Biochemically-Inspired Emergent Computation

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1 Artificial Chemistries for Pervasive Adaptation

Pervasive Adaptation software systems are expected to exhibit life-like properties such as robust operation in uncertain environments, adaptive immunity against foreign attackers, self-maintenance, and so on. The traditional software design model based on top-down human engineering fails in this context, where new, bottom-up *emergent computation* [1, 2] techniques seem more appropriate.

Since chemistry and biochemistry are the basis of life, *Artificial Chemistries* [3] and *Artificial Biochemistries* [4] stand out as natural ways to model such bottom-up life-like software. However, understanding and harnessing the power of emergent behavior in such complex systems is difficult. This position statement highlights some potentially fruitful research directions towards this goal. We advocate that an important research goal within such bottom-up approach is to construct systems able to achieve automatic transitions from lower levels of complexity to higher ones.

2 Towards Life-Like Biochemically-Inspired Software

A bottom-up approach to software construction using artificial (bio-)chemistries would necessarily start at the microscopic level of elementary molecules, and then move up in complexity, to cause molecules to organize into autocatalytic reaction networks forming primitive metabolisms [5], then into protocells [6], and later into more complex cellular structures including a genome and a genetic regulatory network (GRN). The cells would then organize into multicellular organisms relying on morphogenetic mechanisms for building complex structures and dividing tasks among its constituent elements. Some of the cells in such a virtual organism could differentiate into an artificial immune system (AIS) to protect the organism from external aggressions. Several bio-inspired techniques covering each of these complexity levels have been proposed. However, little is known about how the transition from a lower level to an upper one can be achieved in an artificial system in an emergent way. The benefit of a system exhibiting such

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autonomous complexity growth behavior would be *open ended evolution*, leading to continuous and unlimited adaptation potential.

We now briefly discuss some of these levels, and some research issues related to their transitions to upper levels, relating the discussion with our own research experience. We focus on the lower levels that are the foundations for the upper ones, and are more closely related to our experience.

At the bottom level of individual molecules, computation can be performed *in vitro* by encoding information within molecules as in DNA Computing, via concentrations of molecules, or via the propagation of waves of chemicals. Several *in silico* algorithms inspired by chemistry can be found in literature [3]. In [7] we proposed a chemically-inspired technique for self-healing software based on *autocatalytic quines*, self-replicating program fragments that react together to perform some computation and to reproduce. The bimolecular interactions in this model lead to a "survival of the common" outcome, which has two consequences: it makes the population resistant to invasion, conferring an immunity to attacks and harmful mutants; but it also shows poor evolutionary capabilities, any potential improvement being quickly washed out. A transition to an upper level of organization is therefore difficult to achieve with such system.

In [8] we proposed an energy model to be used for computations with artificial chemistries. We showed that this model is able to control the otherwise spontaneous elongation of autocatalytic quine strings. Moreover, clusters of cooperating quines exhibiting controlled and localized autocatalytic activity emerged under the right amount of energy inflow. In [9], we use a similar energy model to obtain *catalytic search*, a new optimization algorithm that makes use of the phenomenon of *catalytic focusing* described in [5] to steer the flow of chemical reactions towards those reactions leading to better-fit products. This could be a step in the direction of coupling the emergence of self-maintaining reaction networks with the computation of products that are fit for a given task. Moreover it could potentially exhibit a transition from a catalytic to a self-reproducing model that could lead to evolution, although we have not been able to demonstrate this yet.

The transition from chemical networks to cells is a difficult one, related to the origins of life and the emergence of protocell structures such as the *chemoton* [10]. The use of such cellular structures for computation is definitely worth further exploration. Once a basic cellular structure is there, the transition to a multicellular level requires the ability of cells to communicate via signalling mechanisms, to process these signals inside the cell via gene regulation networks, and to use these signals for pattern formation in a morphogenetic process. Recently [11], we have evaluated the robustness of specific morphogenetic algorithms, which can be regarded as another example of chemically-inspired algorithms with self-healing properties.

Finally, combining the lowest with the upper levels, the quines from [7] have been applied in [12] to devise an AIS in an artificial chemistry context.

3 Research Agenda and Outlook

The investigation of transition steps from one level of complexity to the next is definitely an important item in the agenda towards open-ended evolutionary systems capable of unlimited adaptation. In biology the transition mechanisms are also fundamental and not entirely understood [13]. Each transition stage can be studied independently. Currently, we are focusing on the first one: how to design an artificial chemistry that can perform intended computations and at the same time move towards higher levels of complexity when needed.

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