Abstract. The quest for the understanding of the mechanisms of the origin of life on Earth (and by implication elsewhere) could be greatly aided through a synthesis of computer simulation operating at the molecular level and the chemical replication of resultant models in the laboratory. The authors term this synthesis a Cyberbiogenesis. The central technological challenge to computing such an “artificial origin of life” is to design computer models permitting de novo emergence of lifelike virtual structures and processes through multiple levels of complexity. This chapter explores Cyberbiogenesis by investigating its antecedents, engages in a thought experiment rendered in computer graphics, examines results from an early implementation called the EvoGrid, and concludes by looking at the scientific, technical, religious and philosophical conundrums presented by such an endeavor.

1. Introduction

The modern quest for the understanding of possible mechanisms behind the origin of life, or in other words the transformation of nonliving matter into living matter, has been passed down to us from chemistry’s precursors, Middle Ages alchemists (O'Connor, 1994). The mathematician Rene Descartes wrote in the seventeenth century of the then prevalent theory of spontaneous generation that “it is certainly not surprising that so many animals, worms, and insects form spontaneously before our eyes in all putrefying substances” (Margulis and Sagan, 2000, p. 64). Charles Darwin challenged the assertion of spontaneous generation in his seminal volume On the Origin of Species (Darwin, 1859) arguing that species evolved from previous generations through a process of natural selection. In a letter to botanist Joseph Hooker (1871) Darwin contemplated a chemical origin for life in “some warm little pond”. The early twentieth century work of Oparin (Oparin and Morgulis, 1938) and J.B.S. Haldane (Haldane, 1927) regarding the formation of cells and chemical conditions on the early Earth set the stage for the 1953 experiment by Miller and Urey (Miller, 1953) which synthesized of amino acids within a laboratory model of the prebiotic environment.
In the same year of the Miller-Urey experiments, explorations into the origins and evolution of life entered the new medium of digital, electronic computation. In the spring of 1953 researcher Nils Aal Baricelli (Barricelli, 1953) coded one of the first scientific computer programs onto punched cards and fed them into the promethean prototype of all electronic computers just put into operation at the Institute for Advanced Study in Princeton, New Jersey (Dyson, 1997). Calling it an *experiment in bionumeric evolution*, Baricelli was investigating the role of symbiosis in the origin of life and came to believe that while his five kilobyte universe of *numerical symbio-organisms* exhibited criteria of a living, evolving system they would “never become anything more complex than plain numbers” (Barricelli, 1962, p. 73).

Decades later in the 1980s, John von Neumann’s original design for the electronic computer at Princeton had come to dominate the computing world and began appearing on desktops as microcomputers. These tiny machines allowed intellectual successors to Baricelli such as Chris Langton to again work late into the night and code their own renditions of *life as it could be* and along the way creating a new field: *artificial life* (Alife) (Langton, 1986, Levy, 1993). Alife’s close cousin, *artificial intelligence* (AI) had a parallel lineage from the 1950s but was aimed at representing conscious thought. Alife focused on a bottom-up approach, hoping to explore the dynamics of living systems through algorithmic techniques that generated emergent phenomena including the physics of motion (Sims, 1991), and the evolving of competing artificial genomes (Ray, 1991). Great promise was held that in the 1990s increasing computing power would soon support teeming simulated ecosystems which biologists would come to recognize as true living systems. However, it was clear that by the turn of the past century Alife development had stalled as the virtual worlds containing early examples of proto-biota proved too simplistic for the phenomena of open ended growth of complexity to be observed (Rasmussen et al., 2003a).

### 2. A New Synthesis: Cyberbiogenesis

In the early 2000s interest was again growing in creating chemically-based (*in vitro*) experiments in origins of life endeavors which would lead to the formation of so-called *protocells*, chemical structures exhibiting at least some properties of living systems (Rasmussen et al., 2008). In parallel, massively distributed computation and large scale centralized grids and special purpose hardware were hosting viable realistic simulations of very small volumes of interacting molecules over short but biologically significant time scales (Shaw and Dror, 2008). In 2011 a true synthesis of *in silico* simulation as a tool to design and predict the outcomes of *in vitro* experimentation seems to be beckoning to us from just over the horizon. This synthesis holds the promise of new tools for chemistry akin to Computer Aided Design (CAD) enjoyed by other fields such as product manufacturing and architecture. At a not-so-distant date in the future, biochemists should be able to simulate larger biomolecular structures such as proteins yielding a good measure of predictability of outcomes in the test tube (or the Petri dish). Such a synthesis also brings up a new and tantalizing possibility:
Could we actually one day digitally simulate a complete step-by-step chemical scenario for an origin of life on Earth? And if we could carry out such a simulation while remaining faithful to the chemistry, could we then reproduce this particular pathway to life from nonlife on the chemistry workbench?

The computing part of this challenge was perhaps most definitively issued by Richard Gordon in *Divine Action and Natural Selection: Questions of Science and Faith in Biological Evolution* (Gordon, 2008). In his chapter titled “Hoyle’s Tornado Origin of Artificial Life: A Programming Challenge”, Gordon challenges the Alife community to develop a computational environment to simulate an origin of artificial life from artificial non-life (pp. 354-367):

*I would like to suggest that artificial life (Alife) enthusiasts take up Fred Hoyle’s (Hoyle, 1984) challenge, that in a way they simulate a tornado going through a junkyard of parts, and come up with something we would all agree is alive, in the Alife sense, from components that are not alive in the Alife sense...*

This author’s response to Gordon’s challenge was detailed in another chapter “The God Detector” in the same volume (pp. 66-85):

*What I am proposing is to engage all of the best programmers, artists and philosophers of our generation to create a gigantic network of software and computers, working to create a sort of “Evolution Grid” or “EvoGrid”. This EvoGrid would start out as God the Mechanic (like Karl Sims’ creatures) in which we build the simulation, set the initial conditions and then let the artificial ecosystem go from there.*

The chemical fabrication part of this challenge is perhaps best represented by the field of synthetic biology. The recent successful *in vitro* substitution of a synthetically created genome into a living cell (Venter et al., 2001) seems to suggest that the fabrication of significant additional parts of living cells might also be possible.

The term *Cyberbiogenesis* might suffice to capture the complete closing of this circuit from digital simulation to atomic realization. This term could be thought of as a kind of cousin to Mereschkowsky’s word *Symbiogenesis* (Mereschkowsky, 1909) which Margulis argues was a primary driver of evolution (Margulis, 1997). The scope of constructing an end-to-end Cyberbiogenesis system would dwarf the recently completed Human Genome Project (Watson and Cook-Deegan, 1991) but is possibly realizable within this century. To compute an origin of life faithful enough to physical laws of chemistry to be reproducible *in vitro* is perhaps one of the most audacious applications of technology in the history of our species.

The remainder of this chapter will explore Cyberbiogenesis in a thought experiment, then detail one initial attempt at implementing an early computer prototype, and finally enumerate and illuminate some of the many scientific, technological, religious and philosophical conundrums uncovered by such an effort. We hope that these words will lend some shape to Cyberbiogenesis as a grand challenge for the coming
century for those who might choose to take it up. With apologies to readers, we will leave it to others in this volume to provide a decent treatment of the major schools of thought regarding the origin of life.

3. Cyberbiogenesis: A Visually Rendered Thought Experiment

In mid 2008 the author (BD) engaged in a *Gedankenexperiment* (a thought experiment), drew storyboards (Figure 1) and requested a collaborator to produce a short animated movie (Damer et al., 2008) designed to illustrate the concept of cyberbiogenesis.

![Figure 1. The author’s original sketches of the thought experiment](image)

Figure 2 through Figure 11 below depict and describe scenes from the movie which provides a visual cartoon of the thought experiment which imagines a completely realized cyberbiogenesis system.

![Figure 2. The conceptual cyberbiogenesis setup: on the right is the *in silico* molecular simulation space underlain and powered by numerous microprocessors; on the left is the molecular assembler and *in vitro* test beaker](image)
Figure 3. The simulation space renders the physics of an aqueous chemical environment

Figure 4. The formation of virtual molecules and self organization occurs in the simulation space

Figure 5. The formation of a vesicle is observed with the accidental capture of some other molecular machinery (on the lower left center)
Figure 6. The virtual symbiotic entity is capable of a sufficient ensemble of lifelike behaviors including compartmentalization, metabolism and replication with a mechanism for genetic heredity such that Darwinian natural selection has led to its growing sophistication.

Figure 7. A sufficiently evolved entity is selected for digital decomposition perhaps at its embryonic phase and transmitted from the \textit{in silico} simulation to the molecular assembler.

Figure 8. The hypothetical molecular assembler carries out a process akin to 3D printing and combines basic chemical elements to synthesize a molecular rendition of the virtual entity.
Figure 9. The fabricated entity emerges to drop into the beaker of formulated chemicals matching the environment in the original digital simulation.

Figure 10. Within the *in vitro* environment, the molecular version of the entity starts to function as a new form of “living” entity.

Figure 11. The entity advances further and begins to reproduce in the new environment, completing the cyberbiogenesis cycle.
To conclude this thought experiment, we might now ask why have the molecular assembler to fabricate the entity when instead we could simply recreate the same chemical environment as that from which the in silico entity emerged? It may be that the \textit{in vivo} emergence of the parallel chemical entity may not so be easily achieved or may take substantially longer without the shortcuts provided to its computational \textit{in silico} counterpart. We might also ask how realistic and realizable is this thought experiment? According to Nobel laureate Richard E. Smalley a “black box” nano-scale molecular assembler is nowhere near to becoming a reality (Baum, 2003). However recent progress in functional representation of 3D virtual objects (Pasko et al., 2008) paired with digital materialization made possible by universal desktop fabrication (Vilbrandt et al., 2008) shows promise in this direction. In any case, near term progress towards this goal would have to be made in the domain of computational simulation. Given the computing resources available in 2011, it was thought that a reasonable goal might be to produce a prototype that would reach the step depicted in Figure 4 above: a few simple molecules forming from an atomistic soup.

4. One Naïve and Early Cyberbiogenesis Prototype: the EvoGrid

![Figure 12. The architecture of the EvoGrid](image)

How would one begin to construct the computational part of a Cyberbiogenesis system? The author’s company, DigitalSpace, working with the guidance of an energetic international team of advisors undertook to build a first prototype of the EvoGrid. The prototype began preliminary trial operations at the end of 2009 and has engaged in several longer experimental runs in 2010 and 2011 at the University of California at San Diego. Figure 12 depicts the architectural components of the EvoGrid in its first implementation. The EvoGrid is built upon an open source, published framework to allow a larger community to extend it and to permit fully distributed computation on donated networks such as the BOINC environment that supports the “@Home”
experiments (Anderson, 2004). The salient innovation of the EvoGrid is the execution of a large number of small volumes of simulated molecular dynamics over short periods of time. Each of the small volumes is sampled and processed by a search function, which directs whether the simulation should become the starting “seed” for the next branch of simulations or abandoned.

It was hypothesized that the combination of search operating on small simulations would drive the overall system more rapidly toward the emergence of complex molecular structures within branched simulations. As shown at (B) in Figure 13 the storage of the full state tree of the system would permit time-based analysis and backtracking at (C) to re-try promising branches with the hopes to reaching a more complex end state at (D) than would be possible through a simple linear simulation as depicted in (A). This is a stochastic hill-climbing method (E) used commonly in AI (Russell and Norvig, 2003, pp. 111-114) but applied here to molecular dynamics.
Figure 14 illustrates the results of this method applied to an initially random volume of six types of one thousand notional atoms run through a hypothetical nanosecond of simulation time using the GROMACS (van der Spoel et al., 2005) molecular dynamics engine driven by the EvoGrid simulation manager and search functions. Notional molecules were formed through random encounters within the soup of atoms. In several experiments the combination of search functions and back-tracking supported a sustained growth of the population of molecules, shown as a graph of number of observed molecules or yield \( Y \) versus the number of executed simulations \( X \). Momentary declines (the intermittent vertical drops) were overcome through abandonment of these less promising branches.

The results of two experiments are depicted in the figure. Both used the same starting conditions but Experiment #1 (lighter graph on left side) applied a simple hill-climbing method which preserved the gains made by high yielding simulations but only permitted the further exploration of pathways of equal or higher yield. The population of molecules (two or more bonded atoms) quickly climbed to a plateau of sixty (circled) and then no additional growth in “complexity” was observed. The experiment was terminated after two months of computation on a small grid of four servers. Experiment #6 was processed on a larger grid of two dozen cores running at 100% for a two month period ending in June, 2011. This time the search function implemented stochastic hill climbing permitting degradation off local optima and the random selection of new starting simulations from a wider pool. While requiring far more computing resources, this experiment climbed through multiple thresholds (shown circled) arriving at what appeared to be a global maximum of 189 molecules (not shown).
At this point, the richest “soups” had sequestered over half of their total populations of 1,000 free atoms within molecular bonds. Thus the slight change in the search function permitted a “breakthrough” to ever higher complexity through the exploration of a highly rugged fitness landscape. The observed hill-climb in experiment #6 suggests that this landscape is not truly random but is in fact correlated (Kauffman, 1995). A 3D view of one higher yielding simulation is shown in Figure 15. The notional end products of the depicted simulation, which was terminated with over two thousand processed simulations and over two hundred thousand unprocessed simulations in abandoned branches, consisted of 23 kinds of molecules in a total population of 185 in the most populated volume. A control experiment (not shown) involving purely unsearched linear processing produced far fewer types of molecules (6) in fewer quantities (26) with no sustained trend.

The EvoGrid prototype showed that a grid of molecular dynamics simulations could be coupled with a carefully tuned search function such that the yields of experiments would grow rapidly to “interesting” maxima. These simulations were modeled very crudely on the diffuse atomistic regime of interstellar space, where organic and other bio-essential molecules are formed (Deamer and Damer, 2010). In future EvoGrid implementations it is conceivable that more ambitious simulations could be tuned to search their way biologically interesting phenomena such as the formation of vesicles, informational molecules, or autocatalytic sets. It is envisaged that this discovery system of small but rapidly searched simulations working in concert with larger centralized grid-based simulations could provide a combined computing environment rich enough to permit experiments surrounding the origin of life question (Damer et al., 2010). The EvoGrid is only a first step on a very long journey to a full...
system capable of undertaking Cyberbiogenesis. As more realistic chemical interactions are simulated they could inform a whole range of parallel “wet” laboratory experiments not conceivable before (Damer, 2011). The use of combinatorial chemistry techniques automating thousands of parallel experiments with computerized search and robotic reseeding of new experiments could yield a sort of chemical EvoGrid or, more poetically, a “Genesis Engine”. Like the Human Genome Project of the last Century, the Genesis Engines of the 21st Century may well carry us to the brink of a second abiogenesis on the Earth.

5. Conundrums Exposed and Considered

Given the likely distant prospects for any successful Cyberbiogenesis effort, a valuable activity in the interim is to consider the societal impact of such a project on a range of human endeavors. Any enterprise that sets as its goal the emergence of an artificial origin of life, testable in chemistry and therefore ultimately realizable as a new form of chemical life is likely to draw controversy from many quarters. This controversy will in turn expose a number of conundrums that lie at the basis of science, technology, religion, ethics, and philosophy.

5.1 SCIENTIFIC CONUNDRUMS

The goals of Cyberbiogenesis beg many basic questions in science including:
1. How might science define a living entity or indeed an entire living system? When asked to measure aliveness would scientists simply “know it when they see it” when presented candidate lifelike systems?
2. In simulating steps to an origin of life what is the experiment to be undertaken and at what point does it start? Do experiments begin with pre-built components of some complexity but not considered to be living, and proceed from there as suggested by Gordon (2008)? Alternately, should simulation experiments be initiated much further down the ladder with simpler artificial precursor molecules, or even farther down from basic atoms assembling precursor molecules within an ab initio primal soup?
3. How much influence is allowed or required to induce a sufficient measure of emergence? In other words, how much “intelligent design” is required in the setting up and operating of Cyberbiogenesis experiments? What degree of ongoing human guidance should be permitted in both the virtual and chemical experiments which follow?
4. Would an entirely artificially evolved entity pose a current or future threat to any part of the natural environment in the Earth’s biosphere or to technological or biological regimes within human civilization? How could such a threat be mitigated? If such a threat were plausible, would it be grounds for not pursuing this line of research?

5.2 TECHNOLOGICAL CONUNDRUMS

A decade ago the Artificial Life community took stock of their field and proposed a set of “Open problems in Artificial Life” (Bedau et al., 2000) which provide
a clear look at the brickwork of the technological foundations of any serious Cyberbiogenesis effort. The authors set a challenge in the second open problem to solve the challenge of abiogenesis in an artificial chemistry and identified that “[b]etter algorithms and understanding may well accelerate progress… [and] combinations of… simulations… would be more powerful than any single simulation approach” (p. 367-68). The authors also pointed out that while the digital medium is very different from molecular biology, it “has considerable scope to vary the type of ‘physics’ underlying the evolutionary process” and that this would permit researchers to “unlock the full potential of evolution in digital media” (p. 369). Ten years later as projects such as the EvoGrid take aim an in silico abiogenesis, many technological conundrums have come to the fore including:

1. What level(s) do you simulate at, and at what scale? Is molecular dynamics a sufficient level or are quantum dynamical effects required? Alternatively, is a more abstract artificial chemistry which can exhibit desired properties a better starting point than aiming at high fidelity to chemistry?
2. Nature operates in parallel at multiple scales with multiple physical properties emerging at these scales. Therefore, how can von Neumann computers (essentially serial processors) be adapted to meet this substantial computational challenge or does this challenge belong to the domain of special purpose hardware or an amalgam of digital and chemical computing?
3. What computational corners can be cut but still retain plausibility in nature and viability in experimental chemistry? Related to this is the claim by Abel (2009) that any computational simulation is formulaic, subject to predicative knowledge and not based on physicodynamic factors so may never be representative of solutions in vitro. In addressing this question Gordon presents the following possibility for future EvoGrid implementations:
   
   Consider having the EvoGrid simulate a less plausible approximation to chemistry. Allow a more abstract chemistry to be tested which also might be subject to a proof by construction in mathematics. The components will be decent approximations of real chemistry. Allow yourself to introduce all the bias that you want but as long as the program constrains you to do things that are physically realistic then you might argue that you have something artificially alive. You just don’t have the pathway to the end point but you know there is a way back. Decomposed parts could be markers on many paths to life. The important point is proving that one such path exists (Gordon et al., 2010).

4. How much do the search functions and human designed initial conditions and sought after end points to experiments limit their ultimate creativity? This is the problem of systems employing a teleological approach: bias toward the sought-after goals limits the power of the system as an open ended discovery mechanism. As suggested by Dawkins (1986) and others, evolution does not strive toward goals. Even though nature cannot be
praised for the best “designed” solutions to problems it also cannot be faulted for teleological bias. Gordon also makes the following points along this line:

Examine the case of the EvoGrid where you act as the intelligent designer and use the tools to determine the minimal artificial organism. If you could then put one together then you could look for the properties and potential pathways to that minimal artificial organism. You could also consider an experiment where you start with bigger building blocks that are considered to be non alive and see if they assemble into something you would consider to be alive (Gordon et al., 2010).

5.3 RELIGIOUS, ETHICAL AND PHILOSOPHICAL CONUNDRUMS

Any seriously undertaken cyberbiogenesis endeavour will attract the following questions and controversy from the triumvirate magisteria of religion, ethics and philosophy:

1. Does a successful cyberbiogenesis disprove the need for a supernatural creator as an agent in the origin of life and for the guiding of life’s development?
2. What is the consequence for the world’s religions of the creation of an artificially alive (in computer simulations) or a chemically alive entity?
3. Would an artificially sourced living entity be protected as an endangered species? Would only the chemical entity be protected or the virtual one as well?
4. Does the enterprise of cyberbiogenesis represent a willful achievement of human innovation or is it an inevitable expression of the entire biosphere and life itself, with humans as mere agents forwarding life into a new mechanism of evolution? Is this the means by which life is expanding itself out into other parts of our solar system or the universe? Are we willing or unwilling agents of this expansion?

In a discussion of ethical concerns in (Rasmussen et al., 2003b, p. 67) the authors echo some of the above points:

Generating life de novo will create public reactions. The reactions will probably be along two lines: (i) Environmental concerns that the life-producing technology could “get out of control”, and (ii) Religious and moral concerns, based on the beliefs that humankind must restrain from certain endeavors on grounds that they are fundamentally amoral.

Ethical questions arising around the possible creation of cells from existing biology or completely new molecular constructions have a storied history. Non-technical press reaction from announcements in biotechnology and genomics such as the research on minimal cells (Fraser et al., 1995) and the announcement of the sequencing of the human genome (Venter et al., 2001) often turns to talk of “Frankencells”. Concerns about more artificial nanostructures able to survive and reproduce in natural
environments have also been discussed in the nanotechnology community (Merkle, 1992). It is clear that future work on the EvoGrid or any Cyberbiogenesis-oriented system will have to address the above issues. Initially the response to concerns might be to state that lifelike objects in a simulation are merely objects in a simulation and of no threat to people or the biosphere. The argument might be made that these objects might be a threat to computer networks, however, akin to computer viruses. However, virtual environments required to sustain an artificially alive system would be so complex and large that the system would effectively be an isolated island, similar to large multi-player game systems. Once there is an active effort to reproduce these lifelike objects in physical chemistry the alarm will be raised with many in the public and scientific community.

5.4 AN ORIGIN OF ARTIFICIAL LIFE TURING TEST

Related to concerns about Frankencells is the question of: how does the observer know when something is lifelike enough in a computer simulation to declare it “alive”? In his 1950 paper Computing Machinery and Intelligence (Turing, 1950) Alan Turing wrote “I propose to consider the question ‘Can machines think?’ (p. 433) and defined a test of machine intelligence, one variation of which consisted of a human judge conversing through a text interface with an unseen human and a similarly hidden computer (p. 442). If the human judge could not tell the difference between the human and computer conversant then the machine would be deemed to have reached some sort of cognitive equivalence to the human participant.

At some day in the distant future, a test group of biologists, engineers, philosophers and others may assemble in an online virtual space. In another access-controlled space, project specialists would be assembled observing a rich array of lifelike objects moving about in a virtual world running on a greatly advanced EvoGrid. The esteemed guests would then be asked to undertake a kind of Origin of Artificial Life Turing Test, wherein they may read descriptions of the objects and environments being observed but not revealed by the staff. They would also be exposed to descriptions of similar yet real, living entities and their terrestrial environments, such as a termite colony. Over many days or weeks the test group would be able to ask the staff questions about both environments, perhaps even specifying experiments to be performed. If at the end of a long enough period a majority of the test group cannot consistently tell which environment is in fact the real, biological one and which is the one witnessed in the simulation then the simulated environment will have passed this new variant of the Turing Test. Of course there will likely be strong arguments for and against the “aliveness” of these virtual entities, especially if they exist solely in an abstract universe far from the norms of chemistry. If at some later date a chemistry-faithful entity is fabricated with molecules and survives to breed within a physical setting, then the concerns of the doubters may be quelled.

5.5 A VISIONARY VIEW: A LENS ON LIFE IN THE UNIVERSE

Let us now roll forward to some much farther future date when working Cyberbiogenesis systems abound and when a further closure of the loop is in place
whereby the observation of in vitro adaptations feeds directly back to changes in the in silico ecosystem. With this full closure numerous variants on viable biologies could be generated, extending our ability to model origins of life in alien habitats and to cast light onto life as it might be in the universe. Such a system could be used to seed life forms in alien habitats such as the Martian ice cap or the surfaces of near earth objects. Of course there may well be a substantial range of viable artificial living systems for which there would exist no physical medium in which they could be instantiated. In this case the only universe in which that these creatures could be chemically rendered out of the simulation into physical reality is a parallel one possessed of exotic physics. Taking this one step further we might see that nearly infinitely endowed future Cyberbiogenesis systems could serve as a lens into where in this universe or others life might arise and projecting how far it might evolve. Indeed, in the unlikely event that an intelligent higher form of life should arise within a Cyberbiogenesis simulation would we choose to instantiate it physically or seek out where its naturally evolved cousins might be resident? Presumably at that point the new form of life might have its own say in the matter.

7. Conclusions

Recent progress in synthetic biology, the creation of chemical protocells, and models of pathways to the origin of life together with increases in computing power and the ability to accurately model small volumes of molecules suggest that this century may witness a solution to life’s origins emerge in silico and be testable in vitro. A concerted effort or “grand challenge” to create a viable Cyberbiogenesis system might therefore be well worth the effort. The construction of a shared, open and extensible “Primaordial Soup Internet” may serve not only as an experimental environment for origins of life and complexity theory but also provide valuable CAD-type capabilities for biomedical research ultimately simulating the structure and functions of an entire cell.

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