Combinatory Chemistry: Towards a Simple Model of Emergent Evolution

Germn Kruszewski and Tomas Mikolov

1Facebook AI
2CIIRC, Prague, Czech Republic
germank@gmail.com

Abstract

Researching the conditions for the emergence of life—not necessarily as it is, but as it could be—is one of the main goals of Artificial Life. Answering this question requires a model that can first explain the emergence of evolvable units, namely, structures that (1) preserve themselves in time (2) self-reproduce and (3) can tolerate a certain amount of variation when reproducing. To tackle this challenge, here we introduce Combinatory Chemistry, an Algorithmic Artificial Chemistry based on a simple computational paradigm named Combinatory Logic. The dynamics of this system comprise very few rules, it is initialized with an elementary tabula rasa state, and features conservation laws replicating natural resource constraints. Our experiments show that a single run of this dynamical system discovers a wide range of emergent patterns with no external intervention. All these structures rely on acquiring basic constituents from the environment and decomposing them in a process that is remarkably similar to biological metabolisms. These patterns involve autopoietic structures that maintain their organisation, recursive ones that grow in linear chains or binary-branching trees, and most notably, patterns able to reproduce themselves, duplicating their number at each generation.

Introduction

Finding the minimal set of conditions that lead to open-ended evolution in a complex system is a central question in Artificial Life, and a fundamental question of science in general. The main driving hypothesis in this line of research is that living systems emerge from the complex interaction of simple components. Environments like Avida (Ofria and Wilke, 2004) or Tierra (Ray, 1991) have been used to explore this question by allowing self-reproducing programs to mutate and evolve in time. Yet, the reproductive and mutation mechanisms, as well as the organisms’ capacity to tolerate such mutations, depend on the hand-coded design of the human engineers. Instead, Artificial Chemistries try to uncover how such evolvable units emerge in the first place by simulating the properties of natural chemical systems at different levels of abstraction (see Dittrich et al. (2001) for a thorough review). It has been hypothesized that they emerge thanks to self-organising chemical networks forming attractors that preserve their structure in time (Walker and Ashby, 1966; Wuensche et al., 1992; Kauffman, 1993). While some Artificial Chemistries study these questions by mimicking as closely as possible the properties of the chemistry that gave rise to life on Earth (Flamm et al., 2010; Högerl, 2010; Young and Neshatian, 2013), others abstract away from the particularities of natural chemistries to focus only on their hypothesized core computational properties (Fontana and Buss, 1994; di Fenizio and Banzhaf, 2000; Tominaga et al., 2007; Buliga and Kauffman, 2014). In line with this latter line of work, in this paper we introduce an Algorithmic Artificial Chemistry based on Combinatory Logic (Schönfinkel, 1924; Curry et al., 1958) featuring a minimalistic design and three key properties. First, it is Turing-complete, enabling it to express an arbitrary degree of complexity. Second, it is strongly constructive, meaning that as the complex system evolves in time it can create new components that can in turn modify its global dynamics. Third, it features in-
Artificial Chemistries (AC) are models inspired in natural chemical systems that are usually defined by three different components: a set of possible molecules, a set of reactions, and a reactor algorithm describing the reaction vessel and how molecules interact through the available reactions to let the system evolve over time (Dittrich et al., 2001). In the following discussion we will focus on algorithmic chemistries that are the closest to the present work.

Artificial Chemistries

Artificial Chemistries (AC) are models inspired in natural chemical systems that are usually defined by three different components: a set of possible molecules, a set of reactions, and a reactor algorithm describing the reaction vessel and how molecules interact through the available reactions to let the system evolve over time (Dittrich et al., 2001). In the following discussion we will focus on algorithmic chemistries that are the closest to the present work.

In this work, we propose an AC based on Combinatory Logic. This formalism has been explored before in the context of AC by di Fenizio and Banzhaf (2000). While this work shares with us the enforcement of conservation laws, it relies for it on a normalisation process that introduces noise into the system dynamics. Furthermore, as AlChemy, it reduces expressions until they reach their normal forms, explicitly forbidding recursive and other type of expressions that do not converge.

Finally, Chemlambda (Buliga and Kauffman, 2014) is a Turing-complete graph rewriting AC that allows the encoding of $\lambda$-calculus and combinatory logic operators. As such, it is complementary in many ways with the system proposed here. Yet, while both Chemlambda and our system can express similar constructions, we are not aware of any reactor algorithm proposed for Chemlambda, nor about explorations of emerging phenomena with this formalism.
Combinatory Logic

Combinatory Logic (CL) is a minimalistic computational system that was independently invented by Moses Schönfinkel, John Von Neumann and Haskell Curry (Cardone and Hindley, 2006). Other than its relevance to computability theory, it has also been applied in Cognitive Science as a model for a Language of Thought (Piantadosi, 2016). One of the main advantages of CL is its formal simplicity while capturing Turing-complete expressiveness. In contrast to other mathematical formalisms, such as $\lambda$-calculus, it dispenses with the notion of variables and all the necessary bookkeeping that comes with it. For instance, a calculus, it dispenses with the notion of variables and all the necessary bookkeeping that comes with it. It.

In order to form a Turing-complete basis, we rely on a function $f$ and the following rewriting rules:

\[
\begin{align*}
If & \rightarrow f \\
Kfg & \rightarrow f \\
Sfgx & \rightarrow fx(gx)
\end{align*}
\]

An expression that contains a term of the form given in the left hand side of the rules above is called a “reducible expression” or redex. Otherwise, it is said to be in normal form. The application of these rules to any redex within an expression is called a (weak) reduction. For example, the expression $SII(SII)$ could be reduced as follows (underlining the corresponding redexes being rewritten):

\[
(SII(SII)) \rightarrow I(SII)(I(SII)) \rightarrow SII(I(SII)) \rightarrow SII(SII).
\]

Thus, this expression reduces to itself. We will later see that expressions such as this one will be important for the self-organizing behaviour of the system introduced here. Also note that $I(SII)(I(SII))$ has two redexes that can be rewritten, namely, the outermost and the innermost identity combinator $I$. Even though many different evaluation order strategies have been defined (Pierce, 2002), here we opt for picking a redex at random\(^1\), both because this is more natural for a chemical system and to avoid limitations that would come from following a fixed deterministic evaluation order.

\(^1\)As a matter of fact, $S$ and $K$ suffice because $I$ can be written as $SKK$. The inclusion of $I$ simply allows to express more complex programs with shorter expressions.

Combinatory Chemistry

One of our main contributions deals with reformulating these reduction rules as reactions in a chemical system. For this we postulate the existence of a multiset of CL expressions $P$. Note that if we were to apply plain CL rules to these expressions, the total number of combinators in the system would not be preserved: On one hand, the application of a reduction rule always removes the combinator from the resulting expression. On the other hand, while some a combinator like $K$ discards a part of the expression (the argument $g$), the $S$ combinator duplicates its third argument $x$. Thus, to make a chemical system with conservative laws, we define the following reduce reactions:

\[
\begin{align*}
If & \rightarrow f[+I] \\
Kfg & \rightarrow f[+g + K] \\
Sfgx & \rightarrow fx(gx)[+S]
\end{align*}
\]

The plus symbol denotes a separation between different expressions. An expression in Combinatory Chemistry is said to be reducible if it contains a Combinatory Chemistry redex (CC-redex). A CC-redex is a plain CL redex, except when it involves the reduction of an $S$ combinator, in which case a copy of its third argument $x$ must also be present in the multiset $P$ for it to be a redex in Combinatory Chemistry. For example, the expression $SII(SII)$ is reducible if and only if the third argument of the combinator $S$, namely $(SII)$, is also present in the set. When a reduction operation is applied, the redex is rewritten following the rules of combinatory logic, removing any substrate from $P$ and adding back to it all by-products, as specified in brackets on the right hand side of the reaction. For instance, reducing $SII(SII) + (SII)$ removes these two elements from $P$, adding back $I(SII)(I(SII))$ and $S$ to it. Notably, each of these reduction rules preserves the total number of combinators in the multiset, intrinsically enforcing conservation laws in this chemistry. It is also worth noticing that each of these combinators play different roles in the creation of novel compounds. While the $K$ combinator splits an expression, reducing its total size and complexity, the $S$ combinator is the only one that creates a novel, larger, and possibly more complex expression from smaller parts.

Completing the set of possible reactions in this chemistry, condensations and cleavages can generate novel expressions through random recombination:

\[
x + y \leftrightarrow xy
\]

While other chemistries start from a population of randomly constructed compounds, this system is initialised with elementary combinators only. In this way, diversity materializes only as emergent property rather than through the product of an external intervention. Then, at each step, an expression from $P$ is randomly sampled (in proportion to their corresponding concentrations). If the expression is reducible, then a redex is chosen at random, and the expression replaced with the result of applying the reduction oper-
At the same time, any required substrates are removed from the multiset, while any resulting by-products are added back into it. By applying one reduction at a time, we uniformly distribute the computational budget between all programs living in the system. Therefore, if complex structures emerge, more efficient ones will have a selective advantage. Furthermore, we do not need to take additional precautions to avoid infinitely reducing expressions that never reach a normal form, allowing more interesting functions to form part of our system’s dynamics. The complete algorithm describing the temporal evolution of our system is summarized on Algorithm 1.

Algorithm 1: Reactor Algorithm

Input: Total number of combinators $N_I, N_K, N_S$
Initialize multiset $P \leftarrow \{ I : N_I, K : N_K, S : N_S \}$

while True do
    Let $e \in P$
    if IsReducible($e$) then
        Let $(e \rightarrow \hat{e}) \in \text{Reductions}(e)$
        Remove one $e$ from $P$
        Remove one substrate $x$ from $P$ (if applies)
        Add one $\hat{e}$ and all by-products $y$ to $P$
    else
        Randomly pick cleave or condense
        if cleave then
            Remove one $e = xy$ from $P$
            Add one $x$ and one $y$ to $P$
        else if $e'$ is set then
            Remove one $e$ and one $e'$ from $P$
            Add $e'(e)$ to $P$
        else
            Set $e' \leftarrow e$;
    Function IsReducible($e$):
    if $e \cong 1f$ or $e \cong Kg$ or
    $(e \cong Sfgx$ and $x \in P)$ then
        return True
    else if $|e| = 1$ then
        return False
    else
        return any IsReducible($e'$) : $e' \in e$

Autocatalytic Sets

Emergent order by self-organization in complex systems is hypothesized to be driven by the existence of attracting states in the system’s dynamics (Walker and Ashby, 1966; Wuenische et al., 1992; Kauffman, 1993). Autocatalytic Sets (Kauffman, 1993) were first introduced by Stuart Kauffman in 1971 as one type of such attractors that could help explaining the emergence of life in chemical networks. Similar ideas were introduced before with the concepts of autopoiesis (Varela and Maturana, 1973), and the hypercycle model (Eigen and Schuster, 1978). Autocatalytic Sets (AS) are reaction networks that self-perpetuate in time by relying on a network of catalysed reactions, where every substrate and catalyser of a reaction is produced by at least some reaction in the network, or they are freely available components in the environment. This notion was later formalized in a mathematical form (Hordijk and Steel, 2004; Hordijk et al., 2015) into the concept of Reflexively Autocatalytic Food-generated sets (RAFs). A Chemical Reaction System (CRS) is a mathematical construct defining the set of possible molecules, the set of possible reactions and a catalysis set indicating which reactions are catalysed by which molecules. Furthermore, it assumed to exist a set of molecules freely available in the environment called the “food set”. An autocatalytic set (or RAF set) $S$ of a CRS with associated food set $F$ is a subset of reactions, which is:

1. reflexively autocatalytic (RA): each reaction $r \in S$ is catalysed by at least one molecule that is either present in $F$ or can be formed from $F$ by using a series of reactions in $S$ itself.

2. food-generated (F): each reactant of each reaction in $S$ is either present in $F$ or can be formed by using a series of reactions from $S$ itself.

In our system, all reducing reactions take precedence over random condensations and cleavages without the need of any catalyser. Thus, they are all reflexively autocatalytic (automatically satisfying condition 1), and autocatalytic sets are defined only in terms of reaction subsets that satisfy condition 2: That is, those reaction subsets in which every reactant is formed by a reaction in the set or is freely available in the environment. Because of the dynamics of Combinatory Chemistry, the most common expressions are elementary combinators, which can be randomly combined through random condensations to form longer expressions. Yet, the longer the expression, the exponentially larger systems are required for them to be just as common. To by-pass this latter obstacle, we propose the substrate assemblage mechanism, introduced in the following section.

For example, Figure 2 shows a simple emergent autocatalytic set associated with the expression $(AA) = (SII(SII))$, if $A = (SII)$ belongs to the food set. As shown, when the formula is first reduced on reaction $r_1$, a substrate $A$ is absorbed from the environment. Next, the combinators in this substrate are applied and realised back into the multiset $P$, returning back to the same original expression. We refer to this process as a metabolic cycle because of its strong resemblance to its natural counter-

3We make available our implementation at https://github.com/facebookresearch/CommAI-env/tree/master/projects/combinatory-chemistry

4See Hordijk (2019) for a comprehensive historical review on the topic.
Algorithm 1 is modified at the point of sampling a reduction by the steps in Algorithm 2. By the steps in Algorithm 2, emergent complexity by applying this technique. Therefore, can be observed if the number of freely available atoms start. The number of combinators in the system is limited, ceiling effects ining the required substrates. Furthermore, as the total number of substrates. Here, we introduce a technique that we call substrate assemblage to facilitate the exploration of larger systems without needing to simulate them in full. The central idea is to arbitrarily define a food set containing the expressions that would be freely available had the system been sufficiently large and evolved for long enough. Then, whenever the system needs to reduce an S combinator involving a substrate that is not available in the multiset, the substrate would be constructed on the spot from freely available atomic combinators. In this way, we can can simulate the productivity of sufficiently large environments, without explicitly needing to compute them. On the other hand, this technique does not bypass the need of discovering the main reagent, namely, the expression e being reduced. Instead, it just focuses on creating the required substrates. Furthermore, as the total number of combinators in the system is limited, ceiling effects can be observed if the number of freely available atoms start to dwindle. Even with these concerns in mind, we experimentally show that there are considerable gains in terms of emergent complexity by applying this technique. Therefore, Algorithm 1 is modified at the point of sampling a reduction.

**Algorithm 2: Substrate assemblage**

**Input:** Maximum substrate size F

Let \((e^1[x] \rightarrow e^2[y]) \in \text{Reductions}(e)\)

if \(x \notin P\) and \(|x| \leq F\) then

Let \(n_I, n_K, n_S = \text{Combinators}(x)\)

if \(P[I] \geq n_I\) and \(P[K] \geq n_K\) and \(P[S] \geq n_S\) then

Remove \(n_K\) from \(P\)

Remove \(n_I\) from \(P\)

Remove \(n_S\) from \(P\)

Add one \(x\) to \(P\)

---

**Autopoiesis, recursion and self-reproduction**

While autocatalytic sets provide a compelling formalism to study emergent organization in Artificial Chemistries, it leaves some blind spots for detecting emergent structures of interest. Such is the case for recursive expressions. Consider, for instance, \(e = (S(SI)I(S(SI)I))\). This expression is composed of two copies of \(A = (S(SI)I)\) applied to itself \((AA)\). As shown in Figure 3, its metabolic cycle will use two copies of the element \(A\), metabolising one to perform its computation, and appending the other one to itself, thus \((AA) + 2A \rightarrow (A(AA)) + c(A)\). As time proceeds, the same computation will take place recursively, thus \((A(AA)) + 2A \rightarrow (A(A(AA))) + c(A)\), and so on. While this particular behaviour cannot be detected through autocalytic set, because the resulting expression is not exactly equal to the original one, it still involves a structure that preserves in time its functionality.

![Figure 3: One of the possible pathways in the reduction of the tail-recursive structure \((AA)\) with \(A = (S(SI)I)\). It appends one \(A\) to itself by metabolising another copy absorbed from the environment.](image)

Moreover, while the concept of autocatalytic set captures both patterns that perpetuate themselves in time and patterns that in addition, they also multiply their numbers, it does not explicitly differentiate between them. A pattern with a metabolic cycle of the form \(AA + A \rightarrow AA + c(A)\) (as in Figure 2) keeps its own structure in time by metabolising one \(A\) in the food set, but it does not self-reproduce. We call such patterns simple autopoietic (Varela and Maturana, 1973). In contrast, for a pattern to be self-reproducing it must create...
copies of itself that are later released as new expressions in the environment. For instance, consider a metabolic cycle in Figure 1 with the form \((AA) + 3A \rightarrow 2(AA) + c(A)\). This structure creates a copy of itself from 2 freely available units of \(A\) and metabolises a third one to carry out the process.

All these structures have in common the need to absorb food expressions from the environment to preserve themselves in homoeostasis. Furthermore, because they follow a cyclical process, the types of food expressions upon which they rely will always be the same. Thus, we propose substrate counting as a metric that can capture all these different types of structures. For this, we note that the only operation that allows an expression to incorporate some other expression into its own body is the reduction of the \(S\) combinator. Therefore, counting the number of times each substrate \(A\) has been used in a reaction can serve as a proxy for detecting the existence of a structure relying on this element for food.

**Experiments and Discussion**

We simulated a CRS based on Combinatory Logic for 10M iterations, starting from just 10k evenly distributed \(S\), \(K\), and \(I\) combinators. We applied substrate assemblage with substrate size parameter \(F\) on a range between 1 (corresponding to no substrate assemblage) and 20, repeating the process 10 times with different random seeds for each configuration.

We began by analysing general metrics of the system. Figure 4a shows the expression diversity as a function of the number of performed reactions. As it can be seen, diversity explodes in the first few 200k reactions, before reaching a peak of about 300 expressions. Then, it starts to decline at different speeds, depending on the value of the substrate assemblage parameter \(F\). When this mechanism is disabled \((F = 1)\), the decline occurs at a slow and steady rate. Yet, when this parameter reaches the value \(F = 3\), the decline of diversity becomes much faster, only accelerating after that. This difference could be explained by the fact that reduction expressions involving \(S\) combinators, the only ones that compute increasingly longer expressions, are more likely to be successful thanks to the substrate assemblage mechanism getting into action. Therefore, the limited available combinators tend to be clustered in fewer and longer expressions, as confirmed by Figure 4b. On the other hand, as the number of freely available combinators needed to assemble the substrates becomes scarce, the corresponding reduction operations cannot be executed, and more random operations start to take place instead (Figure 4c). Thus, the system self-regulates the ratio of deterministic operations –as given by reductions– to stochastic ones –as given by random condensations or elevations– occurring in it.

Yet, it is unclear from these results whether the reduction in diversity is driven by emergent complex structures that act as attractors, or some other different reason. To answer this question, we used substrate counting (see above) to detect whether specific substrates where more prominently used, possibly hinting at the existence of expressions that were metabolising them to preserve themselves in time. In particular, we looked at the 10 most frequently used substrates, from which we are selecting a few to simplify the presentation. Results are shown in Figure 5 for five different runs. In each of these, we can see the emergence of different types of structures, including simple autopoietic patterns, recursive structures, and self-reproducing ones. Interestingly, they can emerge at different points in time, co-exist, and sometimes some of them can drive others to extinction.

Notably, we observed that expressions that consume any given substrate \(A\) are typically composed of multiple juxtaposed copies of this substrate, confirming the old adage: “Tell me what you eat and I will tell you what you are”. For instance, in Figure 5a we can appreciate the emergence of the autopoietic pattern \((SI)(SI)\), composed of two copies of the substrate \(A = (SI)\), and a metabolic cycle of the form \((AA) + A \rightarrow (AA) + c(A)\), as shown on Figure 2. Binary substrates such as \((KK)\) and unitary ones such as \(I\) do not form part of any self-preserving structure. Instead, they are only used in the reduction of randomly or semi-randomly produced expressions. Yet, they are used with considerable frequency as any randomly-produced redexes featuring an \(S\) combinator will likely take shorter arguments because of them being more frequent. As unitary substrates are more frequent than binary ones, their consumption levels are also considerably higher. Yet, even though by the same argument the consumption rate of \(A = (SI)\) should be below binary substrates, self-organization into autopoietic patterns drives the usage of this substrate above what would be expected if chance would be the only force at play. At around 2M-3M reactions, the system reaches a point in which the consumption levels of this substrate stabilizes, constrained by free the availability of the substrate: For the consumption levels to increase here, \((SI)(SI)\) structures need to be formed by chance by the collision of two substrate copies, and also kept alive by metabolising freely available substrates. When we start assembling substrates of size at most \(F = 3\) (Figure 5b), we facilitate this second restriction to the extent that \(S\) and \(I\) combinators are freely available in the environment, thus allowing the formation of an even larger number of \((SI)(SI)\) structures. At the same time, rarer autopoietic structures can emerge in this conditions, such as one based on three juxtaposed copies \((AAA)\) of \(A = (SSS)\). This expression has a metabolic cycle of the form \((AAA) + 2A \rightarrow (AAA) + A + c(A)\) (details in Appendix), meaning that it acquires two copies of the substrate from the environment, metabolises one, and releases the other one back intact. We note that this last copy of \(A\) could be construed as an emergent catalyser for the reaction: Even though we can interpret each reduce reaction to be auto-catalysed, multiple reactions taken together can
have emergent properties, such as in this case, where a substrate is just used to complete the metabolic cycle, and then released.

From $F = 4$ we start to see growing structures. In particular, recursive ones. In Figure 5c ($F = 6$) we can observe two such structures. The first one uses the substrate $A = (S(SI)I)$, and follows a tail-recursive cycle that linearly increases the size of the structure: $(AA) + 2A \rightarrow A(AA) + c(A)$ (as shown on Figure 3). The second one is a more complex binary-branching recursive structure, with substrate $A = (S(SSI)K)$. In this case, $(AA)$ follows a somewhat larger metabolic cycle that can end up in each copy of $A$ duplicating so that $(AA)$ becomes $(AA(AA))$ (details in Appendix). When recursive structures come into play, we can see that simple autopoietic patterns are driven into extinction. These extinction events are related to the assemblage mechanism, as it puts recursive and autopoietic structures in direct competition for combinators. Figure 5f displays the amount of freely available combinators in this simulation. As shown, $S$ combinators are exhausted at around $3M$ reactions. At around this point the simple autopoietic structure around the $(SII)$ substrate goes into a slow decline. Yet, when all freely available $I$ combinators are depleted, this structure is driven into a quick extinction: When resources start to dwindle, reductions that rely on a given substrate can fail, and thus the system falls back to either breaking up the expression or combining it with another one. When $(SII(SII))$ is broken into two independent $(SII)$ elements it loses its ability to compute itself. In contrast, recursive structures can cope with conditions of low resources quite effectively, as demonstrated by the fact that they still continue to consume at stable rate their corresponding substrates after $S$ and $I$ combinators are not freely available anymore. A possible reason why this does not bring them into catastrophic failure is their fractal structure: A recursive structure broken up will still have the same function, but it will be smaller. For instance, $A(AA) \rightarrow A + (AA)$ still leaves a functioning $(AA)$ structure. When new resources become available through the continuous influx of combinators released by every computed reduction, it can consume them and grow back again. In the future, to avoid such direct competition for basic resources between all emergent structures, the substrate assemblage could be limited, for instance, to be applied only when there is a minimum buffer of freely available combinators.

Finally, in Figures 5d and 5e we can observe the emergence of a full-fledged self-reproducing structure with substrate $A = (SI(S(SK)I))$. It follows a cycle of the form $(AA) + 3A \rightarrow 2(AA) + c(A)$, thus duplicating itself, and metabolising one substrate in the process. As it replicates exponentially, this structure quickly grows into one of the most active ones. Yet, when resources run out it enters in direct competition with the recursive structure based on the $(S(SI)I)$ substrate. In 5d the substrate consumption rate for this last structure is considerably lower than in 5e, probably due to the fact that the recursive structure $(A(AA))$ can either reduce the internal part, thus consuming one copy of $A$, or at the most external level, consuming $(AA)$, which in this case it is facilitated by substrate assemblage when $F = 8$. On the other hand, the self-reproducing pattern suffers from the same problem of simple autopoietic structures: When it fails to acquire its substrate from the environment it decomposes into an expression that looses its functionality. However, in contrast with simple autopoietic patterns that rely on being produced by chance, self-reproducing ones can recover their population through reproduction. Nevertheless, the recursive structure still keeps an advantage over the self-reproducing one, especially when $F = 8$, where it quickly drives the self-reproducing pattern into extinction.

**Conclusions**

We have introduced Combinatory Chemistry, an Algorithmic Artificial Chemistry based on Combinatory Logic. Even though it has simple dynamics, it gives rise to a wide range of complex structures, including recursive and self-reproducing ones. Thanks to Combinatory Logic being Turing-complete, our system can theoretically represent patterns of arbitrary complexity. Furthermore, the computation
Figure 5: (a-e) Substrate consumption computed over a window of 500k reactions on different runs with different substrate assemblage sizes $F$. Different line styles distinguish substrates used by different types of expressions: Dotted lines represent substrates used by simple non-attracting expressions; Dash-dotted lines are substrates used by simple autopoietic patterns; Dashed lines are substrates used by recursive patterns; Solid lines are substrates used by self-reproducing patterns.

is distributed uniformly across the system thanks to single-step reactions applied at each iteration. As a consequence, emergent structures feature reaction cycles that bear a striking resemblance to natural metabolisms. Moreover, conservation laws keep the system bounded while not introducing any extrinsic source of noise. Finally, our system does not need to start from a random set of initial expressions to kickstart diversity. Instead, this initial diversity is the product of the system’s own dynamics, as it is only initialized with elementary combinators. In this way, we can expect that this first burst of diversity is not just a one-off event, but it is deeply embedded into the mechanics of the system, possibly allowing it to keep on developing novel structures continually. On the other hand, we observed that to keep complex structures functioning, they require a constant influx of specific types of substrates. While only much larger systems would allow for such continual production of these food elements, we bypassed the problem of needing simulate such larger systems by constructing the required substrates on the spot when they were needed. In these way, we have successfully simulated systems where we could observe a large variety of emerging structures, including structures that would self-sustain, but without changing their number (simple autopoietic); recursive expressions that would keep growing until reaching the system’s limit; and self-reproducing patterns that increase their number exponentially. To conclude, we have introduced a simple model of emergent complexity in which self-reproduction emerges autonomously from the system dynamics. It is still to be seen whether this can be used to explain the emergence of evolvability, one of the central questions in Artificial Life. Yet, we believe that the simplicity of our model, the encouraging results, and its dynamics that balance computation with random recombination to creatively search for new forms, leaves it in good standing to tackle this challenge.
Acknowledgements
We would like to especially thank Alessandra Macillo for the idea behind substrate assemblage and feedback, Sebastian Riedel for his invaluable support and feedback, and the rest of FAIR London team and the Complexity Interest Group for all the feedback and interesting discussions.

References
Buliga, M. and Kauffman, L. (2014). Chemlambda, universality and self-multiplication. In Artificial Life Conference Proceedings 14, pages 490–497. MIT Press.

Cardone, F. and Hindley, J. R. (2006). History of lambda-calculus and combinatory logic. Handbook of the History of Logic, 5:723–817.

Curry, H. B., Feys, R., Craig, W., Hindley, J. R., and Seldin, J. P. (1958). Combinatory logic, volume 1. North-Holland Amsterdam.

di Fenizio, P. S. and Banzhaf, W. (2000). A less abstract artificial chemistry. Artificial Life, 7:49–53.

Dittrich, P., Ziegler, J., and Banzhaf, W. (2001). Artificial Chemistries-A Review. Artificial Life, 7:225–275.

Eigen, M. and Schuster, P. (1978). The hypercycle. Naturwissenschaften, 65(1):7–41.

Flamm, C., Ullrich, A., Ekker, H., Mann, M., Högerl, D., Rohrschneider, M., Sauer, S., Scheuermann, G., Klemm, K., Hofacker, I. L., et al. (2010). Evolution of metabolic networks: a computational frame-work. Journal of Systems Chemistry, 1(1):4.

Fontana, W. and Buss, L. W. (1994). What would be conserved if 'the tape were played twice'? Proceedings of the National Academy of Sciences of the United States of America, 91(2):757–761.

Högerl, D. (2010). Simulation of prebiotic chemistries. Master’s thesis, Institute for Theoretical Chemistry, University of Vienna.

Hordijk, W. (2019). A history of autocatalytic sets. Biological Theory, 14(4):224–246.

Hordijk, W., Smith, J. L., and Steel, M. (2015). Algorithms for detecting and analysing autocatalytic sets. Algorithms for Molecular Biology, 10(1):15.

Hordijk, W. and Steel, M. (2004). Detecting autocatalytic, self-sustaining sets in chemical reaction systems. Journal of theoretical biology, 227(4):451–461.

Kauffman, S. A. (1993). The origins of order: Self-organization and selection in evolution. Oxford University Press, USA.

Ofria, C. and Wilke, C. O. (2004). Avida: A software platform for research in computational evolutionary biology. Artificial life, 10(2):191–229.

Piantadosi, S. T. (2016). The computational origin of representation and conceptual change. (under review).

Pierce, B. C. (2002). Types and programming languages. MIT press.

Ray, T. S. (1991). An approach to the synthesis of life. Artificial life II, pages 371–408.

Schönfinkel, M. (1924). Über die bausteine der mathematischen logik. Mathematische annalen, 92(3):305–316.

Tominaga, K., Watanabe, T., Kobayashi, K., Nakamura, M., Kishi, K., and Kazuno, M. (2007). Modeling molecular computing systems by an artificial chemistry its expressive power and application. Artificial Life, 13(3):223–247.

Varela, F. J. and Maturana, H. R. (1973). De máquinas y seres vivos: Una teoría sobre la organización biológica. Santiago de Chile: Editorial Universitaria.

Walker, C. and Ashby, W. R. (1966). On temporal characteristics of behavior in certain complex systems. Kybernetik, 3(2):100–108.

Wuensche, A., Lesser, M., and Lesser, M. J. (1992). Global Dynamics of Cellular Automata: An Atlas of Basin of Attraction Fields of One-Dimensional Cellular Automata, volume 1. Andrew Wuensche.

Young, T. J. and Neshatian, K. (2013). A constructive artificial chemistry to explore open-ended evolution. In Australasian Joint Conference on Artificial Intelligence, pages 228–233. Springer.
Appendix
The following derivations show one of the possible pathways that each of the described structures can undertake as they develop. They demonstrate how these structures preserve their function in time. Note that every expression written as \((fX)Y\) can also be written simply as \(fXY\). This "trick" is known as Uncurrying.

**Metabolic cycle of a simple autopoietic pattern**
Let \(A = (SII)\). Then,
\[
\begin{align*}
(AA) + A & \rightarrow (IA)(IA) + S \\
(IA)(IA) & \rightarrow (AIA) + I \\
(A(IA)) & \rightarrow (AA) + I
\end{align*}
\]

**Metabolic cycle of a ternary autopoietic pattern**
Let \(A = (SSK)\). Then,
\[
\begin{align*}
(AAA) + A & \rightarrow (SADK)} + S \\
(SA(KA)A) + A & \rightarrow (AA(KA)) + S \\
(AA(KA)) & \rightarrow (AAA) + A + K
\end{align*}
\]

**Metabolic cycle of a tail recursive structure**
Let \(A = (S(SI)I)\). Then,
\[
\begin{align*}
(AA) + A & \rightarrow (SIAA) + I \\
(SIAA) & \rightarrow (SIAA) + I \\
(SIAA) + A & \rightarrow (IAAA) + S \\
(AA(AA)) & \rightarrow (AIAA) + I
\end{align*}
\]

**Metabolic cycle of a binary-branching structure**
Let \(A = (S(SSI)K)\). Then \((AA)\) can follow the metabolic pathway:
\[
\begin{align*}
(AA) + A & \rightarrow (SSIA(KA)) + S \\
(SSIA(KA)) + A & \rightarrow (SIAA(KA)) + S \\
(SIAA(KA)) & \rightarrow (SAA(KA)) + I \\
(SAA(KA)) + (KA) & \rightarrow (A(KA)(AA)) + S
\end{align*}
\]
Then each copy of \((A(KA))\) can be reduced as follows
\[
\begin{align*}
(A(KA)) + (KA) & \rightarrow SSIA(KA)(K(KA)) + S \\
(SSIA(KA)(K(KA)) + (KA) & \rightarrow (S(KA)(IA)(K(KA))) + S \\
(S(KA)(IA)(K(KA))) & \rightarrow (S(KA)(KA)(K(KA))) + I \\
(S(KA)(KA)(K(KA))) & \rightarrow (KA(K(KA))(KA(K(KA)))) + S \\
(KA(K(KA))(KA(K(KA)))) & \rightarrow (A(A(K(K(KA)))) + (K(KA)) + K \\
(A(K(K(KA)))) & \rightarrow (AA) + (K(KA)) + K
\end{align*}
\]
Thus, the complete pathway can be summarized as \((AA) + 2A + 5(KA) + (K(KA)) \rightarrow AA(AA) + 4(K(KA)) + 2c(A)\).