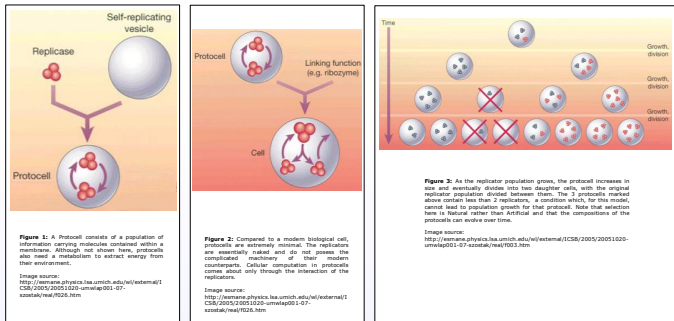


GOAL OF WORK PRESENTED IN THIS POSTER

We are investigating the building of ProtoCells, in silico, using a simplified Classifier System to provide the molecular dynamics. We propose that this classifier system is capable of minimal chemical computation.

INTRODUCTION

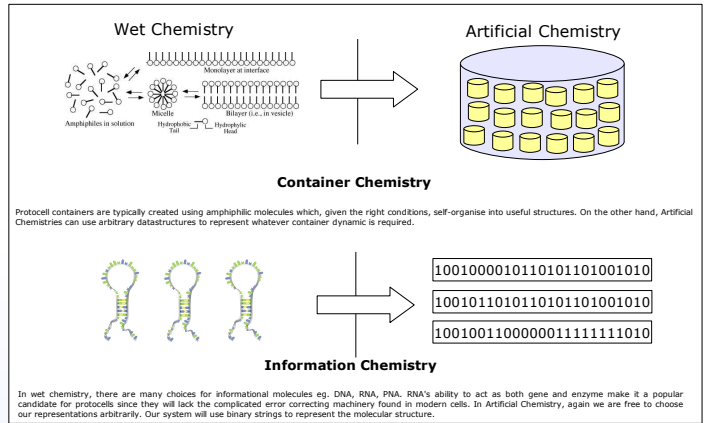
- Other than the complex networks of neurons in the Human Brain, no other biological system is known to be capable of the kind of numerical calculations that we associate with electronic computers.
- Living systems can be thought of as examples of chemical computers performing tasks such as:
 - Cellular chemotaxis,
 - Cell-cycle control,
 - Gene regulation and cognition.
- Such chemical computers may exhibit desirable properties like robustness, the ability to self-repair and constant adaptation to their specific problem domain via Darwinian Natural Selection.
- Chemical or molecular computers are essentially analog computers, precisely designed to model the operation of a target dynamical system by creating an "analogous" system which shares the same dynamics.
- They are composed of microscopic rather than macroscopic components. In terms of this research, we will attempt to build artificial **protocells**, in silico.
- Our future research will examine the kinds of problems that chemical computers are suited to dealing with and also explore new ways to "program" these new computing devices.
- We will focus our attentions on the minimum capacity of protocells to carry out information processing tasks.



BUILDING ARTIFICIAL PROTOCELLS

Research into building ProtoCells is happening both in **wetlab** chemistry and also in **software based artificial chemistry**.

- The wetlab approach to building protocells involves:
- identifying appropriate chemical substrates
 - combining them in the correct quantities and configurations and under the right conditions
- Since artificial protocells are built in software, they give researchers the opportunity to explore many different protocell compositions, including those that could not be realised in wetlab chemistry, with a view to determining the capabilities of physical protocells. This research can then be used by wetlab chemists when they are choosing the chemical components from which to construct protocells so that the underlying chemistry is capable of supporting protocells which resemble the artificial models.
- As mentioned earlier, protocells consist of a container chemistry coupled with an information carrying mechanism and a metabolic chemistry. Research into artificial protocells is not constrained to realisable chemistry but for the most part, artificial protocell research should stay as close as possible to chemically realisable systems.



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Computation

As mentioned above, chemical or molecular computers are suited to certain types of calculation. In our **bottom-up** approach, we are constructing protocells using replicating binary strings which populate a set of containers. Due to the simplicity of the molecules, the kinds of computation we can perform are limited. We propose that evolution at this level is at the cusp of a Major Evolutionary Transition [Maynard-Smith & Szathmari, The Major Transitions in Evolution, 1997], particularly, the Transition from individual replicating molecules to populations of molecules in compartments. To clarify, even though the replicators are now grouped in compartments, they are still operating on an individual level and are as **selfish** now as they were before the compartmentalisation.

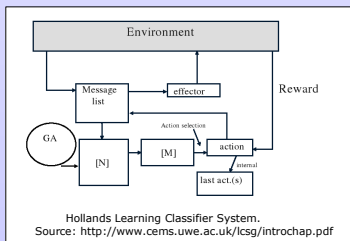
We propose that a form of computation may take place as the protocells evolve to maintain replicators who are less selfish towards their cell-mates. Any more complicated form of computation would not be feasible at this stage due to the evolutionary pressure towards selfishness. Another key limitation in the computational capability of these molecules is Eigens Paradox (Manfred Eigen, 1979). RNA, and thus our artificial simulation of RNA, has a mutation rate of about 0.01 mutations per base pair replicated. This means that RNA can reliably maintain only about 100 base pairs before mutations destroy the information. DNA has evolved complicated error-correcting mechanisms in the form of enzymes which reduce its mutation rate to about 1 mutation every billion base pairs or so. DNA therefore has a much higher computational ability, but we are interested in the evolution of this computation so we start with the simplest form of it.

Molecular Classifier System

To implement our model of computation, we are designing a rudimentary Classifier System based on Hollands alpha-Universes. This string-rewriting system will be different from Hollands original model in that we make no separation between the rules and the messages. In our molecular classifier system, the rules are the messages. In their normal form, the molecules form the messages. When we want to treat a message as a rule however, we perform a decoding translation which produces the rule. The rule is composed of codons from a different alphabet than that of the message structure.

At the moment, our model consists of binary string messages which are decoded using a four-letter alphabet. We use this secondary structure as a regular expression and attempt to find another molecule which satisfies the pattern. If we find a suitable molecule, we replicate it with a certain mutation rate.

By increasing the size of the secondary alphabet, we could explicitly describe the replication process using the extra operators. Of course, it may not be a complete replication that happens, but even partial replications could work together to build longer strings. Extra symbols could also add redundancy to the regular expression language.



FUTURE WORK

Since this model is still in development, our future work will be aimed at gaining an understanding of the peculiarities of such a system. We hope to keep the design as simple as possible to increase the chances that it could be realised in a wet chemical system.

- We are particularly interested in the following:
- How can the replicators interact with the containers to affect their growth?
 - What methods can we use to mine data from the system and get a better view of what is going on?
 - How can we apply evolutionary principles to implement some sort of programming for the system?

THE PACE PROJECT

Life revolves around real-world information processing, but the gap between computers and living systems is still formidable. The European Commission has approved an **Integrated Project PACE** that will create the foundation for a new generation of embedded information technology using programmable, self-assembling artificial cells.

Distributed intelligent technical systems with self-organizing and evolvable life-like properties are required both to make the next generation of self-repairing computer and robotics technology and to direct all kinds of production and remediation on the nanoscale. The integrated project PACE will focus on the IT potential of truly artificial cells: addressing both the technical opportunities of programmable artificial cells and an evolutionary roadmap to producing them under the control of current computers. Such artificial cells will be useful because of their distinctness from, rather than similarity to current biology.

A consortium of some 13 partners and 2 cooperating groups from 8 European countries, including Switzerland and Lithuania, and several USA organizations will pioneer this new approach under the IST-FET section of the EU 6th Framework Program (FP6).

PARTNERS:

- UNIVERSITA' CA' FOSCARI DI VENEZIA
- UNIVERSITY OF COPENHAGEN, FACULTY OF HEALTH SCIENCES
- CHALMERS TEKNISKA HOGSKOLA AB
- UNIVERSITAT POMPEU FABRA
- UNIVERSITY OF ZURICH
- VILNIUS UNIVERSITY INSTITUTE OF THEORETICAL PHYSICS AND ASTRONOMY
- TELECOM ITALIA LEARNING SERVICES S.P.A.
- PROTO LIFE S.R.L.
- UNIVERSITY OF SOUTHERN DENMARK
- DUBLIN CITY UNIVERSITY
- REED INSTITUTE D.B.A. REED COLLEGE
- COMUNE DI VENEZIA
- LOS ALAMOS NATIONAL LABORATORY
- ARGONNE NATIONAL LABORATORY

