Design of a P System based Artificial Graph Chemistry

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Abstract

Artificial Chemistries (ACs) are symbolic chemical metaphors for the exploration of Artificial Life, with specific focus on the origin of life. In this work we define a P system based artificial graph chemistry to understand the principles leading to the evolution of life-like structures in an AC set up and to develop a unified framework to characterize and classify symbolic artificial chemistries by devising appropriate formalism to capture semantic and organizational information. An extension of P system is considered by associating probabilities with the rules providing the topological framework for the evolution of a labeled undirected graph based molecular reaction semantics.

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.

*Work done when author was in NUS (2002-2005).
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 nonliving 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 behavior 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 “neighborhood” 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 'λ', 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 flexibility 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 differential equations. Replicator equations of Lotka-Volterra type \[\text{[Font92, JK98]}\] 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 constructive 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 organizations. While level-0 organization consists of only self replicating molecules whose frequencies are modelled using replicator equations, level-1 organization has strong element 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 interdependent 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 counterpart. 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 calculus...
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 $\pi$ - 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 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 cellu-
lar 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 forge new bonds or break up can be fully modelled 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 neighboring 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 neighboring 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 membrane structures.

**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 P System based Artificial Graph Chemistry

In the previous section we reviewed some examples of ACs with discussion on their positive and negative aspects from the point of view of pre-biotic evolution of life ranging from the level of abstractions of essential molecular properties from real chemistry to the nature of emerging organizational structures.

In this section we will propose a new AC to address the problem of lack of structural abstraction in molecular structures and reaction rules. Again as discussed in the previous section topological constraints play significant role in emergence of certain phenomena in ACs, for example emergence of membrane type structure, which limits the scope of molecular interactions and promote local interactions. Nature of reaction rule space as well has fundamental effect on the possible emerging structures. We use extension of P system, explained next, to capture the spatial membrane type topology for our AC. This should enable us to understand better the role played by topological constraints in emergence of life-like structures. [Sujuki01] has discussion on use of P-system to model pre biotic phenomena with molecular structure and reaction rules as in case of ARMS (Section 1.2.2).

2.1 P System

G. Paun [Paun00] (ref [Paun02]) introduced membrane system as a model of parallel and distributed computation with “membrane” type structure. P system is a basic model of a mem-
brane systems with membranes arranged in a hierarchical structure, as in a cell, and processing multisets of symbol-objects.

**Definition**

The main components of a membrane system are the *membrane structure*, *multisets of objects*, and the *evolution rules*. A membrane structure describes the mutual relationship between membranes, the relations of adjacency, of being in and out.

Formally a membrane structure is defined as follows. Consider a context free language $D$ defined over the alphabet $\{[,]\}$ and generated by following the grammar

$$S \rightarrow \epsilon | [S] | SS$$

Then language $MS$ over alphabet $\{[,]\}$ is defined as

$$MS = [D]$$

that is, $MS$ consists of any string of correctly matching pair of parentheses $[, ]$ with a matching pair at the end. $[1[2][3][4][5][6][7]]$ is one such example where brackets are numbered (with subscripts) to match the correct pairing.

Let $\overline{MS}$ be the set of all equivalence classes of $MS$ with respect to reflexive and transitive closure of the relation $\sim$ defined over $MS$ such that for $x, y \in MS$, $x \sim y$ if and only if $x$ and $y$ can be made same when two pairs of parentheses which are not contained in each other are interchanged, together with their contents. The elements of $\overline{MS}$ are called *membrane structures*.

Each matching pair of parentheses is called a *membrane*. There is a unique external membrane called *skin*. For a membrane structure $\mu$, any closed space delimited by a membrane is called a *region* of $\mu$. Alternately if we consider a membrane structure as a directed unordered rooted tree then the depth of any membrane from the root (the skin) is called its *degree*. A membrane structure of degree $n$ contains $n$ regions, one associated with each membrane.

Consider $U$ as denumerable set of objects. Let $\mu$ be a membrane structure of degree $n(\geq 1)$, with the membranes labelled in a one to one manner, for instance, with the numbers from 1 to $n$. In this way, the regions of $\mu$ are also identified by the numbers from 1 to $n$. If a multiset $M_i : U \rightarrow N$ is associated with each region $i$ of $\mu$, $1 < i < n$, then we say that we have a *supercell*.

In other words a super-cell is defined as $(V, \mu, M_1, \ldots, M_n)$, where $V$ is an alphabet; its elements are called objects.

Super cell extended to a *P system* of degree $n; n \geq 1$, is a construct

$$\Pi = (V, \mu, M_1, \ldots, M_n, R_1, \ldots, R_n; i_0),$$

where:

(i) $\mu$ is a membrane structure of degree $n$, with the membranes and the regions labelled in a one to one manner with elements in a given set $\Lambda$, which can be assumed to be just $\{1, 2, \ldots, n\}$;

(ii) $M_i$, $1 \leq i \leq n$, are multisets over $V$ associated with the regions 1, 2, $\ldots$, $n$ of $\mu$;

(iv) $R_i$, $1 \leq i \leq n$, are finite sets of evolution rules over $V$. An evolution rule is of the form

$$u \rightarrow v,$$

where $u$ is a string over $V$ and $v = v' | v' \delta$, where $v'$ is a string over

$$(V \times \{\text{here, out}\}) \cup (V \times \{\text{in}_j|1 \leq j \leq n\}),$$

and $\delta$ is a special symbol not in $V$.

(v) $i_0$ is a number between 1 and $n$ which specifies the output membrane of $\Pi$.

The symbols *here, out, in}_j$, $1 \leq j \leq n$ are called *target commands* or *target indicators*. Length of $u$ in $u \rightarrow v$ is called the *radius* of the rule. These rules are explained in the next section.
Evolution of a P System

The above defined P system evolves as follows. Consider a rule $u \rightarrow v$ in a set $R_i$. We look to the region associated with the membrane $i$. If the objects mentioned by $u$, with the multiplicities specified by $u$, appear in $M_i$, then these objects can evolve according to the rule. The rule can be used only if it can use the objects in $u$. More precisely, we start to examine the rules nondeterministically and assign objects to them. A rule can be used only when there are enough copies of the objects as specified by the definition of the rule, left after application of other rules chosen non deterministically before this rule. Therefore, all objects to which a rule can be applied must be the subject of a rule application. All objects in $u$ are consumed by using the rule $u \rightarrow v$, that is, the multiset identified by $u$ is subtracted from $M_i$.

The result of using the rule is determined by $v$. If an object appears in $v$ in a pair $(a, \text{here})$, then it will remain in the same region $i$. If an object appears in $v$ in a pair $(a, \text{out})$, then $a$ will exit the membrane $i$ and will become an element of the region immediately outside it (thus, it will be adjacent to the membrane $i$ from which it was expelled). In this way, it is possible that an object leaves the supercell itself: if it goes outside the skin of the supercell, then it never comes back. If an object appears in a pair $(a, \text{in}_q)$, then $a$ will be added to the multiset $M_q$, providing that $a$ is adjacent to the membrane $q$. If $(a, \text{in}_q)$ appears in $v$ and the membrane $q$ is not one of the membranes delimiting “from below” the region $i$, then the application of the rule is not allowed.

If the symbol $\delta$ appears in $v$, then the membrane $i$ is removed (said dissolved) and at the same time the set of rules $R_i$ is removed. The multiset $M_i$ is added (in the sense of multisets union) to the multiset associated with the region which was immediately external to the membrane $i$. We do not allow the dissolving of the skin, the outermost membrane because this means that the supercell is lost, we do no longer have a correct configuration of the system.

A P system evolves as a whole unit with all possible applications of rules at the same time. That means, all the operations are done in parallel, for all possible applicable rules $u \rightarrow v$, for all occurrences of multisets specified by $u$ in the region associated with the rule and all regions are considered at the same time.

If there are rules in a supercell system $\Pi$ with the radius at least two, then the system is said to be cooperative; in the opposite case, it is called noncooperative. A system is said to be catalytic if there are certain objects $c_1, \ldots, c_n$ specified in advance, called catalysts, such that the rules of the system are either of the form $a \rightarrow v$, or of the form $c_i a \rightarrow c_i v$, where $a$ is a noncatalysts object and $v$ contains no catalyst. (So, the only cooperative rules involve catalysts, which are reproduced by the rule application, and left in the same place. There are no rules for the separate evolution of catalysts.

Biological analogy of Super Cell system. The mode of evolving of objects in a supercell provided with evolution rules as described above can be interpreted in the following - idealized - biochemical way. We have an organism, delimited by a skin (the skin membrane). Inside, there are free molecules, organized hierarchically. The molecules float randomly in the “cytoplasmic liquid” of each membrane. Under specific conditions, the molecules evolve, alone or with the help of certain catalysts. This is done in parallel, synchronously for all molecules. The new molecules can remain in the same region where they have appeared, or can pass through the membranes delimiting this space, selectively. Some reactions not only modify molecules, but also break membranes. When a membrane is broken, the molecules previously placed inside it will remain free in the larger space newly created, but the evolution rules of the former membrane are lost. The assumption is that the reaction conditions from the previous membrane are modified by the disparition of the membrane and in the newly created space, only the rules specific to this space can act. When the external membrane is broken, then the organism ceases to exist.
2.2 Design of the Chemistry

Having defined the basic concepts of P System, we will now discuss the basic components of the P system based artificial graph chemistry (AGC) by defining an extension of the P System and the molecules as labelled graph.

2.2.1 A Probabilistic Extension of P System

We extend a P system by associating probabilities with rules. These probabilities can be interpreted as relative frequencies of rule applications on the molecules over the course of evolution. This happens in real chemistries as well, where in a large pool of several chemical compounds (which was supposedly the situation in pre-biotic world) the reactions which take place are largely random and possibly only affected by the neighborhood of a molecule to some extent. The advantage of associating probabilities is to capture more clearly how relative frequencies of application of certain rules affects the kind of emerging structure in later states of evolution. The main role of this extension comes into picture when an AC on P system is evolved. Under this scheme molecules will be distributed in regions and during the long course of evolution of these regions and populations inside them, reaction rules are applied based upon the probabilities associated with them. This differs from the original static structure of rule space and resemble more like naturally occurring processes.

Another main modification on the basic definition of P system is that to suit an AC set up, we modify the basic P system with multisets of symbols and rewriting rules to a P system with multisets of molecules with the reaction rules. The structure of molecules with reaction semantics is presented next.

2.2.2 Molecular Structure Representation and Reaction Semantics

We represent a molecule as undirected labelled graph and develop reaction semantics to represent molecular reactions. The main motivation behind the selection of a graph comes from the observation on the lack of the structural abstractions in ACs like lambda chemistry, chemical abstract machine etc.

Formally a molecule is represented as a *undirected labelled graph* $G = (V, E)$ with mapping $w : E \rightarrow R$ associating weights with edges $e \in E$, where $R$ is the set of real numbers. $G$ can also be represented as weighted symmetric matrix. Each node of the graph can be thought of as an “atom” and an edge as “chemical bond” such that label/weight associated with an edge determines the relative strength of the bond between these atoms. These weights will be used to decide the possible structural changes (substitution etc) during reactions.

Each reaction rule is a *mapping* from a subset of molecules called *reactants* to another subset of molecules called *products*. In other words a reaction can be thought of as a *n*-ary ($n \geq 2$) *graph transformation operator*. Reactions are constrained by *guards*, which are used to capture the thermodynamic conditions controlling the real chemical reactions.

We can consider two cases. In the first case the set of possible reaction rules is fixed and determined priori. Only the guards are evaluated later. Secondly we can have some generic laws controlling the nature of possible reactions, which actually happens in the case of real world, where concentration, temperature, pressure, velocity and other kinetic properties determine what will be the result of the reactions. We need to understand how different choices of these reaction rules affect the information processing, computational structure and what kind of organizational structures emerge during the course of evolution.

Initially we choose no specific spatial structure on distribution of molecules. Thus in essence each molecule can potentially react with any other molecule. The dynamics is controlled stochastically, that is, we randomly select the rules and see if they can be carried out, if yes, we select random concentration of the molecules for reaction. Though we have no explicit spatial structure but we want that not all the reactants get over with single rule application, so we choose
this strategy of choice of random concentrations. We replace the reactant molecules with the 
products in the reactor. Like CHAM we consider the heating and the cooling rules, which re-
result in braking up of the molecule-graph into smaller components, and joining of smaller graphs 
respectively.

A spatial structure can be imposed on the molecules using our extended probabilistic P-
system, where sets of molecules will be encapsulated inside membranes for local reactions, with 
possible migration of molecules across membranes.

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 defined a probabilistic P system based AGC with the aim of understanding 
the principles leading to the evolution of life-like structures in an AC set up. We need to explore 
it further by carrying out detailed experiments with varying parameters such as definitions of 
reaction rules, presence and nature of topological constraints, distribution of molecules, and 
population dynamics.

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 be 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.

This is where this proposal is expected to contribute most by explaining issues like what 
are the fundamental ingredients of an AC set up which will lead to interesting emergent or-
ganizations? Can these ingredients be related to information and/or computation? Is an AC 
able to create information? Does “information processing” emerge by way of evolution? Can 
molecules be interpreted as computational units which evolve in computational power during 
the course of evolution of an AC? What kind of complex computational structures emerge and 
how? Has communication any role to play in origin of organizational structures? What kind of 
limits one can put on the basis of the basic structure defined in an AC on the possible level and 
type emerging organizations? Thus as conclusion we expect that the proposal will contribute 
significantly in the research on ACs.

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