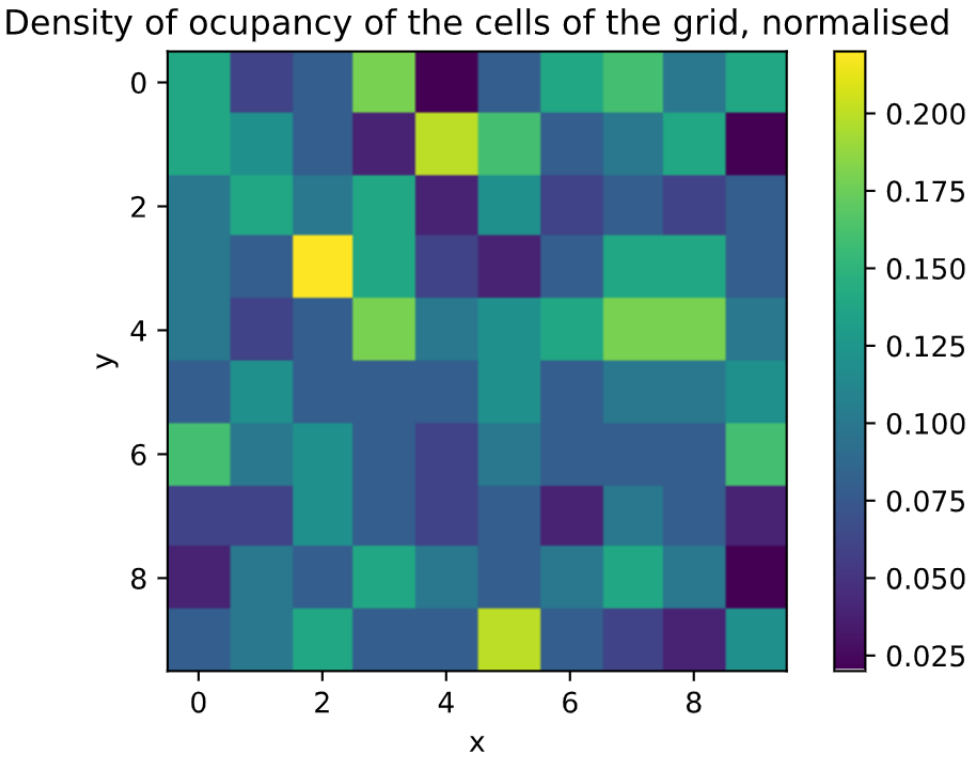

Figure 6: Here we have a grid of 10×10 and 500 agents in the system with the same unbiased initial state. This plot shows the occupancy after 20 steps where we know the distribution has been established

This thought to be analogous to the formation of economic hubs of trade such as cities within countries. The agents in this model have the strong tendency to cluster

together.

This simulation would be best compared to former Soviet states distribution of income across their population in the first few years after the fall of the Soviet Union. Introducing market economy. Obviously the society in these states were far from perfect equality, but is thought to best represent the initial state of our model before allowing stochastic trade.

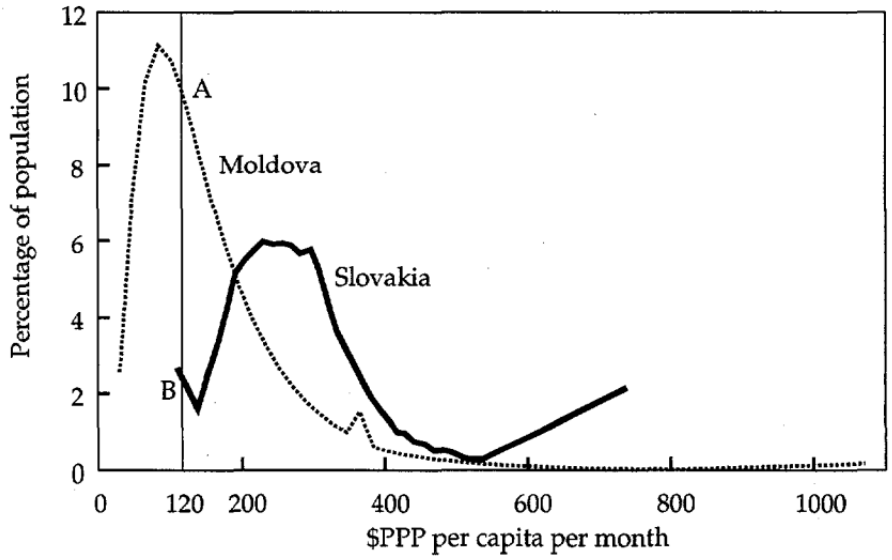

Figure 7: Here we have the income distribution of two former Soviet states from 1993, two years after the fall of socialism in this region. Image sourced by World Bank publication of 1998[13]

The formation of this very unequal wealth distribution happens after such a short amount of time. The distribution for Moldova is very similar to the shape predicted by the simple model constructed. This importantly verifies that the formation of such distribution does indeed happen on very short time scales as was seen in simulation. The feature which does not correspond to the model is the model predicts a the large portion of the population has wealth about zero. But this is not data from the wealth of everyone in the economy. It is the income distribution amongst people that are in fact earning money to even be included in the data set. It would not account for informal workers or the unemployed as data points. This means the prediction close to zero in the model is not applicable this real economic distribution. The rest of the model is however very representative.

The code used to simulate this agent based model is based on a tutorial on building

the foundation of this model. It is available on[11]

5 The Ising model

Moving from the macro-scale example of trade. Let's consider another multi-component complex system. This time our active agents are on the quantum mechanical scale. Classically, a magnetic field arises as a result of a moving electric charge. A single electron orbiting a nucleus gives rise to a magnetic dipole. Magnetism can be induced in some materials by using an external magnetic field to align these dipoles moments belonging to electrons. I.e. the orbital speed of the electrons is affected.

In particles such as electrons, this is not the only source of their magnetism. An electron also possesses a spin magnetic moment as a result of its spin belonging to the electron. Electrons belong to the set of elementary particles Fermions which have half spin. This spin can be found in one of two states, spin "up" or spin "down", i.e. the direction of the resulting magnetic field.

When we typically think of magnetism, we consider Ferromagentism. Ferromagnetism occurs on the macro-scale when the spin's of the atoms comprising the material are aligned and remain aligned without the presence of an external magnetic field.

It must be noted, that by Pauli's exclusion principle - no two Fermions may be in the same state[9]. In other words, two electrons may not exist in the same orbital with the same spin orientation. In some materials, the identical atoms comprising the material have un-paired electrons in valence shells. Another part of Pauli's exclusion principle is that as electrons fill the different states of a nucleus, the lower energy orbitals get fulled up first, in the case of a stable un-excited atom. Two atoms with un-paired spin in overlapping vicinity, will be further apart when their un-paired electrons have the same (parallel) spin. As a result of Pauli's exclusion principle, when the electrons' spins are opposite but all other quantum numbers are the same[9], there will be attraction bringing the atoms closer together - increasing electrostatic energy in the system. Thus the material is in a lower energy state when the spins are parallel compared to other orientations. This proporty of a material results in Ferromagnetism [9]. Relating to this is the Curie temperature[9] of a

Ferromagnetic material, above which the material is too energetic for neighbouring spins to be in parallel. Often in naturally Ferromagnetic materials, the volume is divided into sub domains of these spins in parallel, the magnetic field from these different subsets of the volume of the material tend to add up to a net zero magnetic field. A permanent magnet can be made by heating this type of material to a high enough temperature - un-aligning any of the neighbourhoods of parallel spins. The material is then placed into an external magnetic field. As the material cools and the magnetic field is removed, the spins in the material are now "permanently" aligned[9].

The aim of this section is to build an Ising model simulating Ferromagnetism. Ferromagnetic materials are most commonly metals, i.e. Iron. For this reason, it is appropriate to model the atoms comprising the material as a rigid lattice. This allows a similar architecture to be used for simulation as we had before. Now though, the atoms which we could consider agents do not move, the only thing we are modelling is the individual spins of the atoms making up the lattice and anticipate rectified behaviour to emerge. The model built could either represent a permanent magnet or a neighbourhood of atoms with a preferred axis.

Let's start defining notation for this model. Let's consider our metal to be represented by a lattice of its N atoms. Let the index i correspond to the i^{th} point in the lattice, and j, the j^{th} immediate neighbour of i. Consider state $s_i = 1$ an atom with its dipole as a result of its spin pointing upwards and $s_i = -1$ for downwards. If the i^{th} atom is parallel to one of its neighbours, it has already been explained that their exchange frees up energy $-\epsilon$ in the system, where as if they are anti-parallel, more energy $+\epsilon$ is taken up in the system. This exchange can therefore be given by[9]:

$$U_i = -\epsilon \sum_j s_i s_j$$

Now it is relatively easy to solve this system in one dimension. I.e. each atom will only have two neighbours. Doing this we should be able to infer properties of this simplified Ferromagnetic model. It will however be limited as real Ferromagnetic lattices such as iron takes the form of a body centered cubic lattice at lower temperatures including room temperature. This form of structure has eight nearest neighbours for every atom. Since the thermodynamic properties are dependant on the nearest neighbours for each atom - a one dimensional solution is hardly practical

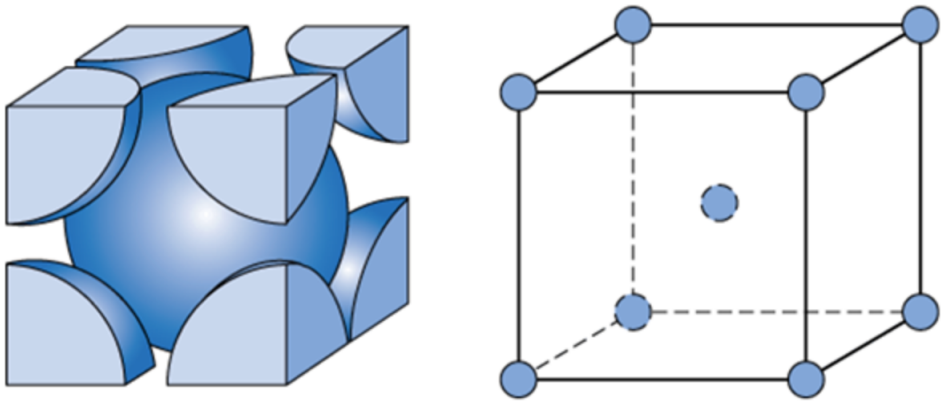

Figure 8: Picture showing a body centered lattice, picture sourced from [15]

5.1 One dimensional solution

The partition function of a system is the sum of all possible states. This is given by[2]:

$$\mathbf{Z} = \int d\Gamma e^{-H\beta}$$

Where H is the Hamiltonian / total energy function of the system and $\beta \equiv \frac{1}{k_B T}$, where k_B is the Boltzmann factor and T is the temperature of the system. For the one dimensional case, this is easily simplified to[9]:

$$\mathbf{Z} = \sum_{s_1} \sum_{s_2} \cdots \sum_{s_N} e^{\beta \epsilon s_1 s_2} \cdots e^{\beta \epsilon s_{N-1} s_N}$$

Knowing each of these states may have spins 1 or -1, each summation in the above expression may be simplified to:

$$\sum_{s_N} e^{\beta \epsilon s_{N-1} s_N} = e^{\beta \epsilon} + e^{-\beta \epsilon} = 2 \cosh \beta \epsilon$$

We can therefore give a nice expression for $\mathbb{Z}$ in one dimension:

$$\mathbf{Z} = 2^N (\cosh \beta\epsilon)^{N-1}$$

Since N is the number of atoms in the system, we assume N is very large. With this, the following approximation can be made[9]:

$$\mathbf{Z} = (2 \cosh \beta\epsilon)^N$$

We can use the following formula for expectation value of the energy of the system[2]:

$$\langle E \rangle = -\partial_\beta \log \mathbf{Z}$$

$$\implies \langle E \rangle = -N\partial_\beta \log 2 \cosh \beta\epsilon$$

$$\implies \langle E \rangle = -N\epsilon \tanh \beta\epsilon$$

This expectation value tends to zero as β tends to infinity. In other words - temperature tending to zero. Now as β tends to zero, we have $\langle E \rangle = -N\epsilon$. From what we know of the energy interactions in a Ferromagnet, this implies that there are equal numbers of atoms with opposite spins - net zero magnetisation.

As it stands, the simulation problem is that with two possible states for each point in the lattice, there are 2^N different possible macrostates. Thus the random sampling of states using a number this large is not computationally friendly. Analytical solutions in one dimension are not that intimidating but are not accurate to nature at low temperatures[9]. In two dimensions case was famously solved by Lars Onsager in 1943[14]. This model behaves like a real Ferromagnet in that - there is a critical temperature such that the net magnetic field drastically increases. The reason for this being is that each node in the lattice will have four nearest neighbours in the two dimensional case - compared to two in the one dimensional case[9]. Thus it follows from intuition that the more neighbours each atom has in the lattice/metal, the greater the tendency there to be a larger net magnetic field, provided the temperature is not too high.

The naive brute force to the problem of trying to solve the system via simulation would be to calculate all of the different 2^N macrostates and then calculate expected values for energy, magnetic spin alignment etc. In a realistically large system - this calculation is far from feasible.

5.2 Simulation solution

What we have here is an agent based system. Where the agents are atoms and they make their decisions based on the spin of their immediate neighbours. In the last simulation of a simple economy, thermodynamic properties appeared globally after enough iterations of the simulation. That however was not a thermodynamic system and such, thermodynamic properties were not used to create the simulation. Here however we do have a thermodynamic system. We simplify the complexity of the simulation (complexity referring to the total number of operations needed for the simulation) using the principles of thermodynamics. All combinations of spins for the lattice are possible, but we know that the total energy in the lattice is the same as the net temperature of the lattice. We also know that with time - the system will tend towards equilibrium. This is the foundation for the Metropolis algorithm - which is coded in Python using the LLVM compiler library Numba[16] to speed up computation time.

Consider a single iteration of the simulation of a lattice of arbitrary structure with each lattice point/ atom/ agent having n nearest neighbours. For a single iteration we choose one point in the lattice at random. Then we calculate the energy difference ΔE (before and after) if this atom were to change to opposite spin. If the energy difference is less than or equal to zero, the algorithm has the condition that then the spin of this atom will change sign. Doing this not non physical since we know the system tends towards equilibrium. To build on this more rigorously, consider two different energy states for the whole lattice E_1,E_2, which vary only by the fact that a single atom's spin is flipped between these two states. The probability of choosing the atom in the lattice of N points, that by changing its spin alignment results in a lower energy state is:

$$P(\Delta E) = \frac{1}{N} e^{-\Delta E \beta}$$

Now considering this energy change is not absurd and proportional to its relatively small number of immediate neighbours:

$$P(\Delta E \leq 0) \approx \frac{1}{N}$$

In other words sampling - at random out of all N atoms in the lattice. If however this energy change increases the energy of the system that was initially in a lower energy state, we have[9]:

$$P(\Delta E > 0) = \frac{1}{N} e^{-\Delta E \beta}$$

In the case of low temperatures, the probability of this happening is far less than the case of a net decrease in the state's energy. Crucially for the algorithm, the factor of $\frac{1}{N}$ is already accounted for by the fact that for every iteration - we choose the atom at random. Of course we can only say that this is physically accurate after an infinite number of iterations/ samplings. If the algorithm only runs for small number of iterations (say one thousand) - only a small subset of states will be simulated. For low temperatures the lattice should tend towards total alignment very fast as this would be very likely for the dipoles to flip accordingly such that there is total magnetisation. This is another realistic aspect of the algorithm. The system does not have time to explore all possible micro states before reaching equilibrium[9]. A building blocks pseudo code on implementing the Metropolis algorithm is given on page 349 of[9].

The structure of this system is in the form of a two dimensional array - representing a 10×10 grid. Boundary conditions implemented are equivalent to the torus topology of the previous agent based model, only here this was hard coded and not a call of a function of an existing package. For each temperature in the range zero to four, ten million iterations of the Metropolis algorithm were executed.

For the sake of simplicity, ϵ is set to a natural unit of one in the simulations. The temperature is therefore in units of $\frac{\epsilon}{k_B}$. In the subject of solid state physics, the nomenclature of the number of nearest neighbours of an atom in a lattice is the co-ordination number.

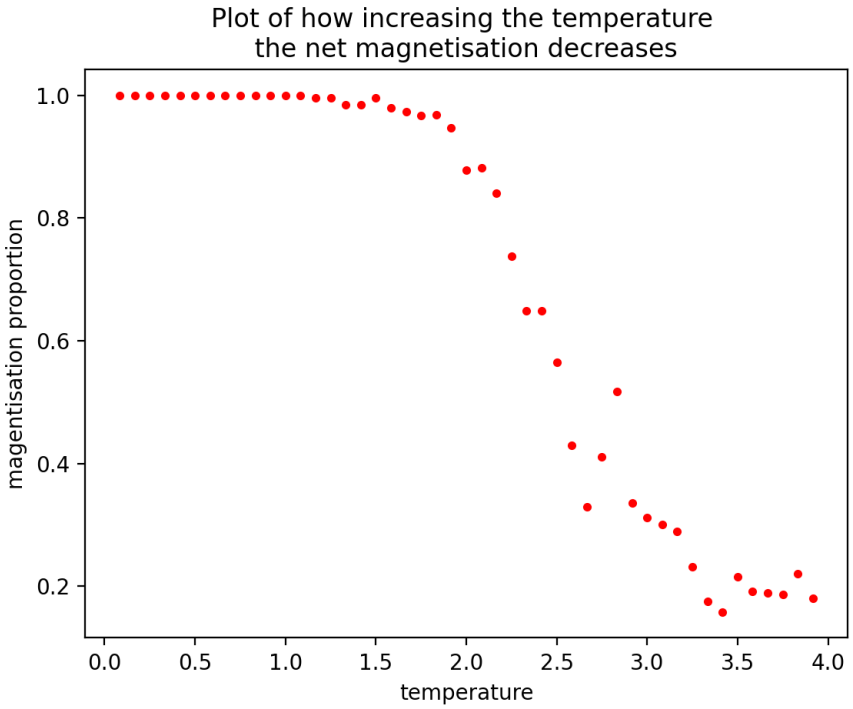

Figure 9: Plot showing the net magnetisation of the lattice were each agent has a co-ordination number of four, over a range of dimensionless temperatures.

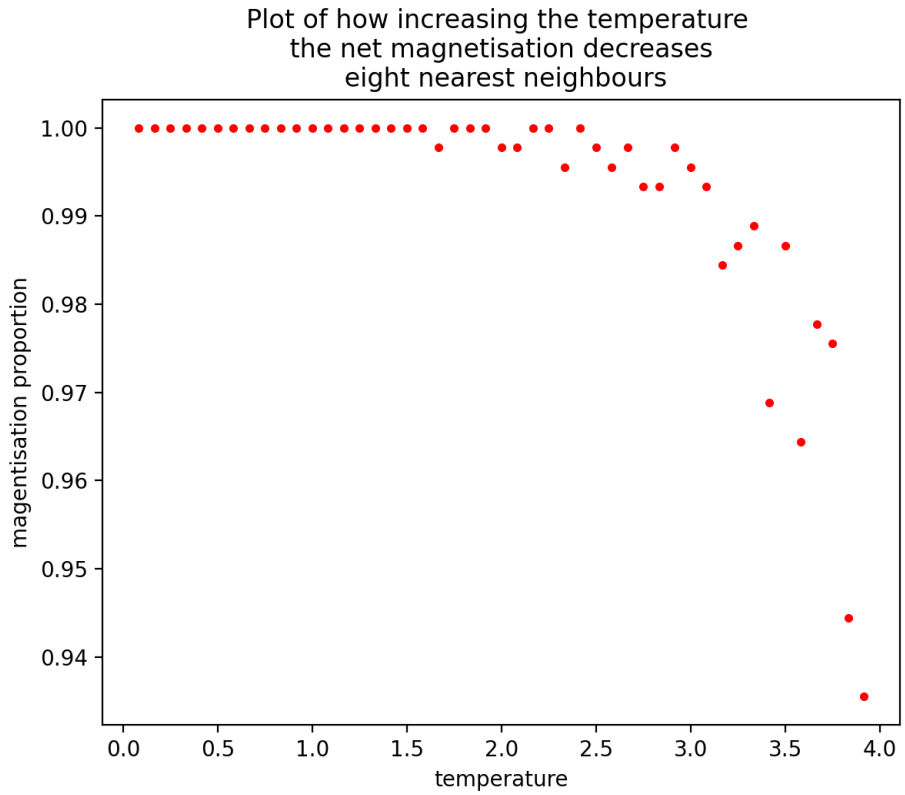

Figure 10: Plot showing the net magnetisation of the lattice were each agent has a co-ordination number of eight, over a range of dimensionless temperatures.

The results from the simulation confirm the analytical solution famously obtained by Lars Onsager, where the critical temperature for a two dimensional lattice with each atom having four nearest neighbours being $T_C \approx 2.27$. What is interesting is by increasing the co-ordination number for each agent in the lattice - we significantly increase the critical temperature. This directly relates to physical ferromagnetic lattices. The Curie temperature of Nickel is around $627K$ (Kelvin) - Nickel compounds typically have a co-ordination number of six[17]. The most known Ferromagnetic lattice is Iron, which has a Curie temperature of $1043K$ - which has a co-ordination number of eight. This difference in Curie temperature corresponds to our numerical results above.

Next, we explore the astronomic number of different possible states that a tiny lattice (30×30) may take on. This is done exploring lattice states at different total temperatures. Considering how much larger the lattice of a macro Ferromagnet, we can really appreciate the shear variety of possible states the lattice can take on. We examine the states for different temperatures after a million flips.

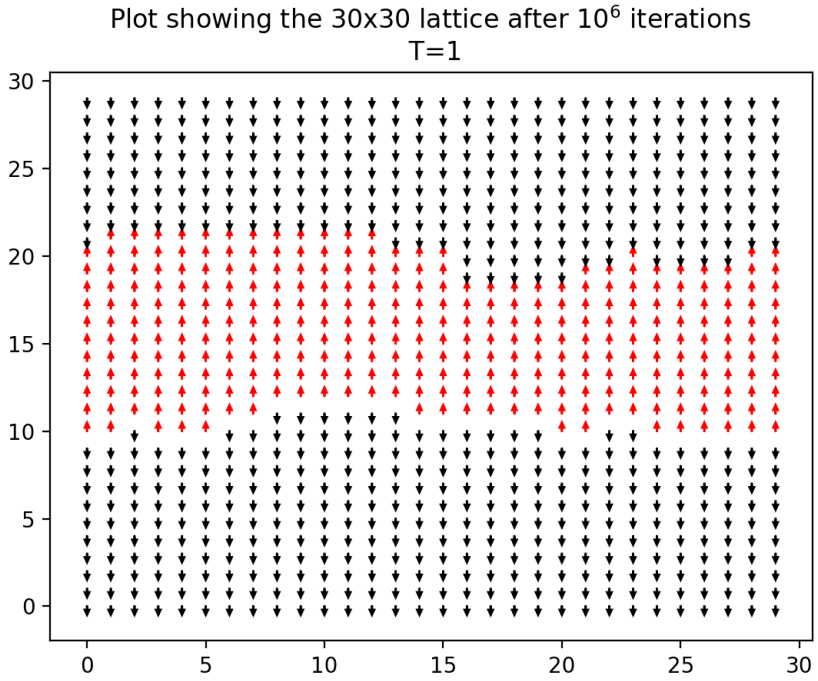

Figure 11: 30×30 lattice in state of uniformly partitioned magnetic field.

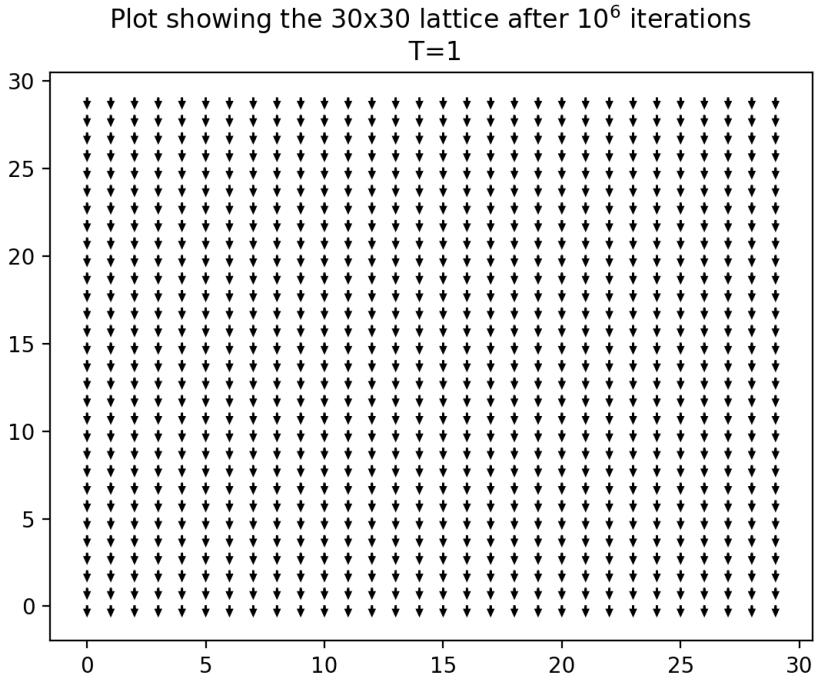

Figure 12: 30×30 lattice in state of uniform magnetic field.

Figure 13: Lattice close to critical temperature.

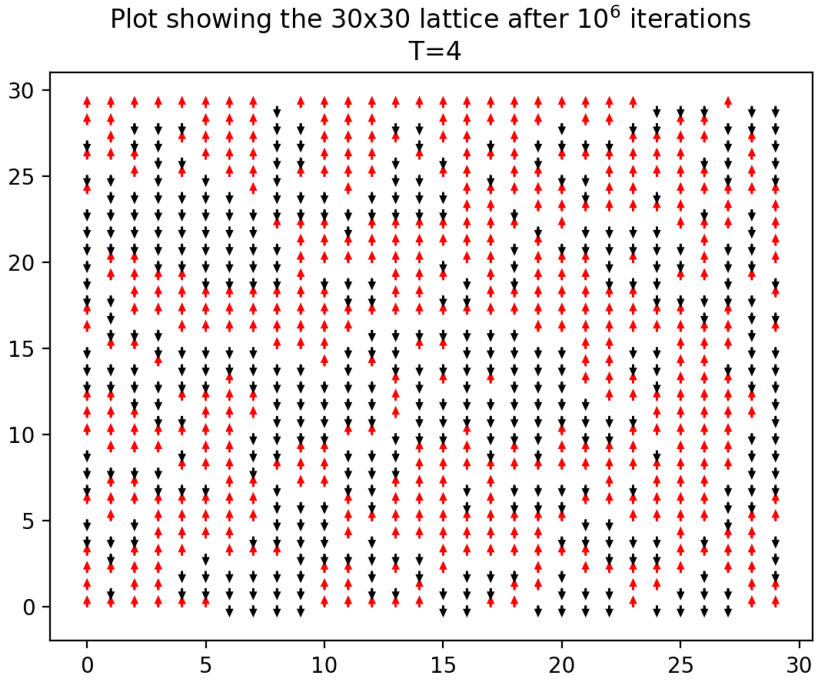

Figure 14: Lattice far past critical temperature. No net magnetic field.

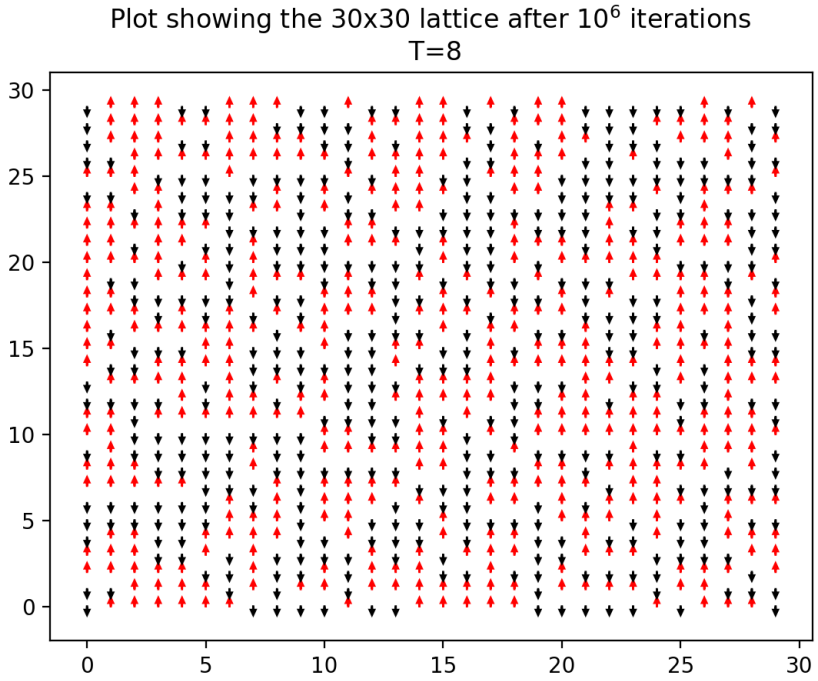

Figure 15: Lattice far past critical temperature. No net magnetic field.

Although simple - the figures above pin point a lot of the described features of Ferromagnetism. Figures 11 and 12 are both states after a million flips. Both have distinct aligned magnetic fields. What is interesting is that figure 10 has converged to a state where the top third is aligned downwards, the middle - upwards, and the last third downwards. In figure 12, the state is one of the two most likely states for this Ferromagnetic type lattice for this temperature. I.e. the other most likely state is the field pointing uniformly upwards. What figure 11 shows is two distinct partitioning "lines" where the atoms on either side will be in a higher energy state. Although this particular state is extremely unlikely, it is still possible for this temperature. If we lowered the temperature even further, this state would not be realisable.

Figure 13 shows a lattice close to its critical temperature. There is still a distinct net magnetic field, but there are single spins in opposite direction to their neighbours. There are too small domains of atoms with opposite spins to their surroundings. This is indicative of how naturally occurring Ferromagnetic materials have domains of alignment. Indeed when we increase the temperature to four, there is no longer a net magnetic field. What there are though is domains of various sizes of aligned spins. Despite there being no net magnetic field though out the lattice, the align-

ment of the spins still serves as keeping the lattice in a state of equilibrium. This observation is backed up by figure 15. The lattice here has double the temperature of figure 14. On top of there being no net magnetic field, the domains are significantly smaller than the lattice with half its temperature.

On the subject of system rectification. By decreasing the temperature the magnetic spins of the individual atoms become rectified into a unified direction.

6 Conclusion

Agent based modelling forms a mechanism for simulating the behaviour of ensembles of agents. One of the biggest obstacles is simplifying computations, since most systems will comprise of many different agents and therefore there is a high order of magnitude of different possible states. As shown in this paper, many agent based systems, where all interactions are accounted for - the laws of Thermodynamics arise. Most important from this is that the state tends towards an equilibrium, low energy state. Results of this simulated were one: how simple market economies tend towards an unequal wealth distribution. Secondly, an agent based model was used to model a characteristically Ferromagnetic lattice. In this example the system also tends to a state of equilibrium which is dependent on the lattice's total (conserved) energy.

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