Abstracts

Molecular Replicator Dynamics

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Template-dependent replication at the molecular level is the basis of reproduction in nature. A detailed understanding of the peculiarities of the chemical reaction kinetics associated with replication processes is therefore an indispensable prerequisite for any understanding of evolution at the molecular level. Networks of interacting self-replicating species can give rise to a wealth of different dynamical phenomena, from competitive exclusion to permanent coexistence, from global stability to multi-stability and chaotic dynamics. Nevertheless, there are some general principles that govern their overall behavior.

We use RNA secondary structures as a biophysically realistic model for a fitness landscape. The existence of neutral and the shape space covering property determine the basic features of adaptation: interplay of neutral exploration in sequence space and short adaptive periods. We then extend this paradigm to interacting self-replicators and show that similar mechanisms as in the landscape case govern the dynamical behavior.

Extra-Solar Planets and Life: Present and Future Space Missions

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Planet hunting has begun, seriously, in the late 20th century. So far, much of it is done from the ground but there are several ambitious plans for space-borne missions that will change the state of this field when launched after 2010. These include new technologies to directly observe Earth-size planets and to detect signs of life, like ozon, in their atmosphere. The talk will review some of these plans with special emphasis on the space-mission Darwin.

Fermi's Paradox and Astrobiology

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If extraterrestrial planets are common, it is plausible that there are millions planets with conditions favorable for the evolution of life. The Fermi Paradox poses the question "if intelligent life is common, where are they?" the lack of evidence for visits of extraterrestrial beings on Earth suggests that there are none, so perhaps we are alone after all. Astrobiology in the solar system and tools such as Space Telescope, the Terrestrial Planet Finder and spectral signature of life on extrasolar planets put the Fermi Paradox in more specific terms.

The elusive nature of the concept of homochirality

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Homochirality is a central issue in evolutionary studies. It requires a clear-cut definition of handedness (left or right), and requires also that this definition holds for all members of the group of molecules, which is labeled as “homochiral”. We show that handedness labeling is inherently problematic: For any given definition of left/right there must be a chiral object for which it is not possible to assign handedness under that definition. Furthermore, we show cases where within a gradually changing group of molecules/objects, which would have been labeled as a homochiral group, there is actually a flip from left-handedness to right-handedness. Some of the specific examples to be presented include chiral clusters of water molecules, helical objects, chiral diffusion limited aggregates, and chiral tetrahedral molecules of the general formula AB_4, such as SiO_4 which is the building block of quartz.

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Early and Contemporary Metabolism

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I will show how seemingly unrelated results in the fields of contemporary bacterial metabolism and early prebiotic chemistry can be interpreted as different aspects of the same biochemical organization principles.

Both contemporary bacterial cells and early protocellular structures involve the nonequilibrium propagation and evolution of self-sustaining compositions of chemical species [1]. In both cases, biochemical networks seem to often operate at the edge of their optimal growth capacity. This assertion is supported by comparison between predictions and experimental data for bacterial cell growth [2], and it is explored by computer models of prebiotic mutually catalytic networks [3]. At the prebiotic level, maximal growth capacity can be understood as the inherent outcome of a set of equations describing the dynamics of the system [3]. Conversely, in contemporary cells, such optimal adaptation is the result of natural selection in the classical sense, and may depend strongly on environmental and genetic constraints [2].

Despite the several differences between early and contemporary metabolic networks, the analogies explored here reveal a common fundamental thread of optimal metabolic adaptability. The explored scenario poses new questions about chance versus necessity in determining the details of self-sustaining prebiotic chemistries [4], as well as about the properties of present ecosystem dynamics [5]. Many of these questions could be addressed using novel large scale computational methods.

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Complexity Feeds on Order: Schrodinger's Negentropy after Sixty Years

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In his classic "What is Life?" Schrodinger (1944) has introduced an odd notion, Negentropy, on which the organism is supposed to feed. This notion has been severely criticized. We present a new and simple twist to it. Order, from both the mathematical and thermodynamic perspectives, must be the initial state for any process which produces complexity and/or information and therefore must be produced by any organism as a reservoir for its future development. We apply this formulation to show how a population adapts to its environment and generalize it to address the origin of the genetic code.

Explicit Collision Simulation of Chemical Reactions

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A Toy Model was implemented for the study of random chemical reaction networks and prebiotic chemistry [1]. Experimental research in prebiotic chemistry is limited by feasibility. The difficulties range from obtaining a sufficient quantity of products to analyze an experiment, or attaining the necessary conditions, for example temperature and pressure, to very long experiment durations. Those problems were tackled using a simulation framework with given generic reactions in the form of graph rewriting rules. In order to avoid a possible bias by given generic reactions, the reactions are now simulated from scratch. An approach is implemented in which molecules collide and interact/react explicitly. More specifically, the original energy calculation of the Toy Model can be extended to intermediary

structures occurring during a collision.

[1] J. Chem. Inf. Comput. Sci. 43(4): 1085-1093 2003

Early Systems Biology and Prebiotic Networks

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Systems Biology constitutes tools and approaches aimed at deciphering complex biological entities. It is assumed that such complexity arose gradually, beginning from a few relatively simple molecules at life's inception, and culminating with the emergence of composite multicellular organisms billions of years later. We argue that in fact very early in the evolution of life, molecular ensembles with high complexity may have arisen, which are best described and analyzed by the tools of Systems Biology. We show that modeled prebiotic mutually catalytic pathways have network attributes similar to those of present-day living cells. This includes network motifs and robustness attributes. We point out that early networks are weighted (graded), but that using a cutoff formalism one may probe their degree distribution and show that it approximates that of a random network. A question is then posed regarding the potential evolutionary mechanisms that may have led to the emergence of scale-free networks en-route to modern cells. Specifically, we are carrying out Graded Autocatalysis Replication Domain (GARD) simulations aimed at tracing how the gradual appearance of larger molecules (oligomers and polymers) may have contribute to such a process.

Reconstruction of the earliest biological peptides

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Recently reconstructed evolutionary chart of the triplet code has strong predictive power. Several important predictions have been confirmed, in particular - conservation of protein sequences in their binary form. That is, the binary version of modern protein sequence or motif is its evolutionarily earliest version. That allows to reconstruct the oldest sequence motifs. It is found that the earliest peptides had the size 6 or 7 residues. Their sequence structure displays features of complementarity that suggest that at some early stage the respective minigenes (18 or 21 bases) had a hairpin structure.

The Coevolution of Genes and Genetic Codes Explains the Redundancy and Error-Correcting Properties of the Standard Genetic Code

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The standard genetic code is the nearly universal system for the translation of genes into proteins. The code exhibits two salient structural characteristics. It is extremely efficient in reducing the impact of errors in translated proteins by creating interchangeable elements: the code assigns functionally similar amino acids to codons that are frequently interchanged for one another in replication and translation. And, it is highly redundant: 61 codons code for only 20 amino acids. Here we show that both properties can be explained by the coevolution of genetic codes and genes. At any stage of the evolution of the code, genes were under selection to produce useful proteins when they were translated according to a given code, and in turn, changes in the code were under selection to produce useful proteins with the genes presented to them. Our work builds upon a mathematical framework that captures the essential coevolutionary relations between genes and genetic codes. We show that the coevolution of genes and genetic codes, which begins from a highly ambiguous initial code, gives rise to rules of code modification that generate a transient annealing type of convergence to a code that is both error-correcting and redundant. When we assume the qualitative characteristics of errors known today, the process of code-message coevolution reproduces the error-correcting patterns observed in the standard genetic code.

A Colorful Origin for the Genetic Code

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The genetic code maps the sixty-four nucleotide triplets to twenty amino-acids. Several scenarios argue that the code with its twenty amino-acids depends finely on the specifics of primordial chemical interactions or evolutionary adaptation. Others argue that the code is a 'frozen accident' because of the overwhelming effects of any change. The recently observed variant genetic codes all encode the same twenty amino-acids, suggesting that this number is a universal invariant. This motivates us to study the implications of evolution on the code within a minimal, generic model. The forces that shape the code are the interplay of the needs for diverse amino-acids and for minimal impact of errors. Our model suggests that the number twenty is a fundamental topological feature of the code that stems solely from its four letter triplet structure and is related to the map-coloring problem.