Thoughts on an Unified Framework for Artificial Chemistries

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Contents

1 Basic Framework of Artificial Chemistries ............................................ 2
   1.1 Introduction .................................................................................. 2
   1.2 Examples .................................................................................. 3
      1.2.1 Algorithmic Chemistry - AlChemy ................................... 3
      1.2.2 The Chemical Abstract Machine ......................................... 5
      1.2.3 Artificial Chemistry on a Planar Graph .............................. 6
   1.3 More Discussion on Artificial Chemistries ................................. 7

2 An Abstract Framework for Artificial Chemistries ......................... 8
   2.1 Do Artificial Chemistries Correctly Abstract the Real Chemistry? .......... 8
   2.2 Need and Structure of a Unified Framework ................................. 8
   2.3 Analysis of the Notions of Information ...................................... 10
      2.3.1 Shannon’s Information Entropy ......................................... 10
      2.3.2 Algorithmic Information ................................................ 11
   2.4 Towards an Abstract Framework ............................................. 12
   2.5 Discussion ............................................................................. 13

3 Final Discussion ............................................................................. 15

Abstract

Artificial Chemistries (ACs) are symbolic chemical metaphors for the exploration of Artificial Life, with specific focus on the problem of biogenesis or the origin of life. This paper presents authors thoughts towards defining a unified framework to characterize and classify symbolic artificial chemistries by devising appropriate formalism to capture semantic and organizational information. We identify three basic high level abstractions in initial proposal for this framework viz., information, computation, and communication. We present an analysis of two important notions of information, namely, Shannon’s Entropy and Algorithmic Information, and discuss inductive and deductive approaches for defining the framework.

*Work done when author was in NUS (2002-2005).
1 Basic Framework of Artificial Chemistries

Aim of this section is to present a brief introduction to artificial chemistries. We will start with a discussion on the epistemological foundations of the area and will illustrate further details using examples relevant to this proposal. The examples are followed by discussions to motivate the main theme of the proposal which is elaborated in coming sections.

1.1 Introduction

It is a long held topic of scientific debate whether there are any biological principles of life and other complex biological phenomena, which are not directly reducible to physical and chemical laws. Living beings, however small and consisting of the same molecular components as non living things, nonetheless exhibit qualitatively different characteristics. This may be in part due to the complex organizational structure which distinguishes them or it could be because of their quantitatively complex structure which gives rise to difficulty in analyzing properties using currently available tools.

The direct ways to understand this complex biological phenomena are usually difficult and error prone because living structures are by default complex and hard to manipulate. Even cellular level experiments are difficult to carry out and their simulations are quite cumbersome.

Artificial life (AL) is a tool to study principles explaining this complex phenomena of life without directly getting involved with the real biological systems. The fundamental assumption here is that principles of life are independent of the medium and carbon based life on earth is just one example of the possible forms of life. This means even artificial environments like digital media can also exhibit life-like behaviour under certain conditions. This way AL complements the main stream biological studies by synthesizing life-like systems using digital media. There are several such examples where these artificial life forms exhibit properties remarkably close to higher forms of life, e.g., Tierra [Ray91], Avida [Adami98].

Living phenomena has several aspects to study, one such is the origin of life or biogenesis. Here the problem is to understand how first primitive form of life such as metabolism and self replicating structures could have come into existence starting from non living chemical compounds. Artificial chemistries (AC) are the primary tools in AL studies aimed at understanding this origin of life and other complex emergent phenomena. ACs follow chemical metaphor. Like real chemical reactions between molecules, which give rise to new molecules, ACs as well define abstract molecules and reactions and study what emerges during the course of reactions.

An AC has three main components, a set of objects or molecules, a set of reaction rules or collision rules, and a definition of population dynamics.

Objects can be abstract symbols, numbers, lambda expressions, binary strings, character sequences, abstract data structures etc. Reaction rules might be string matching, string concatenation, reduction rules, abstract finite state machines, Turing machines, matrix multiplication, simple arithmetic operation, cellular automata, boolean networks etc. Dynamics can be specified in terms of ordinary differential equation, difference equation, meta dynamics, explicit collision simulation, well stirred reactor, self organizing topology, etc.

A survey on various ACs is given in [Ditt01], which also has some broad classification of
ACs based upon the kind of molecular abstractions (explicit or implicit), type of reaction rules (constructive or non constructive), and population dynamics.

To illustrate, we take examples from two kinds of ACs. One where no spatial structures are considered, that is, all molecules evolve as a whole in a reactor tube and all molecules can interact with each other according to the collision rules. The examples of AlChemy (Section 1.2.1) and CHAM/ARMS (Section 1.2.2) are of this type. Second kind of AC systems impose some sort of spatial structures on the molecules thus limiting the possible reactions between molecules to their “neighbourhood” only. Planar graph (Section 1.2.3) based AC is of this type.

It seems, during the pre-biotic evolution of life, spatial structures (e.g., membranes etc) emerged starting from the open reactor type system without any spatiality. This spatial structure based classification is one of the main motivations for P system based AC definition, we propose in the next section.

1.2 Examples

Next we illustrate the common design of ACs using examples. Each example is followed by a discussion on the relative strengths and limitations of it w.r.t. real chemistry.

1.2.1 Algorithmic Chemistry - AlChemy

We consider λ expression based AC proposed in [Font92, Font94] called AlChemy.

Molecules - λ Terms: The object space consists of abstract lambda expressions (also called terms). These terms are generated as follows: There is an infinite supply of variable names \( V = \{x, y, z, \ldots\} \). Other than \( V \), the alphabet consists of a lambda symbol ‘\( \lambda \)’, dot ‘.’, and encapsulating brackets ‘(‘, ‘)’.

The set of terms, \( \Lambda \), is defined inductively:

1. \( x \in V \Rightarrow x \in \Lambda \)
2. \( x \in V; M \in \Lambda \Rightarrow \lambda x.M \in \Lambda \) (abstraction)
3. \( M \in \Lambda; N \in \Lambda \Rightarrow (M)N \in \Lambda \) (application)

A variable \( x \) is said to be bound if it occurs inside a sub-term with the form \( \lambda x.P \), otherwise it is free. The set of free variables in an expression \( P \) is denoted by \( f(P) \).

Syntactical Transformation: The schemes of transformation are oriented rewrite rules. Structures on the left hand side are replaced by structures on the right hand side. More precisely,

Substitution
4. \( (\lambda x.x)Q \rightarrow Q \)
5. \( (\lambda x.E)Q \rightarrow E; \) if \( x \notin f(E) \)
6. \( (\lambda x.\lambda y.E)Q \rightarrow \lambda y.(\lambda x.E)Q; \) if \( x \neq y \) and \( (x \notin f(E) \lor y \notin f(Q)) \)
7. \( (\lambda x.(E_1)E_2)Q \rightarrow ((\lambda x.E_1)Q)(\lambda x.E_2)Q \)

Renaming
8. \( \lambda x.E \rightarrow \lambda z.(\lambda x.E)z; \) \( z \notin f(E) \)

Reaction Rules - Function Composition and Normal Form Reduction: The reaction rules in Alchemy consist of application of one lambda term over the other, which is then reduced to a normal form. The choice of lambda calculus allows the abstract formulation of chemical substitution during chemical reactions. Normalization is used to
get equivalence classes based on functional equivalence. Since normal form reduction is
undecidable in case of lambda calculus, reduction steps are finitely bounded [Font94].

Formally a reaction between molecules \(A\) and \(B\) can be written as a binary operation \((+\Phi)\) defined as

\[
A +\Phi B \rightarrow A + B + nf(((\Phi)A)B)
\]

Where + is used from the convention of writing chemical equations to represent that
the molecules are present in reactor. \(nf()\) uses some consistent reduction strategy to
reduce the term in finitely many steps to a normal form. This choice of finite step normal
form reduction actually results in equivalence classes consisting of all the expressions
which are functionally same modulo finite execution steps. The choice of \(\Phi\) gives flexi-
bility in the way molecules can react.

**Population Dynamics - Stochastic Molecular Collisions:** Initially a large pool
of random lambda terms of finite lengths is generated. Only those terms, which are in
normal form are considered. In each iteration two molecules are chosen at random and
one is applied to the other (function composition) according to \(\Phi\), which is fixed at the
beginning. Result is reduced to its normal form in finite steps. Filtering conditions are
applied, for example, before collision takes place if the operator molecule does not start
with symbol \('\lambda'\) then it is discarded. These filter conditions are basically meant to ensure
consistency in results as per the lambda calculus semantics and to give diversity to the
emerging organizational structures. Flow is maintained by randomly selecting molecules
and removing them from the reactor.

The relative quantitative dynamics of various molecules is captured in terms of dif-
ferential equations. Replicator equations of Lotka-Volterra type [Font92, JK98] are used
to describe the relative concentration of self replicating molecules.

**Discussion:** In actual chemistry, especially in case of organic compounds with chains of
carbon atoms and possible branching, chemical reactions substitute parts of one molecule
with other molecule thus leading to structural rearrangement in the chemical composition
of these molecules. This is the main motivation behind the choice of lambda terms in
AlChemy, where the substitution is abstracted as function composition of lambda terms.
Second motivation is that many chemical reactions can give rise to the same chemical
compound, which is captured by normal form equivalence. The AlChemy is also a con-
structive chemistry like real chemistry. Also the notion of equality leads to formation of
network of molecules.

With stochastic collision dynamics and choice of reaction type \((\Phi)\), the AlChemy gives
rise to some interesting forms of organizations, classified as level-0, level-1, and level-2 or-
ganizations. While level-0 organization consists of only self replicating molecules whose
frequencies are modeled using replicator equations, level-1 organization has strong el-
ement of self-maintenance where any reaction between two molecules produces a new
molecule inside the same population. level-2 organization is a coexistence of two inter-
dependent level-1 organizations which support each other.

Though AlChemy captures certain basic aspects of real chemical compounds and their
reactions, it has its own limitations. Most important of those is related to the choice of
lambda calculus. Even though lambda calculus is computationally universal and has a
consistent reduction strategy (i.e., order of reduction steps does not change the result),
it has no serious bearing on its chemical counter part. Actual chemical reactions are not
only much more complex, they might not follow computationally consistent mechanisms like total substitution.

Thus the first limitation is the lack of selective substitution, which means, in case of actual chemical reactions, new compounds are formed (with substitution) based on the relative strengths of chemical bonds in reactants and relatively higher stability of the products. On the other hand in case of substitution in lambda terms no such conditions apply and instances of free variable are equally substituted everywhere. We propose alternate structure and reaction rules to overcome this limitation in the next section.

Second limitation is the poor abstraction of structural properties of chemical compounds. The only kind of compounds which might be resembling the lambda terms structurally are those which have long carbon chains with possible branching. Double helix structure of DNA with complementarity is difficult to capture using lambda terms. Other geometrical properties like chirality\(^1\) which is so common in living forms\(^2\), as well cannot be captured using lambda terms. The significance of this lack of structural abstraction of geometrical properties is not very clear.

Since chemical reactions are driven by thermodynamic constraints like rate of collision, pressure etc, and the properties of colliding molecules, they are usually symmetrical in nature. Thus the result of collision of the molecules A and B is same as that of B and A since there is no order on A and B. On the other hand, that is not the case with function composition, which is in general asymmetric in its definition. In our view, this presence of asymmetry in lambda chemistry might detach it from the real chemistry significantly.

Functional Equivalence - the kind of functional equivalence defined in case of lambda chemistry does not capture the equivalence which life-like forms demonstrate. In case of living structures, it is the interaction which objects have with external environment or other objects that plays important role. This element of interaction is not captured well. One idea is to consider π - calculus like formalism [Parr01] which has bisimulation kind of equivalence which can be used to capture the equivalence in the objects based upon how they can interact with other objects.

Lack of information abstraction - this is true in general for almost all of the proposed ACs. And that is one of the focus of this proposal to understand the role information plays in the emergence of life-like phenomena in ACs.

### 1.2.2 The Chemical Abstract Machine

The Chemical Abstract Machine (CHAM) was proposed in [Berr96] as an abstract formalism for concurrent computation using closely a metaphor of chemical reactions.

There are two description levels. On the upper level, CHAM abstractly defines a syntactic framework and a simple set of structural behavior laws. An actual machine is defined by adding a specific syntax for molecule and a set of transformation rules that specify how to produce new molecules from old ones.

**Molecules** are *terms of some algebra*. A general membrane construct transforms a solution into a single molecule, and an associated general *airlock* construct makes the

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\(^1\)Many important molecules required for life exist in two forms. These two forms are non-superimposable mirror images of each other, like the left and the right hand. This property is called chirality.

\(^2\)Nearly for all biological polymers to function their component monomers must have the same handedness. All amino acids in proteins are 'left-handed', while all sugars in DNA and RNA, and in the metabolic pathways, are 'right-handed'
membrane somewhat porous to permit communication between an encapsulated solution and its environment. The *generic reactions laws* specify how reactions defined by specific transformation rules can take place and how membranes and airlocks behave. A specific machine is defined by giving the algebra of these terms and the rules. Not all molecules directly exhibit interaction capabilities. Those which do are called *ions*. The interactive capability of an ion is generally determined only by a part of it that is called its *valence*. The *reaction rules* are used to build new molecules from the ions. The non-ion molecules can be heated as per the *heating rules* to break them into simpler sub-molecules. Conversely, a set of molecules can cool down to a complex molecules using reverse *cooling rules*. The presence of membrane type structure gives universal computational power to the model. *Dynamics* of CHAM goes like this - on each iteration a CHAM may perform an arbitrary number of transformations in parallel, provided that no molecule is used more than once to match the left side of a reaction law. A CHAM is non-deterministic if more than one transformation rules may be applied to the population at a time.

Sujuki and Tanaka used CHAM to model chemical systems by defining an ordered abstract rewriting system on multiset called chemical ARMS [Sujuki01]. Molecules are the *abstract symbols*. The *reaction rules* are *multiset rewriting rules*. The reactor is represented by a multiset of symbols with a set of input strings. An optional order is imposed on the rules, which specifies in which order the rules are processed. Different rate constants are modelled by different frequencies of rule application.

The qualitative *dynamics* of ARMS is investigated by generating rewriting rules randomly. This led them to derive a formal criteria for the emergence of cycles [Sujuki96] in terms of an order parameter, which is roughly the relation of the number of heating rules to the number of cooling rules [Sujuki98]. For small and large values of this order parameter, the dynamics remains simple, i.e., the rewriting system terminates and no cycles appear. For intermediate values, cycles emerge.

**Discussion:** Although CHAM was not defined as an AC, it is quite close to actual cellular chemistry in some aspects. The presence of membrane structure gives rise to important resemblance with cellular reactions mediated by membranes. Another significant property of CHAM model is that it is very general hence provides flexibility in the way actual model is defined. Heating and cooling laws closely capture what happens in case of actual chemical reactions under the effect of temperature.

The main limitation of CHAM model is that the allowed abstract terms of algebra are not adequate to capture the structural properties of real chemical compounds, as discussed in case of AlChemy.

Second limitation comes due to nature of rewriting rules, they are actually grammar rules rather than being close to the chemical reactions. Because of this problem with multiset rewriting, in ARMS analysis is done by randomly generating these rewriting laws, and it is not clear whether chemical reactions where molecules actually interact and form new bonds or break up can be fully modeled this way.

### 1.2.3 Artificial Chemistry on a Planar Graph

This model of AC was proposed in [Piet01], where an AC is embedded in a planar triangular graph. Molecules are placed on the vertices of the undirected graph and interact with each other only via the edges. The planar triangular graph can be manipulated by
adding and deleting nodes with a minimal local rearrangement of the edges. The graph based approach provides handle for spatial structures.

**Molecules and Reactions:** There is an (infinite) set of potential molecules $S$ and a reaction mechanism which computes the reaction product for two colliding molecules $x, y \in S$. There may be an arbitrary number of products for each such collision. Molecules are built from different types of substrate of elements called atoms. Each type is associated with a different function. The total number of atoms in the reactor is kept constant during a run. Free atoms (not bounded in molecules) are separately stored and form a global pool.

**Dynamics:** At every step they pick two neighbouring molecules $(x, y)$ and apply the first $x$ to the second $y$ creating a (multi)set of new molecules. These product molecules are randomly inserted in the two faces next to the link between $x$ and $y$. $x$ is replaced with first molecule after the reaction (the result of the combinator reduction) and $y$ is finally deleted. Molecules cannot change their positions in the graph.

In this system, it is observed that clusters of molecules which do not interact with the neighbouring molecules arise. The clusters can be regarded as membranes when they divide the graph into different regions. There also arises a cell organization, that is, a subgraph that can maintain the membranes by themselves.

**Discussion:** As noted in [Ditt01], the presence of spatial topology gives rise to certain phenomena which is not possible to emerge easily in cases where there is no spatial topology present in the model. For example in the case of this planar graph based AC, an emergence of membrane type structure is something which is frequently observed in living systems. This phenomena does not emerge in open reactor type of ACs with no spatial structures. Another important property is the emergence of self organization in the form of maintaining the membrane structures. Choice of ”atom - symbols” as basic molecular unit closely resembles real chemical composition of molecules consisting of atoms.

On the other hand, the choice of planar graph based topology is not something usually present in cellular structures neither it can be a simplified spatial structure for initial chemical environment responsible for emergence of life. Absence of abstraction of geometrical or structural properties is yet another problem.

### 1.3 More Discussion on Artificial Chemistries

ACs are basically motivated by and developed to understand the pre-biotic evolution or the problem of origin of life, which is still an open problem despite lots of advancements in molecular biology [Smith99, Dev00, Dys99]. The problem of pre-biotic evolution differs significantly from the post-biotic phenomena mainly because of the appearance of genetic material. Once the first form of life, a single cell or more primitive forms are available, Darwinian theory of evolution based upon mutation and selection [Smith93] or neutral theory of random drifts [Kimu83], etc can be used to explain the emergence of higher and more complex forms of life. Still the emergence of this genetic material which is so fundamental for the proper functioning of even the simplest forms of life is what makes the problem of pre-biotic evolution so different.

Therefore the kind of problems mainly of focus in ACs and in this proposal are the search for principles governing the emergence of life-like forms from non life-like structures.
in AC systems. This also involves proper level of abstraction from real chemistry without losing generality.

In AC, we primarily consider the qualitative aspects of a problem, before considering the quantitative relations between its components. The quantitative aspect is usually analyzed using reactor flow equations [Yock92]. The stable structures generated by artificial chemistries, the stable sets of molecules, are usually referred to as organizations. Understanding which organization will appear is one such example to understand the qualitative solution of an AC.

Some of the aspects very commonly studied in AC are - given an AC, how to know a priori, which organizations are possible and which are not possible? To know which organizations are probable and which are improbable? To define an AC to generate a particular organization? How stable are organizations? Can the complexity of an organization be defined? If is possible to generate an AC which moves from organization to organization in a never ending growth of complexity? Quantitative questions can also be asked, for example, given an AC, in a particular organization how many stable (attractive) states are present inside it?

[Ditt01] has detailed description of several interesting common phenomena which are observed in different kinds of AC systems such as reduction of diversity, formation of densely coupled stabled networks, syntactic and semantic closure in these networks etc.

2 An Abstract Framework for Artificial Chemistries

One of the pressing needs of AC studies is to develop an unified framework to understand the role of various ACs from the point of view of their basic aim of explaining the possible principles leading to the origin of life-like structures. If we look into the varying nature of molecular abstractions used in various ACs, the varying definitions of reaction rules and population dynamics, we find that it is difficult to understand why only certain phenomena emerges in one AC set up but not the other, which might be emerging with some other AC. There is no single AC which gives rise to all important life-like properties. The role of spatial structures is one such example, where we notice that only the presence of initial topological constraints make it possible the emergence of realistic cellular forms in emerging organizations. Thus the aim of this section is to motivate the need for a new unified framework to characterize and classify symbolic artificial chemistries with appropriate formalism. We explain three basic high level abstract components identified in our initial proposal for this unified framework.

2.1 Do Artificial Chemistries Correctly Abstract the Real Chemistry?

The problem of epistemological cut is deeply present in any branch of AL [Patt95]. This is true in the case of AC as well. The problem is up to what extent the definition of an AC should be based on real chemistry to demonstrate that certain kind of life like phenomena emerges even when molecules or objects are not exactly the real chemical compounds. Thus as we analyze, we consider only those ACs, which are similar to some extent with the real chemical systems, e.g., AlChemy, CHAM, etc. Even in case of these ACs which aim to abstract closely the real chemical environment, we find that they do not come sufficiently close to assert claims in generic sense. In the spectrum of ACs there
are examples of those which demonstrate several of high level organizational properties, for example origin of diversity of life, in Tierra [Ray91], but the power comes out of in-built self replicating and self organizing properties in the basic structures (programs). On the other hand we have examples which closely simulate the bio chemical reactions, e.g., self assembly of protocell structures, but these are complex, time consuming, and do not explain the emergence of complex organizational patterns or life-like properties. This motivates for the need of correctly abstracting the most essential and basic properties from real chemical environment and to explore dynamic structures in an unified way.

2.2 Need and Structure of a Unified Framework

The most basic aspects of emergence of life from non living matter are the emergence of replicative mechanism and the emergence of metabolism. Replicative mechanism emerges as a tool for preserving the structure and function under the disintegrating effect of second law of thermodynamics. This replicative mechanism as we know it, in case of almost all forms of life, consists of two basic and functionally different components [Dev00, Dys99] - one that encodes the instructions how to replicate, and the other, which actually carries out the actual task. These are nucleic acids and proteins respectively. The emergence of metabolism keeps the cells in thermodynamic equilibrium. The metabolism is important because otherwise a cell will disintegrate soon under external perturbations.

Emergence of either the replication or the metabolism as autocatalytic reaction networks [Kuil86] is demonstrated in case of most of the AC systems, along with other complex organizational forms mainly suitable to be compared with post biotic life forms [Ditt01]. Even then the emerging organizations usually do not come very close to the existing cellular structure. The reason might be that either the molecular structure or the collision rules defined in these ACs do not match very well with the real chemistry, as discussed in case of AlChem in the previous section. In cases where real chemical systems are simulated, simulations become quite complex, time consuming and exact analysis of the results is not easy.

At present there is no such standard analytical framework existing, which can be used to understand these aspect in a unified way. To take particular example, we consider the “genetic” information. [Yock92] cites the sequence hypothesis to explain the qualitatively different role played by genetic material inside a cell. The sequence hypothesis states that generation and functioning of certain bio molecules is totally controlled by genetic material and thus, the functioning of cellular processes cannot be explained only in terms of chemical and physical properties of cell compounds. The point is that genetic sequence encodes some very specific instructions which actually direct those processes. Now once we know that this happens, we can try to understand these coded instructions or explain why this works that way using the physical and chemical laws but this does not explain why and how that structure emerged in the first place and why only that way. In AC parlance, this amounts to developing suitable framework which can explain the principles behind all this phenomena without working exactly with real chemistries. In this proposal we aim to address this problem by formally defining the functional and organizational information with sufficiently enough abstractions from real chemistry on the structure of the molecules and/or collision rules.

To illustrate intuitively the role of a analytical framework to analyze emergent phenomena in case of ACs, we consider an AC consisting of two dimensional polygonal tiles as molecules and the reaction rule is, if two colliding tiles fit each other on any of their
sides so that the new joined tile has no gap, the resultant (bigger) tile is included and both of the colliding tiles are removed, otherwise if they do not fit on any side then they are discarded. The colliding tiles are chosen at random.

Given this much we can observe and analyze the population of emerging tiles over a course of time and see if any interesting organization of molecules emerges or not. We can consider the possibility of the emergence of self replicating molecules or organizations. It can be argued that in this AC, self replication is not possible. This is evident when we analyze the reaction rules and then learn that the resultant tile is always different and bigger than the colliding tiles. In this conclusion it is implicitly assumed that self replication is defined as appearance of new tile, which is same in shape and size with either of the tiles participating in the reaction (either in a single step or in series of steps). But if we change the "meaning" of self-replication as only the replication of shape and do not consider the size, we can find example of tiles which result in bigger tile with same shape as one of the colliding tiles. This example highlights the significance of an analytical framework, in this case, the analysis of functional information associated with the tiles as per the reactions rules with respect to meaning of self replication (context) to conclusively determine whether self replication will emerge or not. There is more discussion on self-replication in the section 3.5.

Before we proceed to describe our initial proposal for this framework, we will review the two important known notions of information. They are Shannon’s Entropy of Information and Algorithmic Information. This will motivate us to make the point for the need of a new and broader notion of information.

2.3 Analysis of the Notions of Information

Two well known notions of information in computer science are Shannon’s Entropy notion based on coding theory and Algorithmic Information. Both of these, though, capture certain aspects of what we call information but not everything.

2.3.1 Shannon’s Information Entropy

In Shannon’s information theory [Shan48] the amount of information associated with any symbol is the logarithm of the probability of occurrence of that symbol in a message.

The Shannon’s entropy of a variable $X$ measured in bits is defined as

$$H(X) = -\sum_x P(x) \log_2 P(x)$$

where $P(x)$ is the probability that $X$ is in the state $x$, and $P \log_2 P$ is defined as 0 if $P = 0$. The joint entropy of variables $X_1, \ldots, X_n$ is then defined by

$$H(X_1, \ldots, X_n) = -\sum_{x_1} \ldots \sum_{x_n} P(x_1, \ldots, x_n) \log_2 P(x_1, \ldots, x_n)$$

The mutual information between two discrete random variables $X$ and $Y$ is defined to be

$$I(X;Y) = H(X) + H(Y) - H(X,Y)$$

bits, where $H(X)$ is the entropy of the random variable $X$ and $H(X,Y)$ is the joint entropy of these variables.
The Shannon’s notion of entropy is quite useful in certain aspects in molecular biology such as, mutual information as a measure of the information content of protein families, or statistical properties of genetic material [Yock92]. Still the basic problem is that Shannon’s entropy has nothing to do with the “meaning” of the message as Shannon explained in his original paper in the beginning itself [Shan48]. This absence of meaning in the Shannon’s notion of information makes a fundamental difference when we consider for example the genetic material. Precisely because significance of genetic material is only due to its characteristic functions inside a cell. These functional properties cannot be captured by this measure of entropy which is basically used when information is being transmitted through a channel between a sender and a receiver. In case of information with evolving entities even in pre-biotic evolution, what is important is the formation of information encoding mechanism such as genetic material and this sender, receiver and channel aspect does not arise directly. Still, when considering the communication aspect in our framework, this notion might be of some use.

2.3.2 Algorithmic Information

Algorithmic information is basically the size of the shortest program, which can produce the description of the object as binary string when simulated by a universal computing machine [Chait87]. This notion of information in algorithmic terms was motivated to define the notion of randomness precisely. For a natural number its algorithmic information is equal to its logarithm. Similarly, for any randomly chosen binary string, its expected algorithmic information is roughly equal to its length.

Though algorithmic information is quite useful when dealing with the structural or syntactical aspects of an object’s description, it does not capture the functional properties of the object. For example, two programs written as binary strings as input for a universal computer may have nearly the same algorithmic information but one program may behave be fundamentally different than the other on execution. Thus algorithmic information says nothing of the semantic aspect or the context based functional properties of the object. As another example there might be several molecular structures of high complexity which might have same algorithmic information due to their structures as typical genetic material but may not exhibit same properties when inside a cell as what genetic material exhibits.

This context based functional properties or the semantics specified by the context (environment) is something missing from the current analysis and demands clear formulation. As a remote analogy we can consider this as somewhat similar to program equivalence modulo finite execution steps, whereby two programs executing same way for finitely many steps or structures exhibiting similar reactions are considered equivalent. We consider finite time steps because the more general problem of program equivalence is undecidable and because in real terms it is only finitely many possibilities where an object is expected to function. Thus the presence of genetic code amounts to emergence of an specific kind of structure which can be analyzed correctly only when we consider the specific context based functional information associated with it. [Kupp90] has detailed discussion on the role of information in the origin of life.

Once properly defined this functional information can be evaluated from the structure of reaction rules itself, by computing the change of information from inputs to outputs. In [Sujuki03, Sujuki02] an information space is considered as a fundamental block for
analysis of evolution of complex form of life in artificial life systems. They even consider that presence of structure for programmable information is one of the necessary conditions for evolution of complexity.

2.4 Towards an Abstract Framework

Based upon the analysis of ACs and discussion on the relevance of “context based functional information”, we propose here an initial sketch for a new framework to study the emergent phenomenon such as emergence of self replication in molecules, emergence of hypercycles, metabolic networks, self organization and other life-like properties from a basic AC set-up in a unified way.

We identify three basic high level abstractions in our framework, viz., information, computation, and communication. These notions need to be further refined and clearly formalizes in the context of ACs and in general AL studies. These are discussed next.

Information Among the list of open problems in AL presented in [Bada00] the last problem is - Develop a theory of information processing, information flow, and information generation for evolving systems. Information in the framework will be a way to characterize and compare various structures for their relative functional or semantic aspects. In living systems, this information has very specific role of controlling the way various processes work and transmission of information after replication etc. We need to understand if an AC able to create information. Does “information processing” emerge by way of evolution? Again as noted in [Bada00] it is important to understand the interaction of objects with the environment in terms of information processing and information generation. From the discussion in the previous section on two of the known notions of information, Shannon’s Entropy and Algorithmic Information we know that these might not be adequate to capture completely the kind of information we are interested in.

Computation Extended Chruch - Turing thesis as proposed in [Rasm90] states that all natural processes are basically computational in nature or can be reduced in computational terms, although there can be fundamental differences in the actual model which nature might employ with the known models of computation (e.g., Turing machine, lambda calculus etc.) This essentially means that we can understand the problem of origin or life and complex forms in computational terms. This computational aspect is important because it can be used to understand the generation of information during the course of evolution under the effect of rule space. This way, if we assume that molecules are computational units and their interaction gives rise to new computational units, we can try to understand how the computational dynamics changes and under what conditions life-like forms and other relevant aspects emerge. Self-replication has already been demonstrated to be a computational process [Smi91]. Along the line of computation we can think of the organizational structures emerging in ACs as some kind of (distributed) computing structures and can analyze changes in their structures in terms computational power. Most importantly we expect that it is possibly a powerful computation process which gives rise to the emergence of new forms of information processing like genetic material.

Communication It is not clear if communication in the form of explicit signal passing happens in case of molecular reactions but we may try to capture selective chemical
bonding which is actually determined by geometrical configuration, bond strengths in a molecule, and other thermodynamic constraints using communication analogy. This communication could in turn be used by chemical metaphors for preferential interaction not explicitly defined by interaction rules. The communication pathways can be taken into consideration as a matter of efficiency of evolving of the organization and especially for distributed and collective information processing.

2.5 Discussion

Because of the differences in the basic formulation of various ACs resulting in quite different structures and nature of emergent phenomena, it is not easy to directly formulate the unified framework precisely. Therefore we adopt two broad strategies to achieve the goal, which can be termed as bottom up approach and top down approach.

**Inductive Approach.** This is the approach to formulate first the framework for specific ACs and then combine these individual formulations into more general formulation of the unified model.

To start with, a P system based Artificial Graph Chemistry, discussed in [agr], could be used initially for the formulation of this framework and to do experiments to refine and verify that further. Hence the first step is to carry out experiments with the P system based AC. If life-like structures are observed to be emerging, study the conditions leading to their emergence from the point of unified framework. This step will elaborate the possible principles of emergence of life and will assist in possible refinement and formulation of the framework.

In next step one could work towards generalizing this formulation with respect to essential features in major ACs. This can be done either by attempting to generalize this formulation and then verify it for other ACs or by formulating separately for other ACs and then combining them together to come to a more general formulation. Further experiments could be carried out to refine the formulation. In this approach the main problem is to select right ACs and then to understand them clearly to come to a formulation.

**Deductive Approach.** In this approach we aim to come to a generic formulation first in analytical way by analyzing the essential features of life-like emergent phenomena.

The computation theoretic framework based on cellular automata for self replication is one such example of this kind of top down approach [Smi91]. The quantitative analysis of ACs with self replicating structures is usually done using generic replicator-equations of population dynamics [JK98]. A replicator-equations for a population consisting of \( n \) species with relative frequencies \( x_1, x_2, \ldots, x_n \) is formally given by,

\[
\dot{x}_i = x_i(f_i(x) - \sum_{j=1}^{n} x_j f_j(x))
\]

where for each species \( i \), \( f_i \) describes the fitness of \( i \). These fitness functions are usually taken to be linear. \( x \) is a vector \( (x_1, x_2, \ldots, x_n) \).

As an another example of top down approach, we consider hypercycles, which are roughly the set of small self-replicating molecules where reaction of each molecule feeds the production of some other molecule in a cyclic fashion. This cyclic dependence of the self replicating molecules gives rise to bigger self replicating structures. The hyper cycles
were introduced and formally characterized using reactor flow equations in [Eigen79]. That characterization is general enough to capture any kind of population dynamics. Though again this is quantitative characterization and cannot be used to explain why hyper cycles actually emerge or whether they will emerge at all in an organization where new species keep emerging.

To take this approach further, we identify the following basic elements in emergence of self-replication in an AC set-up.

**Identity** - these are the most elementary entities of replication, that is, which self-replicate itself. Examples of individual cells in an multi-cellular organism are such examples. In real chemistry we notice that, though atoms are the basic components (of self-replicating entities), they do not self-replicate. Thus identification of these self-replicating entities is important to understand any level of self-organization. This is not easy always because there is no bound on the "size” or "type” of these replicating molecules. This might be the case that there are several hierarchies of self-replicating entities, each replicating on its level.

**Self-preservation** - this means structure is robust against perturbations and thus small changes in the structure cannot be taken for dissimilarity. Before talking about replication, the entities need to be able to preserve their own identity. How do we assign an identity to the entities that is preserved over time?

**Causality** Let us say a new entity appears somehow. How do we establish that the new entity arises from an existing entity? Only if we establish a causal relationship between the old and new entity, we would be able to talk about self-replication.

**Equivalence Relation** - This relation is used to correctly formulate the characteristics, which will be used to determine the presence of replication. To clarify the point, again consider the case of replicating cells, there not everything replicates itself during cell division, therefore similarity in overall chemical composition or equal cell sizes cannot be the basis of characterizing self-replication. In fact it is mainly genetic material which replicates during cell division and we treat it as cell replication.

A working equivalence relation can be functional equivalence using some measure of “context based functional information”, that is, if two structures can function the same way then they are treated equivalent. The problem, as we discussed in last section correct formulation of this information.

**Period of replication** - this is measured to find out after how many reaction steps, a self-replicating structure will replicate itself. In most of the simple cases it is just one reaction period, which means structures maintain and replicate themselves for each reaction. It need not to be the case for a larger self-replicating organization, which might involve gradual replication of its components across several reaction cycles.

As second step we will verify and refine this generic formulation based upon the experiments with individual ACs, for example to see whether this formulation can be used for analyzing the emerging structures in P system based AC.
3 Final Discussion

Objective of this section is to summarize main goals of the proposal and discuss the broader picture where these goals may fit in an AC research.

To summarize, we aim to develop a unified formal framework to characterize and classify symbolic ACs based upon three high level abstractions viz., information, computation and communication. This framework will be used to understand the aspect of information processing and computation in an AC environment.

There are two major approaches to develop the unified framework. The bottom-up or inductive approach is by formulating analytical framework for individual ACs and then combining them to more general one. Second top-down or deductive approach is to work for general formulation with later refinement and verification using actual AC set-ups.

ACs are basically designed to complement the main stream AL research. This is primarily because major AL studies presume the prior existence of basic structure of life-like entities and develop over them. This leaves the question of origin of these basic structures open and that is where ACs come into picture.

Because the main theme of AL research is to discover the possible biological principles which might be working independent of physical laws, AL studies mainly draw motivation from real-life biological phenomena. Theory of evolution based on random mutations and fitness based natural selection is one such source of motivation in many AL studies [Adami98]. Similarly ACs also draw motivation from real chemistry. The main conceptual motivation ACs borrow from real chemistries is not the actual chemical structures or reactions but the abstract concept that life originated as a result of complex dynamical interplay between the rule space consisting of reaction rules or semantics and the object space consisting of the molecules which react. This is what is the prime source of differences in various ACs in their definition and structures, since there is no such generic framework which can used by ACs to define the basic structure of molecules or reactions. Most often what is clear is only the end results, that is, an AC set up is expected to lead to the emergence of certain basic characteristics of life, e.g., self-replication, metabolism etc.

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