An algorithmic chemistry as a toy model for the origin of life[1]

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Ingredients

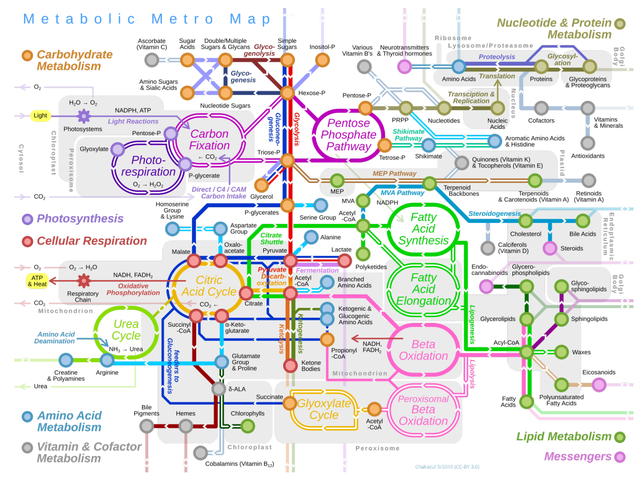
What is Life?

"*...living matter, while not eluding the "laws of physics" as established up to date, is likely to involve "other laws of physics" hitherto unknown, which however, once they have been revealed, will form just as integral a part of science as the former.*"
Erwin Schrödinger [5]

"*The human body completely changes the matter it is made of roughly every 8 weeks, through metabolism, replication and repair. Yet, you're still you –with all your memories, your personality.. If science insists on chasing particles, they will follow them right through an organism and miss the organism entirely.*"
Robert Rosen [6]

"*An autopoietic system is a network of processes which produces all the components whose internal production is necessary to maintain the network operating as a unit.*" Maturana and Varela [7]

Metabolic Networks



Minimal Properties for Artificial Life

- **Computational Unboundness (Algorithms)**: the system must be capable of building arbitrarily complex functions. In terms of algorithms this is equivalent to Turing completeness (e.g. Cellular automata, programming languages, lambda calculus). Computational unboundness is essential to have a system that is really open-ended, in the sense that its evolution can potentially bring it to always new functions and strategies.
- **Efficiency (Thermodynamics)**: for each scale of complexity, the system should require minimal computational resources to sustain its organization. It is not enough to be potentially open-ended to become effectively open-ended. Each subpart of the system need to be able to perpetuate itself in a minimal fashion, with minimal resources, in order to have left enough ordered energy to explore new possibilities (i.e. every metabolic cycles has its own efficiency, and only most efficient cycles –if we compare cycles with similar functioning– will dominate the system).

A Toy Model for the Origin of Life

A Soup of Functions

We consider a toy model of functions that interact with each other by random encounters (non spatial Gillespie dyanmics) to build new functions. Two basic operations are considered:

- **Application**: $x + y = x(y)$
  $+$ is a non-commutative operator, i.e. $x + y \neq y + x$. x and y can be any functions.
- **Evaluation**: e.g. $\mathbf{A}(x)(y)(z) \to x(y(x))$
  the function **A** has its own *evaluation rule* which recomposes its arguments.
  A is agnostic of x, y, z, it is only recomposing them.
  Each function has its own evaluation rule which takes k arguments and recomposes them in a well-definded fashion.

Atoms (aka Combinators)

The soup is composed of a finite set of atomic functons (aka combinators), which defines the *base* of the system. To each of these atoms correspond an evaluation rule.
For example the **S-K-I** base is composed of three atoms with the following evaluation rules:

- **I-rule**: $\mathbf{I}(x) \to x$
- **K-rule**: $\mathbf{K}(x)(y) \to x$
- **S-rule**: $\mathbf{S}(x)(y)(z) \to x(z)(y(z))$

This base is Turing complete, i.e. any function can be written only with these three combinators. Recently combinators were also used to suggest that universal computation is well within the reach of molecular biology [3].

Combinatory Chemistry

The soup is initially composed of just atomic functions (e.g. **S**,**K**,**I**) and thought *random recombination* (application and its inverse) and *rule-evaluation* it evolves towards more complex functions. The dynamics for each possible reactions follows two properties:

- **detailed balance**
- **conservation of the number of atoms**

In the chemistry we call applications and its inverse respectively ligation and cleavage:

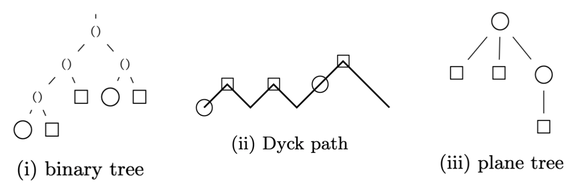
$$x + y \rightleftarrows x(y)$$

While rule-evaluations that conserve the number of atoms are called reductions. We have the following reduction constructed from the respective evaluation-rules:

- **S-reduction**: $\alpha\mathbf{S}(x)(y)(z)\beta + z \to \alpha x(z)(y(z))\beta + \mathbf{S}$
- **K-reduction**: $\alpha\mathbf{K}(x)(y)\beta \to \alpha x\beta + y + \mathbf{K}$
- **I-reduction**: $\alpha\mathbf{I}(x)\beta \to \alpha x\beta + \mathbf{I}$

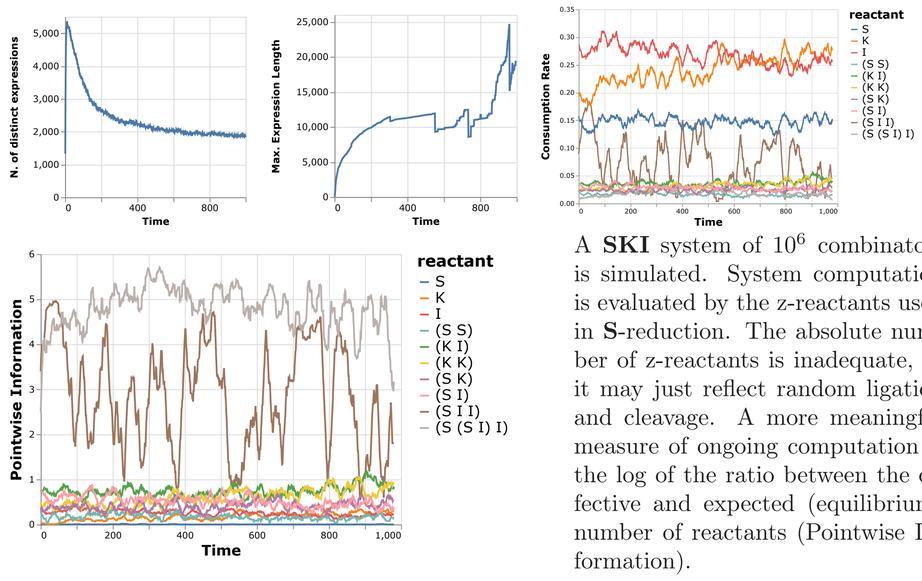
where $\alpha \ldots \beta$ indicates that the reduction is evaluated inside a larger expression.

Equivalent Representations of $\bigcirc(\square)(\square)(\bigcirc(\square))$



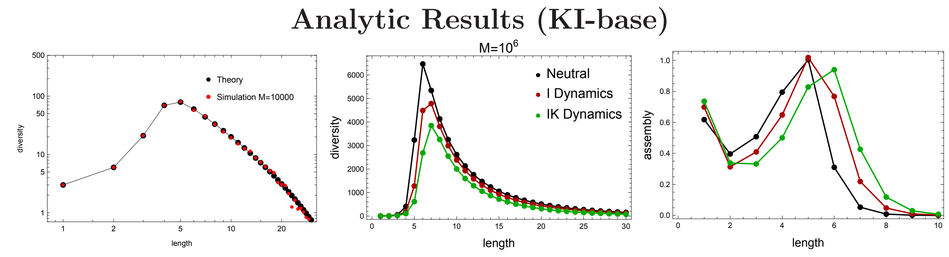
(i) binary tree (ii) Dyck path (iii) plane tree

Simulations (SKI-base)[1]



A **SKI** system of 10^6 combinators is simulated. System computation is evaluated by the z-reactants used in **S**-reduction. The absolute number of z-reactants is inadequate, as it may just reflect random ligation and cleavage. A more meaningful measure of ongoing computation is the log of the ratio between the effective and expected (equilibrium) number of reactants (Pointwise Information).

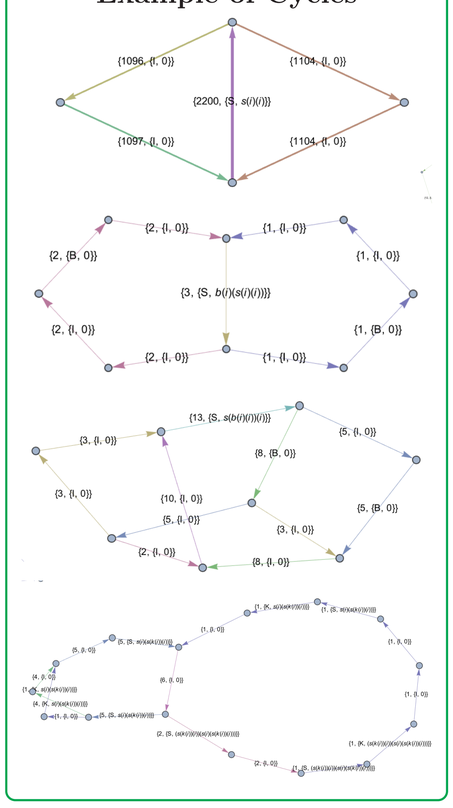
Analytic Results (KI-base)



In the case of a **KI**-base, since the reductions are only contractive, the system reaches equilibrium, allowing for exact evaluation of the probability of each expression in the system. Consequently, many mean-observables can be assessed, such as the number of distinct expressions (diversity) and the assembly, which measures the complexity of each expression.

Emergenge of Cycles (i.e. dynamical attractors)

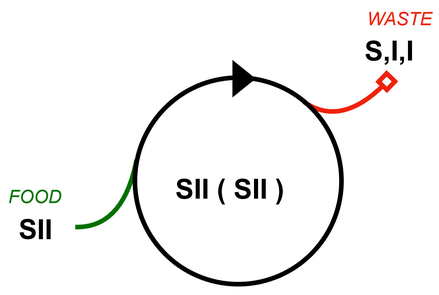
Example of Cycles



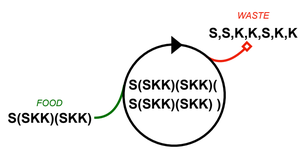
3-node Cycle [1]

1. $\mathbf{SII(\ SII\ ) + SII \to I(\ SII\ )(\ I\ (\ SII\ )\ ) + S}$
2. $\mathbf{I(\ SII\ )(\ I(\ SII\ )\ ) \to SII\ (\ I(\ SII\ )\ ) + I}$
3. $\mathbf{SII(\ I(\ SII\ )\ ) \to SII(\ SII\ ) + I}$

This 3-node cycle can be tought as a minimal metabolism that absorbs the food **SII** and release the waste **S,I,I**.



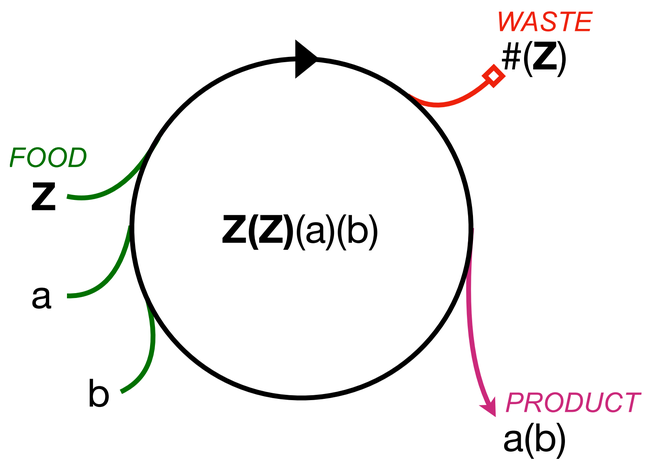
Given the functional equivalence $\mathbf{I} \sim \mathbf{SKK}$, the same cycle can be represented only in terms of **S** and **K** as the 7-node cycle,



... but it is is less efficient. More in general this cycle can be represented with an infinite set of equivalent expressions, depending on the chosen base. Some are more efficient then others.

Enzyme Cycle [2]

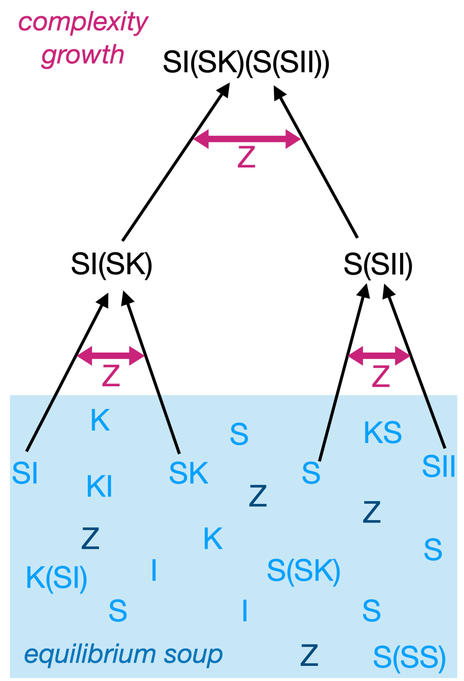
The simplest cycle that can catalyze a reaction $a + b \to a(b)$ is the enzyme cycle



where **Z** is an abstract function, which has different representations depending on the chosen base of atoms. For example in the **SKI**-base
$\mathbf{Z = S(\ K(\ S(\ S(\ KS\ )K\ )\ )\ )\ (\ S(\ K(\ S(\ K(\ SK\ )\ )\ )\ )(\ SII\ )}$
this is a quite long expression which requires very large simulations to emerge, but changing the base the same function can be expressed in shorter forms, such as $\mathbf{Z = B(\ SB\ )(\ B(\ B(\ SK\ )\ )\ )(\ M\ )}$ or even $\mathbf{Z = W(\ V\ M\ )}$ (where $\mathbf{B, M, V, W}$ are properly defined combinators). It is evident the role of the chosen base in the emergence of cycles.

Autocatalytic Networks [4]

Given the emergence of enzymes it is possible to forecast that the system will become able to sustain the structure of a structured complex dynamics of interacting cycles. Each cycle can participate to a larger autocatalytic network



Perspectives

Combinatory chemistry serves as a minimal toy model designed to explore the functional space related to the origin of (artificial) life. This system possesses the potential for unbounded computability (Turing completeness), which is essential for open-ended evolution. By introducing dynamics that preserve the number of atoms, the system facilitates the emergence of simple cycles that are efficient enough to persist. Can these dynamics employ these cycles to construct an autocatalytic network capable of fostering the growth of complexity? The system's simplicity allows for analytical study in certain stationary regimes. Our aim is to use stochastic thermodynamics tools to explore the cycles that emerge, quantify their efficiency, and examine the relationship between local entropy production and the growth of complexity.

References

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