

A Meta-Atom Based Sub-Symbolic Artificial Chemistry

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Abstract

We introduce a new sub-symbolic Artificial Chemistry, called the Meta-Atom Artificial Chemistry. It treats composite particles (composites of random boolean networks, RBN) as a new type of higher level atom, a *meta-atom*. These complex structures, together with a new kind of link, then form even larger, multi-level, structures. We show that Meta-Atom Artificial Chemistry exhibits rich behaviour, including reaction pathways that resemble catalytic reactions.

Introduction

We wish to use Artificial Chemistries to build and investigate open-ended systems. As such, we wish to minimise the number of explicit rules and properties needed, yet still get rich behaviours. For this reason we have developed *sub-symbolic artificial chemistries* (Faulkner et al., 2018), where the properties and dynamics of atomic and composite particles emerge from the underlying structure of the particles themselves. This is in contrast to more traditional AChems (Dittrich et al., 2001; Banzhaf and Yamamoto, 2015), in which the atomic particles have no underlying structure.

Spiky-RBN AChem (Krastev et al., 2016, 2017) is one such sub-symbolic artificial chemistry. In the original Spiky-RBN AChem, the lowest level structure, an atomic particle, is a random boolean network (RBN) (Gershenson, 2004; Drossel, 2008). An RBN has N nodes; at initialisation each node is assigned K inputs selected at random from K of the N nodes (possibly including the node itself), and a randomly generated Boolean function of these inputs; each node has a Boolean-valued state. The node's function is used to update the state of the node from the states of its input nodes at each timestep. When started from some initial state, the dynamics of the RBN goes through two phases: a *transient* phase of progressing through states, followed by an *attractor cycle* where states that are periodically revisited (Wuensche, 1998). The transient phase and attractor cycle have a rich variety of emergent properties; for $K = 2$ both these phases are relatively short, so calculating the properties is computationally tractable.

In Spiky-RBN, the RBN nodes are assigned to functional groupings known as *spikes*, which act as *bonding sites* for

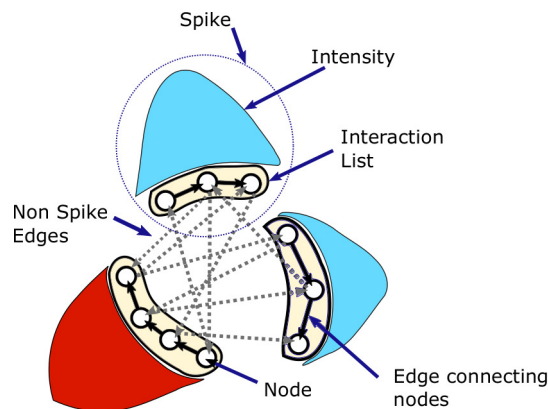


Figure 1: Spiky-RBN atomic particle. The specific node functions and connections of the underlying RBN result in emergent properties captured as *spikes*. Blue spikes have a positive intensity value and red spikes have a negative intensity value. After (Krastev et al., 2016)

the particle. Spikes consist of an interaction list, which is a list of all the nodes in the spike, and an intensity, which is a signed integer value related to the states of the nodes in the interaction list. These spikes, and hence the particle's bonding properties, are emergent properties of the underlying structure and dynamics of the underlying RBN; for details of how they are calculated from the properties of the RBN, see Krastev et al. (2016). An atomic particle is shown in Figure 1.

Particles can form a link (bond) if they have spike intensities of equal and opposite magnitude; the nodes in each particle have their inputs redirected to link together to form a composite particle (Figure 2). A composite particle may decompose, or may react with another particle. This leads to reaction pathways in which novel composite particles form from the reactions of an initial set of particles in a reactor. Krastev et al. (2016, 2017) show that the Spiky-RBN AChem has a rich behaviour and is able to form composite particles of varying sizes and structures through complex reaction pathways.

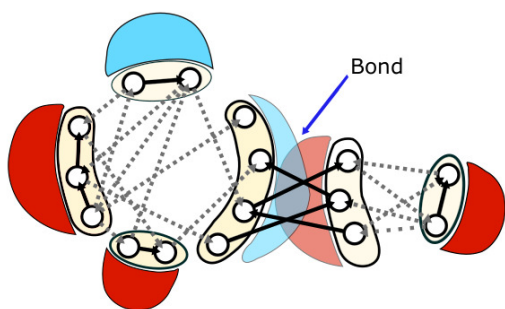


Figure 2: A composite particle composed of two atomic particles. After (Krastev et al., 2016)

Here we introduce two variants of the original Spiky-RBN AChem. Firstly, we define Frozen-Node-Spiky-RBN (FN-SRBN), in order to explore how further emergent properties of RBNs can be exploited as bonding properties. Secondly, we use this new variant as the basis of Meta-Atom Artificial Chemistry. This Meta-Atom AChem reacts composite particles through a higher level kind of bond, using ‘dangling nodes’ in lower level bonds as the bonding criterion. As with Spiky-RBN AChem, the aim is to build an AChem where the bonding properties emerge from its underlying structure and dynamics. Here the underlying structure is that of the lower level bonds in composite particles formed in FN-SRBN.

The Frozen-Node-Spiky-RBN AChem

In this section we introduce a modified version of the Spiky-RBN AChem, the Frozen-Node-Spiky-RBN (FN-SRBN) AChem. We discuss why this AChem has been developed, and describe the structure of atomic particles and the new bonding process. We conclude the section with the introduction of a special composite particle called a *ring*, and an experiment to generate ring structures, which will be used as the basis of the later Meta-Atom AChem experiments.

Atomic Particles in the FN-SRBN AChem

FN-SRBN AChem is used to explore if other emergent properties of RBNs, here *frozen nodes* (see later), can be used as part of an AChem, and to see how other approaches to generating the interaction lists affect the behaviour of the AChem. This allows us to explore new Spiky-RBN AChems and to see if they have the rich behaviour which is required for a useful AChem.

Spiky-RBN AChem generates interaction lists by following the connections of the nodes in the RBN ordered by their ‘influence’ (number of outgoing connections). In the FN-SRBN AChem we instead follow the connection of randomly selected nodes. The algorithm which builds the interaction list is shown below in Algorithm 1.

Spiky-RBN AChem calculates the intensity of the spikes as a function of the state changes of the nodes over the

```

Data: N: List of all nodes in the RBN
while N is not empty do
  Create new empty Interaction List  $IL_i$ ;
  Remove random node  $n$  from N;
  Append  $n$  to  $IL_i$ ;
  while  $\exists n' \in N$  where  $n'$  is an input to  $n$  do
    Remove  $n'$  from N;
    Add  $n'$  to  $IL_i$ ;
     $n \leftarrow n'$ ;
  end
   $i++$ ;

```

end

Algorithm 1: Building interaction lists for an RBN

RBN’s attractor cycle. In the FN-SRBN AChem the intensity of the spike is instead dependent on the states of the ‘frozen’ nodes in the attractor cycle. Frozen nodes are nodes whose states remain constant over the attractor cycle, and are a prominent feature of RBNs. Each node n in a spike S is assigned a weighting n_w :

$$n_w = \begin{cases} 1 & \text{if node frozen in True state} \\ -1 & \text{if node frozen in False state} \\ 0 & \text{if node is not frozen} \end{cases} \quad (1)$$

The intensity of an FN-SRBN spike S_i is the sum of weightings for each node in the interaction list IL_i of the spike:

$$S_i = \sum_{n \in IL_i} n_w \quad (2)$$

As with Spiky-RBN AChem, this gives a spike with a magnitude and a sign. The intensity is constrained by the length of the interaction list:

$$-\#IL_i \leq S_i \leq \#IL_i \quad (3)$$

FN-SRBN AChem introduces a new parameter called spike type S_T which influences how easy it is for two spikes to bond. The spike type ranges from 1 to 3 and is a function of the length of the interaction list of the spike

$$S_T = \begin{cases} 1 & \text{if } \#IL_i < 5 \\ 2 & \text{if } 5 \leq \#IL_i < 10 \\ 3 & \text{if } 10 \leq \#IL_i \end{cases} \quad (4)$$

The attractor cycle is found from an initial state of all nodes being false, and the number of inputs each node takes is $K = 2$ in order to obtain stable rather than chaotic behaviour (Wuensche, 2008).

Bonding Atomic Particles

FN-SRBN AChem forms bonds in the same manner as Spiky-RBN AChem, with two spikes from different atomic

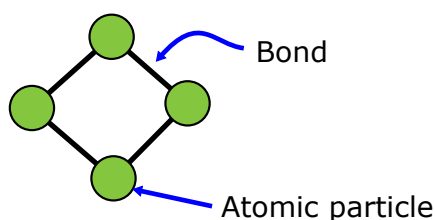


Figure 3: A *ring* of four atomic particles. The green circles are atomic particles, each with exactly two spikes, and the lines between atomic particles are bonds.

particles linking together as in Figure 2. Spiky-RBN AChem requires that the intensity of both spikes must sum to zero before bonding for the bond to form, and after bonding for the bond to remain stable (the intensity may change on bonding since the linked RBNs have a different dynamics from the unlinked ones; this decomposition property arises naturally from the emergent intensity property).

In FN-SRBN AChem the bonding condition depends on both the intensity and the spike type. Let the spike from the first particle be S^1 with intensity S_i^1 and type S_T^1 , and the spike from the second particle be S^2 with intensity S_i^2 and type S_T^2 . Then the two particles can bond if the spikes meet the appropriate condition specified in eqn. 5:

$$|S_i^1 + S_i^2| = 0 \text{ and } S_T^1 = 1 \vee S_T^2 = 1 \quad (5a)$$

$$|S_i^1 + S_i^2| \leq 1 \text{ and } 2 < S_T^1 + S_T^2 < 6 \quad (5b)$$

$$|S_i^1 + S_i^2| \leq 2 \text{ and } S_T^1 = 3 \wedge S_T^2 = 3 \quad (5c)$$

This condition reduces to the Spiky-RBN AChem behaviour if either IL is very short (just one node), but becomes more relaxed as the ILs get longer. This more relaxed behaviour is needed to ensure sufficiently rich behaviour, to compensate for the different distribution of spike intensities in FN-SRBN.

If the condition continues to be met after bonding, then the bond is stable. If the bond is unstable, it breaks.

Rings of Atomic Particles

A *ring* is a special composite particle consisting of atomic particles each of which have two bonded spikes and no unbonded spikes. A ring of four atomic particles is shown in Figure 3.

This ring structure can be considered an ‘inert’ composite particle. Since all its spikes are bonded, it cannot bond to any other particles. We use this structure for our initial Meta-Atom AChem studies here, since we do not need to consider any lower level reactions between these inert rings.

Experiment: Growing a Set of Rings

The aim of this experiment is to generate a set of rings using FN-SRBN AChem. The set can then be used as the basis for a higher level AChem.

```

while true do
  // Phase 1 – find atomic set
  chain := empty
  while empty chain do
    R := 20 randomly created atoms
    tries := 0
    while empty chain and tries < 95 do
      a1, a2 ∈ R
      if a1, a2 can bond then
        | chain := bonded (a1a2)
      end
      ++tries
    end
  end
  // Phase 2 – build a ring
  if head,tail of chain can bond then
    | ring := bonded chain
    | exit
  end
  tries := 0
  while tries < 700 do
    a ∈ R
    if a, chain can bond then
      chain := bonded (a,chain)
      if head,tail of chain can bond then
        | ring := bonded chain
        | exit
      end
    end
    ++tries
  end
end

```

Algorithm 2: Building a ring from random atoms

This is done using a well stirred reactor with no spatial component. The reaction contains a set of 20 atomic particles. To form this set, atoms are randomly generated with a size N chosen uniformly between 2 and 15 nodes. An atom is kept provided it has exactly two spikes, which it needs to be a link in a ring. Atoms are randomly generated in this manner until there is a set of size 20.

The algorithm to build a ring has two phases, see algorithm 2.

Phase one finds a suitable atomic set, by producing a short chain of two atoms. The reactor is initialised with 20 randomly generated atoms. Two atoms are selected at random, and a bond is attempted. Selection of pairs of atoms continues until a bond is formed. If after 95 attempts no initial bond is formed, another set of atomic particles is generated.

Phase 2 generates a ring. It starts with the initial pair of bonded atoms, and the atomic set, from Phase 1. A bonding attempt is made between the head and tail of this chain of two atoms, attempting to form a minimal ring. If no ring forms, a further atom is selected at random from the set,

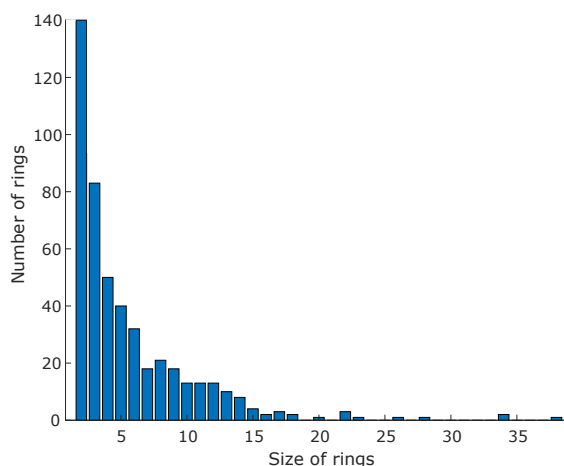


Figure 4: Chart showing size of rings against number of rings of this size. Total number of rings is 625, smallest size is 2, largest is 38.

and a bond is attempted with the short chain. This random selection is continued until the chain is lengthened by one atom. Each time the chain is lengthened, there is an attempt to bond the head and tail to form a ring. If no ring forms, the chain is further lengthened. If no ring has been created after 700 lengthening attempts, then entire process is started again.

Using this algorithm, 625 rings were generated. The distribution of ring sizes for atomic particles consisting of up to 15 nodes and an attractor cycle length of 3 is shown in Figure 4. The figure shows that the majority of rings consist of less than five atomic particles.

It is possible to obtain much larger rings, up to size 38 in this experiment, although this is rarer. There are two reasons for this rarity. Firstly, the algorithm is biased towards smaller rings, since it incrementally increases ring size, and stops once a stable ring forms. Secondly, larger rings have more bonds, increasing the likelihood of an existing bond becoming unstable and breaking when a further bond is formed during lengthening.

The Meta-Atom Artificial Chemistry

In this section we introduce the Meta-Atom AChem.

Meta-Atoms

FN-SRBN AChem can be used to bond particles with one kind of bond, as demonstrated above. Meta-Atom AChem introduces a new kind of bond, to bond composite particles formed in FN-SRBN in a new manner. Meta-Atom AChem has its own ‘atomic particles’, called *meta-atoms*. A meta-atom’s behaviour and dynamics emerge from its underlying structure, which here is that of a ring of bonded FN-SRBN AChem atomic particles. We can consider the Meta-Atom AChem as a higher level sub-symbolic artificial chemistry,

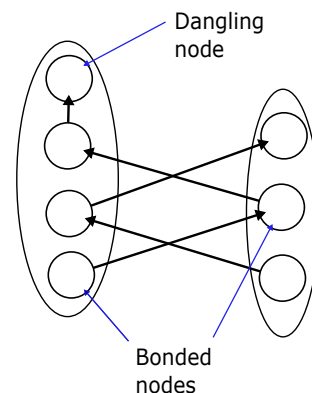


Figure 5: Two spikes bonded together resulting in a single dangling node. The colours of the spikes and connections to nodes outside of the interaction list have been removed for clarity.

as its properties and dynamics emerge from a lower level sub-symbolic artificial chemistry.

We use FN-SRBN rings as meta-atoms in this initial study, as they are inert at the FN-SRBN level, and so reactions between low level particles does not need to be considered. In principle, composite particles that are not inert could be used as a basis for meta-atoms. Meta-atoms of reactive composite particles will be added in future iterations of our Meta-Atom AChem, where we will investigate the interaction of the two bonding mechanisms. Such interaction could result in new reaction pathways and new products emerging.

Dangling nodes

Figure 2 shows a composite particle composed of two atomic particles. Figure 5 shows a zoomed view of the bond between the two particles. Figure 5 shows that when two spikes bond, not all of the nodes in a spikes need to be rewired to connect to the other spike. Such nodes play no direct part in the bond; we refer to these as *dangling nodes*. If there are multiple dangling nodes in a bond, we refer to this as a *dangling tail*. Nodes that are directly involved in the bond are referred to as *bonded nodes*.

Dangling nodes and tails are an emergent property of the bonding process between atomic particles. Dangling nodes and tails arise when the lengths of the ILs of the two bonded spikes are unequal. The number of dangling nodes, γ , in a bond is the difference in the lengths of the ILs of the two spikes:

$$\gamma = |\#IL_1 - \#IL_2| \quad (6)$$

Each dangling node is associated with a spike, which has an intensity and type. We assign the dangling node an intensity and type equal to the intensity and type of its spike.

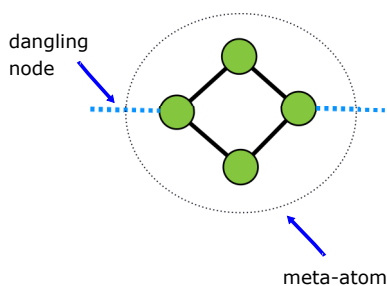


Figure 6: A meta-atom consisting of a ring of size four and two dangling nodes. The green circles are atomic particles; black lines are bonds between atomic particles; the light blue dashed lines emerging from two of the atomic particles represent bonding possibilities via dangling nodes, or dangling tails.

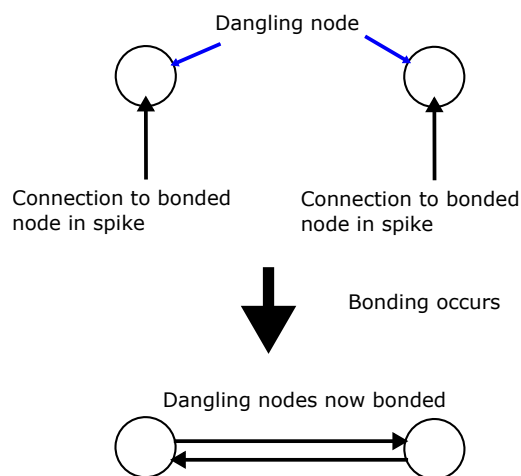


Figure 7: Dangling nodes bonding. This causes bonds in the low level structure of the atomic particle to break.

Meta-Atom bonding

As with the FN-SRBN AChem, there needs to be a mechanism that allows meta-atoms to bond in order to generate larger structures. To bond meta-atoms, we use the emergent dangling nodes within bonded spikes. We represent a meta-atom diagrammatically as a ring of atomic particles with dangling nodes (Figure 6).

Here FN-SRBN AChem is used as the lower level AChem to generate rings for meta-atoms. Future work will extend Meta-Atom AChem so that the low level structure of meta-atoms can be made up of composite particles generated by other Spiky-RBN AChems (Krastev et al., 2016).

For dangling nodes to attempt to bond, as with bonding spikes, we need to see if the intensity and type obey the bonding criterion (eqn. 5). If the condition is met, the dangling nodes swap connections (Figure 7). We refer to bonded meta-atoms as a meta-molecule.

The swapping of connections alters the underlying struc-

tures of the atomic particles in the ring. This means that higher level bonding alters the lower level structure of both meta-atoms involved in the bonding. Hence the properties of every spike in the ring need to be recalculated after a higher level bond has occurred. Bonding at the higher level can lead to intensities of the spikes changing (and thus the intensity of dangling nodes). This can cause the bond between dangling nodes to break and can also cause bonds in the low level structure to become unstable and break. A change in higher level bonding can perturb the low-level structure and alter it. A change in the low-level structure can then affect the higher level bonds in turn. Thus after meta-atoms bond to form a meta-molecule, there can be a period of instability in which the meta-atom's internal structure and the higher level bonds can change.

This period of instability post meta-atom bonding means that the structure of a meta-molecule needs to be reanalysed until all of its meta-atoms are stable. A stable meta-molecule is one in which all of its composite meta-atoms bond. Both high-level and low-level particles must meet the appropriate stability criteria as defined in eqn. 5. If the higher-level bonds between meta-atoms break, the meta-molecule is checked for meta-atoms which no longer have high-level bonding with other meta-atoms. If a meta-atom with no bonds to the meta-molecule is found, it is removed from the meta-molecule as it has 'broken away' from the meta-molecule.

Experimental Implementation

The FN-SRBN and Meta-Atom AChem were implemented using the Python programming language and the NumPy numerical library. An object-oriented design approach is used and the software is available on GitHub¹.

Analysis of Meta-Atom Bonding

The simplest case of meta-atom bonding is two meta-atoms M_1 , M_2 , each with one dangling node, coming together and attempting to bond. The eight possible outcomes of this reaction are shown in Table 1. In this table, R1 (Ring 1) Stable shows whether the underlying structure of M_1 is affected by the higher-level bonding between the meta-atoms. If R1 Stable is false, the underlying structure is affected by the bonding, and the ring will break one or more low-level bonds. MB Stable indicates whether the Meta-Bond is stable. For example, a type 5 reaction results in the low level structure M_1 changing, but the bond between M_1 and M_2 is stable and the low level structure of M_2 is stable. An example of a possible meta-molecule formed through a type 5 reaction is shown in Figure 8.

From Table 1 we can see that there is a symmetry between reaction types 3 and 5, and that there is also a symmetry between reaction types 4 and 6. Figure 8 is a pictorial repre-

¹github.com/iw596/Meta-AChem

Type	R1 Stable	R2 Stable	MB Stable
1	True	True	True
2	True	True	False
3	True	False	True
4	True	False	False
5	False	True	True
6	False	True	False
7	False	False	True
8	False	False	False

Table 1: Reaction types between two meta-atoms with a single bond between them.

sentation of Table 1, showing the resulting product of each reaction type.

Type 1 Reaction

A type 1 reaction results in a meta-molecule as there is stable bond between the two meta-atoms. The internal structure of both meta-atoms is unchanged by the reaction. This reaction type is analogous to a standard successful collision in the lower-level FN-SRBN AChem where two atomic particles react together to form a composite particles. Instead of atomic particles forming composite particles, now meta-atoms form meta-molecules.

Type 2 Reaction

Type 2 reactions are elastic collisions between meta-atoms. This reaction results in no stable bond between the two meta-atoms and the internal structure of both meta-atoms are not altered by this elastic collision. This is analogous to an elastic collision in the lower level FN-SRBN AChem.

Type 3 & 5 Reactions

Both type 3 and type 5 reactions result in a meta-molecule consisting of two meta-atoms. One of the meta-atoms is unchanged by this bond but the other meta-atom is altered by the bond. The alteration to the meta-atom could be small, e.g a single low level bond breaking. The alteration could be large, e.g many atomic particles breaking away from the ring. This reaction type results in the previously inert lower-level structure becoming reactive. This means that it is now possible to have further reactions in the lower-level structure. With meta-atoms with more than one higher level bonding site, a type 3 or 5 reaction could result in a meta-molecule which is reactive at both the higher and lower levels.

Type 4 & 6 Reactions

Both type 4 and 6 reactions result in the meta-atoms being temporarily bonded. This in turn results in one meta-atom being altered while the other is unchanged. This change one

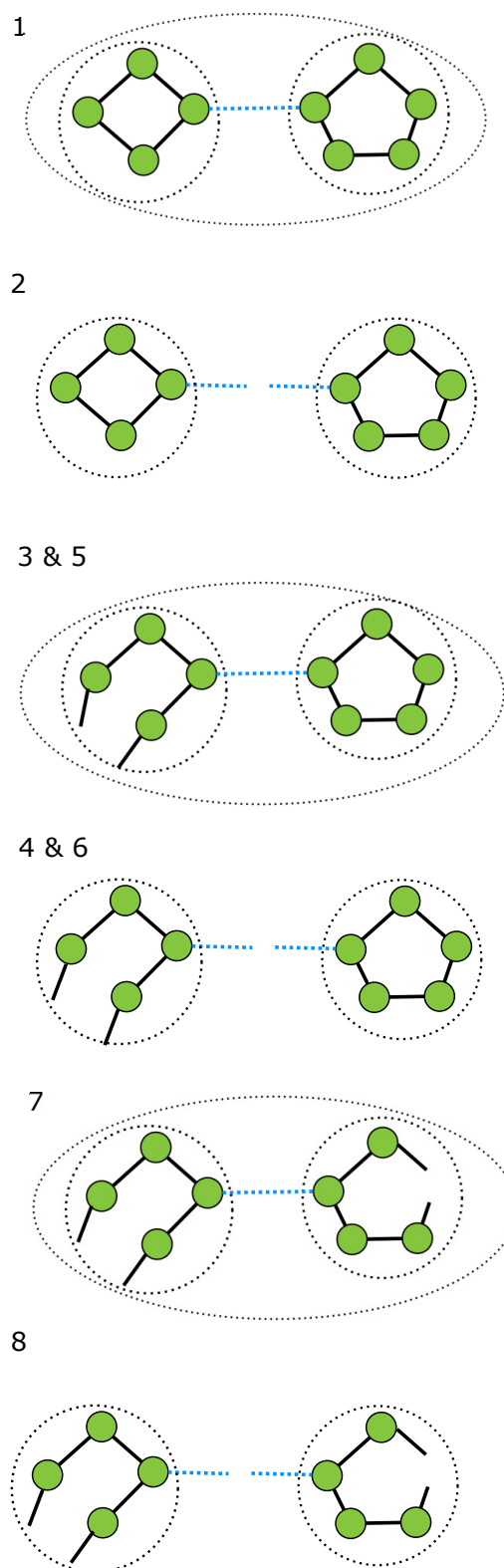


Figure 8: A potential product from each reaction type 1 to 8 listed in Table 1. Symmetric reaction types are grouped together.

meta-atom's structure causes the high-level bond between the meta-atoms to become unstable and break. A type 6 reaction is shown in Figure 9 in more detail. These reactions are interesting as they can be viewed as analogous to reactions between a reagent and a catalyst. The reagent is changed but the catalyst is not. Catalysts are thought to be important in the origin of life (Belmonte and Mansy, 2016; Russell, 2018), so having analogous behaviour in the Meta-Atom AChem shows that the AChem has some emergent properties which are potentially similar to real world systems. It further shows that this AChem has rich behaviour and warrants further exploration. These reaction types are a partially destructive collision, as no meta-molecule is formed and one of the meta-atoms has been altered by the reaction.

Type 7 Reaction

Type 7 reactions are similar to type 3 and 5 reactions in they result in a stable meta-molecule. The underlying structure here of both meta-atoms has been altered, and it is now possible to have further reactions in the lower-level structure of the meta-atoms.

Type 8 Reaction

A type 8 reaction is a fully destructive collision as the meta-atoms do not form a stable bond and both meta-atoms have their internal structure altered by the attempt to bond. This reaction type moves from having two meta-atoms that are inert at the lower level to having two meta-atoms that are reactive at both the lower and the higher level. This reaction type could be useful as it provides a way of creating very reactive meta-atoms, which could be used as a building block for generating complex meta-molecules.

Analysis

Our experimental tests have generated all of the reaction types in Table 1. These tests were performed using the set of rings shown in Figure 4. This shows that the Meta-Atom AChem has a rich behaviour as it exhibits all the possible reaction paths. These results also show that the AChem is capable of generating new structures.

Further tests, of bonding dangling tails rather than single dangling nodes, show that meta-atoms with dangling tails also can exhibit all the reaction pathways shown in Table 1. Reactions between meta-atoms that have two dangling nodes (or tails) on separate spikes result in products such as the one shown in Figure 10. One of the dangling nodes has bonded, which here has resulted in one of the rings in a meta-atom to break. Since there are still dangling nodes available, this meta-molecule could continue to bond with other meta-atoms to generate yet more complex products. With each meta-atom made up of composite particles, large composite particles consisting of many atomic particles can be generated in this way.

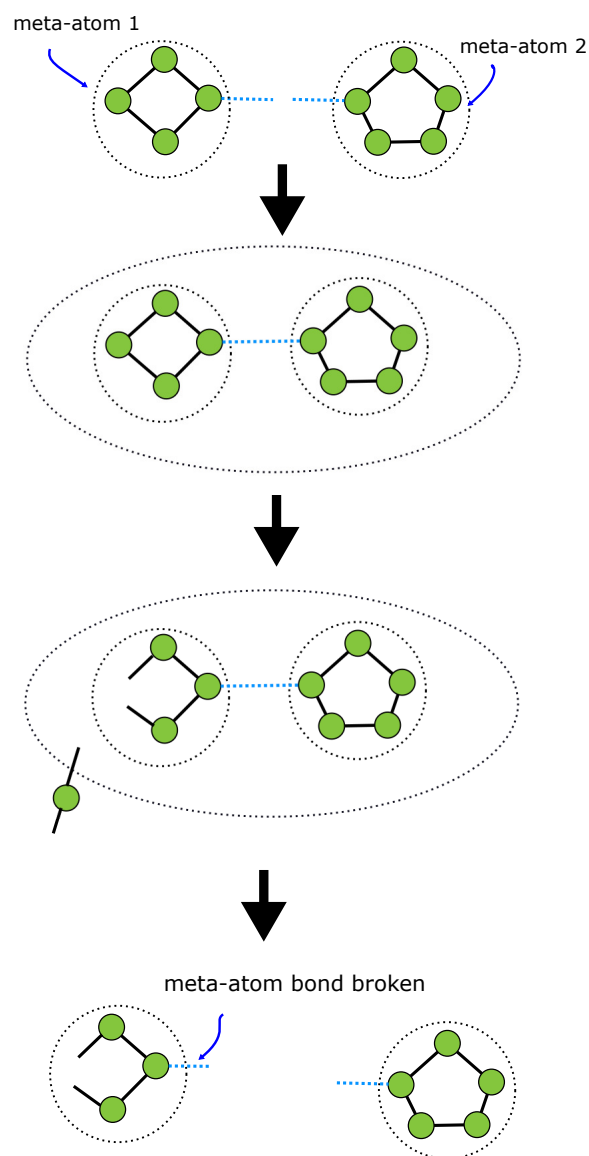


Figure 9: Reaction pathway for a type 6 catalytic reaction.

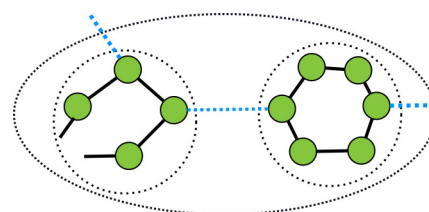


Figure 10: A meta-molecule with unbonded dangling nodes.

Conclusion & Outlook

We present a novel multi-level sub-symbolic AChem, Meta-Atom AChem, in which the structure and dynamics emerge from a lower level Spiky-RBN AChem (Krastev et al., 2016, 2017). Bonding in this Meta-Atom AChem exhibits a wide range of reaction pathways (Figure 8). Examples of these pathways include a catalytic reaction pathway. Meta-Atom AChem may be a way to analyse the structure, dynamics and stability of large composite particles.

Further analysis of bonding in the Meta-Atom AChem is required. For example, the distribution of reaction types between meta-atoms to determine the most frequent reactions is necessary. Furthermore, it needs to be investigated how the structure of a meta-atom affects the likelihood of a reaction pathway occurring. This would assist in the prediction of products from a reaction. To fully understand the dynamics of this new AChem, further work is also required in analysing the difference in strength between higher and lower-level bonds. Understanding this property would also aid in the prediction of products from a reaction.

Future work will involve extending the functionality of this AChem. Two main areas of interest are energetics and spatiality. By adding these features the Meta-Atom AChem may increase its richness.

Adding energetics could lead to new reaction pathways emerging. Energetics would modify the set of all possible reactions with a probability of occurrence at the current temperature. The effects of a reaction may cause a change in temperature. As the temperature varies, the probabilities vary, and so we would get a feedback coupling between reactions that occur and the probabilities of subsequent reactions.

Currently the AChem has no spatial components to bonding. Introducing emergent spatial properties to bonds could lead to interesting products being formed.

Additionally, further work will investigate if this high-level AChem could form the basis of another, even higher-level AChem. The possibility of using the Meta-Atom AChem as the basis of a higher level AChem will also need to be explored once functionality such as energetics are introduced. Emergent behaviours due to these extensions may occur and could be a natural property to form a higher level AChem.

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