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Information and Negentropy: a basis for Ecoinformatics

Enzo Tiezzi, Department of Chemical and Biosystems Sciences, University of Siena, Italy, tiezzienzo@unisi.it ;
Nadia Marchettini, Department of Chemical and Biosystems Sciences, University of Siena, Italy, marchettini@unisi.it ;
Elisa B.Tiezzi, Department of Mathematic and Informatic Sciences, University of Siena, Italy, tiezzie@unisi.it .

Abstract

This paper is an attempt to develop the new discipline of ecodynamics as a quest for evolutionary physics and ecoinformatics.
Particular attention is devoted to goal functions, to relation of conceptualizations surrounding matter, energy, space and time and to the interdisciplinary approach connecting thermodynamics and biology.
The evolutionary dynamics of complex systems, ranging from open physical and chemical systems (strange attractors, oscillating reactions, dissipative structures) to ecosystems has to be investigated in terms of far from equilibrium thermodynamics (Prigogine).
The theory of probability is discussed at the light of new theoretical findings related to the role of events, also in terms of entropy and evolutionary thermodynamics.

Introduction

More than a hundred years ago, in 1886, Ludwig Boltzmann [1], one of the fathers of modern physical chemistry, was concerned with the relation between energy and matter in scientific terms. According to Boltzmann, the struggle for life is not a struggle for basic elements or energy but for the entropy (negative) available in the transfer from the hot sun to the cold Earth. Utilizing this transfer to a maximum, plants force solar energy to perform chemical reactions before it reaches the thermal level of the Earth's surface.

To live and reproduce, plants and animals need a continuous flow of energy. The energy of the biosphere, which originates in the luminous energy of the sun, is captured by plants and passes from one living form to another along the food chain. The energy captured by chlorophyll is stored in carbohydrates (molecules rich in energy), and by means of photosynthesis, a term that means "to make things with light". This radiant pathway that provides us with great quantities of food, fibers, and energy—all of solar origin—has existed for about four billion years, a long time if we think that hominids appeared on the earth only three million years ago and that known history covers only two thousand years. Our ancestor, the blue alga, began to photosynthesize, thus assuming a fundamental role in biological evolution.

The organization of living beings in mature ecosystems slows the dispersal of energy fixed by plants to a minimum, enabling them to use it completely for their own complex mechanisms of regulation. This is made possible by large "reservoirs" of energy (biomasses) and by the diversification of living species. The stability of natural ecosystems, however, means that the final energy yield is zero, except for a relatively small quantity of biomass that is buried underground to form fossils for the future.

Photosynthesis counteracts entropic degradation insofar as it orders disordered matter: the plant takes up disordered material (low energy molecules of water and carbon dioxide in disorderly agitation) and orders it using solar energy. It organizes the material by building it into complex structures. Photosynthesis is therefore the process that, by capturing solar energy and decreasing the entropy of the planet, paved the way for evolution.

It is important to emphasize that biological activity is a planetary property, a continuous interaction of atmospheres, oceans, plants, animals, microorganisms, molecules, electrons, energies, and matter, all part of a global whole. The role of each of these components is essential for the maintenance of life.

The relations and activities of the global biogeochemical system are life. The aim of science is to maintain these relations and characteristics; to live in harmony with nature, not to conquer it. This type of science comprehends complexity and uncertainty, and moves away from a deterministic-mechanistic view of the world in favor of a holistic and evolutionary view. It refers to the "clinamen" of Lucretius and to the "disciples of Sais" of Novalis rather than to the clockwork world of Descartes and the reversible time of Newtonian mechanics. It considers the constraints not as halters or chains but as conditions that create diversity and mutations, all of which amounts to biological evolution: constraints as sources of creativity and presuppositions for evolution.

The basic laws of physics from Newton to the present day have been time reversible; on the contrary, reality is constituted by phenomenological aspects: macromolecular organization, cellular differentiation, life processes, characterized by irreversibility of time. The reason for this lies in dynamical interactions that take place in complex systems. The analysis of reality requires major modification of current physical chemistry equations and theories. What is now clear is that complex systems and their behaviour can only be analyzed by means of relations including time as directional factor.

On one hand, the use of time-reversible classical and quantum physical chemistry approaches for studying matter at the molecular level and the behaviour of simple molecular systems has greatly improved man's understanding. On the other hand, we need new approaches and new time-irreversible theories able to describe the behaviour of complex systems.

As Thomas Khun [2] remarks, the passing of time often brings anomalies which existing theories are no longer able to explain. The divergence between theory and reality may become enormous and consequently a source of serious problems. This is exactly what is happening today between current scientific theories and the natural situation of the planet. For this reason the sustainability theory needs this type of approach.

In Khun's terms this means a shift toward a new paradigm. As Palomar in Italo Calvino's novel observed: "if the model does not succeed in transforming reality, reality must succeed in transforming the model".

Based on the .assumption that the interaction between biophysical constraints and evolution is not satisfactorily described by current scientific theories, this paper is an attempt to present a new model to be used in ecological physical chemistry as concerns entropy, energy and time fluctuations in biological and ecological systems.

The epistemology of the model derives from interdisciplinary cross-fertilization between physical chemistry, mainly thermodynamics, and ecology, mainly systems ecology. The logical consequence is a complete change of point of view or a "gestalt" shift in modelling the relationship between biophysico-chemical parameters and the global environment.

Professor Ilya Prigogine, Nobel prize winner in chemistry, founded the basis of this new discipline. We do like to call this new discipline Ecodynamics or Evolutionary Physics.

Dissipative structures

In the framework of evolutionary physics we deal with goal functions instead of state functions, the ecodynamic models have to be based on relations evolving in time; “far from equilibrium thermodynamics” (Prigogine) assumes upon itself the role of foundation of a new description of nature.

Prigogine introduces the concept of the arrow of time to describe irreversible changes. The main issue derived from the theory of dissipative structures is that the evolution and maintenance of open systems far from equilibrium are possible only if irreversible thermodynamic processes occur. Such processes dissipate energy and matter, increasing Entropy in the environment.

The evolutionary process is such that systems become more and more complex and organized. Biological diversity is the product of long-term interactions at a genealogical and ecological level: the genealogical interactions regard the dissipation of Entropy by irreversible biological processes; the ecological interactions regard Entropy gradients in the environment.

There are also chemical systems that show phenomena of self-organization such as the formation of stationary spatial structures or periodic oscillatory states. Self-organizing chemical systems have been of relevant importance for the development of the theoretical biology, and nowadays they cover an important role in the evolution of systems biology. This science has been originated from the confluence between molecular biology, with its emphasis on individual macromolecules (DNA, proteins, enzymes…), and the molecular self-organization theories, in which thermodynamics plays the key role

[3]. In his seminal work "*The Chemical Basis of Morphogenesis (1952)*" [4], Alan Turing theorized that tissues differentiation in the development of an organism starting from similar cells, could be due to a reaction-diffusion process in the cellar environment.

Under a theoretical point of view pattern formation can be modelled by the interaction between two diffusing biologically active chemical species. A process of this form is described by a pair of coupled reaction-diffusion equations:

$$\begin{aligned} \dot{u} &= F(u,v) + \nabla^2 u, \\ \dot{v} &= G(u,v) + \nabla^2 v, \end{aligned} \tag{1}$$

Where *u* and *v* are the scaled concentrations of the two diffusing and reacting chemical species, with *u* being the activator and *v* the inhibitor. *F(u,v)* and *G(u,v)* represent the interaction kinetics. Turing showed that a spatially homogeneus steady state of eq. (1) may become unstable via a simmetry breaking bifurcation if $\delta > 1$, that is when the inhibitor diffuses more rapidly that the activator. Associated with the instability is a critical wave number that determines tha wave length of the resulting pattern.

This intuition remained only a theoretical speculation until 90s, when Dekepper's group in Paris found this kind of structure in an oscillating chemical system performed on a gel substrate [5]. Nowadays, the chemical pattern formation is deeply studied for its implications in biological systems, in particular a relatively simple chemical model can be used to explicate a lot of behaviors in cellar and tissue development. We performed a great number of experiments studying the Belousov-Zhabotinsky (BZ) oscillating reaction in membranes used as model for biological systems [6], and the figures 1 and 2 explain the similarities between the laboratory model and biological systems of several orders of complexity.

In particular, figure 1a shows the *Labyrinthine* structures obtained in our experiments. These structures are also obtained by Cartwright [7], who obtained this specific pattern choosing for *F(u,v)* and *G(u,v)* the form of the van der Pol-FitzHug-Nagumo equations with diffusive coupling of both variables:

$$\begin{aligned} \dot{\psi} &= \gamma(\eta - \psi^3/3 + \psi) + \nabla^2\psi, \\ \dot{\eta} &= -\gamma^{-1}(\psi + \nu + \beta\eta) + \delta\nabla^2\eta, \end{aligned} \tag{2}$$

Here ψ represents the concentrations of activator, and η the concentration of inhibitor, of an autocatalytic reaction whose kinetics are determined by γ. This model has a homogeneus equlibrium state that is unstable to spatial oscillation via a Turing bifurcation for

$$|\nu| = \frac{\sqrt{\delta(\delta\gamma^2 - \beta)}(3\delta\gamma^2 - 2\delta\gamma^2\beta - \beta^2)}{3\delta^2\gamma^3} \tag{3}$$

and in addition is unstable to temporal oscillations via a Hopf bifurcation for

$$|\nu| < \frac{\sqrt{\gamma^2 - \beta}\left(3\gamma^2 - 2\gamma^2\beta - \beta^2\right)}{3\gamma^3} \tag{4}$$

The integration of these equations led to the formation of Labyrinthine patterns shown in figure 1b. The phenomenon is clearly related to the role of entropy in dissipative structures and to the input-output entropy flows.

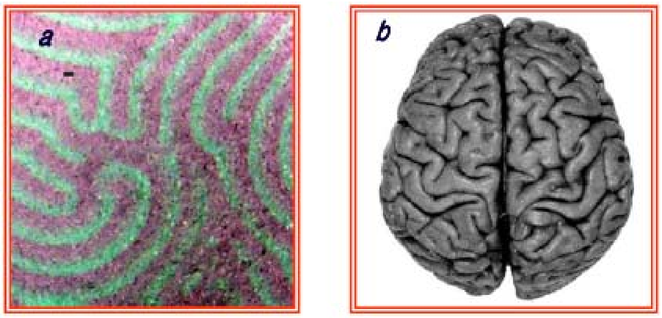

Figure 1 a)*Labyrinthine* chemical structure obtained with our reaction diffusion system (the Belousov-Zhabotinsky reaction) in lipid membrane b)Human brain

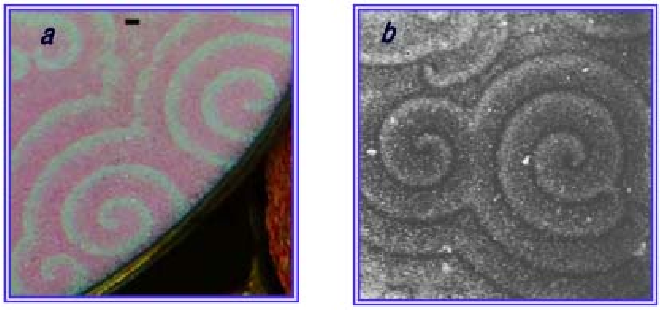

Figure 2 a)Spiral patterns obtained in our chemical systems b) A colony of *Dictyostelium Discoideum* [8]. The spirals shown are caused by the movement of cells in response to cAMP waves periodically initiated by the aggregation center.

Entropy and information

In the far from equilibrium thermodynamics the role of entropy is fundamental. We may say that entropy exist *per se*, is a non-conservative function and is related to evolution. This conclusion is a big step because it overcomes the old dilemma of whether entropy was the shadow of energy or vice versa, and does not reduce the ingenious invention of entropy to a purely energy dogma. The First Principle formulates the concept of energy in a conservation framework; the Second formulates that of entropy in an evolutionary framework. This is where evolutionary biology and mechanics meet. Schrödinger's introduction of the concept of negentropy was an inspired one: a living system absorbs negentropy from the external environment, structuring itself and evolving on the basis of this interaction. In other words, energy and entropy can be related, as is done in classical thermodynamics and statistical thermodynamics, but from the point of view of time, the two concepts are irreducible and different. In an evolutionary Gestalt, entropy has an extra gear which is the key necessary for studying living systems and ecology. It is important to study flows of energy and matter, quantities which are intrinsically conserved; it is also important to study entropy flows, an intrinsically evolutionary and non conserved quantity. The appearance of a term of entropy production, or "source term" as Aoki [8] calls it, is the watershed dividing the evolutionary world from the special case of conserved energy and mass. *But if energy and mass are intrinsically conserved and entropy is intrinsically evolutionary, how can entropy* *be calculated on the basis of energy and mass quantities (entropy paradox)?* This question is still unanswered [8] and all we can do is to note that the ecodynamic viewpoint is different from that of classical physics and classical ecology.

Let us observe the different relations of energy and entropy vs. information.

An energy flow can lead to destruction (increase in entropy, for example a cannon ball) or organization (decrease in entropy, for example photosynthesis). The same quantity of energy can destroy a wall or kill a man; obviously the loss of information and negentropy is much greater in the second case. Energy and information are never equivalent.

Entropy has the broken time symmetry of which Prigogine speaks. In other words, entropy has an energy term plus a time term that energy does not have.

Entropy has an intrinsic temporal parameter. Energy obeys spatial and material constraints; entropy obeys spatial, material and temporal constraints.

If history and the succession of events are of scientific relevance, the concept of function of state should be revised at a higher level of complexity. The singularity of an event also becomes of particular importance: if a certain quantity of energy is spent to kill a caterpillar, we lose the information embodied in the caterpillar. But were this the last caterpillar, we should lose its unique genetic information forever. The last caterpillar is different from the nth caterpillar.

Stories take place in a setting, the details of which are not irrelevant to the story. What happens in the biosphere, the story of life, depends on the constraints of the biosphere itself. Hence it is important to have global models of the biosphere in terms of space, time, matter, energy, entropy, information, and their respective relations.

Finally if we consider the evolutionary transition from anaerobic to aerobic living systems, the ratio of energy to stored information is clearly different. The information that led to an evolution and organization of the two types of system is not proportional to the flow of energy.

Thus entropy breaks the symmetry of time and can change irrespective of changes of energy, being energy a conservative and reversible property, whereas entropy is evolutionary and irreversible *per se*. The flow of a non-conservative quantity, negentropy, makes life go and the occurrence of a negentropic production term is just the point that differs from analysis based on merely conservative terms (energy and matter).

The situation is explained in *table 1* “The death of the deer”: mass and energy do not change, whereas entropy does. There is an entropic *watershed* between far from equilibrium (living) systems and classical systems (the dead deer or any inorganic-not living system).

Table 1: The death of the Deer

Far from thermodynamic equilibrium	ENTROPIC WATERSHED	Towards thermodynamic equilibrium
m		m
E		E
S		+ΔS
-ΔS		-ΔS_{lost}
information		Information lost

We may conclude that in the far from thermodynamics equilibrium systems (biology and ecology) *entropy is not a state function, since has intrinsic evolutionary properties*, strikingly at variance with classical thermodynamics.

The probability paradox

An event occurs in a stochastic manner because it is preceded by others. There are genetic and environmental constraints. Evolutionary events proceed in a manner that depends on time: they show a direction of time; they are irreversible.

Past time has determined the constraints; the future is largely unpredictable, and always has a stochastic or probable element.

Previously unobserved events cannot be predictable; rare and extreme events may completely change the dynamics of complex systems.

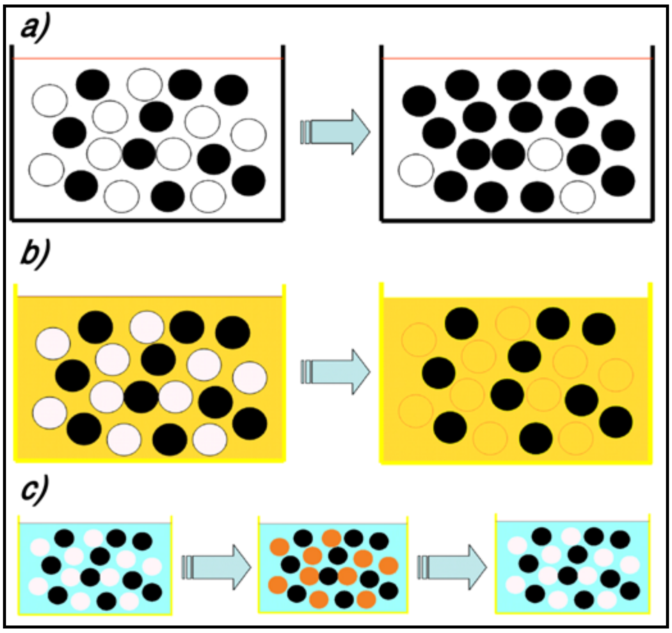

Figure 3 Unexpected events that may occur in living systems: a) oxidation; b) chameleon effect; c) oscillating reaction;

Figures 3 shows the *emergence* of a probability paradox in the presence of events:

a) suppose that an oxidation (chemical event), unknown to the observer, arises in the classic “white and black spheres” game: the probability white/black is no more fifty-fifty (only if the oxidation is changing the white sphere to grey, I may know what happened),

b) suppose that an evolutionary event also occurs , related to the *“chameleon” effect* (sensible to the environment): again the probability is no more fifty-fifty; moreover the event’s interval depends on the “chameleon”;

c) suppose an oscillating event occurs, similar to the previously observed BZ reaction: the situation is more complex and depends on many parameters. Again the observer has no possibility to predict which sphere will be picked up from the container.

It is possible to conclude that in the far from equilibrium framework a classical probability approach does not apply and new models have probably to be developed for the Boltzmann’s relation S = k lnW.

Conclusions

> *“in order to understand reality, let us divide it into parts, as many as possible”*
> *CARTESIO*

> *“the whole is more than the sum of its parts”*
> *PASCAL*

We may conclude that:
- In classical science:
  - geometric rules and mechanistic laws apply;
  - Newton's laws are reversible deterministic laws.

Prigogine adds and counterpoises the concept of "events" to "laws of nature" of this kind. We know that such laws are not true for living systems, ecosystems, and the events of biology and ecology.

Far from equilibrium we witness new states of matter having properties sharply at variance with those of equilibrium states. This suggest that irreversibility plays a fundamental role in nature.

We must therefore introduce the foundations of irreversibility into our basic description of nature (evolutionary thermodynamics).

It is also important to underline that:

- *Space is, by its structure, reversible*;
- *Time is, by its structure, irreversible*.

In order to achieve an ecodynamic description we need to shift our attention from state functions to goal functions.

We may conclude also with the following two statements by Sven Jørgensen:

“The presence of irreducible systems is consistent with Gödel’s theorem, according to which it will never be possible to give a detailed, comprehensive, complete and comprehensible description of the world. Most natural systems are irreducible, which places profound restrictions of the inherent reductionism of science.”;

“Many ordered systems have emergent properties defined as properties that a system possesses in addition to the sum of properties of the components – the system is more than the sum of its components. S. Wolfram [10] (1984) calls these *irreducible systems* because their properties cannot be revealed by a reduction to some observations of the behaviour of the components.”; and we may refer to the last Jørgensen’s book [11] for a complete review of Thermodynamic Theory for Ecosystems.

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