View metadata, citation and similar papers at core.ac.uk
brought to you by CORE
provided by Repositório Aberto da Universidade do Porto

A biochemistry-inspired artificial chemistry: LAC

José A. Pereira

***Abstract*—A computational artificial chemistry (AC) system, called LAC, was developed bearing in mind the major biochemistry principles. Basic elements may be interpreted as small carbon molecules capable of bonding by nucleophilic substitution or nucleophilic addition. Reactions similar to hydrolysis and oxidation-reduction complete the present set of LAC site interaction rules. Reaction extension is governed by artificial thermodynamic principles and the reaction rate is controlled by specific catalysts made of the same kind of basic elements they act upon. The preliminary results of LAC experiments show the ability to mimic enzyme regulation and oscillatory reactions.**

***Index Terms*—Artificial chemistry, catalysis, Lotka-Volterra mechanism, oscillating reactions.**

I. Introduction

Last century's breakthrough on biochemistry research, leading to an in-depth knowledge of cell's molecular organization, coincided with the development of new epistemological and formal approaches to explain the phenomenon of life, from Erwin Schrödinger's 1944 text "What is life" to the self-reproducing automata of John von Newmann [1], the Universal Turing Machines [2], Hofstadter's Typogenetics [3] and the autopoiesis theory of Maturana, Varela and Uribe [4]. The autopoiesis theory was perhaps the first wide-range attempt to develop formal criteria to generally define living systems. In this theory life is a system property, characterized by an organized component production network that also includes a physical boundary that individualizes it. This organization is operationally closed, depending on a number of specific internal relational constraints and it has the special ability of reproducing itself. Autopoiesis is a convenient guiding framework to use in the development of computational artificial life and it is applicable to an artificial chemistry setup [4, 5].

A variety of computational AC approaches have been used to investigate the fundamental aspects of living systems, reviewed in [6] and more recently analysed for some cases in [7]. To design an AC system it is necessary to decide on the nature of its three general components: the basic elements set, the set of rules that define interactions between elements and an algorithm for the time evolution of the whole system in a space. In some cases the criteria for the design of the AC components are purely abstract but in other cases the essential features of a preexisting system inspire the creation of the AC model components so that some isomorphism can be established, giving a more precise meaning to, and a straightforward interpretation of, the results [3]. As we prefer the latter approach, our aim was to develop an artificial chemistry closely inspired in the basic principles of chemistry and of biochemistry, that we called LAC, making as many parallels as possible to biological molecules functions and the general cell metabolic strategy. Although the autopoiesis theory has a formulation independent of thermodynamical criteria the question of energy was recognized as essential for the development of LAC and was addressed quantitatively.

Manuscript received August 29, 2005.

J. A. Pereira is with the Universidade do Porto at ICBAS - Instituto de Ciências Biomédicas de Abel Salazar, Largo Prof. Abel Salazar, 2, 4099-003 Porto, Portugal (phone: +351 222 062 288; fax: +351 222 062 232; e-mail: jpereira@icbas.up.pt).

II. Specifications for LAC

A. Basic elements

The basic elements should not represent anything more complex than a macromolecule although the small molecule level or the atom level would be better because it provides a finer description. Also, in biochemistry the shape of molecules is a most important feature because the whole cellular organization depends on specific interactions selected by molecular recognition. The aggregates of the basic elements, or compounds, should therefore be represented by some kind of data structure bearing interconnecting flags and internal coordinates for each element, like a simplified molecular graph [8], and should be recognized by its shape using pattern matching. This can be a source of novelty, in the sense defined in [9], if new shapes are interpreted by an AC system algorithm as corresponding to new functions. Such genotype-phenotype relationship insures closure between (bottom-up) compound construction and (top-down) chemical activity, in line with the concepts of self-reproducing automata or Turing machines.

B. Reaction rules

Still with biochemistry in mind, the LAC reaction rules have to account for at least two types of general interactions: