IS THE EMERGENCE OF LIFE AN EXPECTED PHASE TRANSITION IN THE EVOLVING UNIVERSE?

STUART KAUFFMAN AND ANDREA ROLI,

September, 2024

We propose a novel definition of life in terms of which its emergence in the universe is expected, and its ever-creative open-ended evolution is entailed by no law. Living organisms are Kantian Wholes that achieve Catalytic Closure, Constraint Closure, and Spatial Closure. We here unite two established mathematical theories. Together these imply that life is expected as a phase transition in the evolving universe. Beyond this, **we discover that we can use no mathematics based on Set Theory to deduce the evolution of the biosphere**. We propose new astronomical ways to search for life on exoplanets and in the solar system, new experiments to seek the emergence of the most rudimentary life, and the hint of a coherent testable pathway to prokaryotes

The Emergence of Life

Introduction

Erwin Schrödinger, in his famous 1944 book, What is Life?, brilliantly proposed the aperiodic crystal as the source of order in organisms. But he did not answer his question. Eighty years later we hope to do so. The universe may hold a million trillion habitable planets. **If we are right, the emergence of life in the universe is a miracle, but an expected one. Once life emerged, its evolution is radically creative and cannot be based on physics alone. Strong reductionism fails. No Laws entail the evolution of the biosphere.**

Life is a double miracle.

. A Novel Definition of Life

losures: Catalytic, Constraint, Spatial, Kantian

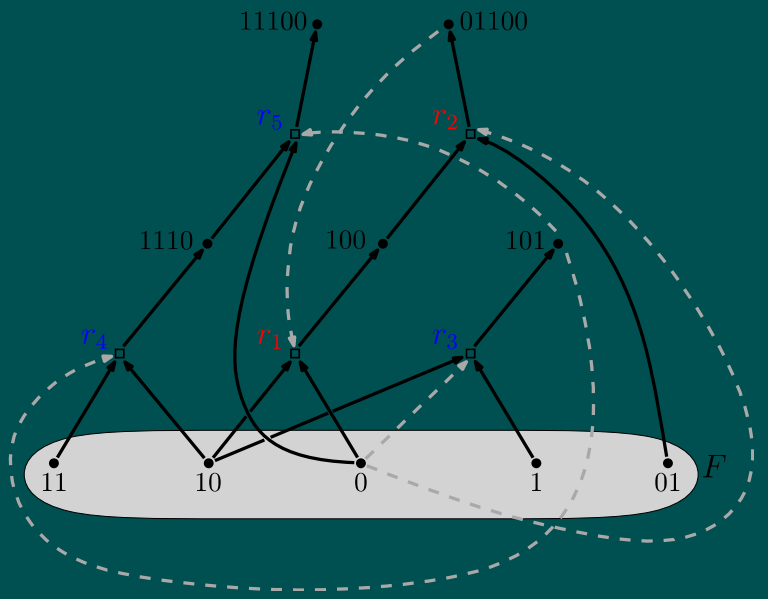
e no agreed-upon definition of life. We here build toward the following:

a non-equilibrium, self-reproducing chemical reaction system that achi
ctive autocatalysis.
straint Closure.
tial Closure.
such, living entities are Kantian Wholes. We explain these concepts bel

ely Autocatalytic Sets

**ely autocatalytic set, CAS, is an open chemical reaction system fed wit
s molecular and energetic building blocks, having the property that at l
cal reaction step forming each molecule in the set is catalyzed by at lea
n the set or by one molecule in the food set.**

hows a simple example of a collectively autocatalytic set:

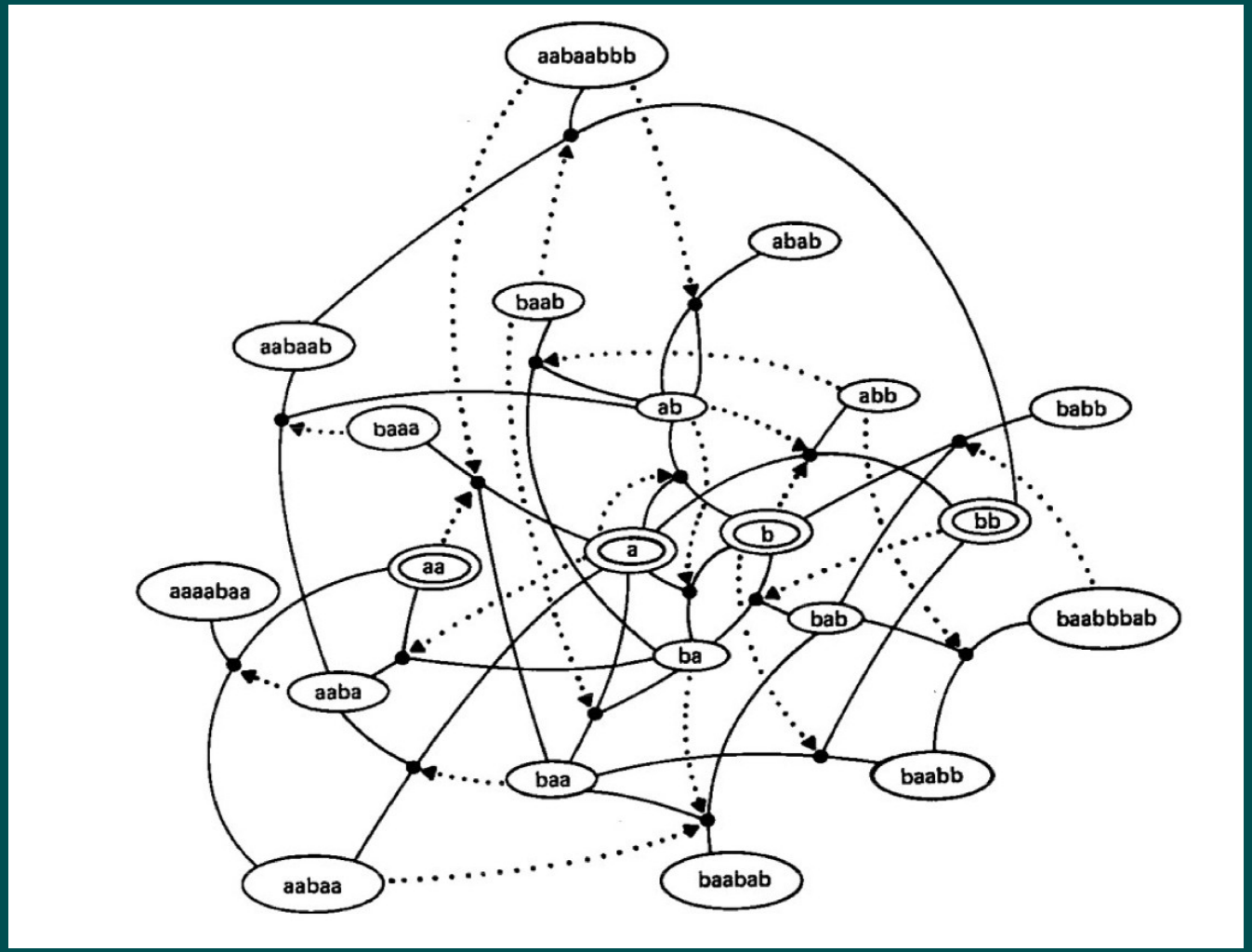


Bipartitie hypergraph:

Digits, 1 and 0, are molecules. Dots are reactions. White dotted arrows show which molecule catalyzes which reaction.

Binary small molecules, elements 1 and 0. The four dimers in the white zone are the foot set

The Emergence of Peptide Collectively Autocatalytic Sets, 1986



Bipartitie Hypergraph:

Digits, 1 and 0, in ovals are small peptides.

Dots are reactions.

Dotted arrows show which Peptide catalyzes which reaction.

Double ovals are the food set

Farmer, Kauffman Packard 1986

Peptide Collectively Autocatalytic Sets. J. Theoret. Biol. 1986

TEMPLATE REPLICATION

The concept that life must be based on template replicating polynucleotides has dominated the origin of life field for some 50 years. Yet replication of a “nude replicating RNA gene” has not yet been achieved. Nevertheless, this goal may be achieved.

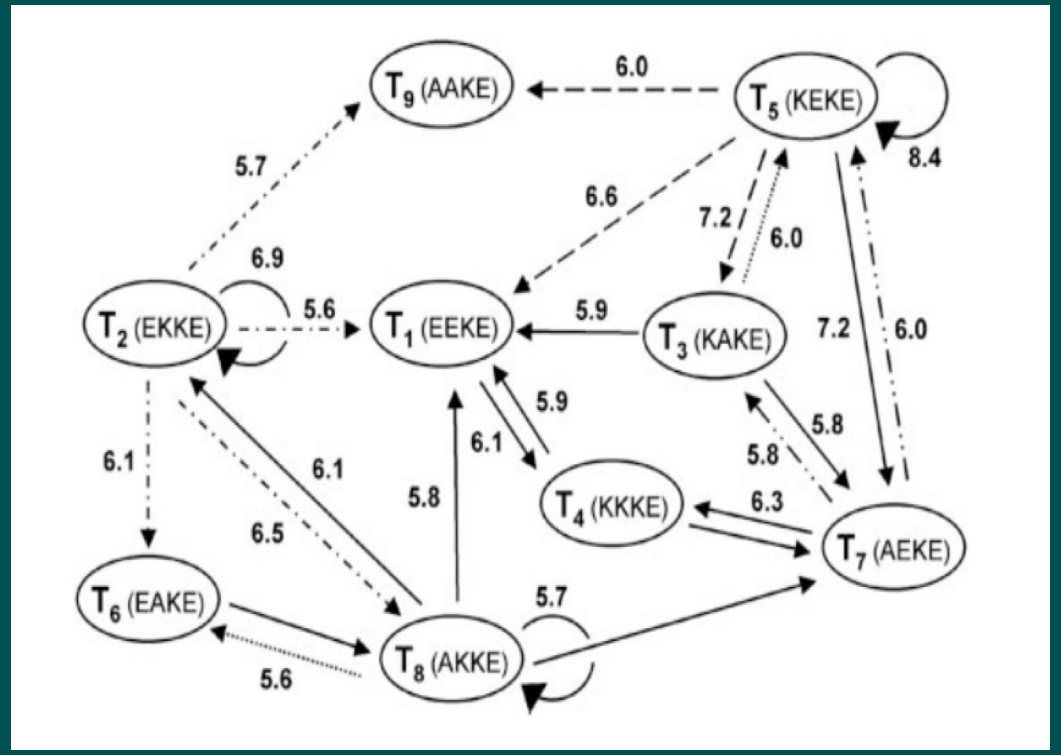
The familiar concept of a template replication double stranded RNA sequence is a specific example of a collectively autocatalytic set. Each strand is a template catalyst for the synthesis of the other strand. However, the concept of collective autocatalysis is far broader.

Collectively Autocatalytic Sets

In sharp contrast to the hopes for a template replicating RNA sequence, collectively autocatalytic sets of DNA, of RNA, and of peptides have been constructed. The first, a DNA collectively autocatalytic set, was constructed by G. von Kiedrowski. An RNA collectively autocatalytic set was achieved by N. Lehman and colleagues. This set spontaneously self organizes given its building blocks. A collectively autocatalytic set of nine peptides constructed by G. Ashkenasy, is shown in Figure 2, next. Autocatalytic sets of lipids have been considered.

These results are of fundamental importance. **Creating self-reproducing open chemical reaction systems is achieved.**

A Nine Peptide Collectively Autocatalytic Set



The nine peptide collectively autocatalytic set created by G. Ashkenasy. The ovals show the molecules, the arrows show the transitions among the molecules and the relative rates.

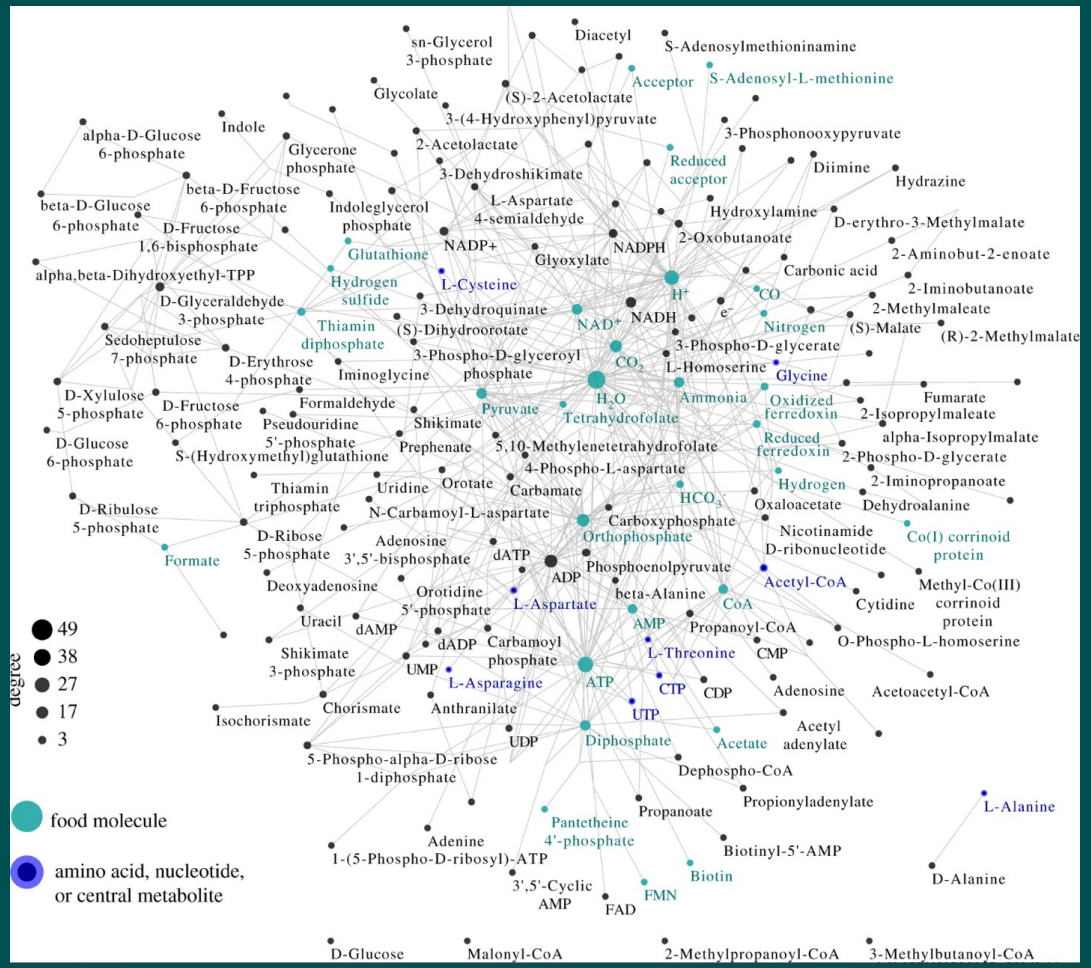
Small Molecule Collectively Autocatalytic Sets in All 6700 Prokaryotes

Joana Xavier 2018 2024

Stunning evidence now demonstrates the presence of small molecule collectively autocatalytic sets containing no DNA, RNA, or peptide polymers, in all 6700 prokaryotes, Figure 3. These small molecule self-reproducing sets contain from tens to hundreds of small molecules and reactions among them. These autocatalytic sets synthesize several amino acids and ATP. They link ATP and Redox energy metabolism. The sets are identified computationally. It remains to be shown that they reproduce in vitro.

The presence of small molecule collectively autocatalytic sets in all 6700 prokaryotes strongly suggests that the first chemical systems capable of self- reproduction in the universe were precisely such sets. We show below that the emergence of such sets is expected.

A Small Molecule Collectively Autocatalytic Set: Joana Xavier 2024



hall molecule collectively autocatalytic set with no DNA, RNA, or peptide polyme
prokaryote. Similar small molecule autocatalytic sets are found in all 6700 proka
umably the phylogeny among these is part of the evolution of metabolism.

Life: Kantian Wholes, Catalytic Closure, Constraint Closure, Spatial Closure.

Kantian Wholes:

In the 1790s, philosopher Immanuel Kant introduced a fundamental concept: **An organized being has the property that the Parts exist for and by means of the Whole,** (13). Kant's insight has lain dormant for 230 years. **All living beings are Kantian Wholes** that exist for and by means of their Parts. You are a ***Kantian Whole***. You exist by means of your Parts – heart, liver, kidneys, lungs, brain. Your Parts exist by means of you, the Whole. You reproduce, and your children inherit your Parts.

Kantian Wholes are a special class of dynamical physical systems. **A crystal is not a Kantian whole**. The atoms of the crystal can exist without being parts of the crystal. A brick is not a Kantian Whole. A cell is a Kantian Whole.

Catalytic Closure

A collectively autocatalytic set such as the 9-peptide set in Figure 2, achieves *Catalytic Closure*. Each reaction in the system is catalyzed by at least one molecule in the system. All living cells achieve catalytic closure. No molecule in a living cell catalyzes its own formation. The set molecules in a living cell, a Whole, achieves catalytic closure as the cell reproduces, (14,15,16).

Systems that achieve catalytic closure are also Kantian Wholes. Each of the peptides in the 9-peptide collectively autocatalytic set in Figure 2 is a Part that exists for and by means of the Whole set of nine peptides whose mutual catalysis enables all the Parts to exist.

CONSTRAINT CLOSURE

Living cells, including a small molecule collectively autocatalytic set of the type found in all 6700 prokaryotes, achieve a newly recognized and profound property: ***Constraint Closure***. **Thermodynamic *work* is the constrained release of energy into a few degrees of freedom**. An example is a cannon with powder at its base and a cannon ball nestled next to the powder. When the power explodes, the cannon, that is both a boundary condition and a constraint, constrains the release of energy to blast the cannon ball down the bore of the cannon. Thermodynamic work is done on the cannon ball. **In the absence of constraints on the release of energy in a non-equilibrium process, no thermodynamic work can be done.**

Newton does not tell us where the boundary conditions come from. The cannon in the example is the boundary condition. But where did the cannon come from? The critical answer is that

Maël Montévil and Mateo Mossio in 2015 first defined Constraint Closure:

Consider a system with three non-equilibrium processes, 1, 2, and 3. Consider three constraints, A, B, and C. Let A constrain the release of energy in process 1 to construct a B. Let B constrain the release of energy in process 2 to construct a C. Let C constrain the release of energy in process 3 to construct an A, Figures 1a, 1b and 2.

The above system achieves a remarkable property: *Constraint Closure.* The set of constraints, here A, B, and C, constrain the release of energy of a set of processes, here 1, 2 and 3, into the few degrees of freedom that therefore do thermodynamic work construct the very same set of constraints, A, B, and C! This system literally does the thermodynamic work to construct itself by constructing its own boundary condition constraints on the release of energy that construct the same boundary conditions.

Spatial Closure

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Living cells are abounded spatially. The common hypothesis is that these arose by the
spontaneous formation of li;posomes that enclosure the rest of the self-reproducing
system.

Part III. The First Miracle: The Emergence of Life is an Expected Phase Transition – TAP and RAF.

In this Part III we show that the emergence of collectively autocatalytic sets is an expected phase transition in chemical reaction networks as the diversity of molecular species in the system increases, and the diversity of the reactions among them increases even faster. We discuss first the phase transition to collective autocatalysis, RAF, in sufficiently rich chemical reaction networks. Then we marry the RAF theory to the TAP theory that yields the increasing diversity of chemical species in which the RAF phase transition must eventually occur. This TAP RAF union is new.

Random Graph Theory

In 1959, two mathematicians, Erdos and Renyi, published a seminal paper on the properties of random graphs. **A graph is a set of dots or nodes or vertices. Each dot may be connected by a line to no other dots, one other dot, or some number of other dots.**

Erdos and Renyi asked a wonderful question: Start with N nodes. Randomly pick up a pair of nodes and connect them by a line. Iteratively keep picking up random pairs of nodes and connecting them with lines.

Let N be the number of Nodes. At any step in this process let the number of lines connecting nodes be L. Consider the ratio: L/N. What happens to the graph as L increases for fixed N?

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Magic Happens when N/L =0.5

When N/L = 0.5 a Giant Component emerges as a first order phase transition:

In the Giant Component finite fraction if the N nodes are mutually connected, directly or indirectly.

Cycles of all lengths form.

As L increases beyond 0.5, the Giant Component grows larger

The First Miracle - Part I:
The Emergence of Molecular Reproduction as a First Order Phase Transition

The emergence of collectively autocatalytic sets, also called RAFs, arises as the same phase transition in bipartite chemical reaction hypergraphs. Consider a given bipartite chemical reaction graph. Consider increasing the probability, Pcat, that any molecule catalyzes any given reaction. For each value Pcat assign at random according to Pcat which molecules catalyze which reactions. Does the system contain a collectively autocatalytic set? **At some value of Pcat so many reactions are catalyzed that they form a giant component that is now collectively autocatalytic.**

***Keep Pcat constant and increase the number and atomic complexity of the molecules in the system*. The ratio of reactions to molecules, R/M, must increase**. At some

The First Miracle - Part II.
The Expected Emergence of Molecular Reproduction in the Evolving Universe.

A first-order phase transition to molecular reproduction is expected in the chemical evolution of the universe where the diversity and complexity of molecules increased. At the earliest stage there were the fundamental particles, quarks, gluons, electrons, positrons. As the universe cooled, hadrons formed. Then the first elements, hydrogen, beryllium, formed. Later, in supernovae, the rest of the 98 stable atoms formed.

The emergence of simple then ever-more complex molecules followed the same pattern from simple molecules and low diversity upward. The diversity, atomic complexity of the molecules, and the potential reactions among them increased. The Murchison meteorite, formed five billion years ago with our solar system, has hundreds of thousands of molecular species and potential reactions among them.

The New Mathematical Theory – TAP and RAF

The theory of the emergence of collectively autocatalytic sets, RAFs, is well established. We here marry that RAF theory to an independent theory, TAP, that can explain the increasing diversity of molecular species in the evolving universe.

The TAP Equatio and Behavior:

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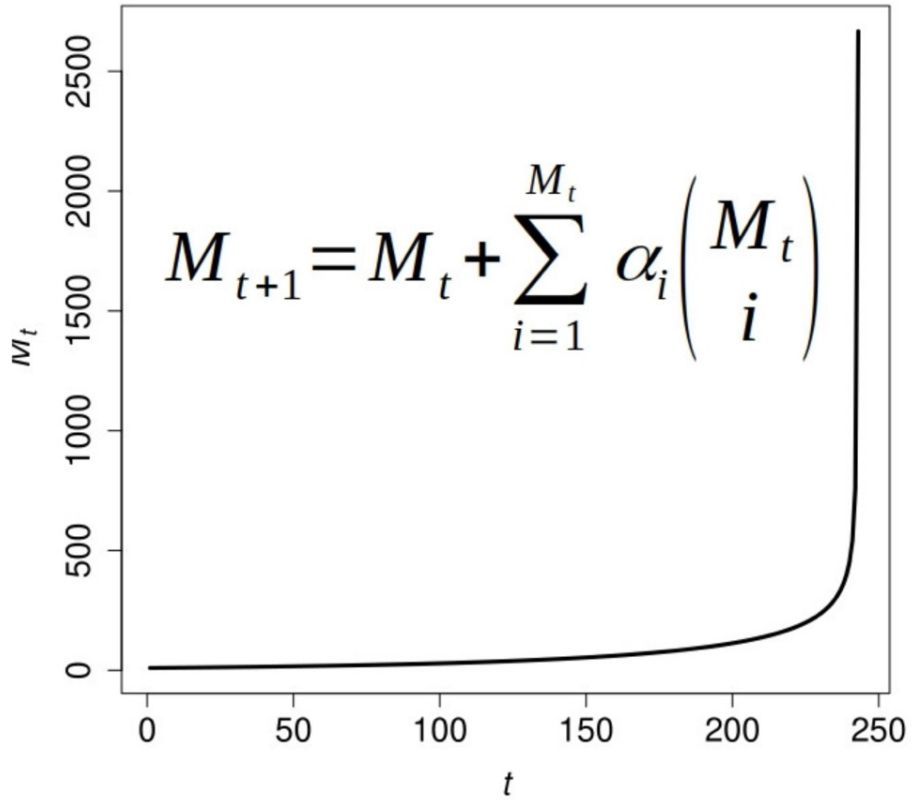
$$M_{t+1} = M_t + \sum_{i=1}^{M_t} \alpha_i \binom{M_t}{i}$$



Hockey stick growth

The TAP process is a crude model of the increasing chemical diversity of the universe.

We now unite TAP and RAF. This union hopes to explain the expected emergence of collectively autocatalytic systems as a first order phase transition in the evolving universe. The simple step is to allow each molecule in TAP to catalyze each reaction in TAP at random with a fixed probability Pcat. The first results with respect to technological evolution were just published. **As time passes, the diversity of entities increases, then the first order phase transition to the emergence of collectively autocatalytic sets arises with probability 1.0**

This united TAP-RAF theory demonstrates a basic truth. In the chemical evolution of the universe, molecular diversity increased by some analogue of the TAP process. As this occurred, the complexity of molecules increased, thus the number of reactions increased as did the ratio of reactions, R to molecules, M, R/M. But the same set molecules,

Part IV. The Second Miracle: The evolution of the biosphere is a propagating, non-deducible construction, not an entailed deduction. There is no Law. Evolution is ever-creative.

All classical physics, the physics of Newton, lives within the Newtonian Paradigm: i. State the relevant variables, for example position and momentum. ii. State the Laws of Motion in differential form connecting the relevant variables. Newton's three laws of motion are an example. iii. Define the boundary conditions. These define the phase space of all possible combinations of values of the relevant variable. iv. State the initial conditions. v. Integrate the equations of motion to obtain the entailed determined single trajectory in the system's phase space, (41,42,43).

The Newtonian Paradigm is unchanged in Quantum Mechanics. Schrödinger's wave equation is integrated to obtain the entailed trajectory of a probability distribution. Then measurement, typically held ontologically random, occurs.

The Failure of the Newtonian Paradigm

We show next that the evolving biosphere of Kantian Wholes persistently creates novel phase spaces that cannot be deduced or determined ahead of time. The entire Newtonian paradigm collapses. The evolving biosphere cannot be explained by physics alone. Appeal to “function” is necessary. There is no “Final Theory” that entails the evolution of the Universe

These issues are basic:

Once we have defined a Kantian Whole, the non-circular definition of the “function” of a Part is clear. **The function of a part is *that subset* of its causal consequences that sustains the Whole**. The function of your heart is to pump blood, not make heart sounds or jiggle water in your pericardial sac.

Selection acts at the level of the Kantian Whole organism, not its Parts. Selection does not directly select for hearts that are more efficient at pumping blood. Organisms that inherit such improved hearts are more likely to have offspring, thus improved hearts are indirectly selected.

These issues are basic:

Because the function of a Part is that *subset* of its causal properties that sustains the Whole, the *function of the very same part can change*. Some new, unused, subset of causal properties of the same Part can come to sustain the Whole. These are called Darwinian pre-adaptations, or by Gould and Verba, **exaptations.** Examples include the co-opting of scales that evolved for thermoregulation on some dinosaurs to evolve into flight feathers on birds. Other examples include the co-opting of normal enzymes to become transparent lens proteins. A superb example is the evolution of swim bladders from the lungs of lung fish.

A remarkable and fundamental feature of such exaptations is that they cannot be deduced. Consider a hypothetical example. An engine block can be used as a paper weight. The same engine block has sharp corners that can be used to crack open a coconut. But from the fact that an engine

These issues are basic:

Such new uses of the same object are “Jury Rigging.”
There is no deductive theory of Jury Rigging.

The truly profound implication is that such *non-deducible jury-rigged exaptations are the source of functional novelty and the open-ended evolution of the biosphere*.

The evolution of the biosphere is a non-deducible construction not an entailed deduction. No entailing laws govern the evolution of the biosphere.

The further implication is equally profound**. We *cannot list* all the uses of an engine block alone or with other things. We also *cannot list* all the uses of a screwdriver alone or with other things. *Therefore, we cannot use Set Theory or any mathematics based on set theory:***

The First Axiom of Set Theory is the Axiom of Extentionality: **"Two sets are equal if and only if they contain the same members"*. But we cannot prove that the un-listable uses of an engine block are identical to the un-listable uses of a screwdriver.*** *More the **Axiom of Choice fails** as well. The implication is huge:* ***We can use no mathematics based on Set Theory – essentially all of mathematics – to deduce the future evolution of the biosphere****.*

No union and intersection of Sets. No First Order Logic. No numbers via Russell). No numbers via Peano). No equations. No

These issues are basic:

The entire Newtonian Paradigm that is the basis of all physics, requires a prestated phase space. **But we can neither deduce nor prestate the evolving phase space of the evolving biosphere. *Evolution is beyond the Newtonian Paradigm*.**

We cannot explain the evolving biosphere with physics alone. The heart evolved by virtue of its function pumping blood. Natural selection of heritable variation acts on the Kantian Whole, not directly on its Parts. Such selection is Downward Causation. Here, the explanatory arrows point upward.

Strong reductionism, the dream of many, fails. If the Final Theory to be inscribed on the famous T shirt is to include the deduction of the evolving biosphere, there is no final theory.

These issues are basic:

Profound Negative Results and the Transformations of Mathematics

I Euclid: Mathematics is discoverable by mind alone, is certain given the axioms, and is true of the world. Mathematics is the Queen of the Sciences.

II. Lobachevski: Non Euclidian Geometries. Mathematics is discoverable by mind alone, it is certain given the axioms, but may not be about the world.

III Godel's Incompleteness Theorems: Mathematics is discoverable by mind alone, need not be about the world, and is not even certain.

IV Kauffman and Rolit: The real evolving biosphere is not

These issues are basic:

Heisenberg's demonstration of the Uncertainty Relation demanded that we abandon Classical Physics.

If we must abandon Set Theory with respect to biological evolution, what are the implications? We hardly begin to know.

We now enter the Third Transition in Science. The new fundamental questions surely include: How does the evolving biosphere create, and seize by heritable variation and Natural Selection, or genetic drift, the ever-new possibility bubbles of ways organisms can co-exist for some period as the burgeoning wave of life flowers onward. What a stunning adventure.

Part V. New Observations and Experiments: Is There Life in the Cosmos?

We are discovering ever more exoplanets. **We seek evidence of life in the atmospheres of these planets. We seek life elsewhere in our solar system**. The results discussed here suggest a potent new hope. If we establish that the small molecule collectively autocatalytic sets in all 6700 prokaryotes do reproduce chemically in vitro, we can then seek evidence in the atmospheres of exoplanets, or in our solar system. For example, **can we find such small molecule collectively autocatalytic sets in the ancient Mudrocks on Mars?** These sets are plausibly the most rudimentary form of life in the universe. If Yes in the Mudrocks we may be seeing ancient life on Mars.

Can we demonstrate experimentally the spontaneous formation of small molecule autocatalytic sets?

It is now feasible to create high diversity small molecule libraries. For example, work by Ott running the Miller Urey experiment starting with only four molecular species for a month yields thousands of small molecules, identified by mass spectrometry. **We can now ask if in such systems, small molecule collectively autocatalytic sets can emerge**. This is a “Go or No Go” experiment. If No, the theory is probably wrong.

If Yes, we can begin to envision testable pathways beyond small molecule collectively autocatalytic sets to such sets becoming the metabolism of peptide RNA autocatalytic sets with which they co-evolve as new Kantian Wholes. In turn these might evolve to template replication, and even to genetic coding. Real experiments are needed.

CONCLUSION

We have sought the source of life in all our creation myths among all the peoples of the earth, perhaps back to Neanderthal 500,000 years ago. The issue of the Origin of Life as a scientific problem arose with Pasture's claim: Life only comes from life.

Experimental efforts have been underway since Haldane and Oparin, then the famous Miller Urey experiments in 1953. Intense efforts based on the conviction that life must be based on template replication of polynucleotides have been carried out. So far, no case of molecular reproduction has been found on this sensible pathway.

Since Newton, basic science has rested on the powerful Newtonian Paradigm. This paradigm requires a prestated and knowable phase space of all the values of the relevant variables. But living organisms are Kantian Wholes that achieve Catalytic Closure, Constraint Closure, and Spatial Closure. Stunningly, we can use no mathematics based on Set Theory – all of mathematics it seems – to deduce the ever-creative evolution of the biosphere.

Life is an expected miracle in the universe whose ways of becoming are literally numberless.

The 20th Century saw the emergence of the atomic Age, the mushroom cloud, and mutually assured destruction. With Gödel, the 20th century also saw the End of Certainty, (59). In this, the first quarter of the 21st Century, we begin barely to glimpse the astonishing blossoming creativity of the biosphere of which we are members.

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https://doi.org/10.31219/osf.io/6rvjs

2) Link: “A third transition in science?”, Stuart Kauffman and Andrea Roli, J Roy. Soc. Interface 4/14/2023

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THANK YOU