Building Virtual Ecosystems from Artificial Chemistry

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Abstract. This paper adopts an interdisciplinary view of the significant elements of ecosystems and the methods by which these might be simulated to explore theoretical issues of relevance to Artificial Life and Ecology. Artificial Life has largely been concerned with evolutionary ecosystems of agents in trivial environments. Ecology commonly produces models of specific habitats and organism populations unsuited to general exploration of theoretical issues. We propose that limitations of the simulations in these disciplines can be overcome by simulating ecosystems from the level of artificial chemistry. We demonstrate the approach's feasibility by describing several virtual organisms represented at this level. The organisms automatically adopt trophic levels, generate energy from chemical bonds and transform material elements in the process. Virtual organisms may interact with one another and their abiotic environment using the same chemistry. Biosynthesis and decay may also be simulated through this mechanism.

1 Introduction

> "This paper discusses a computer model of living organisms and the **ecology** they exist in called PolyWorld." — Yaeger, 1992
>
> "The memory, the CPU, and the computer's operating system are viewed as elements of the **'abiotic' environment**." — Ray, 1991
>
> "A hierarchical computer program has been developed with genetic, organismic and population levels embedded in an **ecosystem**." — Conrad and Pattee, 1970

The terms *ecology*, *ecosystem* and *environment* have been employed extensively within the field of Artificial Life to refer to simulations. To date, virtual ecosystems (the authors' preferred terminology) have been utilized primarily for general studies of evolutionary processes within Artificial Life. For instance, Ray's *Tierra* [1] and Yaeger's *Polyworld* [2] are two early systems that fall into this category. Epstein and Axtell have used a similar system, *Sugarscape*, to study the emergence of social behaviour [3]. Dorin has employed evolutionary virtual ecosystems for aesthetic purposes [4]. In the field of Ecology, individual-based models are more typically non-evolutionary and represent particular, real species and landscapes [5]. The aim of these ecological models is to shed light on specific ecologies where spatially explicit models are required or where the phenomenon under study emerges through the heterogeneity of a population.

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The different agendas of Artificial Life and Ecology have to some extent determined the path through which virtual ecosystems in each field have been developed. This paper suggests an approach that melds the interests of Artificial Life researchers and Ecologists. The aim is to demonstrate that a simple artificial chemistry can support the existence of autotrophic and heterotrophic organisms, their interactions with one another and with the abiotic environment. A virtual ecosystem emergent from the simulation can then incorporate natural cycles of matter and energy between organisms of different trophic levels and their abiotic environment. The approach offers an alternative conceptualization of the virtual ecosystem that incorporates the benefits of artificial chemistry and Ecology's individual-based simulations of sub-evolutionary time scales.

The remainder of section 1 explains the significant features of the approach. Section 2 introduces one means of building such a simulation. Section 3 details various organism types and their operation based in the artificial chemistry.

1.1 The Ecosystem

The concept of the ecosystem first appeared in an article by ecologist Tansley [6], whose interest was in the relations amongst organisms and between organisms and their environment. He debated the merits of applying the term *organism* to communities of creatures and their physical habitat. Tansley preferred to refer to this whole as a "system", or to be specific, an *ecosystem*.

Insilico there is no theoretical reason to distinguish between biota and an abiotic environment unless the programmer wishes it. However, there are often practical reasons for making such a distinction — it has thus far proven difficult to simulate multi-level dynamical hierarchies that could be recognized as simulations of chemicals, organisms and ecosystems, although some examples exist (for instance [7]).

A cursory review of the literature in Artificial Life reveals that by convention we refer to agents with sensory capabilities, internal decision-making and resultant behaviours (such as reproduction) as model *organisms*. The abiotic environment is often understood as a space of some kind, often homogeneous, with rules dictating its change of state, its impact on the organisms and vice-versa. This space may include passive "abiotic furniture" (such as grains of sand or sugar [3]) that agents manipulate, thereby introducing an element of heterogeneity to the landscape. The abiotic furniture and the organisms are not usually implemented using the same data-structures. They are treated as "different stuff" within the simulation framework and in the analysis of results. This works acceptably in Artificial Life, as it does in Ecology, where population dynamics is a frequent subject of study. However, this view has left Artificial Life with a concept of "ecosystem" that differs from that held in Ecology regarding the significance of biogeochemical cycles — cycles of the elements through organisms and environment. Erasing the distinction in simulation between organism and environment allows a model to explore the exchange and transformation of matter and energy.

1.2 The Significance of the Environment

An organism-centric view of the universe defines the interests of Biology. At least since Aristotle, the study of autonomous creatures has dominated over the study of their habitat. In a homocentric circle from dust to dust, "Humanity" (organized dust) would sit at the pinnacle of the circle and "Environment" (disorganized dust) would be relegated to a location far beneath our feet. Perhaps the Fates would drive Time's hand around this circle.

We might nowadays reject the homocentric subjugation and exploitation of the universe by placing organisms (including humans) and the abiotic environment on either side of a more balanced circle. Nevertheless, Artificial Life focuses attention on virtual organisms with little direct study into the significance of their habitats. How many publications model agents trivially in order to study the impact of different sophisticated environmental simulations?

Within Artificial Life this bias is also evident in the field's mission to study "life-as-it-could-be". This is generally understood to refer specifically to organisms, not specifically to their habitats (although sometimes these briefly enter the equation). Within the sub-discipline of Artificial Chemistry researchers ponder the properties of basic building blocks that give rise to virtual organisms [8] or autopoietic entities [9]. Here too the research is organism-centric. The study of the environment has been largely neglected even in Artificial Life! There is nothing surprising about the desire of researchers to comprehend what is arguably the universe's most significant phenomenon. Nevertheless a wider perspective is also beneficial.

1.3 Cycles of Biosynthesis and Decay

An undergraduate level Biology text will explain that ecosystems are significant for their cyclic transformation of elements (carbon, hydrogen, oxygen, nitrogen etc.) and that nearly half of the chemical elements participate in such biogeochemical cycles (e.g. [10, p1248]). As long as the virtual ecosystems of Artificial Life maintain differences between biota and abiotic environment in their underlying implementation, our models will not shed much light on these cycles.

In many simulations, organisms are born and roam their environment to gain energy or resources. However virtual organisms rarely acquire matter from the environment to transform it into biomass through a simulated chemical process that expels waste. Simulated organisms often die, but they seldom *rot* to return materials to their environment. Few model ecosystems incorporate decomposers of biomass although there are some examples [11, 12]. The absence of these phenomena from many models stands in contrast to the fundamental importance granted them in elementary Ecology. A model that incorporates these phenomena will be useful for exploring the interactions of organisms at different trophic levels, their impact on the environment and their requirements for energy and material resources. In order to demonstrate the feasibility of the approach, the following section details one manner in which a simulation of this type may be constructed.

2 Cyclic Ecosystem Simulation

The basis of a virtual ecosystem that simulates all of the elements described above must be the common building block of the abiotic environment and the organism, namely the molecule or its atomic components. Molecules will need to be assembled and disassembled, and energy released or captured in the process. Such artificial chemistries are not new but to date nobody has managed to construct metabolising, replicating structures capable of open-ended evolution — an open problem [13]. Presently we hard-wire some of these processes rather than expecting them to emerge.

One approach is to focus on open-ended evolution and to construct models of self-replicating cells that do not store energy in chemical bonds [7]. In our paper we instead stress the importance of the presence of autotrophs (organisms that produce their own food) and heterotrophs (organisms that consume organic materials produced by other organisms). In particular, the model we propose naturally supports the existence of photosynthetic autotrophs, chemosynthetic autotrophs and decomposers by modelling the storage of chemical energy and its release. In this way the concept of an organism, its energy supply and its interactions with the abiotic environment may emerge from artificial chemistry.

The model is designed to support the interactions between various organism types and the abiotic environment as emergent from the interactions of "dumb" molecules. Agent behaviour need not be hard-wired. In fact, any distinction between agent and molecule is absent from the simulation implementation. Agents emerge in the model as large dynamic "molecules" that transform energy and matter. [1]

2.1 Artificial Chemistry

The system is based upon a set of hypothetical two-dimensional, mobile, non-intersecting, square "atoms" placed on a grid. Atoms may bond to neighbours at their edges by sharing virtual electrons, according to the rules of a virtual chemistry of covalent bonding. Each atom type has a set of electrons in one or more shells. The number of electrons and the fullness of an atom's outer shell determine the bonds in which the atom can participate (for details, see [14]). In all cases, some energy threshold is required to initiate (or break) a bond, and the result of bonding (or breaking a bond) is either the capture of some amount of energy or its release. Additionally, for each type of bond, parameters of the simulation determine the probability of bonds forming or breaking given the availability of the threshold energy.

A catalyst is said to be present at a reaction site when an atom involved in the reaction neighbours an atom of a designated catalyst-type. To support the existence of our virtual organisms, four types of catalyst are required. A chlorophyll-like catalyst is needed that, in the presence of sunlight, manufactures a complex molecule equivalent to sugar. An enzyme that breaks down this sugar, releasing the chemical energy stored in its bond is also needed. For simplicity and clarity, separate enzymes that decompose "organic" bonds that are not sugar and "inorganic" bonds may be added. Further details are given in section 3.

[1] Our model is not concerned with reproduction, evolution or the self-assembly of organisms.

Energy that is released during a reaction is distributed throughout any continuous atomic structure that contacts directly or indirectly (through intermediate neighbours) the reaction site. This energy is available for making or breaking chemical bonds by the atoms that receive it.

2.2 A Simulation Time-Step

The simulation progresses in discrete time-steps. At each step, for each atom, it must be determined stochastically whether each bond should break or join based on the site-types, the presence of catalysts, the availability of energy and the probabilities for bonding. Energy released during a reaction is totalled in each neighbourhood of connected atoms for use in that time-step by reactions that absorb energy. A reaction that requires energy to be expended can only occur if the neighbourhood of atoms involved has accumulated sufficient energy. Reactions occur in random order, consuming or contributing energy to and from the total amount available in their neighbourhood. A reaction that requires more energy than is available cannot proceed. Energy released from a chemical bond must be used in that time-step or it is released in non-recoverable form. The only way energy can be stored is in complex molecules. Sunlight is incident on all atoms at a rate governed by a parameterized sine function for use by the chlorophyll-like catalyst during photosynthesis (section 2.1).

In addition to stochastically determined bonding, within a time-step atoms may be moved one square on the grid in a random direction or they may remain stationary. Bonded atoms (forming molecules) are moved identically to preserve their topology. Collisions are not permitted.

3 Constructing Virtual Organisms from Artificial Chemistry

Our simple artificial chemistry supports the existence of a complete simulated ecosystem of photosynthetic and chemosynthetic autotrophs, heterotrophs (including decomposers) and their abiotic environment. Below we detail the biologically inspired construction of each of these organism types and explain its behaviour. The model obviously abstracts much of the detail of real systems for reasons of practicality.

3.1 The Abiotic Environment

The abiotic environment consists of the same molecules and atoms as constitute the simulation's organisms. Their bond structure and context enables us to label molecules as inorganic or organic, as a component of a metabolic system or as abiotic. Thus the "abiotic environment" is the set of atoms and molecules that are not bonded to a structure identified as an organism.

The abiotic environment consists of virtual atoms from the set {A, B, C, O}. Atoms may also be enzymes for sugar decomposition (break A-B bonds), biomass decomposition (break C-C bonds) or chlorophyll for sugar construction (make A-B

bonds, break A-O and B-O bonds). The probabilities for these significant reactions are given in the simplified reaction table 1.

In order to sustain the required organism forms, the various reactions detailed in the sections below must be supported. Only bonding possibilities of relevance to the discussion are described even though other bonds may also be supported. A line between tiles in the diagrams below indicates a bond between the atoms these represent. Catalysts are labelled *Enz* (enzyme) or more specifically *Chl* (chlorophyll).

Bond	**Make probability**	**Break probability**	**Make probability (catalyst)**	**Break probability (catalyst)**	**Bond energy**
A-B	low	low	high (chl)	high (enzAB)	- high
C-C	moderate	low	—	high (enzCC)	- low
A-O	high	low	—	high (chl, enzAO)	+ low
B-O	high	low	—	high (chl, enzBO)	+ low
C-O	low	moderate	high (enzCC)	—	+ low

Table 1. Simplified reaction table. Bond energy must be supplied to break a specified bond and is released when the bond is made. (Negative bond energy values indicate a release of energy when a bond breaks and energy must be supplied to make the bond.)

3.1.1 Photosynthesis

The process of photosynthesis constructs sugar molecules from water and carbon dioxide, releasing oxygen and water. It requires the presence of the catalyst chlorophyll and incident sunlight. In our virtual chemistry the reaction is represented abstractly as:

$$AO + BO \text{ —(chlorophyll \& sunlight)—> } AB + 2O$$

Reactants A and B may be presented to the catalyst bonded to O atoms or free. The process of photosynthesis may be represented in many potential atom arrangements. An example is given in figure 2.

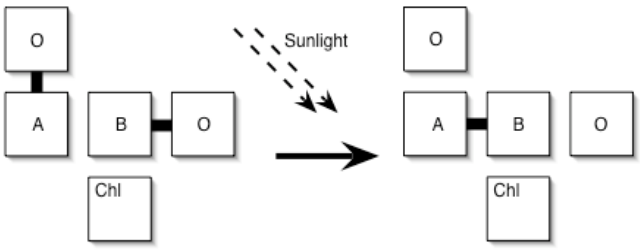

Figure 2. *Virtual photosynthesis* breaks A-O and B-O bonds (on the left of the figure) to manufacture an A-B molecule (on the right) employing a chlorophyll catalyst and sunlight.

3.1.2 Respiration

Real sugar molecules may be broken down in a process of respiration to release energy. The process utilizes oxygen and an enzyme to break down the sugar. Carbon dioxide and water are released. In our virtual chemistry the reaction is represented abstractly:

$$O + AB \ —(enzyme)—> A + BO + energy$$

An example respiration reaction is given in figure 3.

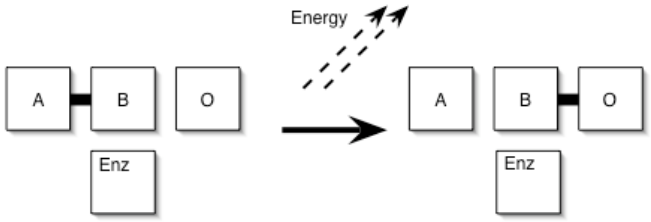

Figure 3. *Virtual respiration* breaks an A-B bond (on the left of the figure), employing an enzyme and releasing energy, A and B-O (on the right).

3.1.3 Biosynthesis

Organisms are able to add to their biomass by constructing bio-molecules from those they ingest. Growth occurs when a structure binds to atoms employing a reaction that requires energy. These bonds would not normally form in the absence of the energy required to create them (or the presence of a suitable catalyst). Such bonds may also break down spontaneously with probabilities as indicated in table 1. Hence an "organic" structure formed of these bonds must produce sufficient energy to sustain itself against natural decay by rebuilding broken bonds and by adding new material in a breach. When an organic bond is broken energy is released into the neighbouring structure. The amount that may be captured by a particular neighbouring atom will be insufficient to remake the bond instantaneously without an additional energy source. In our virtual chemistry the biosynthesis reaction is represented abstractly:

$$C + C \ —(energy)—> C_2$$

One possible configuration for the biosynthesis reaction is depicted in figure 4.

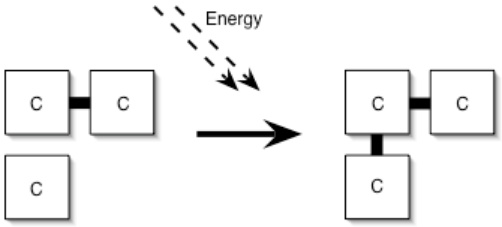

Figure 4. *Virtual biosynthesis* forms C-C bonds by consuming energy.

3.2 Photosynthetic Autotroph

A photosynthetic autotroph requires chlorophyll, an enzyme to decompose sugar and possibly a space in which to manufacture and store it. One structure suited to this role is given in figure 5. Countless variations on this design are possible but not all

will capture the sugar molecules within a vacuole (cavity). They may survive nevertheless if they maintain sufficient sugar concentration in their vicinity.

In the design presented, one internal wall of the vacuole anchors chlorophyll. Any A-O and B-O molecules that contact it will be converted into sugar but remain trapped. By chance an A-B molecule may later touch the opposite enzyme-laced wall where it will participate in respiration, releasing energy through the structure and allowing biosynthesis.

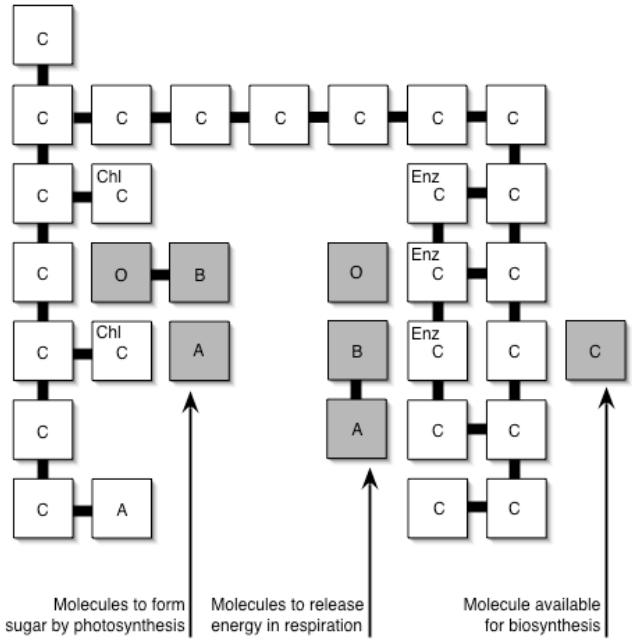

Figure 5. *Photosynthetic autotroph.*

3.3 Chemosynthetic Autotroph

A chemosynthetic autotroph generates its energy from inorganic molecules without the need for sunlight. In the chemical system described, one way to achieve this is by obtaining free O atoms and binding them to available A or B atoms. Given the natural affinity of A and B for O in the model, suitable atoms may be scarce unless a catalyst is employed to split A-O and B-O. The elements may then rejoin against the surface of the structure. In this case almost any structure containing a suitable catalyst on its surface would suffice in the role.

3.4 Heterotroph

A heterotroph in the present model breaks down A-B sugars produced by other organisms using an enzyme. Alternatively, a heterotroph may act as a decomposer if it possesses a catalyst to break down the C-C bonds of another structure. This catalyst

must be isolated from its own organic C-C structure. One way to achieve this is with an intermediate O atom bonded to C with the aid of a catalyst (figure 6).

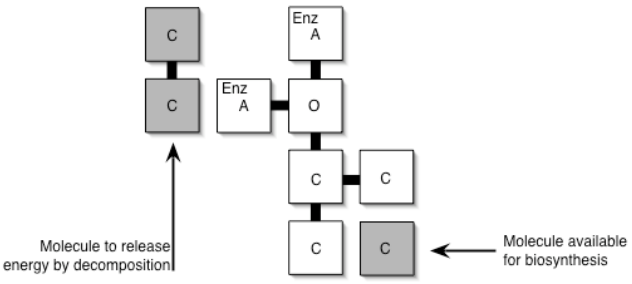

Figure 6. *Decomposer.*

4 Conclusions and Future Work

At the time of writing, a simulation run with all organism types present simultaneously remains to be performed. Since each is based upon the same set of chemical rules, at least in principle there is nothing preventing this from being successful. In the future we hope to adjust the chemical rules to facilitate the self-assembly and eventually, the replication and evolution of structures within the virtual ecosystem.

The host of organism structures presented here demonstrates the feasibility of constructing a complete virtual ecosystem from even a simple artificial chemistry in which organisms: emerge from the same abiotic elements as their environment; transform these elements in simulated biogeochemical cycles; acquire energy from chemical bonds; produce waste products and utilize the waste and biomass of other organisms.

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