Network Dynamics in the SimSoup Artificial Chemistry

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Abstract

An understanding of the dynamics of chemical networks is important for the development of metabolic theories of the origin of life, and more generally for the explanation of life processes. The purpose of the SimSoup artificial chemistry model is to enable the behaviour of abstract chemical networks to be investigated. The model is outlined, and the concepts of instantaneous and persistent network states are introduced. A recent model enhancement enabling persistent states to be identified using 'Manhattan Distance' plots is described. Results of an investigation into the relationship between connection density and network activity are presented and discussed. It is then shown that persistent states in SimSoup networks can exist for long periods in highly localised regions of the space of possible molecular compositions, and that in some cases they can have an oscillating behaviour. Details of the oscillating behaviour are presented, and an example is shown in which each cycle shows a burst of activity followed by a period of decay, the final stage of which is sometimes very fast.

1 Introduction

1.1 Background

Among the many theories of the origin of life, two major viewpoints can be identified; I refer to these as the Genetic View and the Metabolic View.[1] These can be briefly described as follows:-

- **Genetic View:** Template replicating molecules or crystals were crucial for the origin of life, and have from the outset been the carriers of inherited information that makes evolution possible
- **Metabolic View:** The first living entities were metabolic systems, and they evolved by exploring the possibilities for new kinds of metabolic network.

The well known RNA World theory is an example of a Genetic View theory. The clay crystal theory described by Cairns-Smith (1982) can also be regarded as essentially genetic in nature. Examples of Metabolic View theories are those discussed by Oparin (1957), Kauffman (1993), Dyson (1999), Segré et al. (1998, 2000, 2001a, 2001b), Jain and Krishna (1998), and Krishna (2003).

[1] Another important categorisation of viewpoints is the distinction made by Wächtershäuser (1990) between heterotrophic and autotrophic theories.

A key challenge for Metabolic View theories is to explain how an essentially network oriented system can evolve. The conditions for inheritance in such networks have been modelled by Segré et al. (2001b). A model for the appearance of highly non-random organisations in chemical networks on the prebiotic earth has been investigated by Jain and Krishna (1998), and by Krishna (2003).

These models work by representing the catalytic influence of each molecular species on the formation of other molecular species. The modelled species themselves are assumed to be formed from 'food' reactants that have constant concentrations. Krishna (2003) identifies some potential drawbacks of this assumption.

An approach to understanding the dynamics of networks based on an algebraic model is described in the organisation theory of Dittrich and Speroni di Fenizio (2005), and used by Centler and Dittrich (2005) to analyse atmospheric chemistries. In this approach, an organisation is identified as a system that is closed and mass-maintaining for each (type of) molecule in the organisation.

In earlier work by the present author (Gordon-Smith, 2005), the SimSoup artificial chemistry model was introduced. Some preliminary model results were presented, and it was shown that SimSoup networks exhibit some of the properties required for evolution, including the ability to 'remember' new patterns of behaviour.

The purpose of the work described here is to begin a more systematic exploration of the behaviour of SimSoup networks.

1.2 Typographical Convention

In this paper, terms with a specific meaning in the SimSoup model are capitalized. The word 'Molecule' therefore refers to an object in the SimSoup model, whereas the word 'molecule' has the meaning generally used in chemistry.

1.3 The SimSoup Model

The SimSoup model is described in detail in (Gordon-Smith, 2005). An overview sufficient for the purposes of this paper is provided here.

SimSoup is an artificial chemistry model that includes an abstract representation of the static and dynamic properties of a chemical network. The model is designed to enable the dynamic behaviour of such networks to be explored.

SimSoup does not assume a constant concentration of 'food' molecules. However, in its current form it does make the following key simplifications:-

- The detailed structure of molecules is not represented
- Interactions are assumed to take place in a well stirred reactor
- The energy of molecular species is not represented
- There is a fixed number of molecular species.

The following sub-sections describe the logical structure and behaviour of the model in terms of the model entities and the mechanisms by which they interact.

1.3.1 The Static Model

In SimSoup, the laws of Chemistry are represented by a set of Molecule Types and Interaction Types that set a framework within which dynamic behaviour can take place.

A **Molecule Type** is analogous to a molecular species in real chemistry. It has a mass, and can be associated with Interaction Types in which individual Molecules participate as Reactants or Products.

An **Interaction Type** is a category of interaction between Molecule Types. Each Interaction Type has either one or two Reactant Molecule Types, and either one or two Product Molecule Types. In SimSoup there are three forms of Interaction Type, representing the simplest interactions. These are shown in Table 1.

Form of Interaction Type	Interaction Scheme
Construction	$A + B \rightarrow C$
Transformation	$D \rightarrow E$
Fission	$F \rightarrow G + H$

Table 1: The three forms of Interaction Type in SimSoup

The table shows each form of Interaction Type and illustrates its Interaction Scheme. For example, a typical Interaction Scheme for a Construction is $A + B \rightarrow C$. This signifies that when a Construction occurs, it consumes one Molecule of each of types A and B, and produces a single Molecule of type C.

Each Interaction Type has a Rate Constant that is used to determine the Interaction Rate. In addition, each Interaction Type must conserve mass. For example, in the Fission $F \rightarrow G + H$, the mass of Molecule of Type F must be the same as the sum of the masses of G and H.[2]

As a model simplification, Constructions with both Reactants of the same Molecule Type and Fissions with both Products of the same Molecule Type are ruled out.

Interaction Types can be combined to form **Compound Interactions**. For example, a Construction and a Fission can combine to produce a **Catalytic Transformation** as follows:-

- Construction: $A + X \rightarrow B$
- Fission: $B \rightarrow X + C$
- Catalytic Transformation: $A \overset{X}{\longrightarrow} C$.

Here, X is a Reactant for the Construction and a Product in the Fission, and so is not consumed or produced by the overall Catalytic Transformation; it plays the role of a catalyst.

In addition to catalysts, SimSoup Molecule Types can also represent unstable intermediates that are not normally referred to as molecules by chemists. By combining Interaction Types to produce Compound Interactions, reactions of arbitrary complexity can be represented.

[2] Without this restriction, cycles that grow indefinitely can occur.

1.3.2 The Dynamic Model

The SimSoup **Reactor** is envisaged as an enclosed space within which Molecules exist and interact. In the model discussed in this paper, this space is assumed to be three dimensional, with Molecules of each type being evenly distributed throughout the space. An extension of the model to cover situations in which Interactions take place on a surface as envisaged by Wächtershäuser (1997) is possible.[3]

Each **Molecule** in the Reactor is an instance of a Molecule Type. At any point in time, there are a number of **Realisable Interaction Types**. An Interaction Type is Realisable (possible) if there are sufficient Reactants for one Interaction. For example, the Construction $X + Y \rightarrow Z$ is possible if there is at least one Molecule of type X and at least one Molecule of type Y.

The model operates on a timestepping basis. At each timestep the current Realisable Interaction Types are evaluated, Interactions take place according to their Rate Constants, and Molecules of the appropriate types are added to and removed from the Reactor accordingly. In addition, 'food' Molecules are added, and Molecules are removed at random to represent 'leakage' from the Reactor.

2 Network States

2.1 Instantaneous and Persistent States

At any point in time, a SimSoup network has an **Instantaneous State**. This is defined by:-

- **The Static Model:** The set of pre-defined Molecule Types and Interaction Types, and...
- **The Reactor Composition:** This is defined by the number of Molecules of each type present in the Reactor. This can be expressed as a vector $\mathbf{R}$. Each element of $\mathbf{R}$ corresponds to the (integer) number of Molecules of a particular type present in the Reactor. [4]

As Interactions progress in the Reactor, $\mathbf{R}$ may change from one timestep to another so that the overall behaviour of the system is defined by a series of (instantaneous) Reactor Compositions, $\mathbf{R}(t_i)$, where t_i is the time at the i_{th} timestep.

If $\mathbf{R}(t)$ is constant, or is following some repeating pattern, then we can say that the Reactor is in a **Persistent State**.[5]

The following questions arise in regard to Persistent States:-

- How can we recognise that the Reactor is in a Persistent State?
- How can we distinguish one Persistent State from another?

2.2 Manhattan Distance

Both of these questions can be answered to some extent by measuring the **Manhattan Distance** between different Instantaneous States.[6]

Manhattan Distance between two points in a Euclidean space is defined as the sum of the (absolute) differences of their coordinates.

For example, in a plane, the Manhattan distance between the point P1 with coordinates (x_1, y_1) and the point P2 at (x_2, y_2) is

$$|x_1 - x_2| + |y_1 - y_2|.$$

The Manhattan Distance between two points is not dependent on the route taken. This is illustrated in Figure 1.

The Manhattan Distance, D, between two SimSoup Reactor Compositions $\mathbf{R_1}$ and $\mathbf{R_2}$ can be calculated as the sum of the absolute differences between the numbers of Molecules of each Molecule Type. That is:-

$$D = \Sigma_i |r_{1i} - r_{2i}|,$$

where the summation is over all Molecule Types, and r_{1i}, r_{2i} are the i_{th} elements of $\mathbf{R_1}$ and $\mathbf{R_2}$.

For example, if we have a Reactor in which a Fission Interaction, $A \rightarrow B + C$, takes place, then the Manhattan Distance between the Reactor Compositions before and after the Interaction is 3. If a Construction, $B + C \rightarrow D$, then takes place, the Manhattan Distance from the original state before the Fission is now 2.

[3] The assumption of a well stirred Reactor would not apply for a model of surface metabolism, and so the model would need to be extended to represent the locations of Molecules on the surface.

[4] Reactor Volume can also be considered to be part of the Instantaneous State, although in this paper it is assumed to be constant.

[5] The concept of a Persistent State is similar, but not identical to, the organisations described by Dittrich and Speroni di Fenizio (2005). An organisation is a set of molecular species that is closed and mass maintaining. Since this is independent of the number of molecules of each species, it is possible that there could be multiple Persistent States for the same organisation.

[6] Other measures are possible. For example, Segré et al. (2000, 2001b) use the scalar product of normalised compositional vectors.

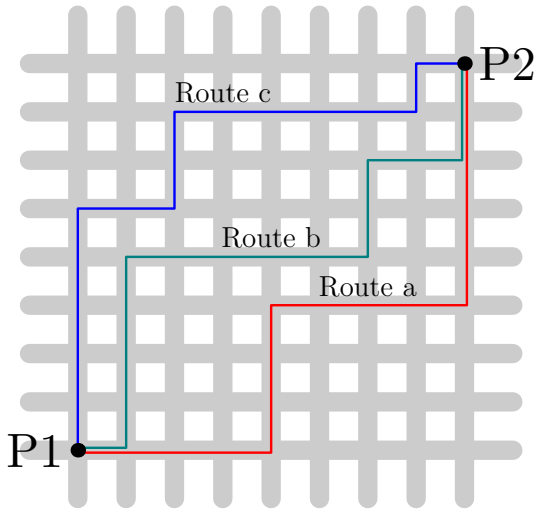

Figure 1: Manhattan Distance. The three routes (a, b, c) between points P1 and P2 have the same length.

2.3 Recognising and Discriminating between Persistent States

If the Manhattan Distance between two Reactor Compositions $\mathbf{R}(t_1)$ and $\mathbf{R}(t_2)$ at times t_1 and t_2 is zero, this indicates that $\mathbf{R}(t_1)$ and $\mathbf{R}(t_2)$ are identical.

If we monitor the Manhattan Distances between Reactor Compositions at different times and find a period during which all of the distances are zero, we can therefore say that the Reactor is in a Persistent State.

It would be unduly restrictive to insist that subsequent states must be identical, and so we can identify a tolerance Manhattan Distance, D_{tol}, and say that the Reactor is in a Persistent State during a period if the Manhattan Distance between any two Reactor Compositions during the period is no greater than D_{tol}.

Reducing D_{tol} can be regarded as increasing the sensitivity to differences between compositions. A series of Reactor Compositions that are regarded as a single Persistent State when a particular value of D_{tol} is used may be separated out into different states if the value of D_{tol} is reduced.

It is possible that $\mathbf{R}(t)$ varies cyclically, such that it traverses a large region in the space of possible compositions, but returns periodically to a composition that is close to (ie within D_{tol} of) the original composition. This situation can also be regarded as a Persistent State.

2.4 The Manhattan Plot in SimSoup

In order to provide a mechanism enabling recognition and discrimination of Persistent States, a 'Manhattan Plot' facility has been added to SimSoup.

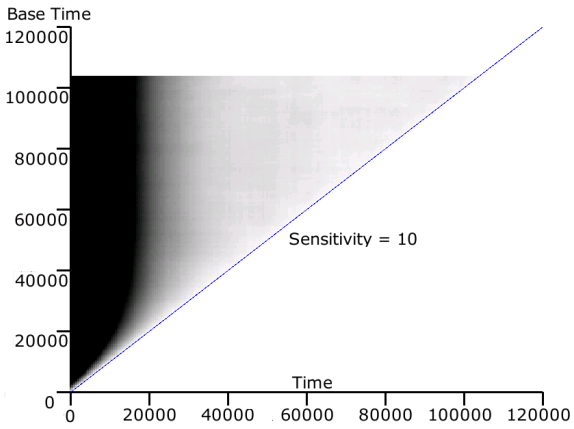

Figure 2: Manhattan Plot Example. The y-axis shows 'Base Time', and the x-axis shows 'Time'. The darkness of the plot at each point indicates the Manhattan Distance between the Reactor Compositions at times 'Base Time' and 'Time'.

An example plot is included in Figure 2. Each point on the triangular plot indicates the normalised Manhattan Distance between Reactor Compositions at times 'Base Time' (y axis) and 'Time' (x axis). A light tone signifies a low distance between the two Instantaneous States. Darker tones signify larger distances.

Two light toned points along a horizontal section have similar Reactor Compositions. 'Sensitivity' determines the darkness of the display for a particular distance. Increasing Sensitivity increases the darkness for a particular value of Manhattan Distance. At Sensitivity = 10, the plot has maximum darkness for any distance above one tenth of the maximum possible distance D_{max}, where D_{max} is calculated as twice the number of Molecules in the Reactor at 'Base Time'.

The plot can be read as follows. The point Base Time = 100,000, Time = 90,000 (towards the top right of the plot) is light grey. This signifies that the Reactor Compositions at these two times are close. Following a horizontal line leftwards from this point, we see that the plot remains light grey until about Time = 30,000. This signifies that at all times between 30,000 and 90,000, the Reactor Composition was close to that at Time = 100,000. Similarly, if we follow the plot to the right, we can see that at times between

90,000 and 100,000, the Reactor Composition was also close to that at time 100,000.

In short, after time 30,000 the Reactor is in a Persistent State in which the Reactor Composition varies only slightly.

Tracing leftwards beyond Time = 30,000, the plot becomes increasingly dark. This signifies that at these times the Reactor Composition was substantially different to that at Time = 100,000.

Note that while a horizontal line of light tone indicates a (roughly) constant Reactor Composition, a horizontal line of black does not indicate constant state; it simply signifies that the Reactor Compositions are substantially different to that at the Base Time. They may or may not be similar to each other.

In the plot of Figure 2, the Reactor Composition is in fact in a considerable state of flux during the period up to Time = 30,000. This can be seen by focusing on the horizontals for Base Time = 30,000 and earlier (bottom left of the figure). These horizontals are black except for all but the latest Times (those that are close to the diagonal). This indicates that whatever Base Time we choose during this period, its Reactor Composition is substantially different to that for earlier times.

2.5 Localisation of Persistent States

The Persistent State in Figure 2 represents a situation in which the Reactor Composition varies by less than $\frac{1}{10}D_{max}$ from a base state over a long period. This clearly represents a stable state in which random variations in Reactor Composition are localised within a limited region of composition space.

The question arises: How limited? The answer is that although the distance travelled through composition space (up to $\frac{1}{10}D_{max}$) is not negligible, the volume of composition space within which this movement takes place is extremely small.

This is because the volume of the space is proportional to $(D_{max})^{N_{Dim}}$, where N_{Dim} is the number of dimensions of the space.

This number of dimensions is the number of Molecule Types (200), and so the Reactor Composition remains within a volume of composition space that occupies $(\frac{1}{10})^{200}$ of the total space.

3 Exploration of Network Dynamics

3.1 Variation of Network Connection Density and the Onset of Network Activity

3.1.1 Description of Scenarios

The dynamic behaviour of a SimSoup network can be expected to be different depending on the number of Interaction Types defined. This section presents the results of a set of model runs to investigate this relationship. For all of the runs, the following aspects of the model setup were kept constant:-

- Number of Molecule Types = 200
- Maximum Rate Constant for Constructions = 0.05
- Maximum Rate Constant for Fissions = 0.05
- Masses for Molecule Types chosen as random integers in the range 1 to 4
- The Reactor is initially empty
- One 'food' Molecule of each of three Maintained Molecule Types introduced to the Reactor at each timestep
- Each Molecule has a removal probability of 0.0001 at each timestep ('leakage')
- Reactor Volume = 1000 (a dimensionless quantity)
- Statistics collection interval = 500 timesteps
- No Interaction Damping: If the Rate Constants in SimSoup are set to high values, this can lead to a situation in which the calculated number of Interactions of a particular type exceeds the supply of Reactant Molecules. SimSoup applies an 'Interaction Damping' mechanism when this occurs. Such situations are not physically realistic and a Reactor Alert is generated. This facility has been used to ensure that Interaction Damping did not occur in the runs described here.

Three series of model runs (denoted A, B and C) were conducted. For each series a different number was used to 'seed' the model's pseudo-random number generator.

For each run within a series, the model was setup with a different number of Catalytic Transformations.

As mentioned in section 1.3.1, a Catalytic Transformation is a pair of Interaction Types consisting of a Construction and a Fission.

The model setup logic is such that within each series, as the number of Catalytic Transformations ($N_{CatTrans}$) is increased, the extra Interaction Types are added to the existing Interaction Types. This means that within each series the network 'grows', rather than being based on a completely different set of Interaction Types for each run.

In addition, the assignment of Masses to Molecule Types is the same for all of the model runs presented here.

3.1.2 Plots of Overall Reactor Activity

The following variables are key indicators of the overall activity in the Reactor:-

- $N_{MolType}$: Number of Molecule Types for which Molecules currently exist in the Reactor (will always be $\leq$ 200, the total number of Molecule Types defined in the setup).
- $Rate_{Int}$: Overall rate of Interactions, averaged over the statistics collection period
- $N_{RIntType}$: Number of Realisable Interaction Types, averaged over the statistics collection period.

Figures 3, 4 and 5 show the behaviour of these variables as $N_{CatTrans}$ increases in Series A, B and C respectively.

Each variable takes a different value at each statistics collection interval during a run. In order to provide an indication of the range of values taken by each variable, maximum and minimum values are recorded for each run. The values taken are based on the maximum and minimum values taken by the variables during the time after the first 50,000 timesteps.

The value of 50,000 is chosen because this represents the end of a transient period during which the Reactor is filling as a result of the addition of 'food' Molecules. The combination of the constant addition of 'food' and the 'leakage' result in a situation in which the number of Molecules in the Reactor typically approaches a limiting value asymptotically. By Time = 50,000, the number of Molecules is typically very close to its long term value.

3.1.3 Observations and Interpretation

The following observations can be made on Figures 3, 4 and 5.

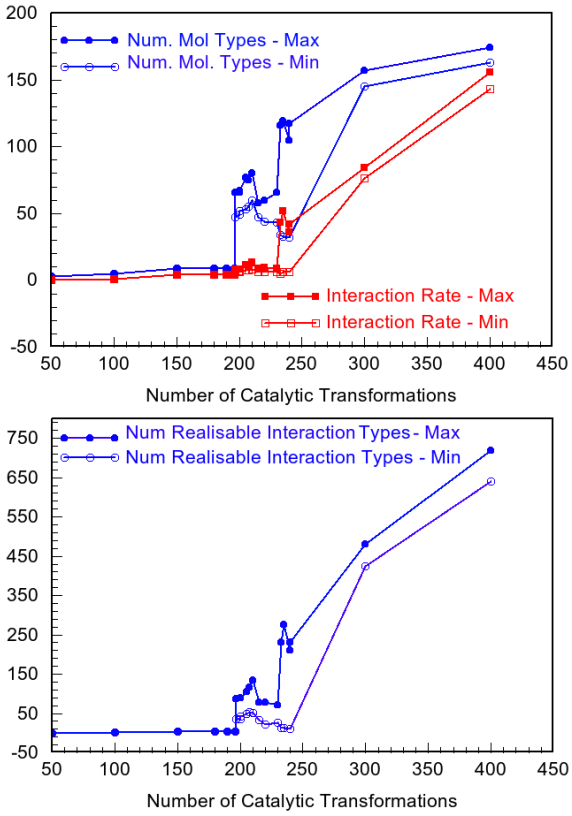

Figure 3: Reactor Activity vs Number of Catalytic Transformations - Series A

Sudden Onset of Reactor Activity: The plots indicate that in all three series there is a sudden onset of Reactor activity when $N_{CatTrans}$ reaches a particular value.

In Series A and C, all three measures begin increasing at roughly the same value of $N_{CatTrans}$ (195 in Series A, 170 in Series C, although in Series A the increase in $Rate_{Int}$ is initially small). In Series B, the increase starts much later (when $N_{CatTrans}$ reaches 318). However, there is then a very much sharper increase than in the other two series.

Figure 4 for Series B shows a linear extrapolation of $N_{RIntType}$ backwards from $N_{CatTrans}$ = 320. The back extrapolation intercepts the line $N_{RIntType} = 0$ when $N_{CatTrans}$ = 190. This is similar to the values of $N_{CatTrans}$ at which the plots begin increasing in the other series.

Change in Network Properties: The above suggests that there may be an important change in network properties that occurs in all three cases in the region $N_{CatTrans}$ = 170 - 195, and that in Series B

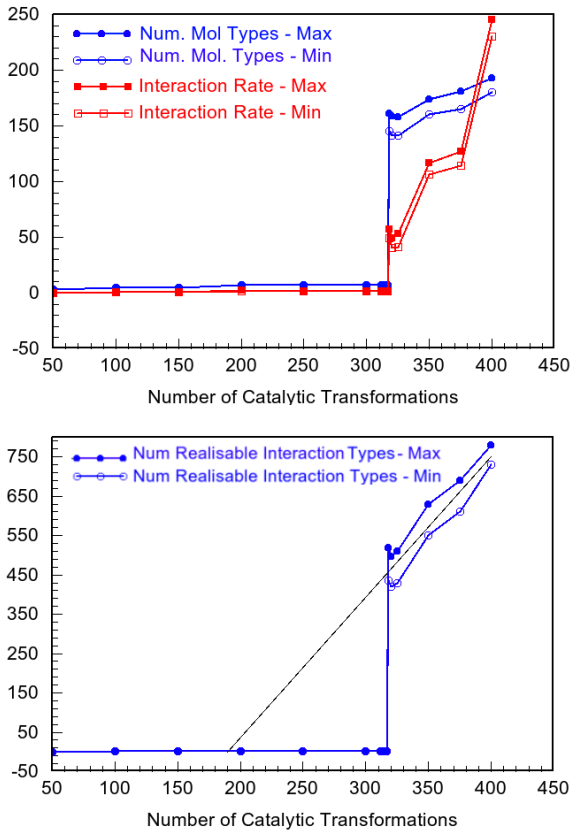

Figure 4: Reactor Activity vs Number of Catalytic Transformations - Series B

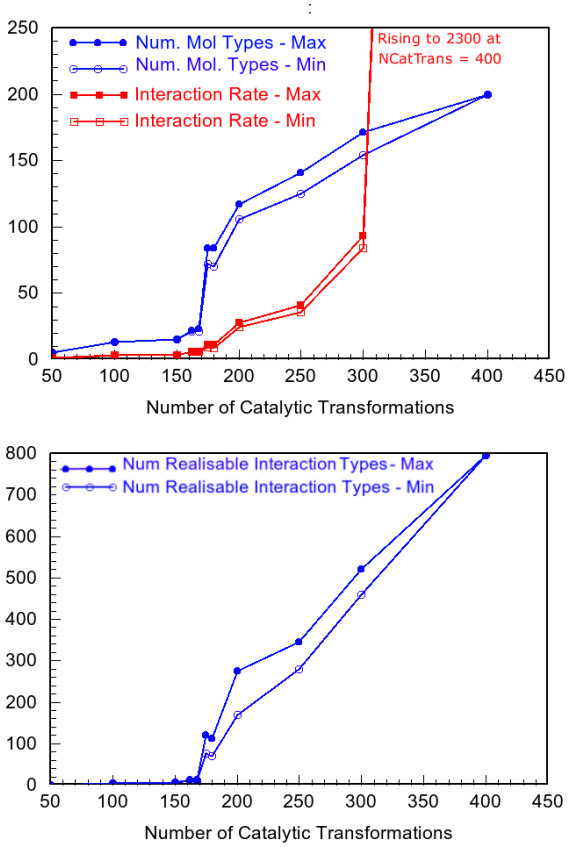

Figure 5: Reactor Activity vs Number of Catalytic Transformations - Series C. The Interaction Rate ($Rate_{Int}$) increases very sharply after $NCatTrans = 300$. It reaches the value 2300 at $NCatTrans = 400$

the effects of this change are delayed until $N_{CatTrans}$ reaches a higher value. A possible reason for this delay is that the overall behaviour of the network is strongly dependent on the details of the Interaction Types having the three 'food' Molecule Types as Reactants; it is these Interaction Types that supply material to the rest of the network. Investigation of the detailed properties of the network shows that the sharp increase in Series B at $N_{CatTrans} = 318$ coincides with the value of $N_{CatTrans}$ at which a second Fission leading from one of the three 'food' Molecule Types is added, and that the Rate Constant for this second Fission is almost nine times that of the first Fission having this Molecule Type as its Reactant.

A Similarity with Random Graphs?: In graph theory, it is well known that sudden changes in the overall properties of random graphs take place as the number of edges connecting nodes increases (see, for example, Albert and Barabási (2002) and Kauffman (1993)). In particular, in a random graph with a large number of nodes (N), as the number of edges (E) increases beyond $0.5N$, the graph changes its topology abruptly from a loose collection of small disconnected clusters to a system dominated by a single giant cluster.

SimSoup networks are not random graphs of the kind to which the above result applies. For example, in SimSoup:-

- Nodes are connected by Interaction Types such as Fissions and Constructions, which each connect three nodes, rather than two
- SimSoup Interaction Types are directional (Reactants result in Products, but not vice versa)
- SimSoup Interaction Types have Rate Constants, and so some are more active than others.

However, it would not be surprising if SimSoup

networks shared similar critical point properties to those exhibited by random graphs.

It is not unreasonable to speculate that if each (directional) Catalytic Transformation were seen as analogous to 'half' of a (bidirectional) edge in a random graph, then the value of 170 - 195 suggested for the critical value of $N_{CatTrans}$ corresponds to 85 - 97.5 edges in a random graph. This is comparable with the value of about 100 for the critical number of edges that would be expected in a random graph with 200 nodes.

Differences in Reactor Variability: The gap between the maximum and minimum values on the plots for Series A are substantially larger than those for the other two series. This means that the behaviour is more variable in this series. The nature of this variability is discussed in the next section.

3.2 Static and Oscillating Behaviour

3.2.1 Static Persistent States

Many SimSoup networks have a behaviour characterised by the appearance of Persistent States that exist over long periods with the same (or nearly the same) Reactor Composition. The Manhattan Plot of Figure 2 presented in section 2.4 is an example of a network that enters such a Persistent State after an initial transient period. The plot shows the behaviour for the Series C run with $N_{CatTrans} = 200$. Other values of $N_{CatTrans}$ for the Series C setup lead to similar behaviour.

3.2.2 Oscillating Persistent States

Manhattan Plots For Series A: Some setup conditions lead to more variable behaviour than that shown in Figure 2. Such variability is evident from the differences in maximum and minimum values for the indicators of overall Reactor activity that are shown in Figure 3 for Series A. Figures 6, 7, 8, 9, 10 and 11 show Manhattan Plots for the Series A runs.

Observations and Interpretation: As mentioned in section 3.1.1, the setup for the three series of runs was the same except for different pseudo-random number seeds. It can be seen from Figures 6 to 11 that the behaviour in Series A is nonetheless substantially different to the static behaviour of Series C shown in Figure 2.

In Figure 6 for $N_{CatTrans} = 197$, we see that there is a variability that is not present in Figure 2. This is indicated not only by the dark lines before Time = 500,000 and Time = 900,000, but also by the many smaller variations in tone.

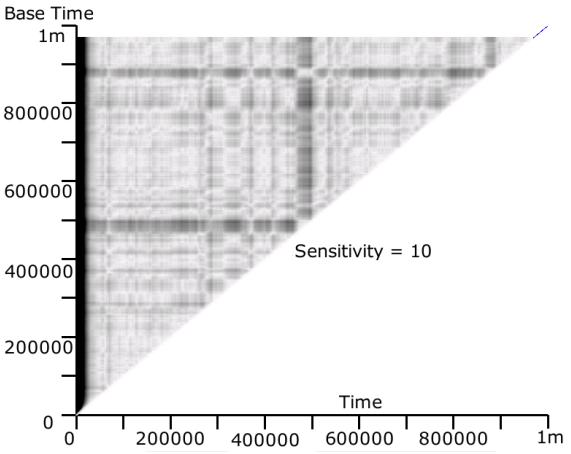

Figure 6: Manhattan Plot for Series A, $N_{CatTrans} = 197$

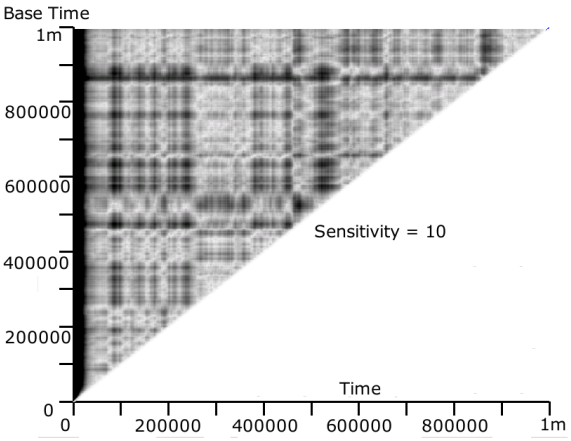

Figure 7: Manhattan Plot for Series A, $N_{CatTrans} = 207$

In Figure 7 for $N_{CatTrans} = 207$, the size of the variability has increased, as indicated by the wider variability of tone. In addition to variability on a timescale of 10,000 to 20,000 timesteps, there also appears to be variability on a longer timescale. This is suggested by the variations in the degree of 'mottling' in different parts of the plot. For example, the pattern of mottling between times 260,000 and 360,000 is noticeably different to that between times 100,000 and 260,000. This suggests that the state of the network is somehow different in these two periods.

Figure 8 for $N_{CatTrans} = 233$ shows a striking pattern of thin diagonal white lines against an

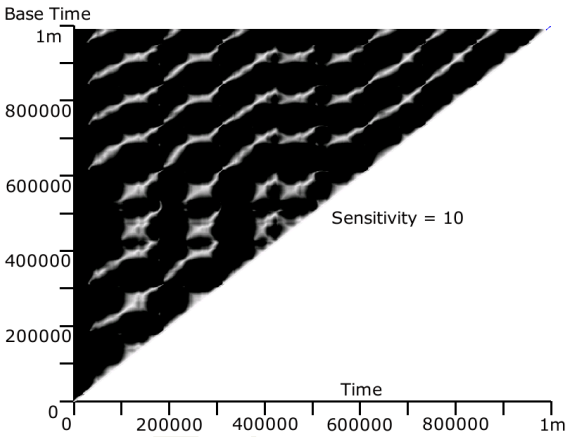

Figure 8: Manhattan Plot for Series A, $N_{CatTrans} = 233$

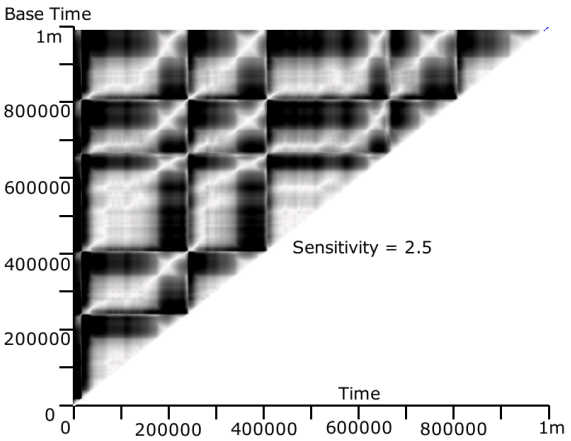

Figure 9: Manhattan Plot for Series A, $N_{CatTrans} = 235$

otherwise completely black background. This indicates that the Reactor Composition is behaving cyclically. Following any horizontal line across the plot, we see that most of the path is black, but that it turns white for a short period approximately every 90,000 timesteps. The white sections along the line indicate periods during which the system had (almost) the same Reactor Composition.

Figure 9 shows that when $N_{CatTrans}$ is increased to 235, and the sensitivity of the plot reduced to 2.5, the behaviour can still be seen to be cyclic. However, there appear to be two distinct periods in each major cycle, with the second lasting typically 50,000 timesteps, and the first lasting longer.

In Figure 10 for $N_{CatTrans} = 240$, the pattern is similar to that in Figure 8 for $N_{CatTrans} = 233$.

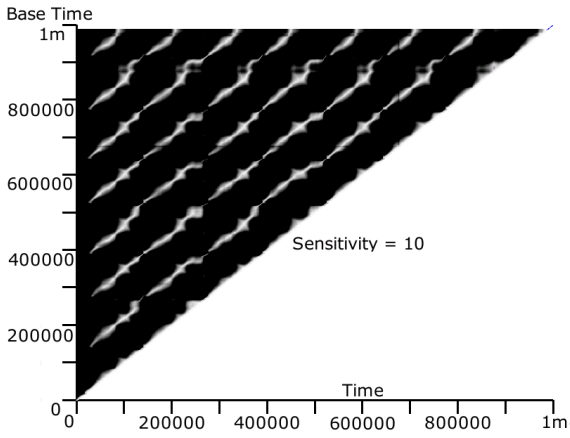

Figure 10: Manhattan Plot for Series A, $N_{CatTrans} = 240$

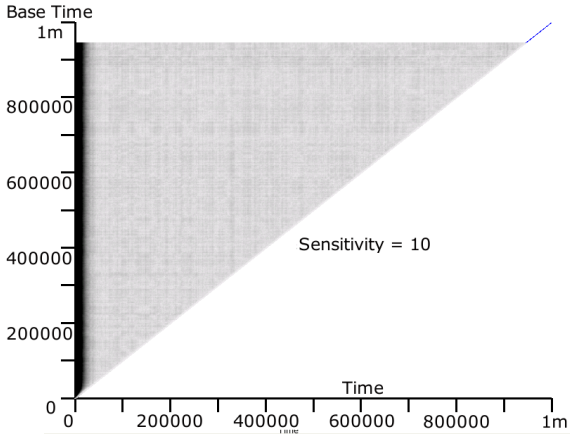

Figure 11: Manhattan Plot for Series A, $N_{CatTrans} = 300$

Finally, Figure 11 for $N_{CatTrans} = 300$ shows a situation in which the network is no longer oscillating, and instead adopts a static Persistent State after the initial transient.

3.2.3 Detailed Behaviour of the Oscillating Network

Sample Plots: Figures 12, 13 and 14 show detailed SimSoup output for the Series A run with $N_{CatTrans} = 235$. They correspond to the Manhattan Plot in Figure 9

Observations and Interpretation: Figure 12 shows that the number of Molecules in the Reactor, the number of Molecule Types that currently exist in

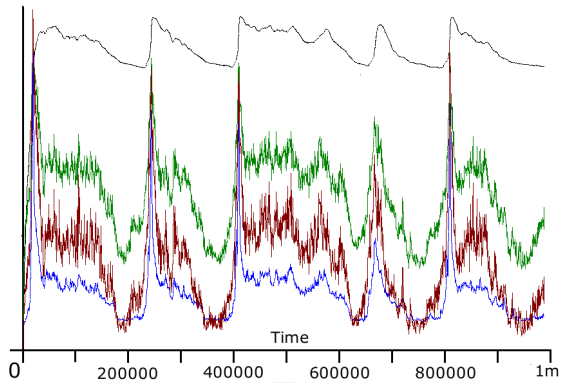

Figure 12: Series A output for $N_{CatTrans} = 235$. The plots, from top to bottom show: Number of Molecules (black plot - top), Number of Molecule Types that exist in the Reactor ($N_{MolType}$, green plot), Number of Realisable Interaction Types ($N_{RIntType}$, brown plot), and Total Interaction Rate ($Rate_{Int}$, blue plot - bottom).

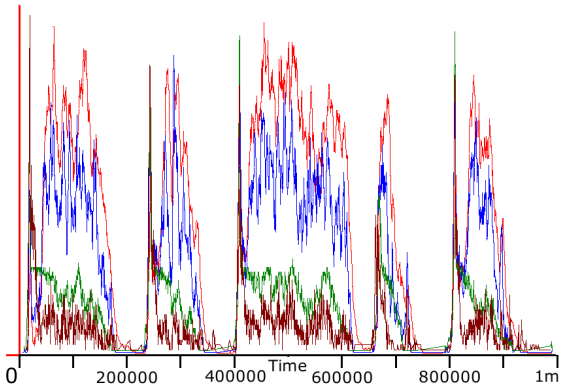

Figure 13: Series A output for $N_{CatTrans} = 235$. The plots, from top to bottom show Number of Molecules of the following types: 163 (red - top), 161 (blue), 158 (green), 83 (brown - bottom)

the Reactor ($N_{MolType}$), the number of Interaction Types that are possible (realisable) in the Reactor ($N_{RIntType}$), and the total rate of Interactions of all types taking place in the Reactor ($Rate_{Int}$) all follow a cyclic pattern. In this pattern, a rapid increase is followed by a period of decay, and then by another rapid increase.

Figure 13 shows the numbers of Molecules of various types in the Reactor. Again, each of these Molecule Types shows a cycling behaviour; the number of Molecules of each type increases rapidly, decays, and then increases rapidly again. It can also be noted that the decay is initially slow, and then accelerates into a much sharper fall.

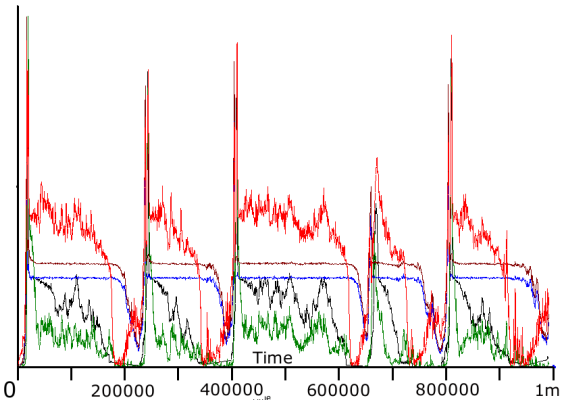

Figure 14: Series A output for $N_{CatTrans} = 235$. The plots, from top to bottom show rates (per timestep) of the following Interaction Types: 385 (red - top), 116 (brown), 117 (blue), 14 (black), 402 (green).

Figure 14 shows the numbers of Interactions of various types in the Reactor. Here a very short and sharp burst is followed by a slow decay, or, in the case of two of the Interaction Types, a period of stability. Again, the fall is much sharper at the end of the period of decay.

Figures 12, 13 and 14 show only a limited sample of the available output. However, it can be suggested that a mechanism exists in which an initial burst of activity takes place and is then inhibited by some products of this burst, such that the next burst cannot take place until the inhibiting products have decayed away, either by being used up by Interactions taking place in the Reactor, or by the constant Reactor leakage.

4 Conclusions and Prospects

4.1 Conclusions

Instantaneous and Persistent States: When considering the behaviour of reaction networks, a distinction needs to be made between Instantaneous and Persistent states.

Manhattan Distance: This measure can be used to recognise and discriminate between Persistent States.

Stability of Persistent States: SimSoup reaction networks often enter Persistent States that are stable over long periods.

Static and Oscillating Persistent States: Persistent States are often static, but can also take on an oscillating behaviour in which they traverse a path through composition space, periodically returning to (almost) the same Reactor Composition.

Localisation of Persistent States: Static Persistent States can be localised within an extremely small region of composition space. Oscillating Persistent States follow a path through composition space, but can return periodically to the same extremely small region of composition space. The Manhattan Plots in section 3.2.2 show networks that are traversing a very 'narrow' corridor through composition space.

Relation between Connection Density and Reactor Activity: For the networks investigated, there is a sudden onset of Reactor activity when $N_{CatTrans}$ reaches a particular value. The results are suggestive of a change in network properties that takes place at a critical value. It is speculated that this may be a similar phenomenon to the sudden changes in the overall properties of random graphs that are known to take place as the number of edges connecting nodes increases.

Bursts and Fallback: The detailed plots of the oscillating persistent state shown in section 3.2.3 show bursts of activity followed by a period of decay. In some cases the final stage of the decay is extremely fast. It is suggested that a possible mechanism for this could be that the initial burst leads to products that inhibit further activity until the inhibiting products have decayed.

4.2 Prospects

Further Exploration: The results presented here represent a start in exploring the behaviour of SimSoup networks. There is considerable scope for investigating the behaviour under different conditions. For example, by varying:-

- Mass of Molecule Types
- Rate Constants
- Mix of Interaction Types
- Network connection scheme (eg using schemes analogous to small world and scale free networks)

The Role of Energy: The networks investigated so far do not embody any concept analogous to energy in real chemistry. While the results are a step in understanding the general properties of networks, including energy in the model will place constraints on the network's behaviour (in addition to the topological constraints already imposed by mass conservation) that will make SimSoup more representative of real chemistry.

Interaction Paths The current version of SimSoup does not record the paths followed by material as it takes place in Interactions that change it from one Molecule Type to another. It will be useful to extend the model to record these paths, and to determine the extent to which material is following 'metabolic cycles' that repetedly return to the same Molecule Type.

Constructive Interactions: In the current version of SimSoup, all Molecule Types and Interaction Types are pre-specified. It will be appropriate to extend the model to enable new Molecule Types and their associated Interaction Types to be produced as the model runs.

The Theoretical Challenge - The Dynamics of Chemical Networks: While there is a large body of theory dealing with networks, this is not generally applicable to SimSoup networks, or to real chemical networks. This is primarily because network theory generally deals with networks of nodes and edges, whereas the fundamental connecting elements in chemical networks include interactions that have the structure of Constructions and Fissions, which are directional connections between three nodes.

An important challenge for researchers in this area is to produce a theoretical model that is applicable to the dynamics of chemical networks.

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