Combinatory Chemistry: Towards a Simple Model of Emergent Evolution

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Abstract

An explanatory model for the emergence of evolvable units must display emerging structures that (1) preserve themselves in time (2) self-reproduce and (3) tolerate a certain amount of variation when reproducing. To tackle this challenge, here we introduce Combinatory Chemistry, an Algorithmic Artificial Chemistry based on a minimalistic 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 with no external intervention discovers a wide range of emergent patterns. 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 include 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. One prominent 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 were fixed by design. 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). The driving hypothesis is that complex organizations emerge thanks to self-organising attractors in chemical networks, which preserve their structure in time (Walker and Ashby, 1966; Wueneschte et al., 1992; Kauffman, 1993). While some

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Artificial Chemistries seek to mimic as closely as possible the properties of the chemistry that gave rise to life on Earth (Flamm et al., 2010; Högerl, 2010; Young and Nes- shitian, 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 (Fontana et al., 1993), meaning that as the system evolves in time it can create new components that can in turn modify its global dynamics. Third, it features intrinsic conservation laws so that the number of atomic elements remains always constant.

Figure 1: Metabolic cycle (showing one of the possible pathways) of a self-reproducing structure that emerges from the dynamics of Combinatory Chemistry. Starting from \((AA)\), where \(A = (ST(S(SK))I)\), it acquires three copies of \(A\) from its environment and uses two to create a copy of itself, metabolising the third one to carry out the process.
Previous work has relied on applying extrinsic conservation laws, such as for instance keeping a maximum number of total elements in the system by randomly removing exceeding ones (Fontana and Buss, 1994; di Fenizio and Banzhaf, 2000). Instead, intrinsic conservation laws allow us to bound the total number of elements without introducing extraneous perturbations. Furthermore, limiting the total amount of basic elements can create selective pressures between emergent structures.

We simulate a Chemical Reaction System (Hordijk et al., 2015; Dittrich et al., 2001) based on Combinatory Logic, which starting from a tabula rasa state consisting of only elementary components, it produces a diversity explosion that develops into a state dominated by self-organized emergent structures, including autopoietic (Varela and Maturana, 1973), recursive and self-replicating ones. Notably, all these types of structures emerge at different points in time during a single run of the system without requiring any external interventions. Furthermore, these structures preserve themselves by absorbing compounds from their environment and decomposing them step-by-step, in a process that has a striking resemblance with the metabolism of biological organisms. Finally, we introduce a heuristic to emulate the effects of having larger systems without having to compute them explicitly. This makes considerably more efficient the search for these complex structures.

The paper is organized as follows. First, we describe earlier work in Artificial Chemistry that is most related to our approach. Then, we explain the basic workings of Combinatory Logic and how we adapted it into an Artificial Chemistry. Third, following earlier work, we discuss how autocatalytic sets can be used to detect emerging phenomena in this system, and propose a novel measure of emergent complexity, which is well-adapted to the introduced system. Finally, we describe our experiments that showcase the emergence of complex structures in Combinatory Chemistry.

**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 with each other (Dittrich et al., 2001). In the following discussion we will focus on algorithmic chemistries that are the closest to the present work.

AlChemy (Fontana and Buss, 1994) is an AC where molecules are given by $\lambda$-calculus expressions. $\lambda$-calculus is a mathematical formalism that, like Turing machines, can describe any computable function. In AlChemy, pairs of randomly sampled expressions are joined through function application, and the corresponding result is added back to the population. To keep the population size bounded, expressions are randomly discarded. Fontana and Buss showed that expressions that computed themselves quickly emerged in this system, which they called level 0 organisations. Furthermore, when these expressions were explicitly prohibited, a more complex organization emerged where every expression in a set was computed by other expressions within the same set (level 1 organisations). Finally, mixing level 1 organisations could lead to higher order interactions between them (level 2 organisations). Yet, this system had some limitations. First, each level of organisation was only reached after external interventions. Also, programs must necessarily reach a normal form, which happens when there are no more $\lambda$-calculus rules than can be applied. Thus, recursive programs, which never reach a normal form, are banned from the system. Furthermore, two processes where introduced as analogues of food and waste, respectively. First, when expressions are combined, they are not removed from the system, allowing the system to temporarily grow in size. Second, expressions which after being combined with existing expressions do not match any $\lambda$-calculus reduction rules are removed. Without these processes, complex organisations fail to emerge. Yet, it is not clear under which circumstances these external interventions would not be needed anymore in order for the system to evolve autonomously. Finally, bounding the total number of expressions by randomly removing excess ones creates perturbations to the system that can arbitrarily affect the dynamics. Fontana and Buss (1996) later proposed MC2, a chemistry based on Linear Logic that addressed some of these limitations (notably, conservation of mass), but we are not aware of empirical work on it.

Here, 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, we are not aware of conservation laws defined within this formalism, nor of any reactor algorithm allowing explorations of emerging phenomena.

**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 function \( f(x) = 1 + x + y \) would be nonsensical, and a function-generating system based on \( \lambda \)-calculus would need to have explicit rules to avoid the formation of such expressions. Instead, CL expressions are built by composing elementary operators called combinators. Here, we restrict to the \( S, K \) and \( I \) combinators, which form a Turing-complete basis\(^1\). Given an expression \( e \) of the form \( e = \alpha X \beta \), it can be rewritten in CL, as follows:

\[
\begin{align*}
\alpha(I\beta) & \rightarrow \alpha f\beta \\
\alpha(K\beta) & \rightarrow \alpha f\beta \\
\alpha(S\beta) & \rightarrow \alpha(fgx)\beta
\end{align*}
\]

When \( \alpha X \beta \) matches the left hand side of any of the rules above, the term \( X \) is called a “reducible expression” or redex. A single expression can contain multiple redexes. If no rule is matched, the expression is said to be in normal form. The application of these rules to rewrite any redex 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. In contrast, \( SII \) is not reducible because it requires three arguments and \( I \) at least one.\(^2\) Also note that \( I(SII)(I(SII)) \) has two redexes that can be rewritten, namely, the outermost or the innermost \( I \) combinators. Even though many different evaluation order strategies have been defined (Pierce, 2002), here we opt for picking a redex at random\(^3\), both because this is more natural for a chemical system and to avoid limitations that would come from following a fixed deterministic evaluation order.

### 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 \( \mathcal{P} \) that react following reduction rules, plus random condensation and cleavages. Note that if we were to apply plain CL rules to reduce these expressions, the total number of combinators in the system would not be preserved. First, because the application of a reduction rule always removes the combinator from the resulting expression. Second, while the \( K \) combinator discards a part of the expression (the argument \( g \)), \( S \) duplicates its third argument \( x \). Thus, to make a chemical system with conservation laws, we define reduce reactions for an expression \( \alpha X \beta \), as follows:

\[
\begin{align*}
\alpha(I\beta) & \rightarrow \alpha f[+I] \\
\alpha(K\beta) & \rightarrow \alpha f[+g + K] \\
\alpha(S\beta) & \rightarrow \alpha(fgx)\beta[+S]
\end{align*}
\]

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 \( x \) (the reactant) must also be present in the multiset \( \mathcal{P} \) 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 reactant from \( \mathcal{P} \) and adding back to it all by-products, as specified in brackets on the right hand size of the reaction. The type of combinator being reduced gives name to the reaction. For instance, the \( S \)-reaction operating on \( SII(SII) + (SII) \) removes these two elements from \( \mathcal{P} \), adding back \( I(SII)(I(SII)) \) and \( SII \) 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 plays different roles in the creation of novel compounds. While \( K \)-reactions split the expression, decreasing its total size and complexity, \( S \)-reactions create larger and possibly more complex expressions from smaller parts.

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

\[
x + y \longleftrightarrow xy
\]

In Combinatory Chemistry, computation takes precedence. This means that whenever an expression admits at least one reduce reaction, this reaction (or one at random, if there are multiple) is immediately applied. Otherwise, if an expression cannot be reduced, it is either cleaved at a random point, or condensed together with another irreducible expression. As reducing reactions take priority over random recombination ones, we construe them as auto-catalysed.

In line with the Gillespie algorithm (Gillespie, 1977), the system is simulated by sampling expressions from \( \mathcal{P} \) with probability proportional to their concentration and applying one reaction at a time. In this way, we uniformly distribute the computational budget between all programs in the system. Moreover, we do not need to take additional precau-

\(^1\)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.

\(^2\)Precedence rules are left-branching, thus \( (SII) = ((SI)I) \) and thus, the second \( I \) is not an argument for the first \( I \) but to \( SI \).

\(^3\)For practical efficiency reasons, we restrict to sampling from the first 100 possible reductions in an outer-to-inner order.
tions to avoid recursive expressions that never reach a normal form, allowing these interesting functions to form part of our system’s dynamics.

Finally, we note that while other chemistries start from a population of randomly constructed compounds, this system can be initialised with elementary combinatorial elements only. In this way, diversity materializes only as emergent property rather than through the product of an external intervention.

The complete algorithm describing the temporal evolution of our system is summarized on Algorithm 1\textsuperscript{4}.

**Algorithm 1: Reactor Algorithm**

**Input:** Total number of combinatorics \(N_I, N_K, N_S\)

Initialize multiset \(\mathcal{P} \leftarrow \{I : N_I, K : N_K, S : N_S\}\)

while \(\text{True}\) do

Sample \(e \in \mathcal{P}\) with \(P(e) = \frac{P(e)}{|\mathcal{P}|}\)

if \(\text{Reducible?}(e)\) then

Let \((e+[x] \rightarrow \tilde{e}+[y]) \in \text{Reductions}(e)\)

Remove one \(e\) from \(\mathcal{P}\)

Remove one reactant \(x\) from \(\mathcal{P}\) (if applicable)

Add one \(\tilde{e}\) and all by-products \(y\) to \(\mathcal{P}\)

else

Randomly pick cleave or condense

if cleave then

Let \(x, y\) such that \(e = (xy)\)

Remove one \(e\) from \(\mathcal{P}\)

Add one \(x\) and one \(y\) to \(\mathcal{P}\)

else if \(e_{\text{LEFT}}\) is defined then

Remove one \(e\) and one \(e_{\text{LEFT}}\) from \(\mathcal{P}\)

Add \((e_{\text{LEFT}} e)\) to \(\mathcal{P}\)

Undefine \(e_{\text{LEFT}}\)

else

Define \(e_{\text{LEFT}} \leftarrow e\)

**Function** \(\text{Reducible?}(e)\):

if \(e = (I f)\) or \(e = (K f g)\) or

\((e = (S f g x)\) and \(x \in \mathcal{P}\) then

return True

else if \(e \in \{S, K, I\}\) then

return False

else return \(\exists e' : e = (ae' \beta)\) and \(\text{Reducible?}(e')\)

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**Emergent Structures**

Having described the dynamics of Combinatory Chemistry, we now turn to discuss how can we characterise emergent structures in this system. For this, we first discuss how can autocatalytic sets be applied for this purpose. Second, we observe that this formalism may not completely account for some emergent structures of interest and thus, we propose to instead track reactant consumption rates as a proxy metric to uncover the presence of these structures. Finally, inspired by the concept of food sets in autocatalytic sets, we propose a heuristic to accelerate their emergence.

**Autocatalytic sets**

Self-organized order in complex systems is hypothesized to be driven by the existence of attracting states in the system’s dynamics (Walker and Ashby, 1966; Wuesche 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. (See Hordijk (2019) for a comprehensive historical review on the topic.) Related notions are the concept of autopoiesis (Varela and Maturana, 1973), and the hypercycle model (Eigen and Schuster, 1978).

Autocatalytic sets (AS) are reaction networks that perpetuate in time by relying on a network of catalysed reactions, where each reactant and catalyst of a reaction is either produced by at least some reaction in the network, or it is freely available in the environment. This notion was later formalized in mathematical form (Hordijk and Steel, 2004; Hordijk et al., 2015) with the name of Reflexively Autocatalytic Food-generated sets (RAFs). Specifically, they define a Chemical Reaction System (CRS) as 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, a set of freely available molecules in the environment, called the “food set”, is assumed to exist. 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.

**Autocatalytic sets in Combinatory Chemistry**

In Combinatory Chemistry, all reducing reactions take precedence over random condensations and cleavages, and thus, they proceed at a higher rate than random reactions without the need of any catalyst (i.e. they are autocatalysed). Therefore, they trivially satisfy condition 1. Thus, autocatalytic sets in this system are defined in terms of subsets of reduce reactions in which every reactant is produced by a reduce reaction in the set or is freely available in the environment (condition 2). For example, if we assume that \(A = (S II)\) is in the food set, Figure 2 shows a simple emergent autocatalytic set associated with the expression

\[\text{some emergent structures of interest and thus, we propose to instead track reactant consumption rates as a proxy metric to uncover the presence of these structures. Finally, inspired by the concept of food sets in autocatalytic sets, we propose a heuristic to accelerate their emergence.} \]

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\(\text{Implementation and supplementary materials at https://germank.github.io/combinatory-chemistry} \)
Figure 2: \( r_1 \)–\( r_5 \) form an autocatalytic set, granted that \((SII)\) belongs to the food set. \((SII(SII))\)’s metabolic cycle starts with \( r_1 \) reducing the \( S \) combinator, while taking \((SII)\) as reactant. Then, the cycle is completed by the reduction of the two identity combinators, in any of the possible orders.

\((AA) = (SII(SII))\). As shown, a chain of reduce reactions keep the expression in a self-sustaining equilibrium: When the formula is first reduced by reaction \( r_1 \), a reactant \( A \) is absorbed from the environment and one \( S \) combinator is released. Over the following steps, two \( I \) combinators are sequentially applied and released back into the multiset \( \mathcal{P} \), with the expression returning back to its original form. We refer to this process as a metabolic cycle because of its strong resemblance to its natural counterpart. For convenience, we write this cycle as \((AA) + A \rightarrow (AA) + \phi(A)\), where \( \phi \) is a function that returns the atomic combinators in \( A \) and the double head arrow means that there exists a pathway of reduction reactions from the reactives in the left hand side to the products in the right hand side.

While autocatalytic sets provide a compelling formalism to study emergent organization in Artificial Chemistries, it also leaves some blind spots for detecting emergent structures of interest. Such is the case for recursively growing 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, during its metabolic cycle it will consume two copies of the element \( A \), metabolising one to perform its computation, and appending the other one to itself, thus \((AA) + 2A \rightarrow (A(AA)) + \phi(A)\). As time proceeds, the same computation will take place recursively, thus \((A(AA)) + 2A \rightarrow (A(A(A(A))))) + \phi(A)\), and so on. While this particular behaviour cannot be detected through autocatalytic sets, because the resulting expression is not exactly equal to the original one, it still involves a structure that preserves in time its functionality.

Moreover, while the concept of autocatalytic set captures both patterns that perpetuate themselves in time and patterns that also multiply their numbers, it does not explicitly differentiate between them. A pattern with a metabolic cycle of the form \( AA + A \rightarrow AA + \phi(A) \) (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 \((AA) + 3A \rightarrow 2(AA) + \phi(A)\). 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 reactants from the environment to preserve themselves in homoeostasis. Furthermore, because they follow a cyclical process, they will continually consume the same types of reactants. Thus, we propose tracking reactants consumption 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 a reactant into its own body is the reduction of the \( S \) combinator, and thus focus on only counting the reactants consumed by \( S \)-reactions.

**Reactant assemblage**

We also note that emergent structures must necessarily rely on freely available expressions that are at least produced by the environment through random collisions. However, longer reactants come in exponentially smaller concentrations, and thus exponentially larger systems should be simulated for them to arise in large numbers. This makes the experimental process considerably inefficient, particularly for allowing the emergence of complex structures that depend on such reactants. Here, we introduce a heuristic that we call reactant 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 in a larger system. For this, we fix a maximum food size \( F \). Then, whenever an \( S \)-reduction requires a reactant that is not present in \( \mathcal{P} \), but is part of this predefined food set, the reactant would be constructed on the spot from freely available atomic combinators. More precisely, we modify Algorithm 1 at the point of sampling a reduction with the steps in Algorithm 2. In this way, we can simulate the productivity of sufficiently large environments, without explicitly needing to compute them. However, this technique does not bypass the need of discov-
ering the substrate, namely, the expression $e$ being reduced. Instead, it just focuses on creating the required reactants. 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 this heuristic facilitates the emergence of more complex patterns.

### Algorithm 2: Reactant assemblage

**Input:** Maximum reactant size $F$

1. Let $(e[x] \rightarrow e'[y]) \in \text{Reductions}(e)$ if $x \notin P$ and $|x| \leq F$ then
   1. Let $n_I, n_K, n_S = \text{Combinators}(x)$
   2. If $P[I] \geq n_I$ and $P[K] \geq n_K$ and $P[S] \geq n_S$ then
      1. Remove $n_K$ from $P$
      2. Remove $n_I I$ from $P$
      3. Remove $n_S S$ from $P$
      4. Add one $x$ to $P$

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### Experiments and Discussion

We initialized $P$ with 10k evenly distributed $S$, $K$, and $I$ combinators and applied reactant assemblage with reactant size parameter $F$ on a range between 1 (corresponding to no reactant assemblage) and 20, simulating 10 different runs of Combinatory Chemistry for 10M iterations.

We then began by analysing general metrics of the system for different values of $F$. 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 different expressions. Then, it starts to decline at different speeds, depending on the value of $F$. When this mechanism is disabled ($F = 1$), the decline occurs at a slow and steady rate. Yet, when $F = 3$, the decline of diversity becomes much faster, only accelerating with higher $F$. This effect could be explained by the fact that $S$-reductions, the only ones that compute increasingly longer expressions, are more likely to be successful thanks to the reactant assemblage mechanism getting into action. Therefore, the limited available combinators tend to be clustered in fewer and longer expressions. This is also consistent with the evolution of the mean expression length shown in Figure 4b. Yet, when $F$ is set to the high end of the range, reduce operations peak, but then start being replaced by random cleavages and condensations as freely available combinators needed to assemble reactants plummet (Figure 4c). Thus, the system self-regulates the ratio of deterministic operations (reductions) to random ones (condensations and cleavages) occurring in it.

However, it is unclear from these results whether the ensuing reduction in diversity is driven by emergent complex structures that act as attractors, or by some other different reason. To answer this question, we tracked reactant consumption rates to detect whether specific reactants where more prominently used. In particular, we looked at the 10 most frequently used reactants, 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, recursively growing, and self-reproducing patterns. Interestingly, they can emerge at different points in time, co-exist, and sometimes some of them can drive others to extinction.

We first observed that expressions that consume any given reactant $A$ are typically composed of multiple juxtaposed copies of this reactant, 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 $(SII(SII))$, composed of two copies of the reactant $A = (SII)$, and a metabolic cycle of the form $(AA) + A \rightarrow (AA) + \phi(A)$, as shown on Figure 2.

Binary reactants such as $(KK)$ and unitary ones such as $I$ do not form part of any stable structure, and the expressions consuming them are produced by chance. Yet, they are used with considerable frequency because $S$ combinators are more likely to be applied to shorter arguments than longer ones. For this reason, the consumption of $I$ is considerably higher than the consumption of $(KK)$. Yet, even though by the same argument the consumption rate of $A = (SII)$ should be below binary reactants, self-organization into autopoietic patterns drives the usage of this reactant above what would be expected would chance be the only force at play. At around 2M-3M reactions, the system reaches a point in which the consumption levels of this reactant stabilizes, constrained by the free availability of the reactant. Yet, when we assemble reactants of size at most $F = 3$ (Figure 5b), the availability of $SII$ reactants is greatly expanded as long as $S$ and $I$ combinators are freely available in the environment, thus allowing the formation of an even larger number of $(SII(SII))$ structures.

At the same time, rarer autopoietic structures can emerge in this condition, such as one based on three juxtaposed copies $(AAA)$ of $A = (SSK)$. This expression has a metabolic cycle of the form $(AAA) + 2A \rightarrow (AAA) + A + \phi(A)^5$. Here, we note that one copy of $A$ is used but then released intact, which could be construed as an emergent catalyst for the reaction: Indeed, even though we can interpret each reduce reaction to be auto-catalysed, reaction chains can have emergent properties, such as in this case, where a reactant is just used to complete the metabolic cycle and then released.

From $F = 4$ we start to see growing structures. In particular, recursively growing ones. In Figure 5c ($F = 6$) we can observe two such structures. The first one uses the react-

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5Derivations are available at the supplementary materials.
A = (S(SI)I), and follows a tail-recursive cycle that linearly increases the size of the structure: (AA) + 2A → A(AA) + φ(A) (Figure 3). The second one is a more complex binary-branching recursive structure, with reactant A = (S(SI)I). 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 atomic 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 consuming the (SII) reactant goes into a slow decline. Yet, when all freely available I combinators are depleted, this structure is driven into a quick extinction: Without the needed reactant S-reactions start to fail, and thus the expression is either cleaved or combined 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 reactants 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) → 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 reactant 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 reactant A = (SI(S(SK)I)). It follows a cycle of the form (AA) + 3A → 2(AA) + φ(A), thus duplicating itself, and metabolising one reactant 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) reactant. In 5d the reactant consumption rate for this last structure is considerably lower than in 5e, seizing less resources for itself. This may be due to the fact that the recursive structure (A(AA)) can either reduce the internal part, consuming one copy of A, or at the most external level, consuming (AA), which in the latter case is facilitated by reactant assemblage when F = 8. Yet, the self-reproducing pattern suffers from the same problem of simple autopoietic structures: When it fails to acquire its reactant from the environment it decomposes into an expression that loses 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 recursively growing and self-reproducing ones. Thanks to Combinatory Logic being Turing-complete, the presented system can theoretically represent patterns of arbitrary complexity. Furthermore, the computation is distributed uniformly across the system thanks to single-step reactions applied at each iteration while conservation laws keep the system bounded without introducing any extrinsic perturbations. The emerging structures that result from these dynamics feature reaction cycles that bear a striking resemblance to natural metabolisms.

Moreover, this system does not need to start from a random set of initial expressions to kick-start diversity. Instead, this initial diversity is the product of the system’s own dy-
Figure 5: (a–e) Reactants consumption computed over a window of 500k reactions on different runs with different reactant assemblage sizes $F$. Different line styles distinguish reactants used by different types of expressions: Dotted lines represent reactants consumed by simple non-attracting expressions; dash-dotted lines are reactants used by simple autopoietic patterns; dashed lines are reactants used by recursively growing patterns; solid lines are reactants used by self-reproducing patterns.

Finally, we noted that emerging structures require a constant influx of specific types of reactants. While only much larger systems than the ones simulated here would allow for such continual production of many of these food elements, we proposed a heuristic to make them available without explicitly simulating them. In this way, we observed a wide variety of emerging structures, including those that would self-sustain, albeit not changing their numbers (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’s own dynamics. In the future, we will seek to apply it to explaining the emergence of evolvability, one of the central questions in Artificial Life. While many challenges lie ahead, we believe that the simplicity of the model, the encouraging results presently obtained, and the creativity obtained from balancing computation with random recombination to search for new forms, leaves it in good standing to tackle this challenge.

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References


