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Astrochemistry and the theory of Complex Systems

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Abstract – This paper wants to highlight some of the links between the science of Complex Systems and Astrochemistry. First, the driving forces that lead the two research fields are presented. Then, it is demonstrated that Astrochemistry investigates Complex Systems. Hence, the features of Complex Systems and the strategies to deal with them are described. An open question concludes this paper.

Keywords: Networks; Out-of-equilibrium Thermodynamics; Emergence; Origin of Life

Riassunto – Questo lavoro vuole evidenziare dei collegamenti tra la scienza dei sistemi complessi e l'astrochimica. In primo luogo, vengono presentate le forze che guidano i due campi di ricerca. Quindi, viene dimostrato che l'astrochimica indaga sistemi complessi. Infine vengono descritte le caratteristiche dei sistemi complessi e le strategie per affrontare la loro descrizione. Il contributo termina con la formulazione di un interrogativo ancora irrisolto.

Parole chiave: Reti; Termodinamica fuori dall'equilibrio; Emergenza; Origine della Vita

INTRODUCTION

Similar driving forces guide the theory of Complex Systems and Astrochemistry.

First, the wonder we feel when we look at the beauty and mystery of nature. Suffice to think about the complex architecture and activity of a cell and the breath-taking astronomical environments. Second, the epistemic curiosity or the so-called "appetite for knowledge". After staring at the beauty of nature, spontaneous questions arise, such as:

"Which are the laws governing the behaviour of Complex Systems?"

"Which is the chemical reactivity in the astronomical environments?"

"How did life originate on Earth?" "Can we find out life outside our planet?"

Third, the will to solve practical problems through the development of technology. For instance, the global population is soaring, and the required amounts of food and energy are growing, as well. We can cope with these rising requests by thinking of colonizing other planets. This problem is just one of the many that humanity has to face in this century. There are other challenges. For instance, human activities should not damage natural ecosystems, shrink their biodiversity, and provoke climate change. We want to predict catastrophic geological events that can cause many sudden deaths. There are incurable diseases that must be defeated, and we must tackle the bacterial resistance to antibiotics. We want to predict the financial and economic crises and eradicate poverty from the Earth. We dream of guaranteeing justice in our societies. These examples make the list of the so-called XXI century challenges [1-3]. Whenever we tackle one of these challenges, we must deal with Complex Systems, such as the geology, the climate of the Earth or other planets; the astronomical environment; the ecosystems; the living beings, and in particular, the human immune and nervous systems; the macro-economy, and the societies. It might seem that these Complex Systems are so diverse. However, they share some common features [4].

Features of Complex Systems

Complex Systems are networks constituted by many nodes and many links or edges. Often, the nodes are diverse. Each node might be unique: suffice to think about single humans, who are the nodes of the Complex System that is a society. The nodes are, usually, strongly interconnected. The distribution of the links among the nodes determines the structure of the network. The presence of mutual interconnections generates feedback actions and high non-linearity.

Complex Systems are networks that work in out-of-equilibrium conditions. If the Complex System involves only inanimate matter, its behaviour is driven by force fields. On the other hand, if the Complex System involves living beings, its behaviour is information-based.

Complex Systems exhibit emergent properties. The integration of the features of the nodes gives rise to properties that belong to the whole network. The whole is more than the sum of its parts. The most striking example of an emergent property is life. If we consider the typical chemical constituents of every living being, we have DNA, RNA, proteins, water, salts, phospholipids, and others. If we take each of them separately, we can never find life. Life emerges only when we consider all the characteristic compounds of a living being, organized in that peculiar spatial and temporal architecture that is a cell.

Therefore, the Complexity (C) of a natural system derives from a peculiar combination ($\subset$) of three properties (see equation 1): (I) Multiplicity (M) of the network; (II) Interconnection (Ic) among the nodes of the network; (III) Integration (Ig) of the features of the nodes of the network [5].

$$C \propto M \subset Ic \subset Ig \tag{1}$$

Another common feature of Complex Systems is that their behavior cannot be described exhaustively. In other words, we find many difficulties in predicting their behavior, especially in the long term. Why? There are three main reasons.

Difficulties in predicting the behaviours of Complex Systems

First of all, many computational problems regarding Complex Systems, such as planning, scheduling, machine-learning, financial-forecasting, are solvable, but intractable when they refer to systems having large dimensions. According to the theory of Computational Complexity, all the solvable problems can be partitioned into two sets: the set of polynomial problems and the set of exponential problems. A problem is polynomial when the number of computational steps (n°c.s.) needed to determine the accurate solution is a polynomial function of the dimension of the problem (N):

$$n°c.s. \propto N^{d} \tag{2}$$

In equation (2), d can be either 1, or 2, or other finite numbers.

A problem is exponential when the number of computational steps is an exponential function of N:

$$n°c.s. \propto x^{N} \tag{3}$$

In (3), x can be 2 or N, as examples.

The accurate solution of any polynomial problem can be found, whatever is the dimension of the problem. The same cannot be said for the exponential problems. When we face exponential problems having large dimensions, their accurate solutions cannot be determined in a reasonable lapse of time. We can make an example if we think about the Schrödinger equation that we use to determine the total energy of a system starting from its ultimate constituents, which are atoms. The Schrödinger equation is an exponential problem, because the number of computational steps depends exponentially on the number of particles (N), according to equation (4):

$$n°c.s. \propto 2^{N} \tag{4}$$

If we consider a system with just 500 particles, the number of computational steps needed to solve the Schrödinger equation is overwhelmingly significant: $2^{500} \approx 3.3\times10^{150}$. Even if we have the fastest supercomputer in the world to make this computation, it is unthinkable to find its accurate solution. According to the TOP500 project [6], in June 2019, the fastest supercomputer in the world is the IBM Summit, reaching the astonishing computational rate of 148 PFlops/s (PFlops/s stands for Peta Floating-point operations per second, i.e., 148×10^{15}). If we use the IBM Summit to solve that Schrödinger equation, the time required to determine its accurate solution is so long, $\approx 7\times10^{125}$ years, that is unreasonable. Suffice to think that the age of the universe has been estimated to be 14 billion years. In similar situations, the accurate solution cannot be determined. Then, we transform the original exponential problem into a non-deterministic polynomial problem. We fix an arbitrary criterion of acceptability for a solution to the problem. Hence, we choose an algorithm that generates, often heuristically, plausible solutions in a reasonable lapse of time. The computation is stopped whenever an acceptable solution is found. However, this solution is not necessarily the exact one.

The second reason why we find difficulties in describing Complex Systems is that they exhibit variable patterns. Variable patterns are entities or events, whose recognition is made difficult by their multiple features, variability, and extreme sensitivity on the context. Examples of variable patterns are human faces and voices, handwritten cursive words and numbers, fingerprints, certain diseases, political, social, and economic events, chaotic time series. When we want to recognize variable patterns, vast amounts of data are collected, stored, and processed. They are the so-called Big Data. However, we still need to formulate universally valid and effective algorithms for recognizing variable patterns.

Finally, the predictive power of science has intrinsic limitations. As far as the microscopic world is concerned, the Heisenberg's Uncertainty Principle holds. According to this principle, it is impossible to determine accurately and simultaneously the position and momentum of a particle. Therefore, the deterministic dream of predicting the dynamics of the universe, based on the properties of its ultimate constituents, which are atoms and molecules, wanes completely. We might think to limit the description of Complex Systems to the macroscopic level. However, Complex Systems can exhibit chaotic dynamics. A dynamic is chaotic when it is aperiodic and extremely sensitive to the initial conditions. Therefore, any chaotic dynamic is unpredictable in the long term, because any initial condition cannot be determined with infinite accuracy. In fact, science is said to be exact, not because it is based on infinitely exact data, but because its rigorous methodology allows estimating the extent of uncertainty associated with any quantitative determination.

It is spontaneous to ask: How can we improve our description of Complex Systems to face the XXI century challenges more effectively?

Strategies to deal with Complex Systems more effectively

According to what has been said so far, it is clear-cut that if we want to deal with Complex Systems more effectively, we need to improve our ways of encoding, processing, memorizing, and transferring data and information. There are two promising strategies to succeed.

One strategy is by improving the performances of current electronic supercomputers that are based on the Von Neumann architecture. In fact, there is a worldwide competition in devising always faster supercomputers, having always larger memory spaces.

The other strategy is the interdisciplinary research line of Natural Computing [7]. Scientists working in the field of Natural Computing draw inspiration from nature to propose (I) new algorithms, (II) new architectures and materials to compute, and (III) new models to interpret the behaviour of Complex Systems. The rationale is that every distinguishable physicochemical state of matter or energy can be used to encode information. Within Natural Computing, there are two programs. In the first program, scientists exploit the physicochemical laws to make computations. In fact, every physicochemical law describes a causal event, and any causal event can be conceived as a computation. The causes are the inputs, the effects are the outputs, and the law governing the transformation is the algorithm of the computation. In the second program, scientists mimic natural information systems. All the natural information systems can be partitioned into four ensembles. The first is composed of the biomolecular information systems that are the cells. The second encompasses the neural information systems that are the nervous systems. The third contains the immune information systems that are the immune systems. Finally, the fourth contains the social information systems that are the societies belonging to the worlds of the micro-organisms, the plants, the animals, and humans. Living beings have peculiar attributes.

Peculiar attributes of life

Scientists and philosophers have been debating for a long time what the term life means [8, 9]. Living beings have distinct features. First, a boundary delimits the living being from the environment. Second, every living being has specific compounds that are fundamental to life. Relevant examples are DNA, RNA, proteins, water, salts, ATP, phospholipids, et cetera. Third, life is a self-propagating chemical system capable of undergoing adaptive evolution [10]. Fourth, a metabolic network self-sustains every living being. Fifth, every living being can protect itself from some intruders and noxious elements. The sixth attribute is teleonomy: the feature of having goals. A living being has the goal of surviving and reproducing. Finally, a living being can use matter and energy to encode, collect, process, store, and send information. Information is essential for life to pursue its goals.

A still open question

The appearance of life on Earth can be described as a phase transition or sudden change in how chemical systems can process and use information. In the beginning, the world was abiotic, and any chemical matter was unable to process information. Then, more than 4 billion years ago, the phase transition from a purely abiotic to the biotic world occurred. It is supposed that all organisms that are present nowadays derive from a unicellular organism, named as LUCA [11], which is an acronym meaning Last Universal Common Ancestor. The question is if this phase transition can still occur in other parts of the universe or it has already occurred. Astrochemistry and the science of Complex Systems can join their efforts and studies to find a plausible answer to this Really Big Question.

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