

December 2020

Thermodynamical properties of Cellular Automata

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Project duration: 2 months

Bachelor of Science thesis supervised by Andrea Idini



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Abstract

Cellular automata are a set of discrete computational models whose evolution is defined by neighbourhood rules and are used to simulate many complex systems in physics and science. In this work, statistical mechanics and thermodynamics in and out of equilibrium are used to develop a five-class classification scheme for two-dimensional cellular automata. Thermodynamical variables and potentials will be derived and computed according to three different approaches to determine if a cellular automaton rule is representing a system akin to the ideal gas, in or out of the thermodynamical equilibrium.

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1 Introduction

1.1 Cellular Automata

A cellular automaton is a computational system which comprises of a set of cells defined on a lattice. Each cell has a state at any given discrete time. The state is updated according to some rules which, depending on the state of the cell's neighbourhood, give the configuration at the next time. Given this simple definition, cellular automata have demonstrated a surprising complexity and range of applications. In fact cellular automata are a typical example of the emergence of complex patterns and behaviours from a simple set of rules.

Most literature focuses on binary cellular automata of one and two dimensions, (with binary we mean that each cell can take one of two values, sometimes also referred to as Boolean). However, in general, the number of available states k does not necessarily need to be $k = 2$. Higher dimensions are very unstable, therefore the fraction of trivial rule outcomes is much higher, they require much higher computational power and have a much larger number of possible rules. As a consequence, higher dimensional cellular automata would require very extensive and expensive studies that are beyond the scope of this thesis. Similarly, the study of non-local cellular automata would massively extend the scope of this thesis.

There has been research on different neighbourhoods definitions for different lattice dimensions [1]. In the last few decades there has also been much research to evaluate the complexity levels of cellular automata, in both qualitative and quantitative ways. Among the qualitative evaluation of complexity emerging from different rules, it is worth mentioning Stephen Wolfram's four-class classification [1] and the six class classification by Li, Packard and Langton [2]. Quantitatively, complexity has been tackled starting from many different assumptions. Most approaches make use of entropy as a measure of complexity [1–3, 6]. Other works use concepts such as mutual information, causal entropic forces, self-organized criticality and $1/f$ noise, compression length as well as the definition of completely new quantities [3–7]. It is important to distinguish between the different uses of entropy as a measure of complexity, since the many definitions coming from both Physics and Information theory can yield different results [2, 3].

Cellular automata have been applied in several contexts [8, 9]. This includes disease spreading, which is a very relevant topic these days, and any system that iterates over local rules. Therefore, the finding of simple reliable metrics for cellular automata can be very beneficial in accelerating the development of these applications. Here metrics is intended as a standard of measurement or evaluation.

Cellular automata have also been studied in relation to statistical mechanics, mainly for

the investigation of phase transition [2] and the Ising model [10]. In a sense, these studies are very straight-forward, since cellular automata offer a lattice grid with two values, which can easily correspond to spin up and spin down. Overall, cellular automata have been used to model physical systems rather than the other way around.

A distinction is usually made between reversible and irreversible rules and between additive and non-additive rules (sometimes also referred to as totalistic/non-totalistic). A rule is reversible if there is a one-to-one mapping between the initial and the final state of the automaton, irreversible if different initial states produce the same final state [1]. A rule is said to be additive if the superposition principle applies, namely if the update is the result of the sum of the neighbourhood instead of the specific values at each neighbourhood site [1]. In this work, it is also relevant to look for a distinction between conservative and non-conservative rules. A rule is said to be conservative if the total energy of the system doesn't change or fluctuates around a stationary value and non-conservative otherwise. Conservation of energy is one of the most universal conservation laws in physics which does not universally hold for cellular automata.

This work studies the problem of the thermodynamics of cellular automata from different perspectives. Different metrics from statistical mechanics and classical thermodynamics are tested to find a way to quantitatively describe the behaviour of different configurations.

The originality and novelty of this approach lies in the premise of using the most basic approaches possible to study the problem of the thermodynamics of cellular automata and in deriving a classification scheme that is quantitative, as opposed to the most used ones to date which are qualitative. Furthermore, the statistical mechanics 'top-down' approach distinguishes itself from the typical approach, which instead derives theorems and statements about cellular automata by inspecting the system at each step in more of a 'bottom-up' fashion, which would include the investigation of the configuration matrix at each step. The former might lack the detail of the latter, but has the great advantage of processing a large number of cellular automata rules in an automated way. The 'top-down' approach is not intended as a substitute for rigorous mathematical analyses of the systems but rather as a complementary approach. The classification obtained can serve as a pre-selection of 'interesting rules' for a more thorough mathematical 'bottom-up' treatment.

1.2 Statistical Mechanics

Statistical mechanics studies the behaviour of large systems by considering the behaviour of the individual components in relation to each other and deriving the global statistical properties of the system from there. Two fundamental concepts are that of microstate, which maps the configuration of the individual components of the system, and that of macrostate, which are the properties of the system as a whole, such as temperature and energy. Statistical mechanics has been successful in the study of the thermodynamics of

mechanical systems such as gases, for which it is fundamentally impossible to solve the equations of motion for every particle involved.

For the case of cellular automata, it is possible to study the state of every single cell at any step. However, an approach based on statistical mechanics can simplify the study of the behaviour of large cellular automata in the same way it simplifies the study of gases and other physical systems. There has been some work in this direction [11, 12], but no comprehensive study of how to directly translate thermodynamical macrostates to the framework of cellular automata.

This thesis covers various aspects of statistical mechanics applied to cellular automata. Therefore, a review of the use of these same concepts in thermodynamics is useful. Note that in this work the Boltzmann constant is kept implicit. The reason behind this choice is that the interest of this thesis lies in the relation between the thermodynamical variables in cellular automata, which are not defined by a natural physical scale such as the Boltzmann constant.

Entropy S is a quantitative measure of the uncertainty or lack of information in a system [13] and it is at the core of many first principle definitions in thermodynamics, thus being of fundamental importance in evaluating thermodynamical metrics for cellular automata. One of the definitions of entropy used in statistical mechanics is the so called Gibbs Entropy S , which is the negative of the expected value of the logarithm of the probability P_s that a system is in the microstate s [13],

$$S = - \sum_s P_s \log P_s. \quad (1.1)$$

Then, temperature can be defined as the partial derivative of the energy E with respect to entropy S ,

$$T = \left(\frac{\partial E}{\partial S} \right)_{\tilde{N}}, \quad (1.2)$$

where the other state variables \tilde{N} (such as the volume and particle number) are kept constant [13].

For a system in thermal equilibrium with a heat bath (or reservoir), the total energy of the system and the reservoir is U_0 , the energy of the system is E_s and the energy of the reservoir is the difference $U_0 - E_s$. The probability that the system is in state s with energy E_s is given, for a very large reservoir in thermodynamical equilibrium, by [13]

$$P(E_s) = \frac{e^{-E_s/T}}{Z}, \quad (1.3)$$

with

$$Z = Z(T) = \sum_s e^{-E_s/T}, \quad (1.4)$$

where Z is called the partition function of the system. Z is very useful in defining the thermodynamical properties of a system. Through the partition function, one can derive the average energy, the Helmholtz free energy and in turn the pressure, the energy fluctuations and the heat capacity of the system at equilibrium.

1.3 Notation, neighbourhoods and boundaries

This work analyses the behaviour of additive rules, so rules that depend only on the total of the values of the cells in a neighborhood. The total number of possible additive rules, which considers the possibility of leaving the cell in its previous state is 3^{n+1} where n is the number of cells in the neighbourhood. The base is three because each configuration of the n cells of the neighbourhood can lead to three outputs, dead, alive or unchanged. The exponent is $n + 1$ because the possibility of zero active neighbours is counted too. The notation to distinguish between the different rules is birth-death, which indicates the number of active sites needed for the activation and the deactivation of a cell. The numbers that are not included in the notation are the ones that leave the cell in its previous state. For example, if a cell is activated at 1 and 2 active neighbours and deactivated at 7 and 8, the rule will be described by 12-78. Recall that these numbers represent the total number of active neighbours and are independent of the position of the cells as long as they are in the neighbourhood. Specifically, using the notation of (1.5) below, 1 and 2 would belong to B , while 7 and 8 would belong to D . The reason why only additive rules are studied is that this selection restricts the study enough for a comprehensive analysis that fits the temporal scope of this thesis. Ideally, given enough time, one would be interested in analysing every kind of cellular automata rules.

Formally, if w and h are the width and the height of the cellular automata (i.e. the number of cells per side) and t is the generation or time, the cellular automata at $t + 1$ can be described as a function of the cellular automata at t as the following $w \times h$ matrix

$$C_{t+1} = E_{x,y,t+1}, \quad x \in \{1, 2, \dots, w\}, \quad y \in \{1, 2, \dots, h\}$$

If B is the set of the number of sites that lead to the activation of the cell and D is the set of number of sites needed for the death of a cell, satisfying the requirement

$$B, D \subset \{0, 1, \dots, 8\} : B \cap D = \{\emptyset\},$$

then $E_{x,y,t+1}$ is defined case wise as follows, with corrections for the boundary cells which depend on the boundary condition:

$$E_{x,y,t+1} = \begin{cases} 1, & \text{if } \sum_{i=-1,0,1} \sum_{j=-1,0,1} E_{x+i,y+j,t} - E_{x,y,t} \in B \\ 0, & \text{if } \sum_{i=-1,0,1} \sum_{j=-1,0,1} E_{x+i,y+j,t} - E_{x,y,t} \in D \\ E_{x,y,t} & \text{otherwise} \end{cases} \quad (1.5)$$

In this work, the focus is mainly in the reduced Moore neighbourhood, corresponding to all cells next to the central cell, including the diagonal and excluding the central cell. The reason behind this is that the Moore neighbourhood is a very common neighbourhood choice, and the limited scope of the work doesn't allow for the testing of several neighbourhoods. With this kind of neighbourhood, the number of rules is $3^9 = 19683$. We now exclude the rules that do not lead to any new birth or any new death, which have a trivial outcome of full population or full starvation, and the number combinations that do not produce any rule, that is both birth and death are empty. Considering these corrections, the number of non-trivial rules is 18150 since the number of rules taken away is $3 \sum_{i=1}^9 \binom{9}{i} = 1533$.

The way the cellular automata is implemented is through the convolution of a neighbourhood matrix along the cellular automata state matrix. In Python this is done as follows for closed boundary conditions:

```

from scipy import signal
import numpy as np
NEWmatrix = np.zeros((w,h), dtype=int)
kernel = np.ones((3, 3), dtype=np.int8) #Neighbourhood
kernel[1, 1] = 0 #Reduced moore neighbourhood
k=signal.convolve(StateMatrix, kernel, mode='same')
for i in range(w):
    for j in range(h):
        n = k[i, j]
        if n in B:
            NEWmatrix[i][j] = 1 #birth
        elif n in D:
            NEWmatrix[i][j] = 0 #death
        else:
            NEWmatrix[i][j] = StateMatrix[i][j] #unaffected

```

This implementation is significantly faster than other algorithms.

Two kinds of boundary conditions are studied, closed and periodic. Periodic boundary conditions lead to the state of a cell at a boundary influencing the state of the cells at the opposite boundary (i.e. a flat torus). Closed boundary conditions do not put value constraints on the cells at the boundaries, but limit their neighbourhood. That is, for a reduced Moore neighbourhood, a cell at the side will have five neighbours and a cell at a corner will only have three.

2 Method

The way the project is carried out is divided into different stages.

- The translation of thermodynamical variables to the cellular automata framework and the effective redefinition of these variables
- The implementation of different rules on different boundary conditions to study, if any, emergent conservation laws. Different choices in the definition of the variables are tested and confronted to evaluate the best way to translate thermodynamical variables to the cellular automata framework.
- The use of the newly defined variables to study the behaviour of different rule outputs.

Subscripts are used to distinguish the quantities derived with the different approaches, to avoid confusing the reader. The benchmark quantities have no subscript (Q), the ideal gas quantities are written as Q_I and the partition function quantities are written as Q_Z .

2.1 Benchmark

Cellular automata lend themselves very well to the framework of statistical mechanics. The system is a partition by construction and the state of each cell can be interpreted as an energy state E_i . In the case of binary cellular automata, this leads to two possible energy states per cell, namely $E_1 = 1$ and $E_0 = 0$. n_i is the number of cells at energy E_i and the total energy of a configuration is given by

$$E_s = \sum_{i=0,1} n_i E_i, \quad (2.1)$$

Considering that the update rules are deterministic, P_s in Eq. (1.1) could be specifically derived for each set of rules. However, deriving the specific probabilities for each cell based on the set of rules is exactly what one attempts to avoid by using a thermodynamical approach. Indeed, this is what this work attempts by studying large cellular automata. Hence the following approach is preferred.

The probability that a cell is in state i is defined as the probability that, if one picks a random cell from the system and checks what state it is in, it is found in state i . This probability corresponds to $P_i = \frac{n_i}{N}$, with N being the total number of cells of the system. By assuming that each microstate at a given energy is equally likely, the expression for entropy (1.1), can be rewritten as $S = -N \sum_i P_i \log P_i$. Following this, by observing that

$n_1 = E_s$ and $n_0 = N - E_s$, one gets

$$S = - \left(E_s \log \frac{E_s}{N} + (N - E_s) \log \left(1 - \frac{E_s}{N} \right) \right) \quad (2.2)$$

for a two level system. Once S and E are established, temperature can be calculated using Eq.(1.2), leading to

$$T = \frac{1}{\log(1 - E_s/N) - \log(E_s/N)} = \frac{1}{\log\left(\frac{N-E_s}{E_s}\right)} \quad (2.3)$$

. Thus the heat capacity C is

$$C = \frac{\partial E_s}{\partial T} = \left(\frac{\partial T}{\partial E_s} \right)^{-1} = - \frac{N}{E_s(E_s - N)(\log(1 - E_s/N) - \log(E_s/N))^2} \quad (2.4)$$

and the Helmholtz free energy A is

$$A = E - TS = N \frac{\log \frac{N-E_s}{N}}{\log \frac{N-E_s}{E_s}}. \quad (2.5)$$

The above expression for S is based on the assumption that all states at the same energy are equally likely. This assumption is known as the principle of equal a priori probability and it is considered to be a postulate of statistical mechanics. It is by no means obvious that this principle is bound to hold for cellular automata as well. In any case, it is a fundamental principle of statistical mechanics, which justifies its use in this work.

Pressure could be calculated from the Helmholtz free energy in relation to a change of volume. In this work, the closest thing to volume/area is the number of cells so $P = -\frac{\partial A}{\partial N}$, this leads to a complex expression for pressure with an asymptotic behaviour at $E_s = N/2$, which is also negative over its whole domain.

$$P = - \frac{N \log(1 - E_s/N) + \log(-1 + N/E_s)(E_s + (N - E_s) \log(1 - E_s/N))}{(N - E_s) \log^2(-1 + N/E_s)}.$$

Alternatively, there is the option of deriving pressure from first principles, via a count of the interactions at the boundaries instead. Namely, as the energy density of the boundaries, which is the energy of the boundary cells divided by the number of boundary cells $4\sqrt{N}$, so

$$P = \sum_{i \in \text{boundaries}} \frac{E_i}{4\sqrt{N}}. \quad (2.6)$$

This way of defining pressure is similar to the microscopic definition of pressure in a thermodynamical system, which takes into account the force that the molecules exert on the boundaries of the system.

For the sake of simplicity, from the next section on, the total energy of a configuration E_s will be denoted by just E .

2.2 Ideal gas

It is demanding to calculate temperature a posteriori as defined in (1.2). Therefore a definition of temperature a priori T_A is used as well. T_A is defined in a way similar to activity in [7] with the addition of a normalization factor $\frac{1}{N}$ to make the variable intensive. By analogy to the concept of the average kinetic energy of the molecules, T_A is the sum of all value changes in the automaton divided by the number of cells.

$$T_A = \frac{1}{N} \sum_{i=1}^N a_i, \quad (2.7)$$

$$a_i = \begin{cases} 1, & \text{if the state of the cell } i \text{ is different from the previous generations} \\ 0, & \text{if not} \end{cases}$$

The interpretation of temperature as the average kinetic energy of the molecules is valid only for an ideal gas model. Its use raises the question of the validity of the assumption of non-interaction in the cellular automata framework. We are going to assume that the ideal gas model can be applied to cellular automata and verify in which cases the assumption of non-interaction holds.

The next step would be to use established results from the ideal gas model to evaluate the thermodynamical properties of cellular automata. With the interpretation of cells as point-like particles, volume and particle number are essentially equivalent (or proportional), both corresponding to N , leading to significant simplifications as shown in the quantities below. In the framework of the ideal gas, energy can be derived from temperature as $E = \frac{3}{2}NT_I$, in the case of a two-dimensional system, this should become $E = NT_I$.

The entropy of an ideal gas is described by the Sackur-Tetrode equation as

$$S_I = k_B N \log \left(\frac{V}{N} \left(\frac{4\pi m E}{3h^2 N} \right)^{3/2} \right) + \frac{5}{2}N,$$

with m being the mass and h the Planck constant and k_B the Boltzmann constant. This is obtained starting from Boltzmann's entropy formula, $S_I = k_B \log(\Omega)$, where Ω is the multiplicity or number of microstates accessible to the system. From equation 2.40 in [14], a three dimensional gas has multiplicity $\Omega \approx \frac{V^N (2\pi m E)^{3N/2}}{h^{3N} N! (3N/2)!}$, where the factor $3N$ accounts for dimensions. Accordingly, to find the two-dimensional multiplicity, one can substitute V with A (the area) and $3N$ with $2N$, leading to $\Omega \approx \frac{(2\pi A m E)^N}{(N!)^2 h^{2N}}$. Using Stirling's approximation, $N! \approx \sqrt{2\pi N} N^N e^{-N}$ one gets $\Omega \approx \frac{(2\pi A m E)^N}{2\pi N^{2N+1} e^{-2N} h^{2N}}$. At large N , $2N+1 \approx 2N$ and $(2\pi)^{N-1} \approx (2\pi)^N$. By using these approximations and taking the logarithm one gets the two-dimensional Sackur-Tetrode equation $S_I = k_B N \log \left(\frac{2\pi m A E}{h^2 N^2} \right) + 2N$.

In our treatment, the area and the particle number correspond both to the number of cells N , and the mass of a cell is not defined. The constants can be grouped as $b = \frac{2\pi m}{h^2}$, which

leads to $S_I = N \log \frac{E}{N} + N(2 + \log(b))$, we can extend b to become $B = 2 + \log(b)$, leading to $S_I = N(\log \frac{E}{N} + B)$.

Here B can be treated in different ways. Generally, one can notice that it should be a large number. The ratio between the mass of the particles and the Planck constant squared becomes a very large number for all gases. In our treatment, it is enough to have B large enough that the entropy is always positive. In general, B can be taken to be $B = \log(N)$. Therefore,

$$S_I = N(\log \frac{E}{N} + \log N) = N \log(E) \quad (2.8)$$

The ideal gas temperature T_I is obtained as $T_I = \frac{\partial E}{\partial S_I} = (\frac{\partial N \log E}{\partial E})^{-1} = E/N$. So

$$T_I = \frac{E}{N} \quad (2.9)$$

This is a very reassuring sanity check, since it reproduces the expression $E = NT_I$ in a rigorous way.

Similarly, the heat capacity $C_I = \frac{\partial E}{\partial T_I}$ becomes $C_I = N$, in accordance to the two dimensional ideal gas. This is an analytical conclusion and a confirmed computational result, the analytical result is shown as

$$C_I = \frac{\partial E}{\partial T} = \frac{\partial E}{\frac{\partial E}{\partial S}} = \frac{\partial E}{\frac{\partial E}{\partial N \log E}} = \frac{dE}{dE/N} = N. \quad (2.10)$$

One could try to derive an ideal gas law for cellular automata, namely finding an analytical expression for pressure, in different ways. A first naive approach could be to start from $P_I V = NT_I$, and by noticing that $V \propto N$, getting to an expression in the form $P_I \propto T_I$. Indeed P_I should be a monotonously increasing function of T_I . This work starts by using $P_I = -\frac{\partial A_I}{\partial V}$, which is interpreted as $P_I = -\frac{\partial A_I}{\partial N}$. From here, one can use the Helmholtz free energy, as it is commonly defined $A_I = E - T_I S_I$.

From the definition, using the ideal gas entropy 2.8, one gets $A_I = E - T_I N \log E$, this can be expressed in different ways using 2.9,

$$A_I = E - E \log(E) = NT_I - NT_I \log(NT_I). \quad (2.11)$$

Thus,

$$P_I = -\frac{\partial A_I}{\partial N} = T_I \log(NT_I).$$

2.3 Partition Function

By having a value for entropy and energy one can calculate the temperature with Eq. (1.2). Thus, the partition function can be evaluated. The expression for the partition function (1.4) in the case of binary cellular automata is very simple and it becomes

$$Z = \sum_s e^{-E_s/T} = \sum_{i=0}^N e^{-i/T}. \quad (2.12)$$

The partition function can be useful in evaluating a whole set of other quantities, at equilibrium. The Helmholtz free energy is $A_Z = -T \log(Z)$, which can be compared to the common definition $A = E - TS$. The average energy is $\langle E \rangle = -\frac{\partial \log(Z)}{\partial \frac{1}{T}} = T^2 \frac{\partial \log Z}{\partial T}$. The variance of the energy is calculated as $(\partial E)^2 = \frac{\partial^2 \log(Z)}{\partial^2 (\frac{1}{T})}$ and it is useful for the heat capacity $C_Z = \frac{(\partial E)^2}{T^2}$, which can be compared to the common definition $C = \frac{\partial E}{\partial T}$ [13]. Entropy can also be calculated from the partition function starting from (1.1) and (1.3), this leads to $S_Z = -\sum_s P_s \cdot (-E_s/T - \log(Z)) = \frac{\langle E \rangle}{T} + \log(Z)$.

As above, using $P_Z = -\frac{\partial A_Z}{\partial N}$ one can use the Helmholtz free energy, as derived from the partition function $A_Z = -T \log Z$ to get to a law for pressure. From the partition function,

$$A_Z = -T \log\left(\sum_{i=0}^N e^{-i/T}\right),$$

for large N one can approximate the sum with an integral,

$$A_Z \approx -T \log\left(\int_0^N e^{-x/T} dx\right) = -T \log T - T \log(1 - e^{-N/T}),$$

which leads to the following formulation for pressure,

$$P_{1,Z} = -\frac{\partial A_Z}{\partial N} \approx \frac{T^2}{N-E} \left(\log T + \log(1 - (N/E - 1)^{-N}) + 1\right) + \frac{(N/E - 1)^{-N} \left(-\frac{N}{N-E} - 1/T\right)}{1 - (N/E - 1)^{-N}}.$$

It can also be shown (i.e. by induction) that Z corresponds to

$$Z = \frac{e^{-N/T} \left(e^{\frac{N+1}{T}} - 1\right)}{e^{1/T} - 1}, \quad (2.13)$$

Proof.

$$\begin{aligned}
N = 1 &\implies Z = 1 + e^{-1/T}, & Z &= \frac{e^{-1/T}(e^{2/T} - 1)}{e^{1/T} - 1} = \frac{(e^{1/T} - 1)(e^{-1/T} + 1)}{e^{1/T} - 1} = 1 + e^{-1/T} \\
N = K &\implies Z = \sum_{i=0}^K e^{-i/T}, & Z &= \frac{e^{-K/T}(e^{\frac{K+1}{T}} - 1)}{e^{1/T} - 1} \\
N = K + 1 &\implies Z = \sum_{i=0}^{K+1} e^{-i/T}, & Z &= \frac{e^{-K/T}(e^{\frac{K+1}{T}} - 1)}{e^{1/T} - 1} + e^{-(K+1)/T} \\
&&&= \frac{e^{-K/T}(e^{\frac{K+1}{T}} - 1) + e^{-(K+1)/T}(e^{1/T} - 1)}{e^{1/T} - 1} \\
&&&= \frac{e^{1/T} - e^{-(K+1)/T}}{e^{1/T} - 1} \\
&&&= \frac{e^{-(K+1)/T}(e^{(K+2)/T} - 1)}{e^{1/T} - 1} \quad \square
\end{aligned}$$

this expression can be used to evaluate some quantities analytically, by using $\log(Z) = -N/T + \log(e^{\frac{N+1}{T}} - 1) - \log(e^{1/T} - 1)$, for large N and $N \gg T$, the first and the second term in the expression cancel out, leading to $\log(Z) = -\log(e^{1/T} - 1)$, thus one can rewrite the aforementioned quantities as

$$\langle E \rangle = \frac{e^{1/T}}{e^{1/T} - 1}, \quad (2.14)$$

$$C_Z = \frac{e^{1/T}}{(e^{1/T} - 1)^2 T^2}, \quad (2.15)$$

$$A_Z = T \log(e^{1/T} - 1), \quad (2.16)$$

and similarly S and P ,

$$S_Z = \frac{e^{1/T}}{T(e^{1/T} - 1)} - \log(e^{1/T} - 1) \quad (2.17)$$

and

$$P_{2,Z} = \frac{\log \frac{N-2E}{E}}{(N-E) \log^2 \frac{N-E}{E}} - \frac{1}{(N-2E) \log \frac{N-E}{E}}, \quad (2.18)$$

which has been obtained using (2.3). One can notice that the two versions of P_Z disagree with each other.

2.4 Non-Equilibrium Thermodynamics

A final approach to the problem of the thermodynamics of cellular automata is provided by the formalism of non-equilibrium thermodynamics, as developed by Prigogine [15]. This approach is based on the concept of local equilibrium. That is, the parts of a thermodynamic system outside of equilibrium are individually in local thermodynamical equilibrium. This allows to define intensive quantities as time and space-dependent, while extensive quantities are substituted by their relative densities, so $T = T(x, t)$, $P = P(x, t)$, $s(x, t) = S(x, t)/N$ and $e(x, t) = E(x, t)/N$. This approach on the thermodynamics of the system assumes that the quantities do not depend on the gradients of the system. That is, the system is not far from equilibrium.

This work attempts to get a qualitative overview of the applicability of the postulate of local equilibrium for some cellular automata rules by partitioning the system into boxes and recursively compute the thermodynamical variables. There is a trade-off when choosing the number of boxes to partition the system into. A high number of boxes gives a better picture of locality but it is a problem in the fact that the quantities are not well defined for small boxes since the thermodynamical limit is not reached. Vice-versa, when there are too few boxes, each box has well defined quantities but the picture of locality is less sharp. A good compromise is found by using 25 boxes, so that each box has 6400 cells, when using a cellular automata of 160000 cells. The output consists of a set of local averages of the variables over the evolution.

The hope is to get some insight into the potential of the non-equilibrium thermodynamics formalism for cellular automata and eventually lay the groundwork for more detailed studies in the future.

Another point of the use of non-equilibrium metrics is the validation of the equilibrium approach and the principle of equal a priori probability. If all the batches in the non-equilibrium study show similar behaviour, then it is justified to use the equilibrium approach developed here. Specifically, if the energy density has similar values across the partition, then the principle of equal a priori probability is valid.

2.5 Classification

Regarding the temperature used in calculating the partition function, one could choose between (2.3), (2.7) and (2.9) which have all been tested with satisfactory results, the quantitative part of this project makes use of the temperature from the benchmark (2.3) since it is the most fundamental definition among the three.

Finally, the rules are classified based on the validity of these three approaches, leading to

five classes:

- Ideal cellular automaton in equilibrium (A)
- Ideal cellular automaton outside of equilibrium (B)
- Non-Ideal cellular automaton in equilibrium (C)
- Non-Ideal cellular automaton outside of equilibrium (D)
- Cellular automaton that reaches zero activity in 'short time', less than 100 iterations (E)

There are several uses to this classification, for example in the applications of cellular automata. By using this classification technique one can restrict the pool of rules among which to choose for a study. If, for instance, one would want to study non-equilibrium behaviour, instead of having to choose among all 18150 rules, it would only need to choose among class B and D rules.

To evaluate the equilibrium, we consider the validity of the partition function approach, this is done by considering the coefficient of variation (the ratio between the standard deviation and the mean) of the first 40 values of the ratio between the Helmholtz free energy as defined from the benchmark and the partition function. If this value is smaller than 0.1, the two values are proportional and are thus equally viable, which means that the partition function is a good approach to the system and we thus consider it to be an equilibrium cellular automata. The reason behind the choice of the Helmholtz free energy is that it is the most direct metrics from the partition function, whereas expected energy and heat capacity require derivatives.

The choice of using the first 40 values only is dictated by the relative short relaxation time of some rules, which could lead to miss-classification if one was to consider all values. The threshold for the coefficient of variation is chosen in a somewhat arbitrary manner. Basically, the lower this value, the more the cellular automata is in equilibrium. The distribution of the coefficient of variations is smooth and didn't show any sharp trend changes, so it had to be chosen in an arbitrary way.

To evaluate if a rule is ideal or not, we consider the variance of the ratio between (2.9) and (2.7). This value doesn't need to be scaled like the former because the ratio between (2.9) and (2.7) is more stable and consistent in its output. If this value is smaller than 1, we say that the two are proportional and thus that temperature can be viewed as an average activity. One could take the threshold to be lower for a more strict classification. However, taking the threshold to be one shows results that are qualitatively satisfying.

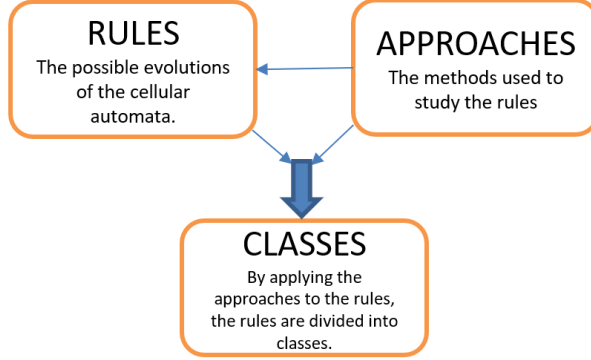


Figure 2.1: A summary of the relations between some key terms used in the thesis.

Table 1: Summary table with the approaches used in this study

	E	S	$\frac{\delta E}{\delta S}$ T	$\frac{\delta E}{\delta T}$ C	$A = E - TS$ A	$\frac{\delta A}{\delta N}$ P
Benchmark	$\sum_{i=0,1} n_i E_i$	$-\sum_s P_s \log P_s$	$\frac{1}{\log(\frac{N-E}{E})}$	$\frac{\delta E}{\delta T}$	$N \frac{\log \frac{N-E}{N}}{\log \frac{N-E}{E}}$	$\sum_{i \in \text{boundaries}} \frac{E_i}{4\sqrt{N}}$
Partition Function	$\sum_{i=0,1} n_i E_i$	$T \frac{\delta \log Z}{\delta T} + \log(z)$	External	$\frac{1}{T^2} \frac{\delta^2 \log(Z)}{\delta^2(\frac{1}{T})}$	$-T \log Z$	-
Ideal gas	$\sum_{i=0,1} n_i E_i$	$N \log(E)$	E/N	N	$E - E \log(E)$	$T \log(NT)$

Finally, alongside the classification, we also investigate if some rules conserve the total energy. A rule is said to be conservative if the difference between initial and final energy is less than a standard deviation of the energy distribution throughout the evolution of the system.

I would not be surprised if the reader was a bit confused at this point, therefore a little diagram that explains the relation between some concepts can be found in figure 2.1. Furthermore, the reader will find a summary of the approaches in table 1.

3 Results

Generally, we have found that cellular automata show the same or similar thermodynamical behaviour with periodic and closed boundary conditions. The results presented in this thesis are obtained with closed boundary conditions. This choice is completely arbitrary. The results are also scale-independent, that is they cannot be compared with each other on the same scale, because of the different underlying assumptions in their derivation and of the different treatment of constants and units. For some of the quantities, constants have been disregarded and the approaches for the derivation of different quantities have been fundamentally different. Therefore, the absolute values of the thermodynamical variables cannot be compared, but quantities that do not depend on scaling can be used for comparison. A way of comparing the results is to normalize them to the same starting value as done in fig 3.1 and fig 3.2. It is most likely possible to solve this scaling problem, but it is non-trivial and beyond the scope of this work.

Generally, the results show some small scale fluctuations, which are a consequence of the finite and limited size of the automata. If they were infinitely large or closer to the thermodynamical limit, the results would be smoother.

Let us now describe the main results and behaviours for each class of rules and thermodynamical quantity.

3.1 Benchmark

The benchmark metrics are well defined for a two-level system [13]. The results obtained are a direct consequence of the energy state E_s , this is shown in Fig. 3.3. This approach also correctly reproduces the transition to negative temperature states for an occupation $E_s > N/2$, with the difference that a system at a given temperature can evolve into a system at its negative temperature. This transition is not allowed in classical thermodynamics [13] in the case of unbounded phase space and energy conservation. In that case, a system at positive temperature will remain positive and a system at negative temperature will remain negative. The transition is accessible to cellular automata because cellular automata do not necessarily obey energy conservation. The entropy of a two-state system is maximized at $E_s = N/2$, So any move from that energy state will cause a decrease in entropy. If the energy increases further, occupying more sites, the temperature is negative.

Regarding the other quantities, the Helmholtz free energy is negative at positive temperature and vice versa for all rules and it is minimized when entropy is maximized, as expected. The heat capacity is always positive but has a somewhat unpredictable behaviour, sometimes stationary, sometimes increasing and sometimes decreasing with each time step. The pressure is generally monotonously increasing with energy, which is a direct consequence of

the fact that the energy tends to distribute evenly across the grid and it offers a weak but reassuring justification of the postulate of equal a priori probability. After all, the pressure (2.6) is defined just as a localized energy density. A more thorough justification of the principle of equal a priori probability is offered by the non-equilibrium approach described in section 3.4.

3.2 Ideal gas

In the case of the ideal gas approach, we start with the same definition of energy as in the previous section but define the other quantities as corrections to the known expressions for the ideal gas. This leads to an entropy (2.8), which is monotonously increasing with respect to energy and temperature taking the form of average energy.

Regarding the other quantities, the Helmholtz free energy, given the simple relationships between the quantities, behaves in a well defined and expected way with respect to energy. This regular behaviour is observed also for the other approaches. The heat capacity is defined as constant. The ideal gas pressure is monotonously increasing with temperature and energy, which is a reasonable result.

This exact behaviour is shown in 3.4 where the monotonously increasing energy leads to monotonously increasing entropy, temperature and pressure and a decreasing Helmholtz free energy towards equilibrium.

3.3 Partition Function

The partition function approach is valid for equilibrium or near equilibrium cellular automata. It is fundamentally different from the previous approaches since it is based on temperature instead of energy. It breaks down if negative temperatures are reached since $\lim_{T \rightarrow 0^-} Z(T) = \infty$.

Overall, the metrics do not show very quick changes. Generally, these equilibrium rules either oscillate around equilibrium, as shown in Fig.3.5 or reach an equilibrium state in a slow and controlled manner, i.e., with small gradients. Specifically, this is generally true for temperature, energy and entropy in the same way. The Helmholtz free energy is generally negative and evolves in opposite direction than the aforementioned quantities. Heat capacity tends to zero at low temperatures and to one at higher temperatures.

Regarding the pressure, $P_{1,Z}$ is only defined for positive temperatures, it is negative for a short part at low energies and then shows a steep increase, tending to infinity for $E = N/2$. This sort of behaviour is very hard, if not impossible to interpret physically. $P_{2,Z}$ is negative for all energy and temperature values. Negative pressure can be hard to consider. Negative pressure is a result that requires more theoretical interpretation for real physical systems [16, 17]. While it is possible to interpret negative pressure for some exotic rules as it is not ruled out by thermodynamics [18], it is not acceptable that it is the case for a whole class of rules and especially it seems unreasonable to be the case for equilibrium rules. Both of these pressure expressions can be therefore disregarded. A substitute can be found with the energy density approach as used in the benchmark, or not found at all. The latter would lead to the conclusion that pressure cannot be defined for these systems.

An example of this approach is found in fig 3.5, where all quantities oscillate around a stable value. It is also to be said that the rule shown in the figure is perhaps one of the most stable, which is also the reason why I choose it to display this approach. Especially outstanding is the behaviour of the pressures, which seem mirrored around zero. This is not a general feature of the pressure expressions but it is only displayed for some rules.

3.4 Non-Equilibrium or Equilibrium?

We find that the energy is evenly distributed among the boxes for all rules examined, and so is entropy. This provides a strong validation of the principle of equal a priori probability. However, when testing the non-equilibrium approach on the rules of different classes, it is observed that some of them deviate from thermal equilibrium. That is, the temperature of the different boxes is different. Sometimes, when the energy of the automaton is close to $E = N/2$, the measures show some boxes at positive temperature and some boxes at negative temperature, which is expected, since the automaton is close to the temperature transition.

For class A and C, that is equilibrium rules, there is no significant temperature gradient, as expected. For class B and D, the results show significant localities in the temperature distribution. This is not always the case, specifically when negative temperatures are reached. Since the partition function breaks down, these rules have been classified as non-equilibrium even though they have an even negative temperature distribution. An example of the temperature distribution for a D class rule is shown in fig 3.6. The same figure is intended as a comparison between the spatial distribution of temperature in class A and class D cellular automata. The reader can notice how the distributions differ in that the class A rule shown is has a very evenly distributed temperature and the class D rule shows strong localities.

3.5 Classification

The developed program has classified the 18150 cellular automata rules considered, in the classes described in section 2.5. The results are shown in Fig. 3.7. One can notice how most of the rules have been classified as out of equilibrium, with the most represented class being that of ideal cellular automata outside of equilibrium and the least represented being that of non-ideal cellular automata in equilibrium. It is also interesting to notice the high amount of rules that 'die out' i.e. class E. In addition to that, 254 rules have been found to be conservative, this doesn't contribute to the classification, but it is helpful in understanding the connections between physics and cellular automata and the lack thereof.

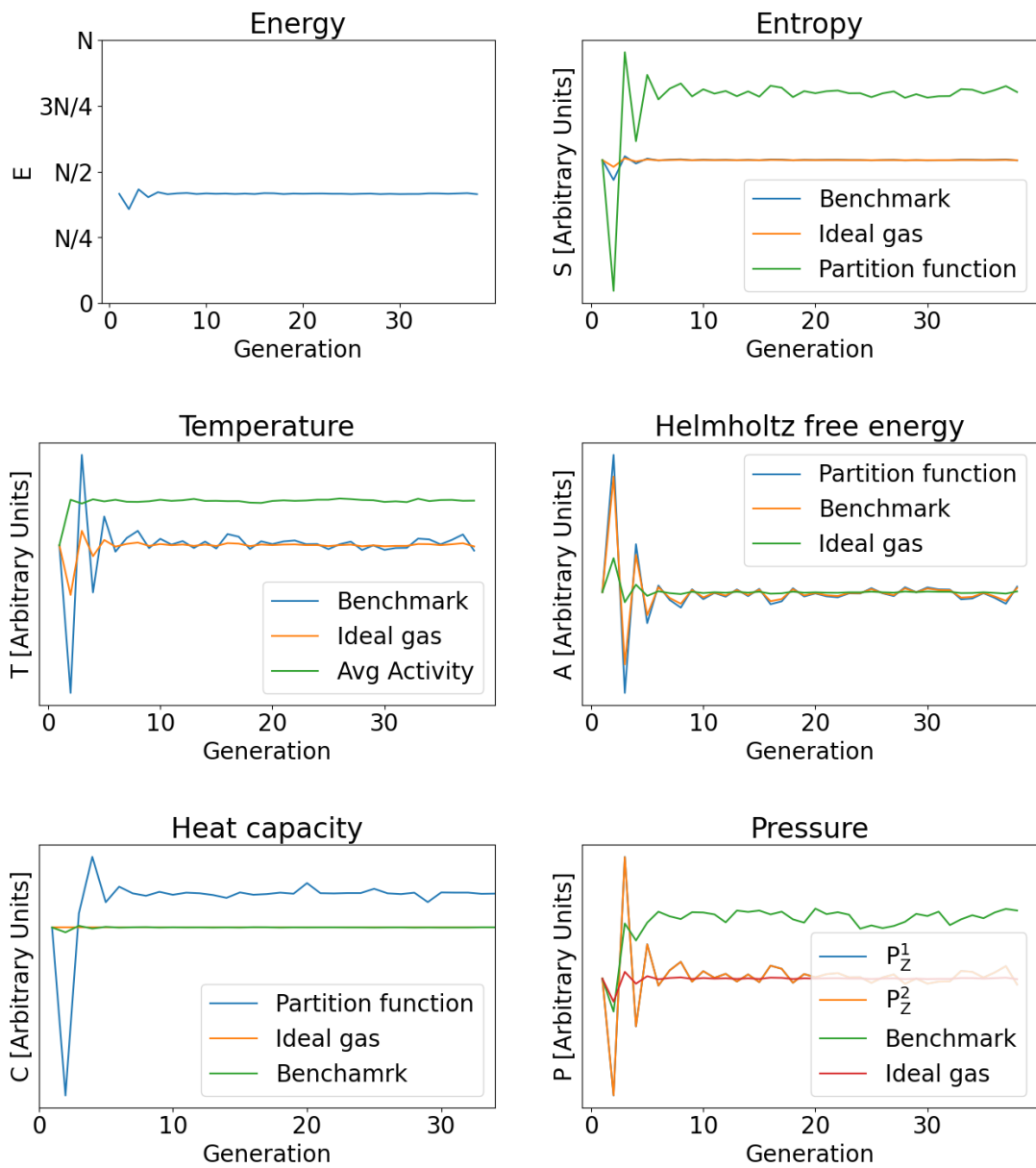


Figure 3.1: Comparison between the variables in a cellular automata evolving according to rule 1367-0245 (class A). All values have been normalized to the same starting point. $P_{1,Z}$ is not visible in the graph, but it behaves as in figure 3.5

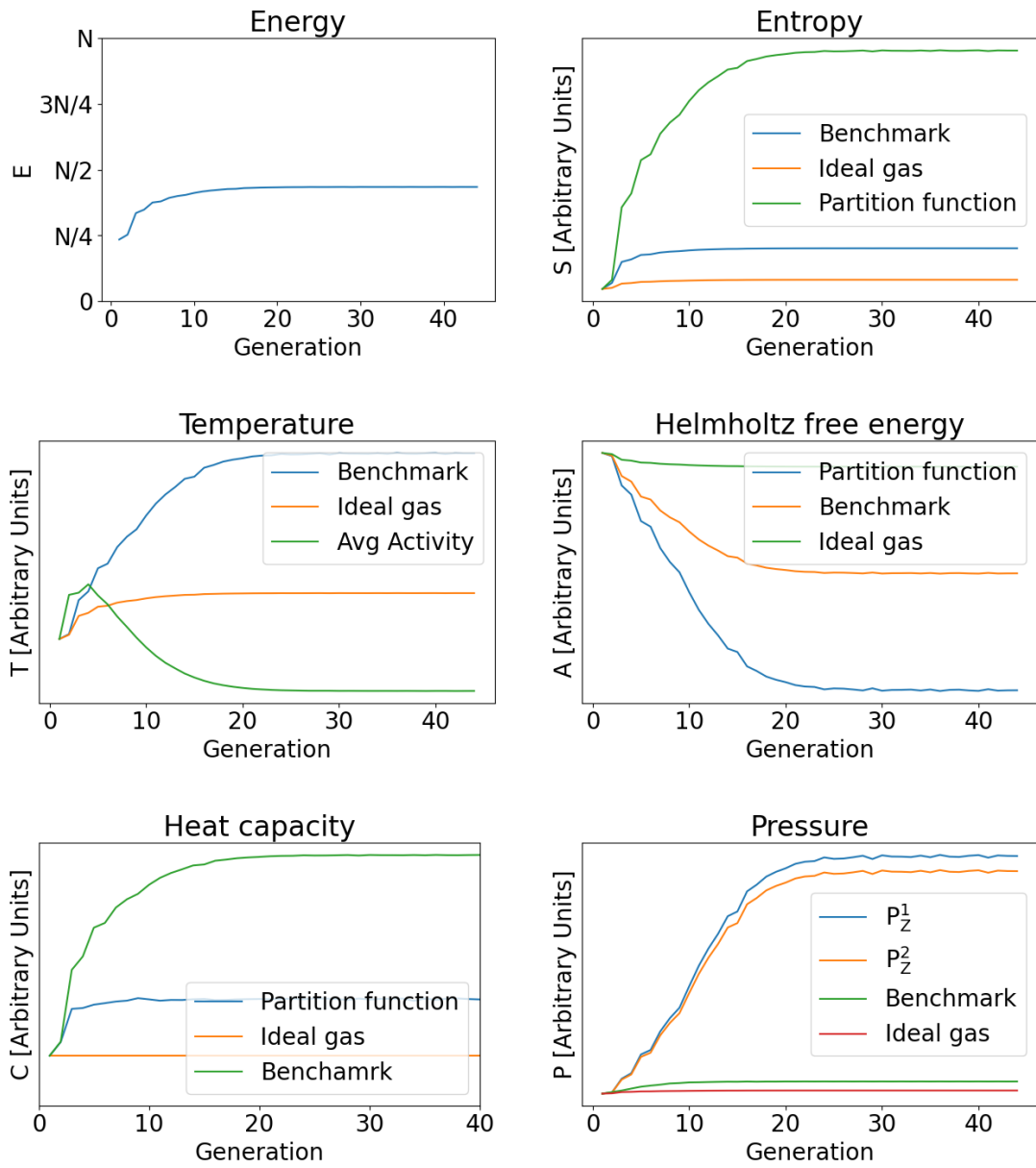


Figure 3.2: Comparison between the variables in a cellular automata evolving according to rule 2-4568 (class D). All values have been normalized to the same starting point.

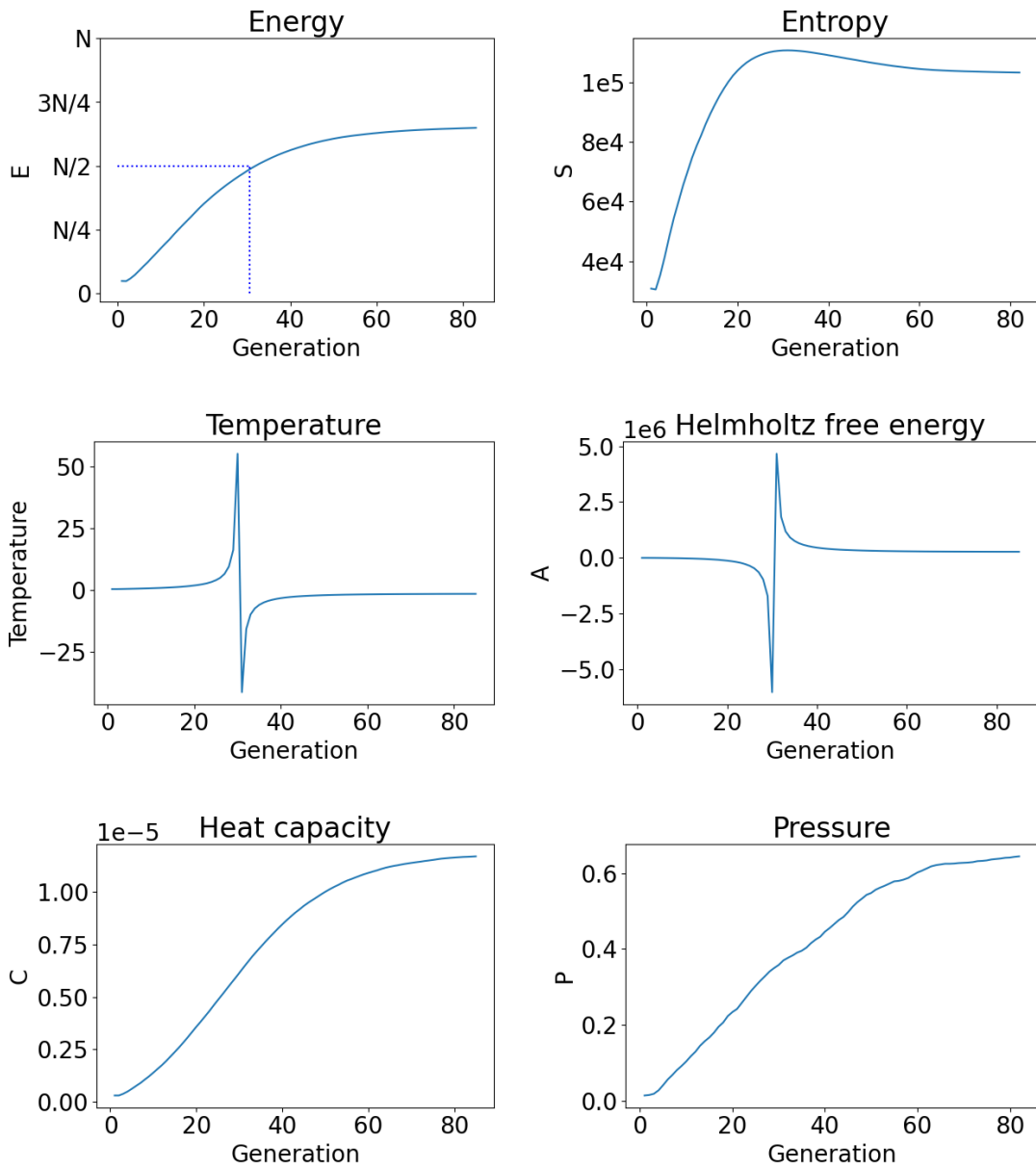


Figure 3.3: The figure shows the energy, entropy, temperature, Helmholtz free energy, heat capacity and pressure as defined in section 2.1 for a cellular automaton with 160000 cells evolving according to the rule 3-0178 (Class D)

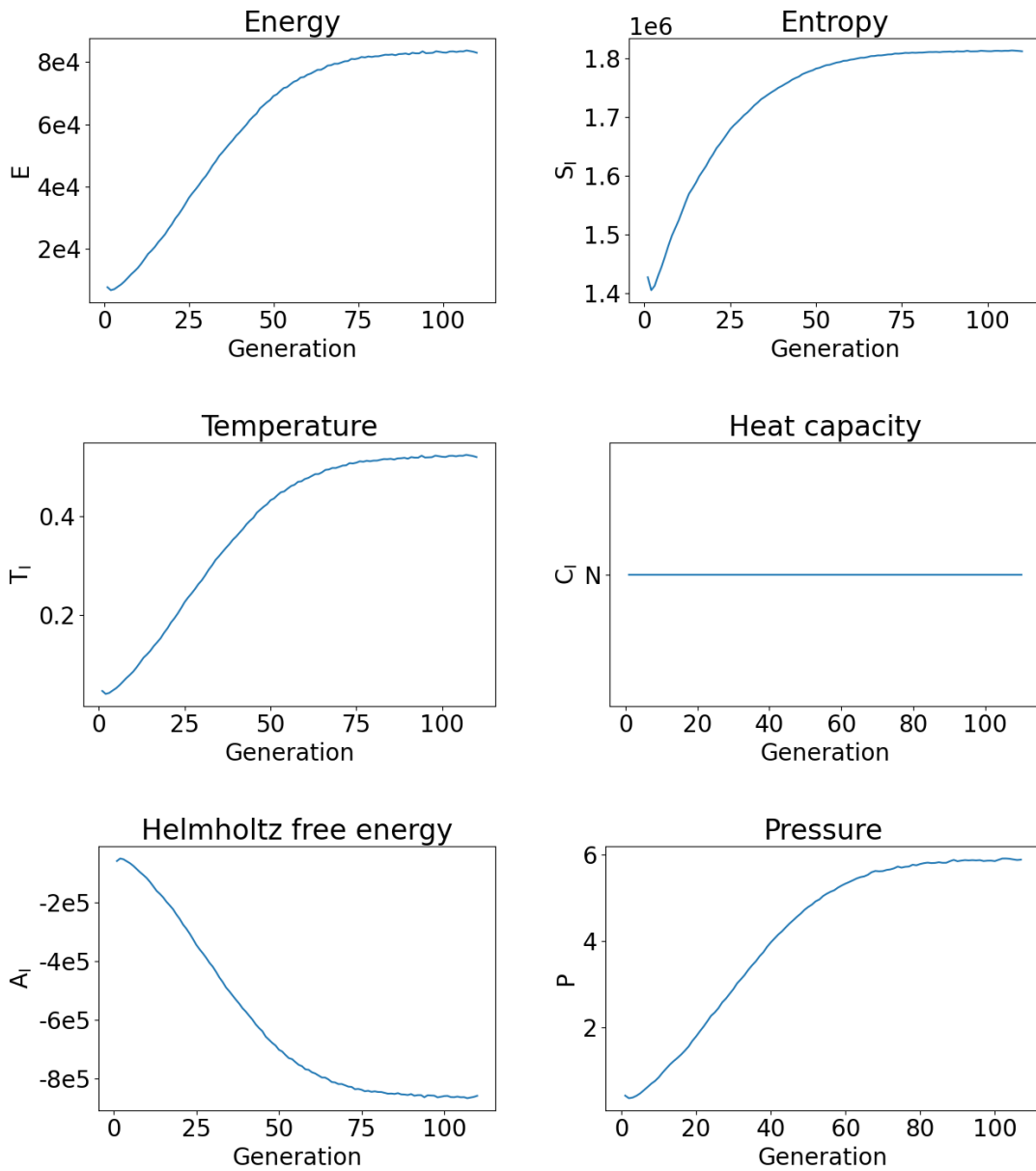


Figure 3.4: The figure shows the ideal gas metrics of energy, entropy, temperature, Helmholtz free energy, heat capacity and pressure from section 2.2 of a cellular automaton with 160000 cells evolving according to the rule 357-0146 (Class B)

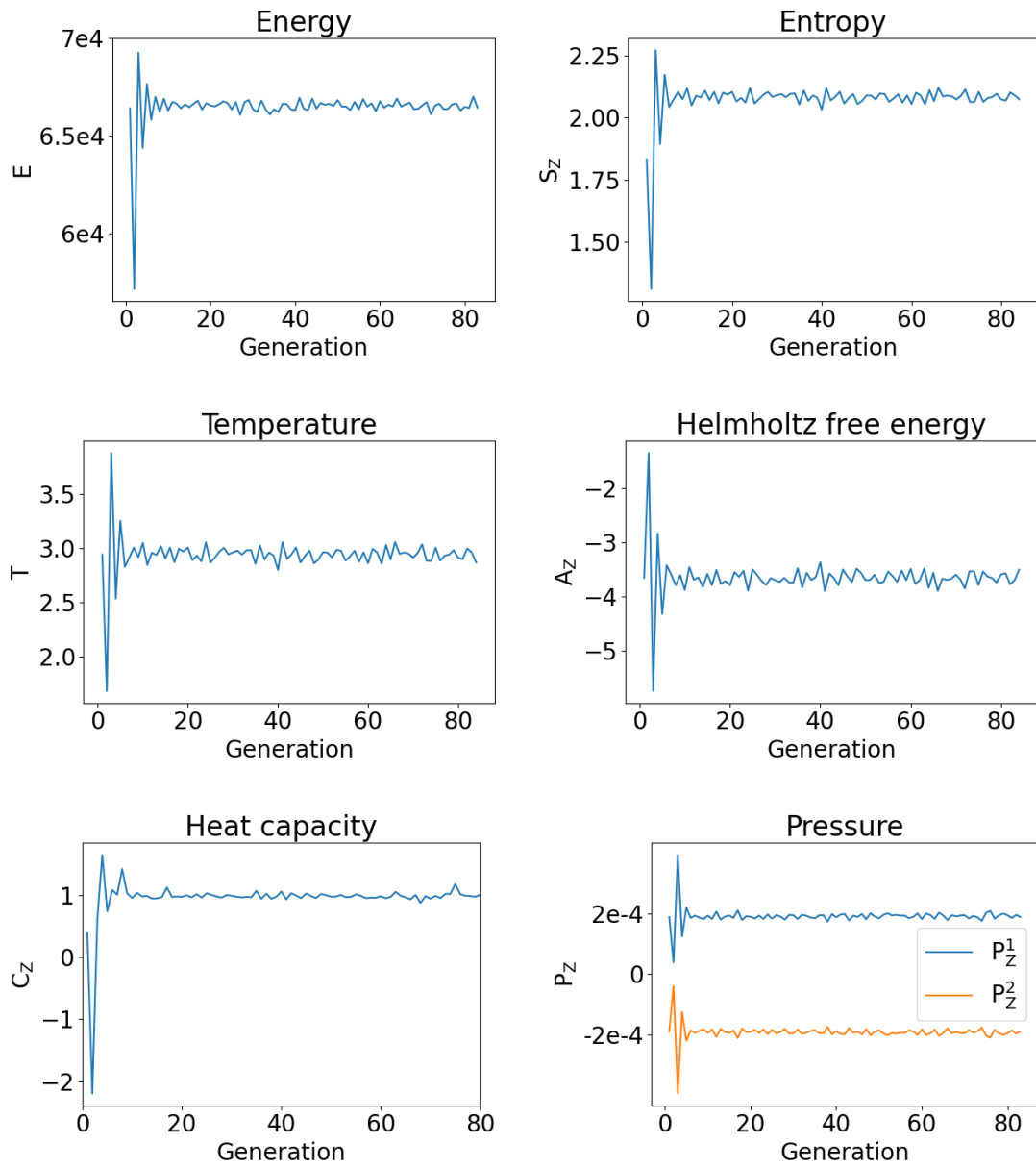


Figure 3.5: The figure shows the energy, entropy, temperature, Helmholtz free energy, heat capacity and pressure from section 2.3 of a cellular automaton with 160000 cells evolving according to the rule 1367-0245 (Class A)

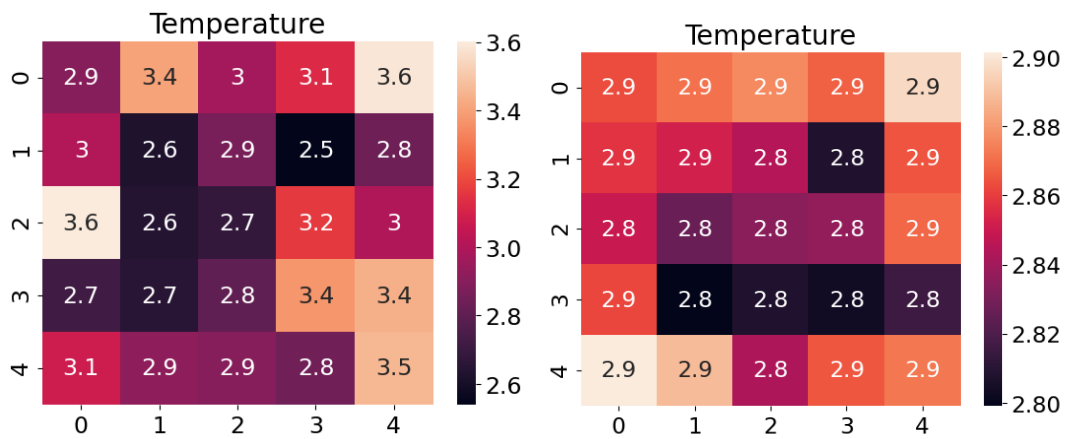


Figure 3.6: Temperature heatmap of a 160000 cells cellular automaton partitioned into 25 subdivisions and evolving according to rule 2-0468 (class D) on the left and rule 1367-0245 (class A) on the right.

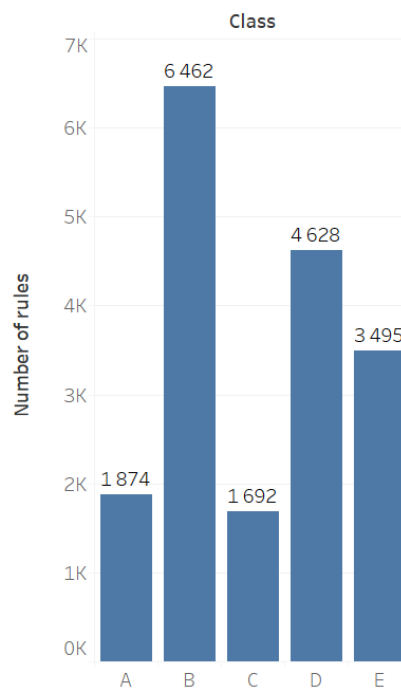


Figure 3.7: Histogram showing the number of cellular automata rules belonging to each class.

4 Outlook

The focus of this thesis has been the exploration of the transferability of basic concepts of equilibrium statistical mechanics to two-dimensional cellular automata. Most results come together comprehensively in both analytical derivations and numerical implementations. That helped define and prove a new quantitative classification scheme based on statistical mechanics. An exception to this is pressure, for which there has not been a correspondence among the different definitions from the partition function, regardless of the use of different approaches. Considering the relative ease and 'beauty' of the coherence shown by the other quantities, it is clear that further study is needed to evaluate the shortcomings of our approach and develop a better definition for pressure. It could be helpful to derive pressure in other ways, without going through the Helmholtz free energy.

The principle of equal a priori probability has been successfully proven right with the non-equilibrium approach and with the benchmark pressure. Both show an even energy density distribution, with the former being a stronger clue than the latter.

The quantities that have been translated successfully could be useful for the simulation and modelling of statistical mechanical systems and the understanding of the equilibrium properties of simple cellular automata. There could be applications of these findings in machine learning and artificial intelligence, since it is not uncommon for the field to borrow concepts from statistical mechanics as done in [19, 20].

The development of a physically derived quantitative classification scheme for two dimensional cellular automata has shown to be successful. Possibly, this work provides a step forward into more rigorous and quantitative classification systems for cellular automata. Whereas the most popular scheme, developed by Stephen Wolfram is qualitative [1]. However, the classification scheme developed here is not directly comparable to Wolfram's since there is a main difference between the two approaches. Wolfram's classification is based on the reaction of the cellular automaton upon perturbation. In this work, the cellular automata develop unperturbed from an initial density

There is also potential in the use of the results of this thesis and the program developed in teaching and didactic at the undergraduate level to offer an intuitive understanding of thermodynamical systems and quantities, which very often is lost in mathematical abstraction [21, 22]. An educator can expand the code to add widgets and offer a visualisation of the microscopic behaviour of a two-state system (the automaton) related to the time evolution of several thermodynamical quantities. It is clearly necessary to mention the tool of molecular dynamics for the same kind of visualization purpose. It would then be up to the educator to choose the most appropriate tool.

A natural next step for this project could be to take the results and methods obtained with equilibrium statistical mechanics and expanding it to the non-equilibrium formalism.

The following steps of this project could be a thorough development and expansion of non-equilibrium thermodynamics methods to study systems of connected cellular automata, subject to different sets of rules and study the non-equilibrium processes associated with them (i.e. heat flow, diffusion and so on). Alternatively, going in the opposite direction, a study could be done into making all the quantities coherent and using first principles to assign relative units to them, incorporating a more rigorous expansion towards the mathematical side. A third possible evolution of this work would consist of a study done with similar methodologies as this one, but focused on probabilistic cellular automata and eventually considering quantum mechanics as well. This approach would present many challenges, among others in the conciliation between the locality of cellular automata and the non-locality of quantum mechanics.

Generally, the classification scheme used can be applied into the prediction of the behaviour of any model system that evolves according to local interactions, by individuating the cellular automata rule that corresponds to the interactions that govern it.

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