

# Computational Approaches for Modelling Complex Systems

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July 12, 2008

## 1 Introduction

Doing research work about complex systems in physics is always bound to the origin works about entropy and the second law of thermodynamics.

In 1865 Rudolf Clausius introduced the term entropy to describe thermodynamical cycles as the change of heat according to the absolute temperature over time.

$$dS = \frac{dQ}{T}$$

Clausius claimed at this point that *“the algebraic sum of all the transformations occurring in a cyclical process can only be positive, or, as an extreme case, equal to nothing.”*<sup>1</sup> This is what we know today as the second law of thermodynamics. According to the term of entropy this means that entropy in a closed thermodynamical system can only increase or – when achieving the so called heat death – become constant at a maximum level. Entropy is often described as the grade of disorder which is scientific not correct. Although there exists no method to measure entropy directly in a system, we must be more careful when dealing with this term. In fact entropy is the number of possible micro states that are achievable by a system in a special macro state. This definition and scientific explanation in the area of statistical mechanics of the second law of thermodynamics has been published by Ludwig Boltzmann. In his work Boltzmann did explain the behaviour of thermodynamical equilibrium systems. But in physics and much more in the area of biology and higher reductive levels equilibrium system models cannot enough to explain observations of the real world.

During the first 60 years of the 20<sup>th</sup> century there was a lively scientific discourse about the meaning of the second law of thermodynamics relating to Charles Darwin’s evolutionary theory. The continuous development in natural

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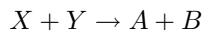
<sup>1</sup>Rudolf Clausius, “Über die bewegende Kraft der Wärme”, 1850.

populations seems to violate this law because no maximum level of entropy is going to be achieved by biological systems but a steady state seems to be the result in most of these systems. Ludwig von Bertalanffy was one of the first scientists who did provide the correct answer to this open question in one of his publications [2] already before it was proved formally by Ilya Prigogine a few years later.

## 2 Calculating Non-Equilibrium States

In this term paper we will deal with easy (Prigogine's Brusselator) and hard (Benard convection) to compute complex systems and some metaphysical considerations about the according effects. To provide the mathematical basics for calculating complex systems we first we will go on with some important milestones in the history of complex systems research.

Let us observe a closed system with the following chemical reaction



where X, Y, A and B are arbitrary molecules. Because the system is closed, no matter but only energy can be interchanged with the environment of the system. The development of such a reaction is known: As long as molecules of X and Y are available, molecules A and B will be produced. To calculate entropy in such a system the reaction rate  $\nu$  and the affinity  $A$  of a chemical reaction (while  $A$  can be described as a coefficient for the chemical potentials) are used. The formula we get for entropy production is based on the results of Gibbs<sup>2</sup>

$$\frac{d_i S}{dt} = \frac{A}{T} \nu \geq 0$$

or in a more general way

$$\frac{d_i S}{dt} = \sum X_j J_j \geq 0$$

while  $J_j$  are rates of different kinds of irreversible processes (chemical reactions, heat transport, etc.) and  $X_j$  are coefficients of the referring forces. Because Gibbs' results are only proven for equilibrium states and states that are 'close' to equilibrium, we are restricted to this area with the formulas from above too. Two important results based on these facts are the Onsager reciprocal<sup>3</sup> relations and the law of minimal entropy production. The second one describes the behaviour of non-equilibrium systems that are close to equilibrium states but cannot achieve these states because of some (external) conditions. In

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<sup>2</sup>Josiah Gibbs, "On the Equilibrium of Heterogeneous Substances", 1878.

<sup>3</sup>Lars Onsager, "Reciprocal Relations in Irreversible Processes", In: Physical Reviews 37, 1930.

this case the system tends to get into a state of minimal dissipation.

Of course it is interesting now what will happen if the system is not close to equilibrium. Prigogine proved in [6] that for characteristics of irritations of a system close to non-equilibrium states the following relation holds

$$\frac{1}{2} \frac{\delta}{\delta t} \delta^2 S = \sum_j \delta J_j \delta X_j$$

while Prigogine defined this as excess entropy. Now we want to know if this excess entropy can influence our system of chemical reactions in a way that the development might differ from a classical equilibrium system. Therefore we want to calculate the effects of irritations of our chemical reaction system with chemical reactions as the only irreversible processes. Using the formula from above

$$\sum_j \delta v_j \delta A_j \geq 0$$

with the stoichiometric coefficient

$$v = XY$$

and the affinity of our system from above

$$A = \log \frac{XY}{AB}$$

we get

$$\delta v \delta A = (Y \delta X) \left( \frac{\delta X}{X} \right) = \frac{Y}{X} (\delta X)^2 > 0$$

as result for the entropy excess in a state close to non-equilibrium for our specific chemical reaction  $X + Y \rightarrow A + B$ .

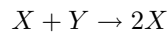
Because the entropy excess in this case is always positive, it can not change the development of the system to the point of heat death even if the system is far away from equilibrium. The next interesting question now is if there exist chemical systems which different behaviour. Describing such systems and proving their thermodynamical behaviour was also part of the work of Ilya Prigogine who did get the nobel prize for his theses about non-equilibrium thermodynamics.

Prigogine did come to the result that such a development of a system is based on autocatalytic reactions within a system. But while an autocatalytic reaction in general is necessary to produce a chaotic development it is not always the case that autocatalytic systems get into such a state. Autocatalytic systems are focused by different scientific works during the last hundred years. Stuart Kauffman actually did write about autocatalytic effects as a possible key

element of the origin of life. In one of his most popular publications<sup>4</sup> he describes algorithms and possible development calculations of theoretical models for autocatalytic chemical reactions as a basic component for the development of living organisms.

An autocatalytic system is a system with at least one catalytic element that supports its own production. In biology one of the most famous examples is the molecule ATP that is used for chemical reactions within photosynthesis.

A much simpler autocatalytic chemical reaction would be



where X works as an autocatalytic element. Doing the same calculation as above we now get

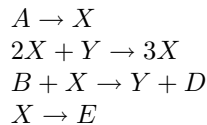
$$A = \log \frac{XY}{X^2} = \log \frac{Y}{X}$$

for the affinity and

$$\delta v \delta A = (Y \delta X) \left(-\frac{\delta X}{X}\right) = -\frac{Y}{X} (\delta X)^2 < 0$$

for the entropy excess. As we can see we now get a negative entropy excess although the only changing within our reaction is that two molecules are producing one of them instead of two complete different molecules. So we did find a way to produce a negative entropy excess within a chemical system. But because Y decreases with time there exists a state in our system where the negative entropy excess will stop and – because we have already shown that other kinds of disturbance might not effect the thermodynamical behaviour – the system will went on to the point of heat death afterwards.

This can only be prevented by switching from the area of closed systems to those of open systems. The system published by Prigogine here is known as the so called Brusselator which is a system of the following chemical reactions:



To get the interesting results – which means to achieve a state close to non-equilibrium – we have to set the relation between the two molecules A and B referring to the relation

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<sup>4</sup>Stuart Kauffman, “The Origins of Order”, Oxford University Press 1993.

$$B > 1 + A^2$$

Such a system will not go on to the point of heat death but continue entropy increasing and decreasing in a cycle.

Another popular example for a similar system is the Belousov-Zhabotinsky reaction that has been discovered twenty years before Prigogine published his theoretical approach and could not be explained by chemistry and physics in the meantime.

### 3 Benard Convection

We now will have a short view on Benard Convection, one of the first examples in practice according to open systems. Movement within fluids or gases is generally known as convection. Following different laws of physics heat and matter is transported within a closed or open system while the molecules of the fluid are moving following the same laws. Convection therefore does not only play an important role in technical developments but is also present in global processes like heat transfer within atmosphere and oceans and in the earth mantle where magma is transported from the mantle to the cooler lithosphere and therefore influences the movement of the plates.

At the beginning of the 20<sup>th</sup> century Henri Benard published the results of his experiments according to convection. For his experiments he took two plates and fluids of a certain viscosity and put it between the two plates.

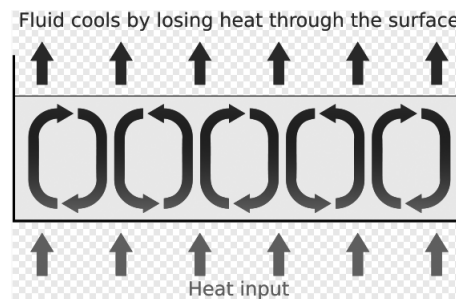


Figure 1: Benard Convection as it works in practice: Heat transfer via convection leads in pattern formation within the fluid. (Source: wikipedia.org under Creative Commons license)

Now the bottom plate is heated. If  $\Delta T = T_2 - T_1$ , where  $T_2$  is the bottom plate and  $T_1$  is the top plate, is quite small, no effect on the macroscopic level will appear. The system in this case is in a state where viscosity forces dom-

inate and only heat is transferred between the two plates without any further effects. If  $\Delta T$  increases and a critical bound  $\Delta T_k$  is exceeded, convection will occur and effects on the macroscopic level emerge – the convection will build up a special pattern, the so called Benard cells. The physical reason in this case is a lower density within the bottom layer of the fluid because of the higher temperature. At the point where  $\Delta T$  reaches the critical bound, viscosity forces are no longer strong enough to avoid movement of the fluid itself. Because the fluid has to move from the bottom plate to the top plate, cools down there and moves downwards again, a movement pattern is build.

It is interesting here that building the convection cells leads to alternating left and right rotating cells, because the molecules rise up on some places, move along the upper plate, decline at some other places and build the cell pattern within this movement. While the building of the cells is deterministic, e.g. we know that the Benard cell pattern will be build in a special experiment when  $\Delta T_k$  is reached, the direction of single cells is not. In detail this means that within the last hundred years it was not possible to define the well known parameters of special experiments in a way that it is possible to say, what kind of rotation will appear in single cells.

If we go on heating the bottom plate and  $\Delta T$  exceeds a second bound  $\Delta T_c$  the pattern will disappear and the system now will be in a so called turbulent or chaotic state. This means that the movement of the particles within the fluid is no longer predictable. Although Benard convection is something difficult to calculate and compute at all, we can calculate the state of pattern forming and the state of chaotic movement for a fluid of a certain viscosity.

One method herefore is to use the Lorenz attractor

$$\begin{aligned} X &= a(Y - X) \\ Y &= X(b - Z) - Y \\ Z &= XY - cZ \end{aligned}$$

where  $a$  is the Prandtl number and  $b$  is the Rayleigh number. For values  $a = 10$ ,  $b = 28$  and  $c = \frac{8}{3}$  we get a chaotic development of Lorenz attractor. During the last hundred years many other approaches to simulate and calculate Benard convection have been implemented. An overview including some interesting simulation results can be found in [4]. The first therotic model was designed by Lord Rayleigh in 1916 as a linear stability analysis assuming stress-free conditions for the velocity – that’s why Benard convection is today also known as Rayleigh-Benard convection. Most mathematical models base on coupled differential equation systems and either focus on the state switch between heat transfer and convection and convection and turbulence or on the surface characteristics during these changes.

### 3.1 Emergence in Benard Convection

Benard convection seems to be something emergent. But while often the whole process including all properties is discussed as emergent or not we will make a more detailed differentiation. Referring to [7] several meanings of the term emergence exist. We will only focus on two special meanings that are described by Stephan as *weak emergence* and *synchronous emergence*. Weak emergence describes a well known characteristics of systems in general: they might have properties or functions which do not succeed from those of the single parts of the system but can be described by knowing the parts of the system and its relations. Reproduction therefore is an example for weak emergence – single cells are not able to produce a new creature, but the creature itself, that consists of single cells, can do and furthermore the process of reproduction can be explained in general. Also think of the special properties of the  $H_2O$  molecule – the characteristics of hydrogen bonds cannot be succeeded from the characteristics of the H and O atoms.

Synchronous emergence now would be something more powerful but also could not be proven in practice so far. A system would have strong emergent characteristics if they cannot be reduced to the properties and relations of the single elements of the system. In general such an effect is described as an emergent step within a development or different layers of a system. The human psyche, political and economical systems or the development of living systems are taken as examples for such kind of synchronous emergence. In fact there is no example in practice where this kind of synchronous emergence can be proven, because all examples for pretended synchronous emergent effects could also be deterministic – we only might not know so far the rules behind them.

Weak emergence can be found within Benard convection when  $\Delta T_k$  is reached and convection and pattern formation start. One argument herefore would be that Benard cells have a different surface than a simple collection of single molecules of our fluid and therefore different physical properties. This is an interesting effect in the area of geology regarding mantle convection and plate tectonics – if Benard cells are built up by the mantle convection the plate movement might have different characteristics than if not.

Now we did say that it is not clear so far if something like strong emergence does exist in reality or not. The rotation property of Benard cells provides a good example to discuss different point of views of such effects.

**Deterministic View.** Referring to a deterministic view an explanation of this effect could be to argue about a very small  $\epsilon$  within some of the property values that cannot be measured but nevertheless influences the rotation in an important way – this in general is known as deterministic chaos (“butterfly effect”) and was explained by Lorenz after calculating some weather prognoses that differ from each other only in some small initial configurations but lead to

drastical different results.

**Indeterministic View.** Instead of a small  $\epsilon$  some kind of real chance could be responsible for different results referring to the rotation value. Quantum effects are sometimes used to explain such an scenario, because if quantum spins are not determined at all they might influence effects on the micro and macro level in a non deterministic way.

**Emergent View.** An emergentist could argue here that the rotation property of Benard cells is a classical emergent property in the meaning of synchronous emergence. This means that for some reason elements involved in such a convection include the set of {right, left} rotation without determining what characteristic will occur in a certain instance. The only fact that we can get our from this view then is that such a system will either develop a right or a left rotation and that a certain development is always emergent. This view is quite difficult to model within a formal system.

As we can see the problem of rotation within Benard cells is quite similar to that of free will. Therefore one could use the same classification to explain this effect than for explaining human brain activities like it is done in [1]. And because of this we also have the same problem here than brain scientists have: As long as we cannot prove a deterministic behaviour within our rotation effect, we have to handle all possible situations, namely deterministic, indeterministic and emergent reasons.

## 4 Cellular Automata Modelling

Modelling of complex systems using cellular automatas did become popular during the last twenty years and was originally introduced by John von Neumann<sup>5</sup>. Von Neumann's approach in the 1950s included a theoretical model for a self-reproducing automata, a so called universal constructor. This approach was quite complex and had to use a lot of different rules and huge computational space to work.

But self-reproduction in cellular automata can be achieved much easier as Langton did prove in 1984. He published a model of a two-dimensional cellular automata using the von Neumann neighborhood and only eight different states. Within a map of 21 x 10 cells a whole self-reproduction cycle can be executed.

Trying to realise self-reproduction was one of the first goals within modelling complex systems using cellular automatas. Today this approach is used in many areas of natural sciences to build up models and simulations of systems. In the area of physics popular examples are crystallization and diffusion processes, in

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<sup>5</sup>John von Neumann 1966, "Theory of Self-Reproducing Automata", 1966

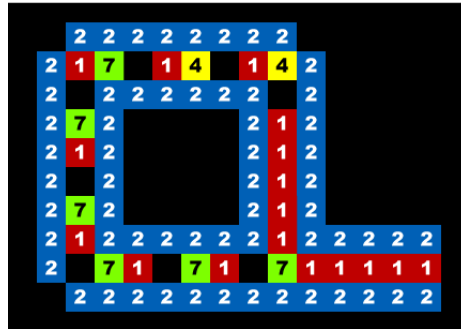


Figure 2: Langton Loop as an example for cellular automata modelled self-reproduction. Within a certain number of steps the loop creates an exact copy of itself.

the area of biology examples are simulations for epidemic development and ants colony development.

#### 4.1 An easy-to-model Complex System: Prigogine's Brusselator

During the work for this term paper a cellular automata model for Prigogine's Brusselator has been designed and implemented. This has been done with the programming language NetLogo<sup>6</sup>, the source code can be found in the appendix. Referring to non-equilibrium systems so far there only exists an implementation for Belousov-Zhabotinsky reaction. But although this application that is embedded in the program archive library of NetLogo seems to produce correct results (mathematical calculation of the development of such an reaction), it does not really follow the idea of cellular automata modelling according to the activities of autonomous agents holding certain properties and communicating with each other to produce special patterns on the macroscopic level.

Therefore a different approach to the example implementation was used for the implementation of Brusselator – here no implementation at all in NetLogo existed so far. In the program implemented, different molecules are modelled as autonomous cells acting with each other following the restricted Brusselator model and reaction rules from [5]. Because of computational random movement and a restricted set of molecules the calculation result is not the same than if we would calculate it using the according differential equation system, but running the simulation<sup>7</sup> shows that such an approach really leads to the same behaviour than the traditional pure mathematical approach.

<sup>6</sup>See <http://ccl.northwestern.edu/netlogo/>.

<sup>7</sup>The simulation can be started at <http://www.systems-everywhere.com>

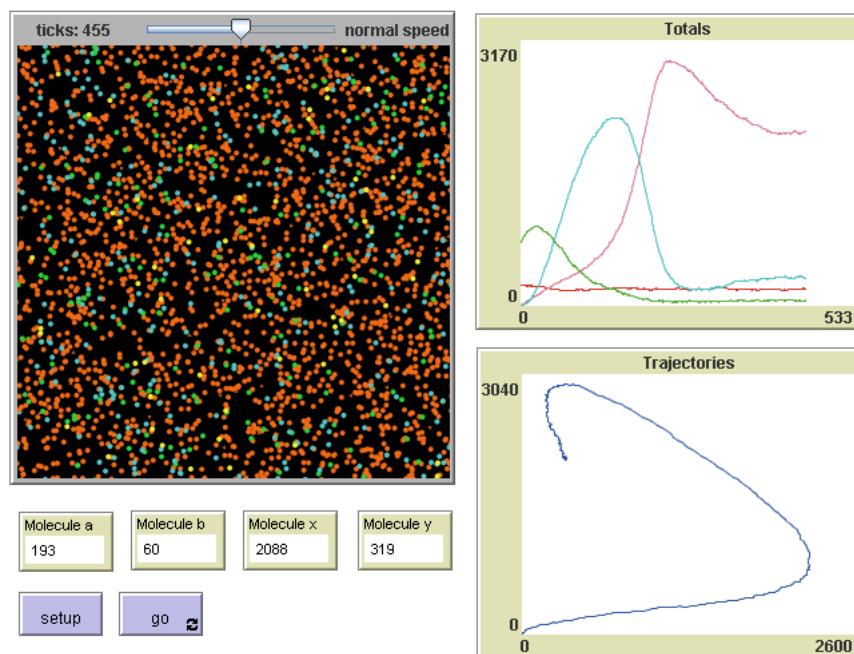


Figure 3: A cellular automata model for Prigogine’s Brusselator at systems-everywhere.com

## 4.2 A hard-to-model Complex System: Benard Convection

So far no comprehensive model for Benard convection using cellular automata exists, because it is quite difficult to model all physical effects within this process. Because of this reason we neither can present such a model. It would be possible to use the Lorenz attractor to provide a simulation that shows at which point the system reaches critical points and how different parts of the system react during this transformation – doing so we would get the results of a Lorenz attractor calculation and additionally a detailed view on the behaviour of the system components over time.

But if we implement such an abstract model approach the two main effects of Benard convection could not be shown: (1) The convection behaviour and development over time and (2) therefore neither the rotation development that would be deterministic simply because of the reason that cellular automata calculation is always deterministic because it is based on deterministic background program logic. One way would be to use randomized states to get different results but then we get a classical indeterministic scenario which is not desir-

able at all. Nevertheless simulating Benard convection using cellular automata would lead to an interesting different point of view on this interesting scientific topic – but in fact this would take a lot of time and exceed the frame of a simple term paper.

Finally we can say that if we assume a deterministic behaviour in all kind of (open) systems, computing complex systems can be done well using cellular automata. If we assume an emergent behaviour so far no computational concepts or models exist to calculate the development of an complex, synchronous emergent system. In this case – as a computer scientist – we would have to refer to Wittgenstein and stop our calculations with the conclusion “What one cannot compute, thereof one must be silent”.

## References

- [1] Mario Bunge, “Das Leib-Seele Problem”, Tübingen 1984.
- [2] Ludwig von Bertalanffy, “Biophysik des Fließgleichgewichts”, Sammlung Vieweg, Braunschweig 1953.
- [3] Bastien Chopard and Michel Droz, “Cellular Automata Modelling of Physical Systems”, Cambridge University Press 1998.
- [4] Innocent Mutabazi et al. (Ed.), “Dynamics of Spatio-Temporal Cellular Structures”, Springer Tracts in Modern Physics 2006.
- [5] Gregoire Nicolis, Ilya Prigogine, “Die Erforschung des Komplexen”, Piper Verlag, München 1987.
- [6] Ilya Prigogine, “Thermodynamics of Irreversible Processes”, 1961.
- [7] Achim Stephan, “Emergenz – Von der Unvorhersehbarkeit zur Selbstorganisation”, Dresden University Press 1999.

## A Brusselator Source Code

```
turtles-own [state]

; molecule to states mapping
; a = 0, b = 1 - 3, x = 4 - 5, y = 6 - 7, d = 8, e = 9

to setup
  clear-all
  create-turtles 1000
  set-default-shape turtles "circle"
  ask turtles [
    setxy random-xcor random-ycor
```

```

        set state random 4
        set-turtle-color
    ]
    do-plots-trajectories
    do-plots

end

to go
    if ticks >= 2000 [ stop ]
    move-turtles
    change-turtles
    manage-molecules
    tick
    do-plots
    do-plots-trajectories
end

to move-turtles
    ask turtles [
        right random 360
        forward 2
    ]
end

to set-turtle-color
    if state = 0 [ set color 65 ]
    if state > 0 and state < 4 [ set color 45 ]
    if state > 3 and state < 6 [ set color 25 ]
    if state > 5 and state < 8 [ set color 85 ]
    if state = 9 [ set color 105 ]
end

to change-turtles
    ask turtles [
        if state = 0 ; a molecule to compute a --> x, k= 0.025
        [
            set state random 40
            ifelse state = 1
            [ set state 4 ]
            [ set state 0 ]
        ]
        if state > 0 and state < 4 ; b molecule to compute b + x --> y + d, k=1
        [
            if count turtles-here with [ state > 3 and state < 6 ] > 0
            [

```

```

        set state random 100
        ifelse state > 50
        [ set state 6 ]
        [ set state 8 ]
    ]
]
if state > 5 and state < 8 ; y molecule to compute 2x + y --> 3x, k=1
[
    if count turtles-here with [ state > 3 and state < 6 ] > 1
    [ set state 4 ]
]
if state > 3 and state < 6 ; x molecule to compute x --> e, k=0.01
[
    set state random 100
    ifelse state = 1
    [ set state 9 ]
    [ set state 4 ]
]
if state = 8 ;; precipitate d with p=0.3
[
    set state random 100
    ifelse state < 30
    [ die ]
    [ set state 8 ]
]
if state = 9 ;; precipitate e with p=0.3
[
    set state random 100
    ifelse state < 30
    [ die ]
    [ set state 9 ]
]
set-turtle-color
]
end

; open system: a and b are put into the system continuous
to manage-molecules
create-turtles 20 [
    setxy random-xcor random-ycor
    set state random 4
    set-turtle-color
]
end

; standard plotting methods

```

```
to do-plots
  set-current-plot "Totals"
  set-current-plot-pen "molecule-a"
  plot count turtles with [ state = 0 ]
  set-current-plot-pen "molecule-b"
  plot count turtles with [ state > 0 and state < 4 ]
  set-current-plot-pen "molecule-x"
  plot count turtles with [ state > 3 and state < 6 ]
  set-current-plot-pen "molecule-y"
  plot count turtles with [ state > 5 and state < 8 ]
end

; plotting dynamic trajectory for x/y
to do-plots-trajectories
  set-current-plot "Trajectories"
  set-current-plot-pen "traj-x"
  plotxy count turtles with [ state > 5 and state < 8 ]
  count turtles with [ state > 3 and state < 6 ]
end
```