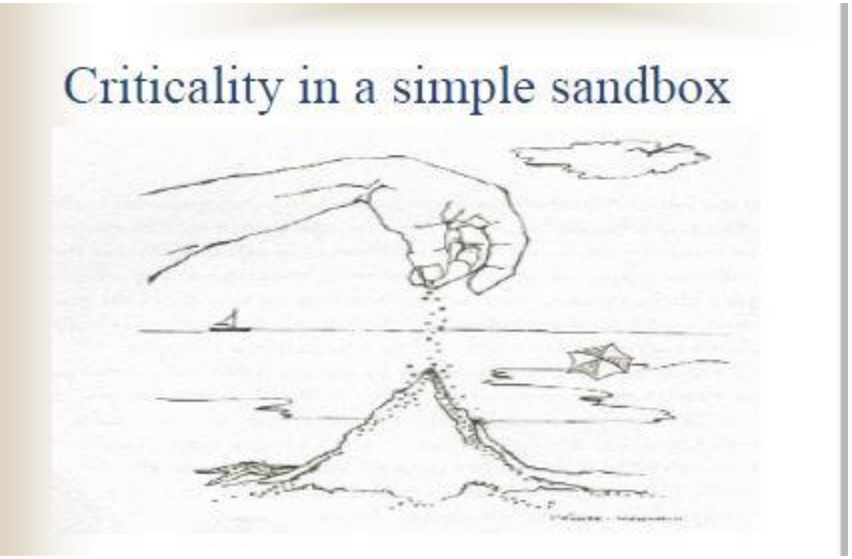
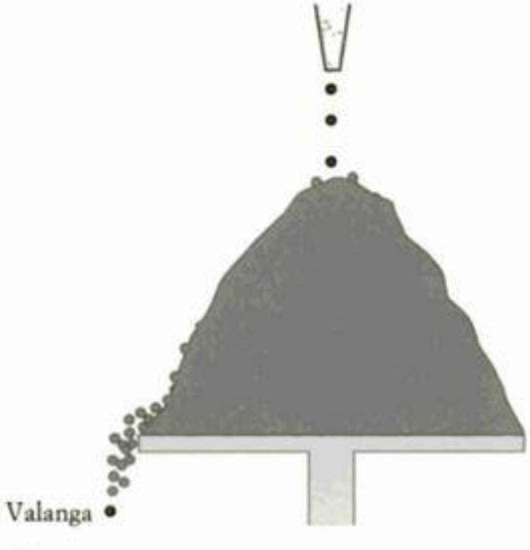
Applications and Examples (selforganization)

►***Improper systems from the complexity point of view***:





Bak and Self Organized Criticality

Per Bak's experiment to illustrate the criticality organized. On a sand pile resting on a circular plate are dropped, one at a time, the grains of sand ; the size of the avalanches that occur in the pile are then recorded.

A swarm-like flock of starlings

Termitarium, only one trivial rule: ants carry a lump of earth impregnated with a hormone that attracts other ants (feedback positive, attractor)

termitarium

►Basic models of flocking behavior are controlled by three simple rules:

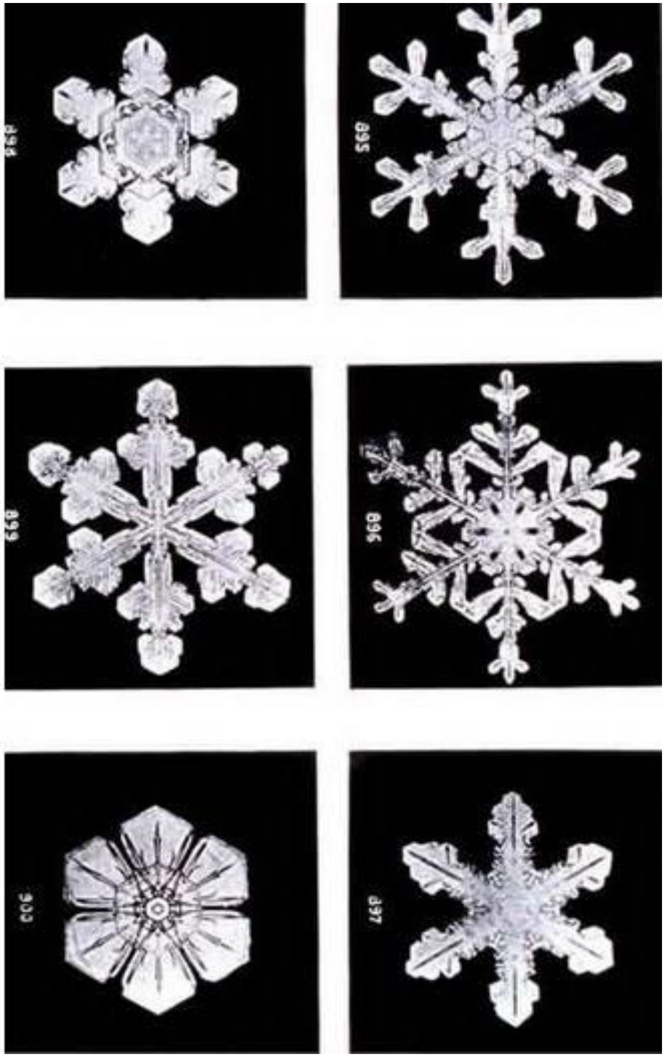
-Separation - avoid crowding neighbors (short range repulsion);

-Alignment - steer towards average heading of neighbors;

-Cohesion - steer towards average position of neighbors (long range attraction).

With these three simple rules, the flock moves in an extremely realistic way, creating complex motion and interaction that would be extremely hard to create otherwise (Craig Reynolds).

Snowflakes and feedback cycles



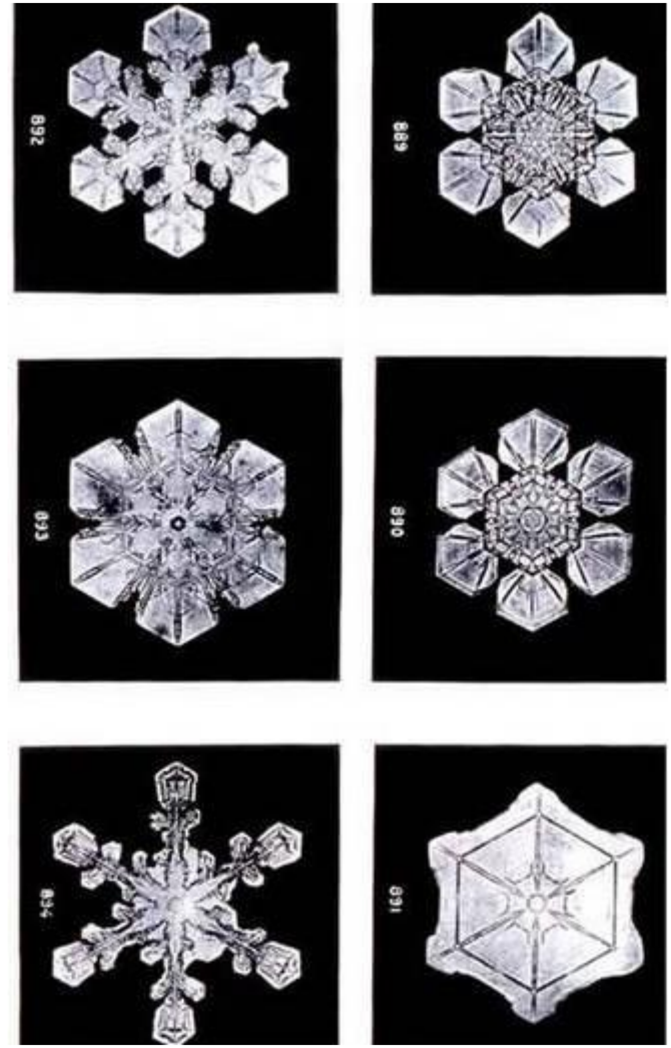
Why ever exagonal structure?

Why ever different?

Wonderful unpredictable laces!

What emergent phenomena implied?

Chance and necessity, entropy and energy.



- Importance of external humidity, temperature and pressure
- Positive and negative feedback cycles produce dendrites

Other strange emergencies at the nanoscales

Study of the fundamental forces: van der Waals, electrostatic, magnetic, capillary, ionic repulsion an frictional forces

- FMA and “Kinetic” hardness (well known macroscopic scale)

We can use the FMA to measure the stiffness and damping of fluids : the stiffness tells us to what extent the liquid layers return to the initial form (how much stored energy), while the damping tells us how much energy is lost in the push exerted on the layers of liquid.
If the probe moves up to 0.8 nm/sec, the water still behaves like a liquid , while beyond that threshold begins to behave as a solid.

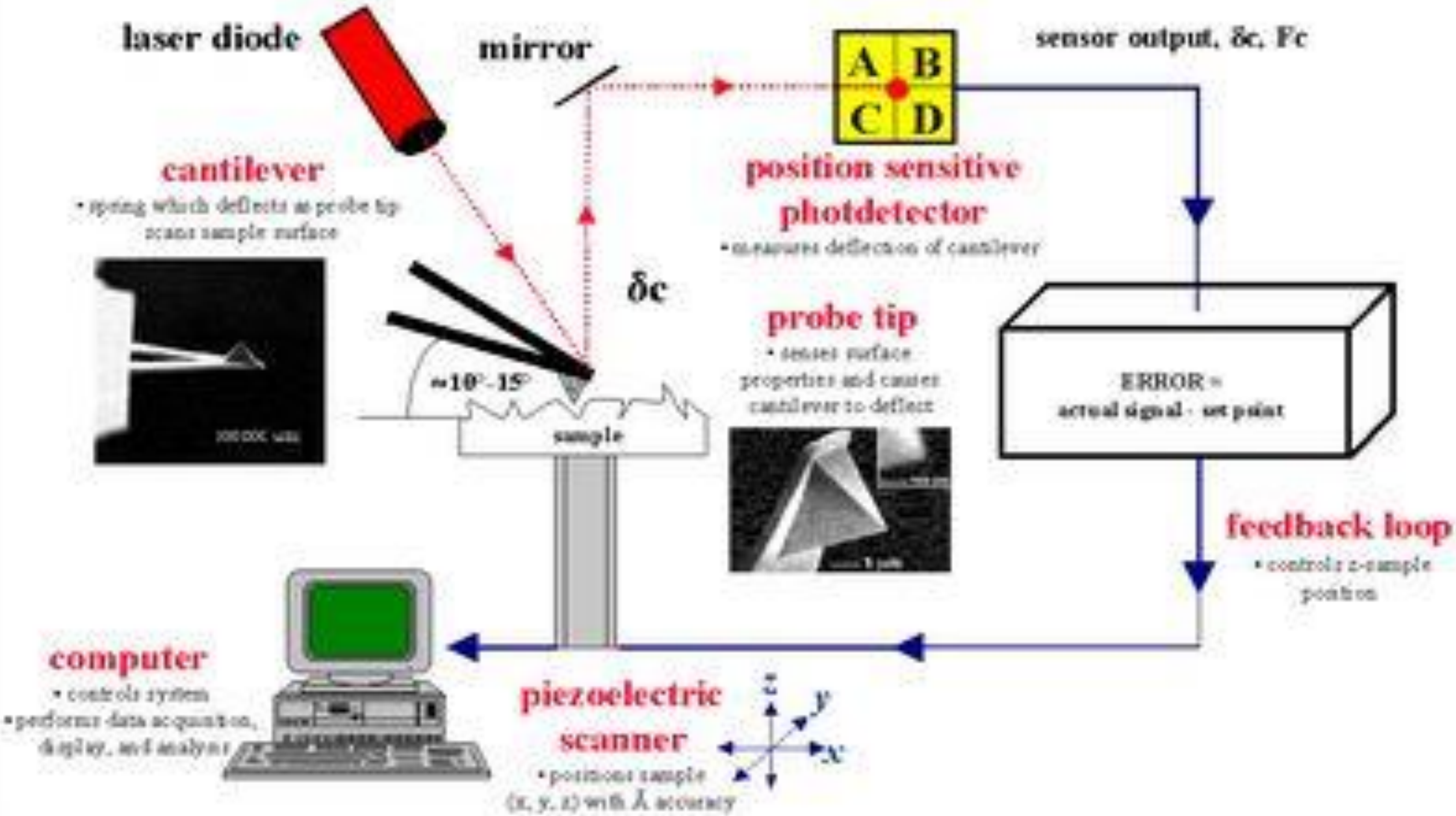
The transition between the two liquid states is sudden: below the critical value, the behavior is always that of a liquid, but over a very short speed range the system answers absolutely comparable like a solid [catastrophic transition, different regime]: why?
The answer is: cooperation!

The cooperation not only causes abrupt transitions but also significant variations in the time scales, making that even a molecular process can last for seconds or even minutes

Cfr Kauffmann, 2012

Atomic Force Microscopy (AFM) :

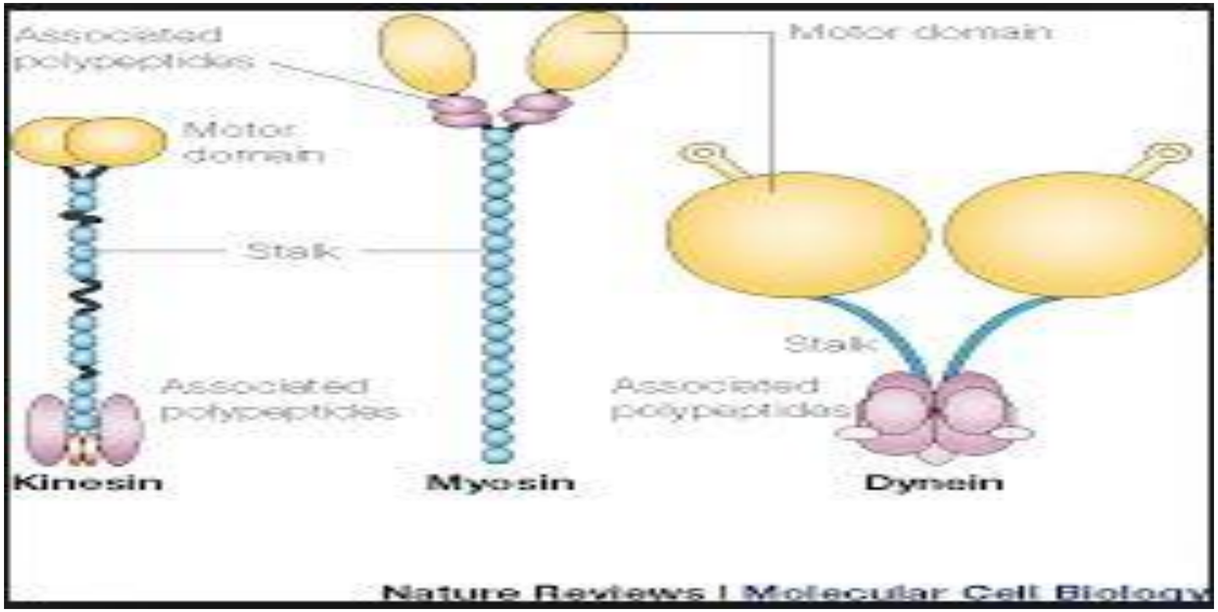
General Components and Their Functions

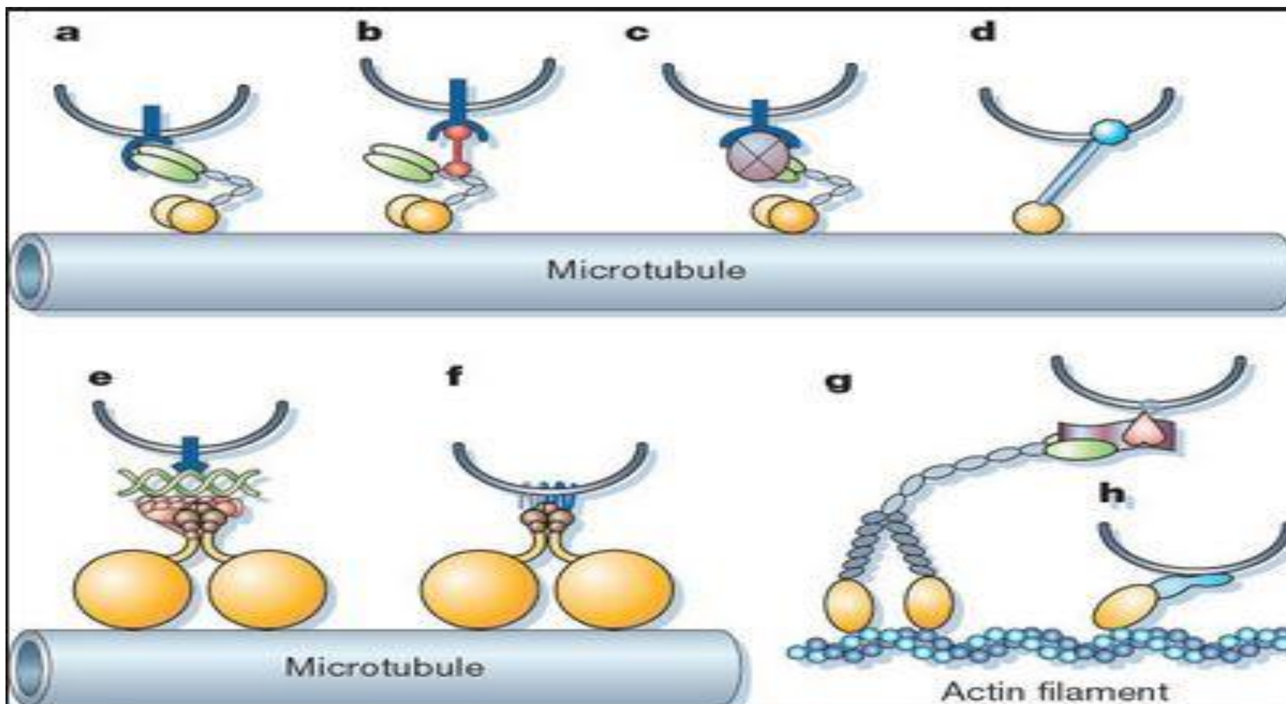


The thermal motion, entropic forces and cooperation are very important to understand the molecular mechanism of life.

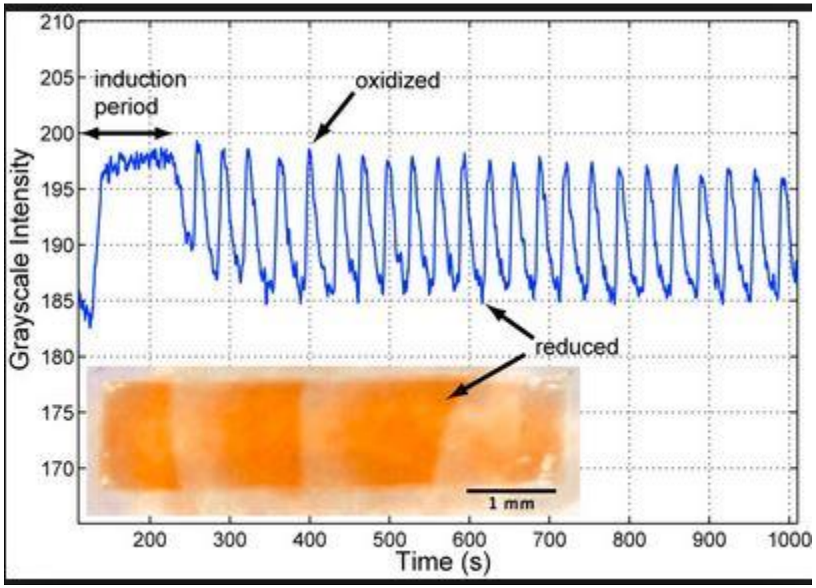
- Molecular machines

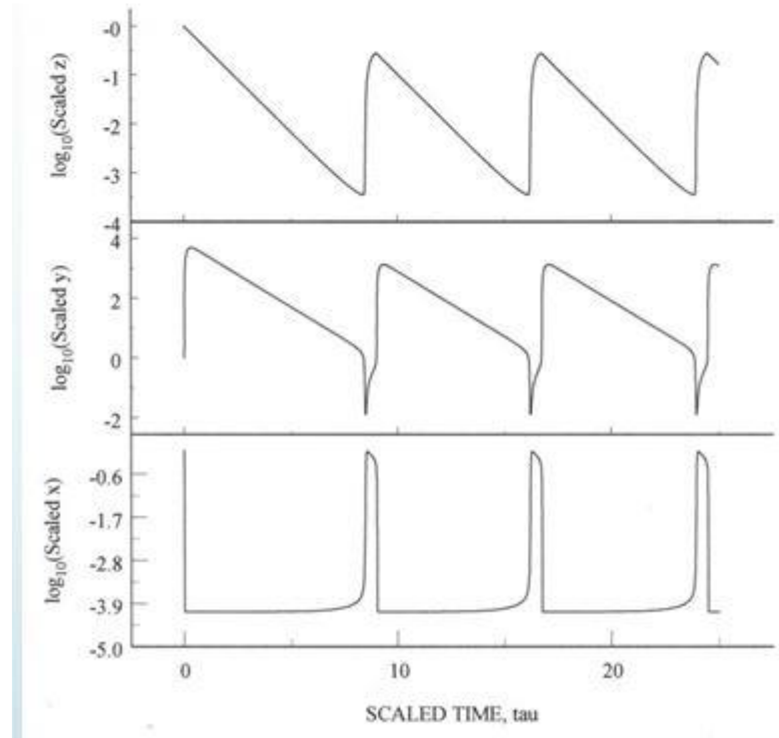
The nanoscale have another truly amazing feature: they know how to convert energy from a form to another one... molecular machines ... Only at the nanoscales many energy forms -from the elastic to mechanical, from chemical and electrostatic to thermal- have more or less the same order of magnitude. It is a fascinating and exciting possibility: the molecules of our body are capable of converting spontaneously many forms of energy among the: nanoscales are really special. Only at the nanoscale the thermal energy values are an order of magnitude such as to allow the formation of complex molecular structures and favor the spontaneous conversion between different forms of energy (self-assembly). Molecular storm do not always leads to chaos as the second law of thermodynamics seemed to indicate: molecular machines of living cells are not traditional molecules; they are small machines and skilled, able ***to extract order from chaos***.


Associated polypeptides
Motor domain
Motor domain
Stalk
Stalk
Associated polypeptides
Associated polypeptides
Kinesin
Myosin
Dynein
Nature Reviews | Molecular Cell Biology


a
b
c
d
Microtubule
e
f
g
h
Microtubule
Actin filament

Oscillating or periodic reactions and morphogenesis





Oregonator

- concentration inhomogeneity (temporal and spatial)
- external energy flux
- conditions far from equilibrium
- non-linear diffusion
- positive feedback (self-catalysis) and negative
- clock reactions
- no first order reactions
- bistability (hysteresis phenomena)

Biology examples:

- action potential propagation
- heart frequency
- glycolysis

Oregonator Model for Belousov- Zhabotinsky reaction

(Zhabotinsky, 1964; Field and Noyes, 1974)

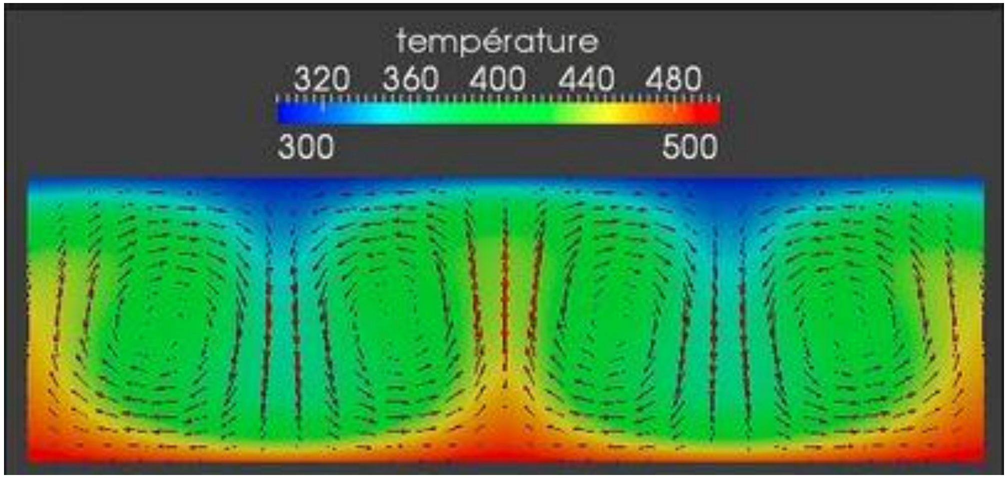
If

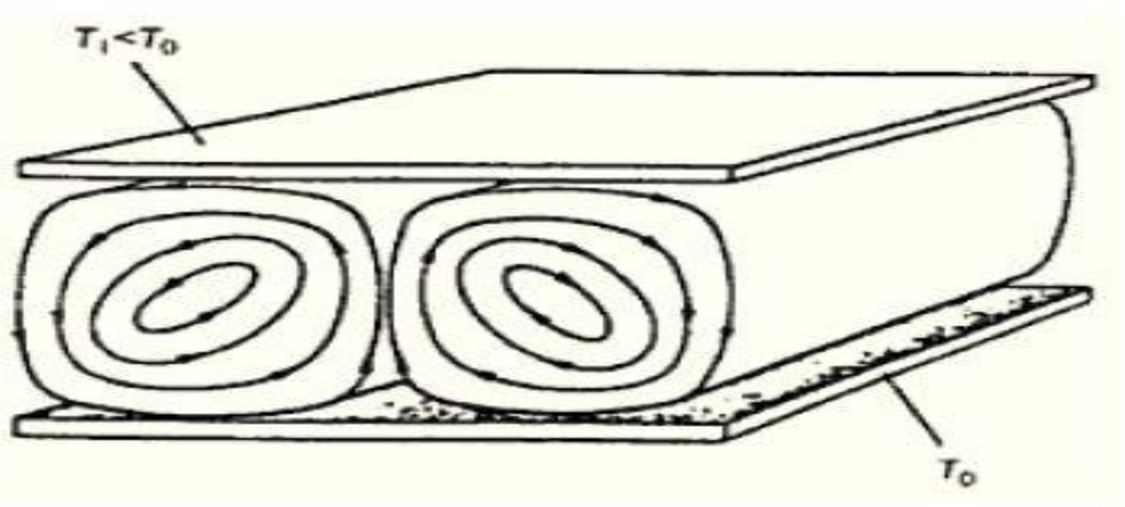
$A = BrO_3^-$
$X = HBrO_2$
$Y = Br^-$
$P = HOBr$
$Z = 2Ce^{4+}$
f= variable stoichiometric factor

$$A + Y \rightarrow X$$
$$X + Y \rightarrow P$$
$$A + X \rightarrow 2X + Z$$
$$2X \rightarrow A + P$$
$$Z \rightarrow f\,Y$$

Morphogenesis in Belousov-Zabotinsky evolving reaction

Bénard cells





Liquid-liquid an liqui-solid diffusion

-First cause: chemical potential gradient, $\mu_i \neq \mu_f$

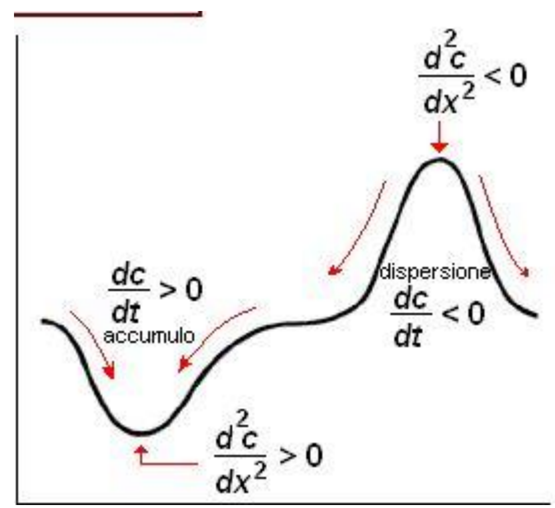
-Fick' s first law : $\boldsymbol{J_i^z = -D_i\, dx_i / dz_i}$ ***or*** $\boldsymbol{dm/dt = -DA\, dc/dz}$ ***z***

(where J_i^z =i-component flux , crossing a surface perpendicular to z; D_i = i-diffusion coefficient in considered phase; dx_i / dz_i =i-molar concentration gradient along z.

-diffusion velocity has an inverse proportionality to respect ionic radius and charge

-Fick's second law**:** $\boldsymbol{dc/dt = -Dd^2c/dz^2}$

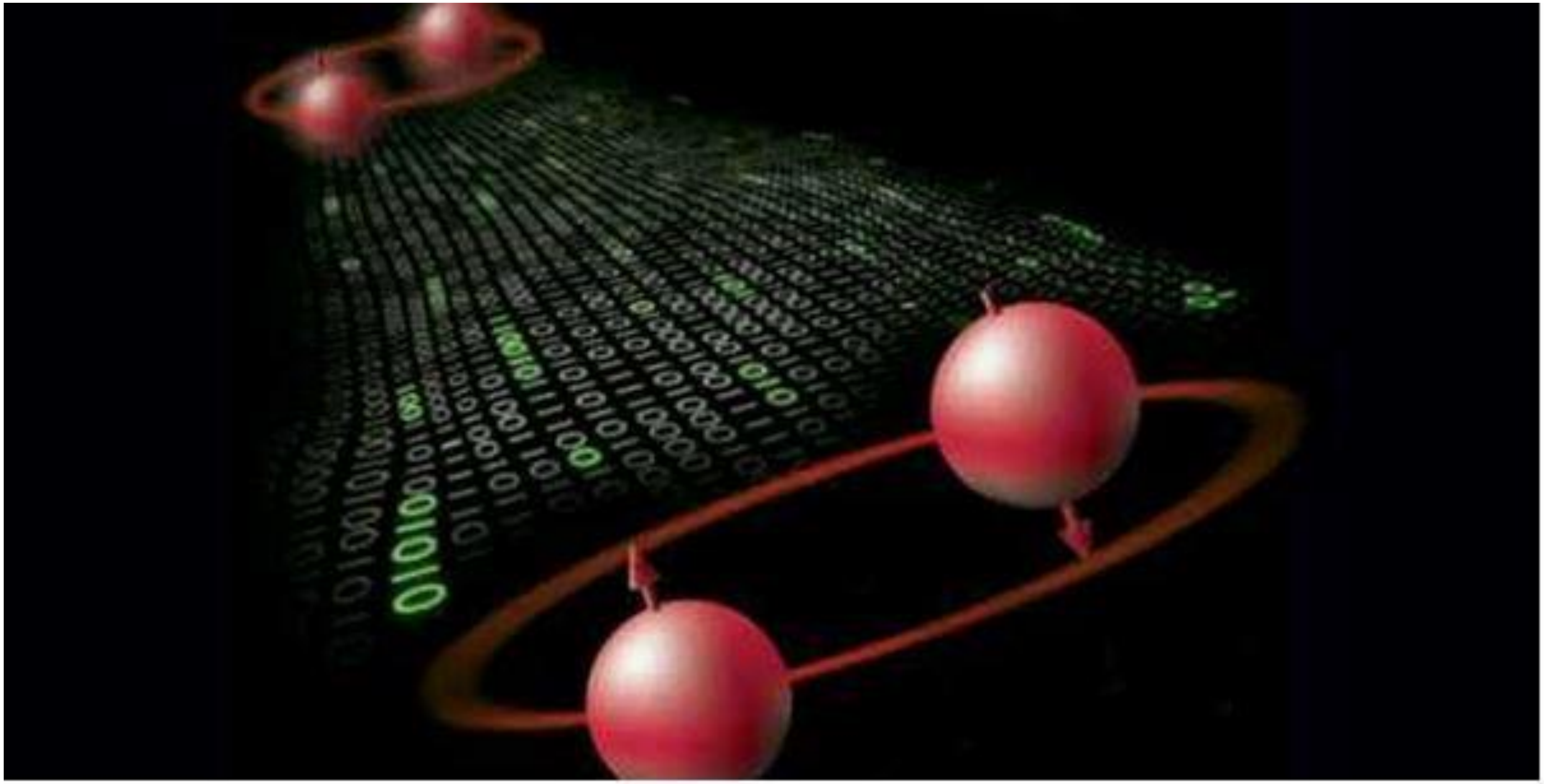
- These laws are important also in dendrites formation: in these case the chemical potential gradient is between two phases.



►***Proper systems from the complexity point of view and*** ***emergence***:

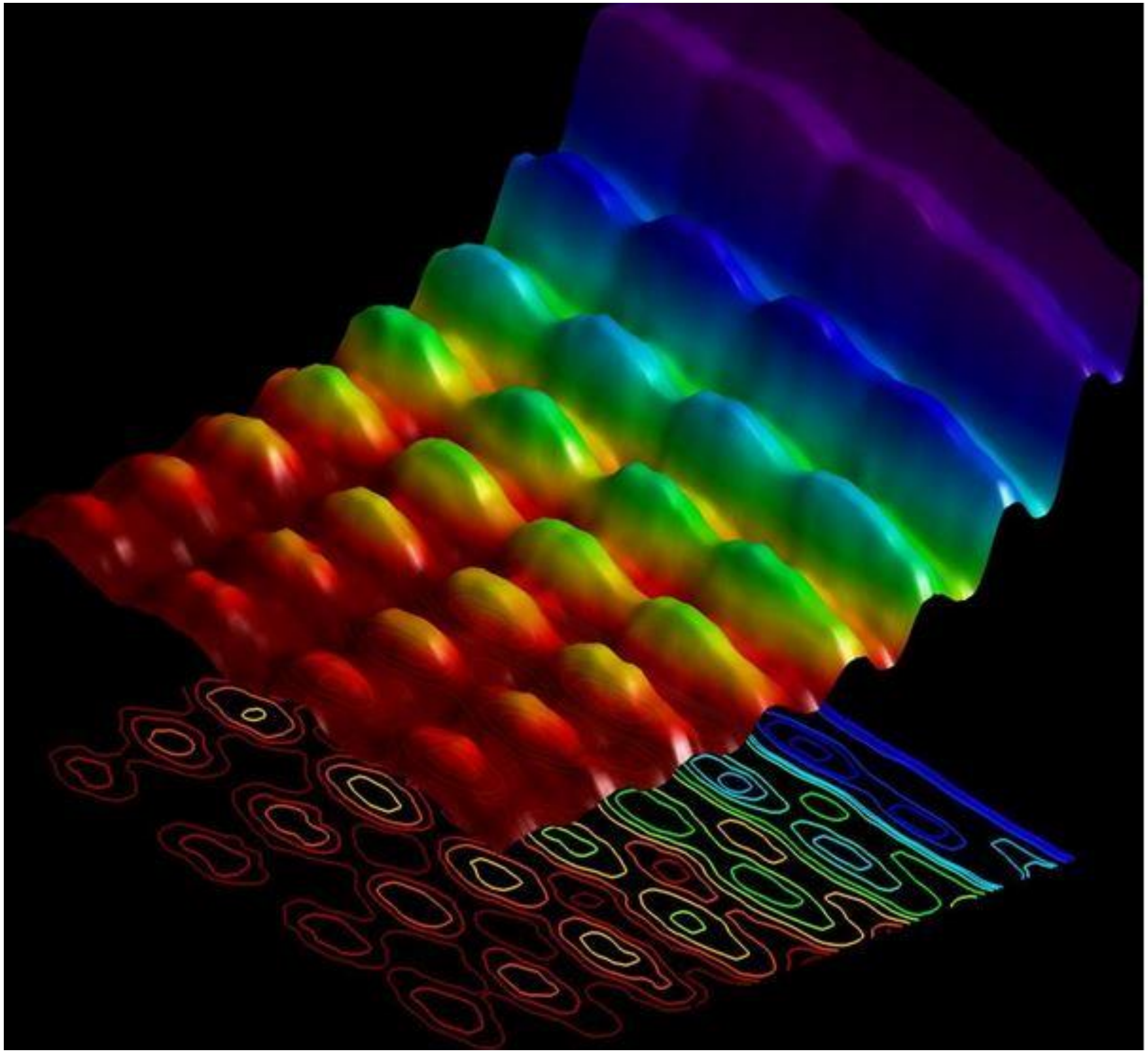
Entanglement: ***"microphysical olism" (?)*****(1935) (EPR-Bell)**

- Two quantum particles are enough! (If previously correlated):
- proton and electron as Hydrogen atom (?)
- non-locality
- photosynthesis and excitons (Fassioli, Olaya-Castro)
- cryptography
- quantum computer
- quantum teleportation (Zeilinger)
- space-time structure as light interconnected network (Einstein)



EPR, 1935
Schrodinger, 1936
Bell, 1964
Aspect et al., 1982

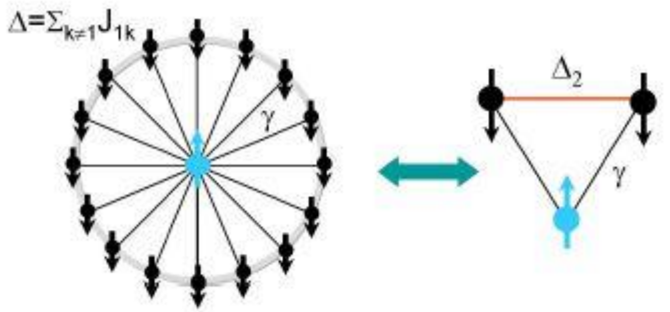
Cfr. Aspect, 1982

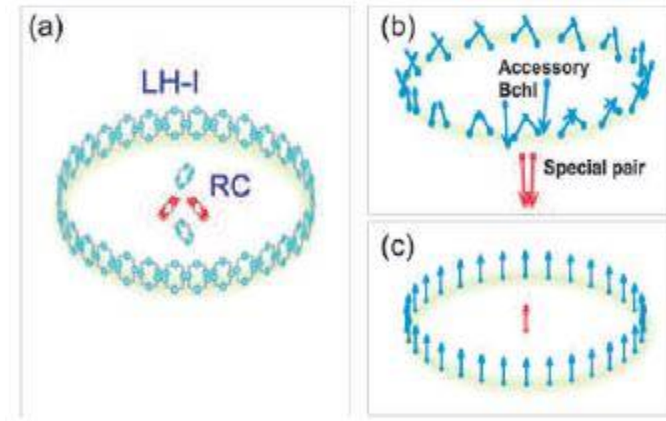


Piazza et al., 2015
Adesso-Girolami, 2012

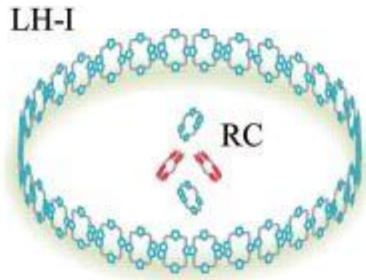
Wave-particle superposition

Photosynthesis and excitons





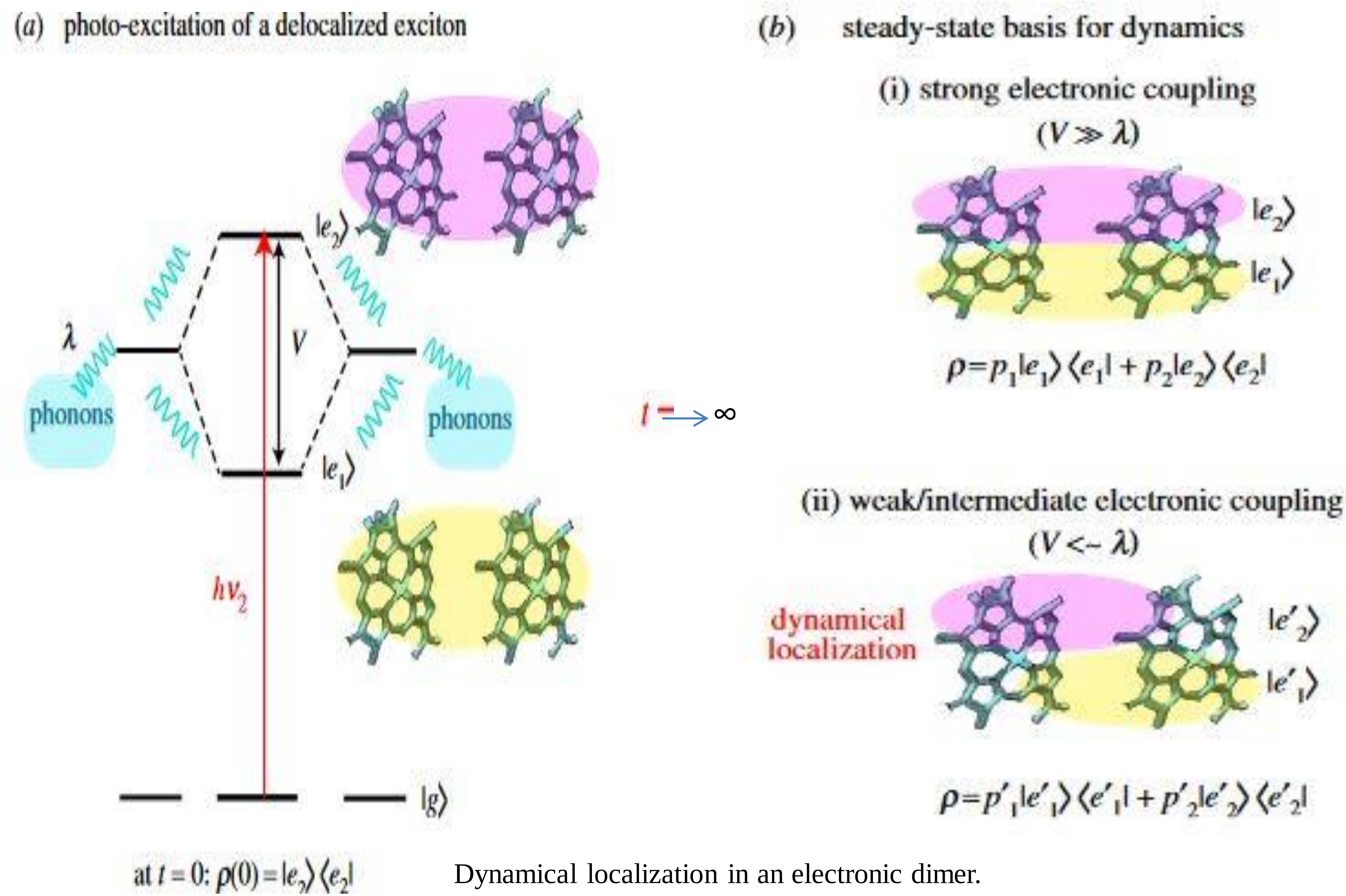
The role of quantum coherence in promoting the efficiency of the initial stages of photosynthesis is an open and intriguing question.



Exciton: an excited electronic state delocalized over several spatially separated molecules, which is the most widely available signature of quantum coherence in light harvesting.

Photosynthesis begins with light harvesting, where specialized pigment–protein complexes transform sunlight into electronic excitations delivered to reaction centers to initiate charge separation. There is evidence that quantum coherence between electronic excited states plays a role in energy transfer.

Olaya-Castro-Fassioli



Dynamical localization in an electronic dimer.

(a) At=0 light excites a fully delocalized electronic state. (b) The interaction with the phonon modes induces relaxation and dephasing, and the steady state of the system corresponds to a statistical mixture of electronic states. In the strong electronic coupling regime (i) the system is in a mixture of the fully delocalized excited states that diagonalize the electronic Hamiltonian. Otherwise (ii), the environment induces dynamical localization such that the excited states that diagonalize the density matrix in the steady state are more localized than the electronic eigenstates.

Cancer

Why it could apply the theory of complex systems to the study of cancer? A complex system can not be encoded in a single formal system. It can be looked at from different points of view, which means that we can build different models to describe different systems of relations: it therefore requires a dynamic management of the models.

Complex systems are open systems, where a continuous reorganization of energy and matter, and in particular information, are present and they are environment sensitive. However, we must not confuse such a environment sensitivity with what happens in chaotic systems (non-linear effects), but that there may be bifurcations, critical points, singularity, that change the history and that can be verified only after they happened. On the other hand a complex system presents different behaviors substantially equivalent from the point of view of energy: the way to use available energy-information is unpredictable.

This particular aspect may be important when the cell energy storage falls below a typical threshold of the optimum behavior of the differentiated cell.

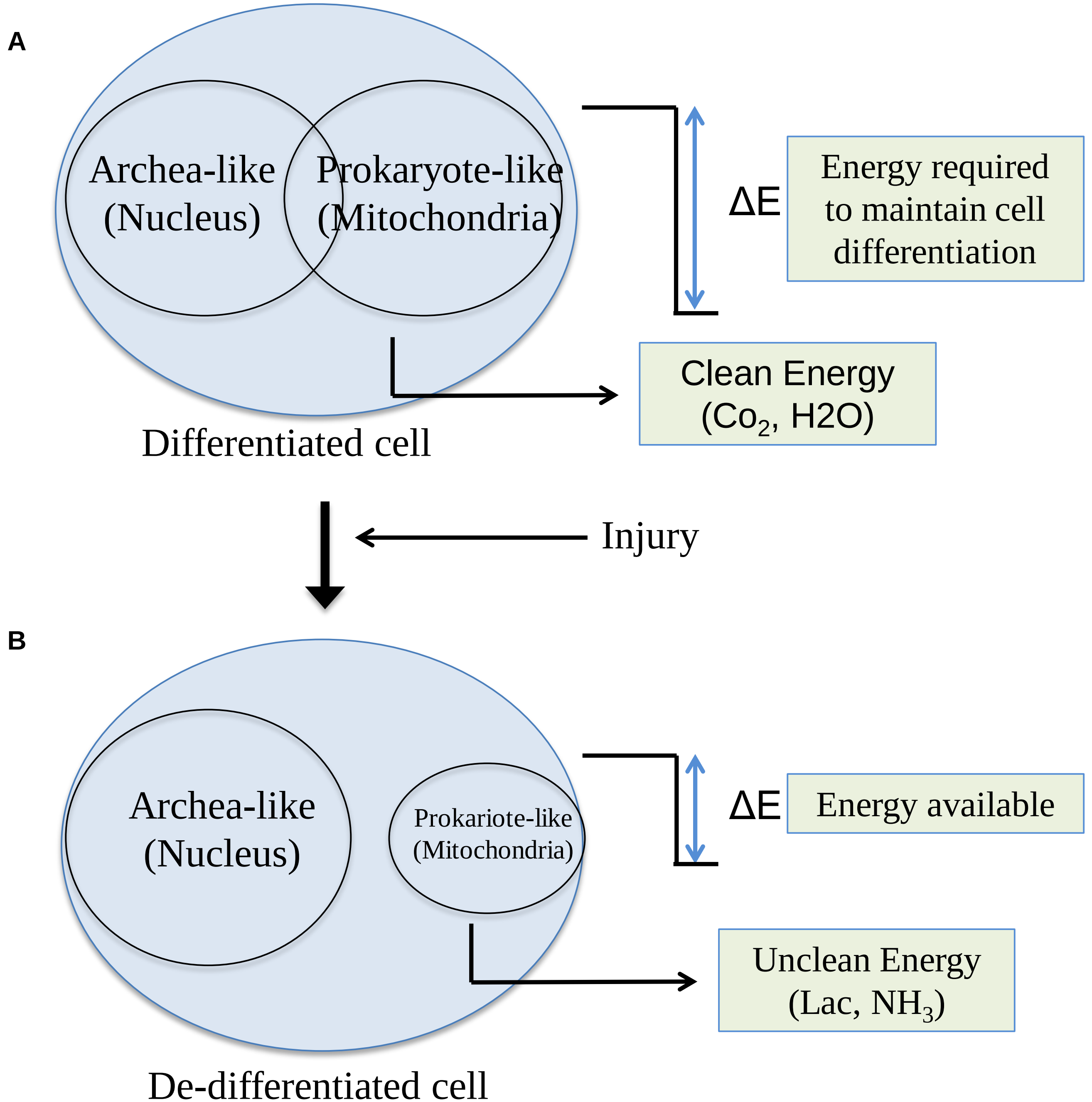

A
Archea-like
(Nucleus)
Prokaryote-like
(Mitochondria)
ΔE
Energy required to maintain cell differentiation
Clean Energy
(Co$_2$, H2O)
Differentiated cell
Injury
B
Archea-like
(Nucleus)
Prokariote-like
(Mitochondria)
ΔE
Energy available
Unclean Energy
(Lac, NH$_3$)
De-differentiated cell

Figure 1

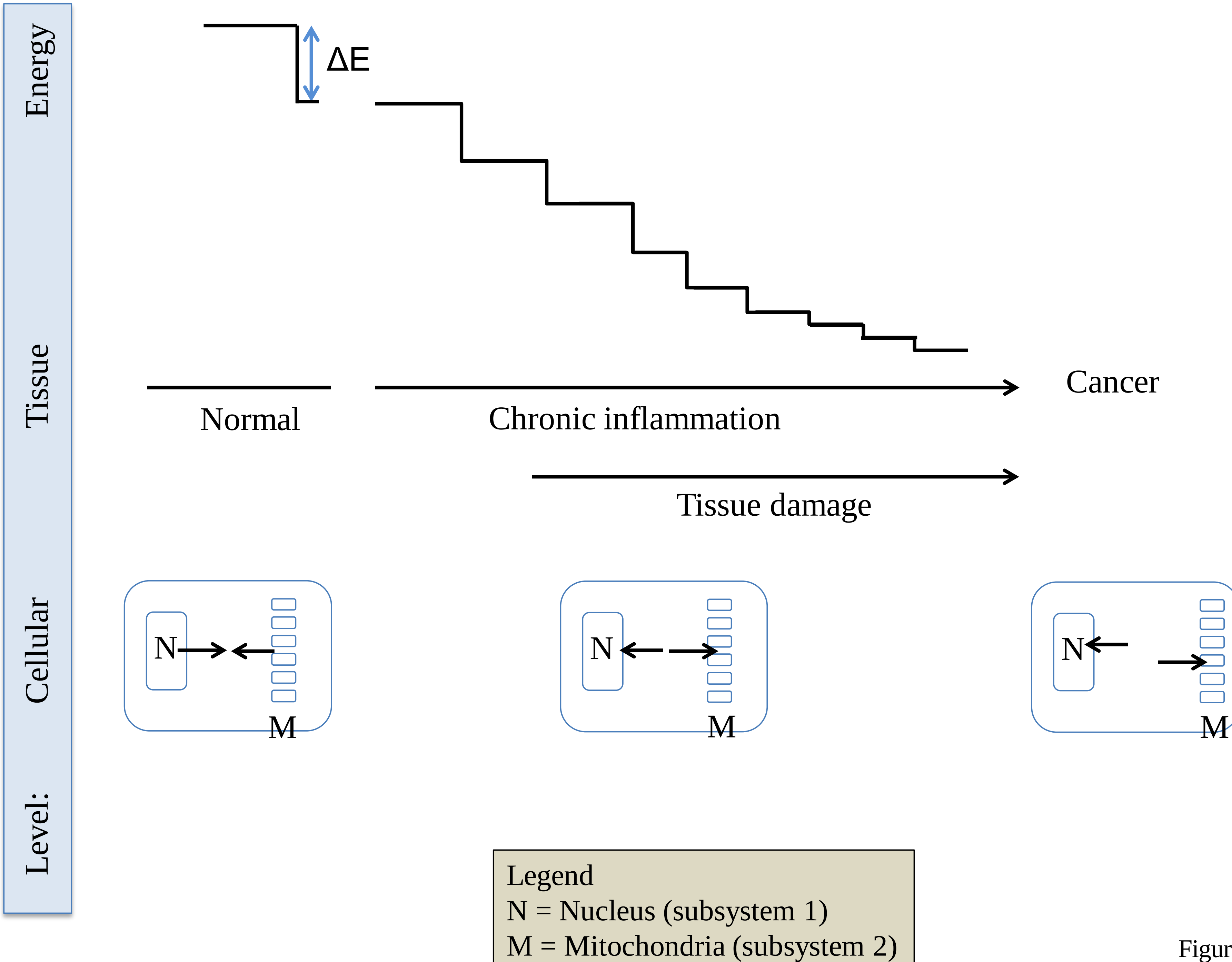

Level:
Cellular
Tissue
Energy
ΔE
Normal
Chronic inflammation
Cancer
Tissue damage
N
M
N
M
N
M
Legend
N = Nucleus (subsystem 1)
M = Mitochondria (subsystem 2)

Figure 2

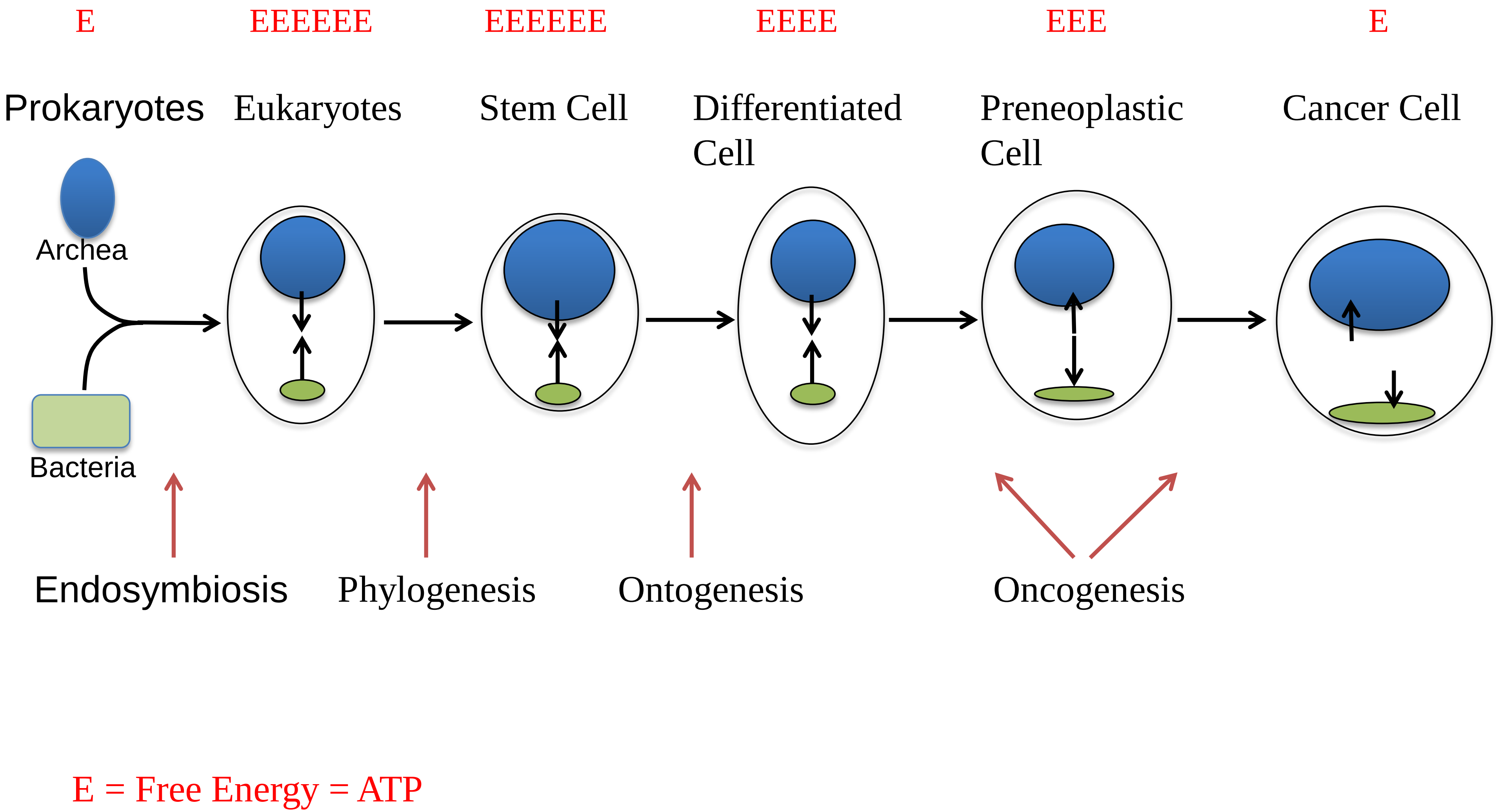
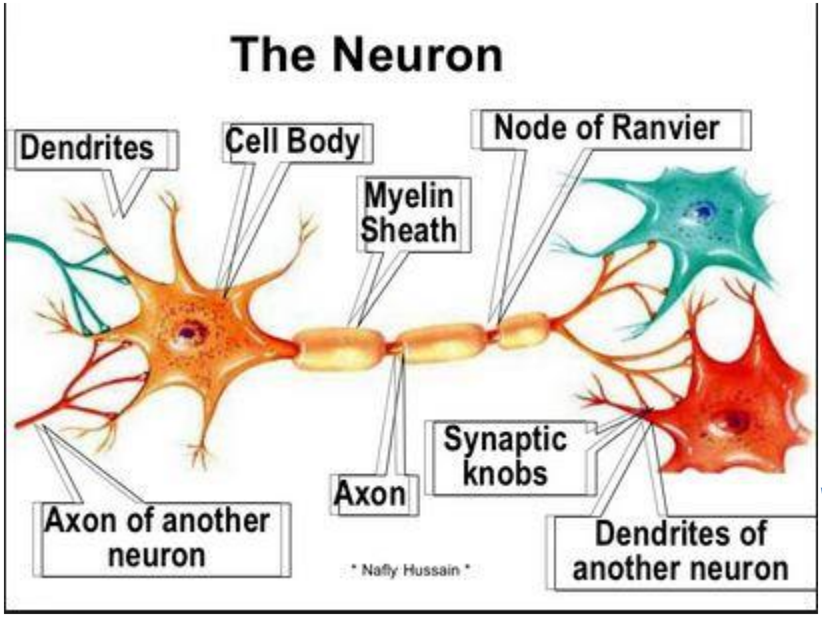

E
EEEEEE
EEEEEE
EEEE
EEE
E
Prokaryotes
Eukaryotes
Stem Cell
Differentiated Cell
Preneoplastic Cell
Cancer Cell
Archea
Bacteria
Endosymbiosis
Phylogenesis
Ontogenesis
Oncogenesis
E = Free Energy = ATP

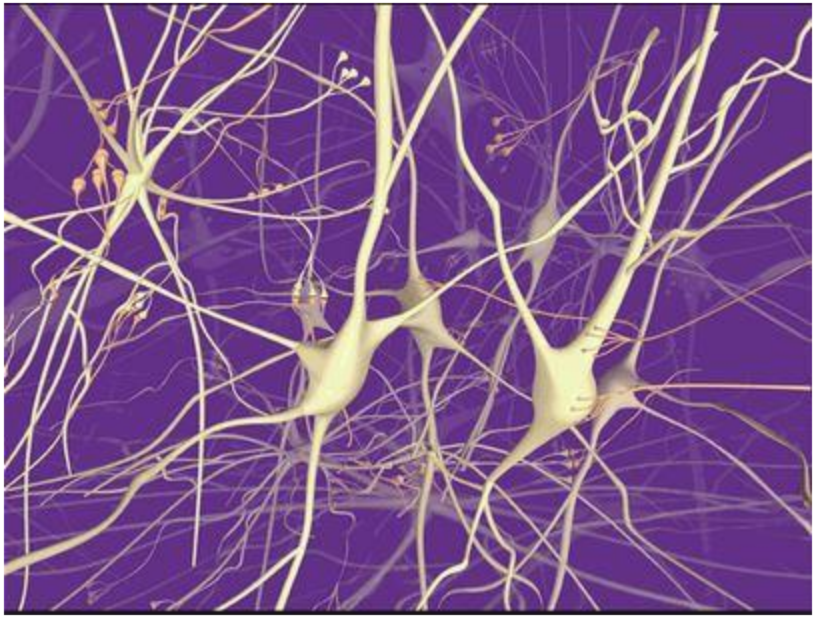
Figure 3

As there is no single model from which to deduce all, we must look at things: the facts determined by the experiments are extremely important. It is therefore important to continuously observe and to observe from different points of view. The reductionist research of fundamental building blocks is absolutely important. Finally, complex systems tend always to position themselves in an area where order and disorder almost coexist, so they have the advantages of both: renew the acquired spatio-temporal configurations by mixing them with the chaos and noise, and by maintaining the autonomy.

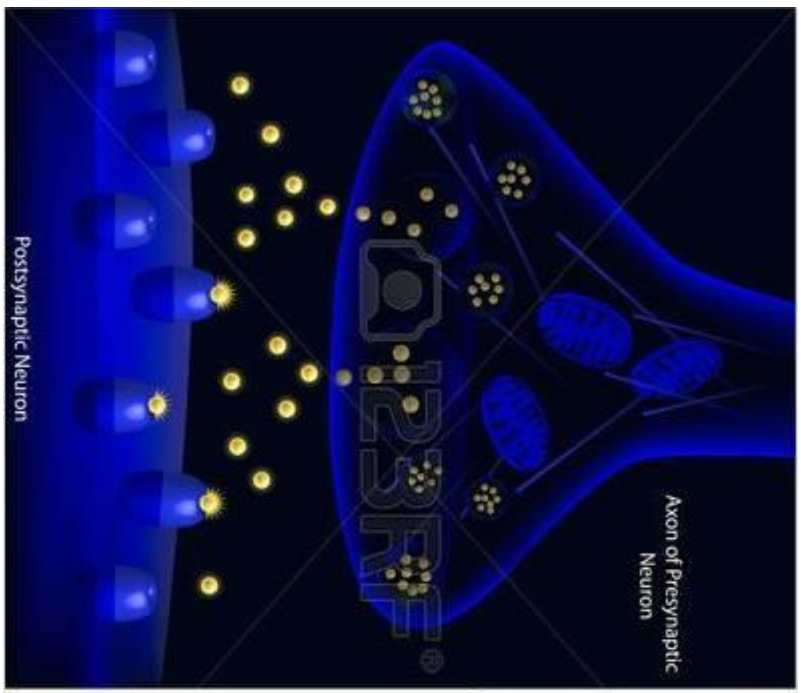
In the case of cancer, for example, from the reductionist point of view, we know almost all the elements and the forces in play, and so we have a very detailed description. But the event as a whole could be the global system emergency effect, where all the elements come into play every time in different way, according to the system-environment boundary conditions: there are several energetically equivalent solutions, and the final one is unpredictable, when for example there is a crucial decrease of energy within a cell.

Neurons and synapsis





Action potential and saltatory condution



Chemical synapsis

Brain

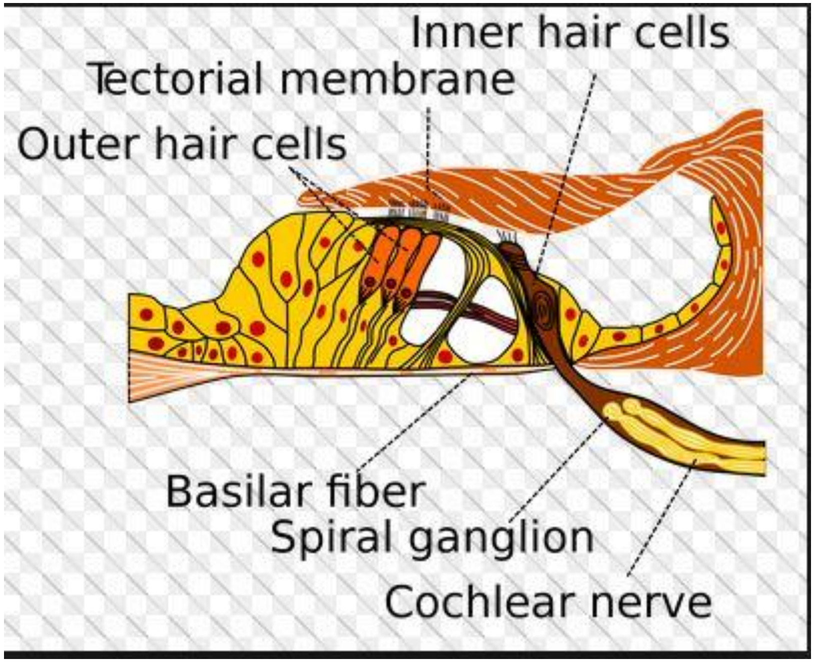
Two contrasting properties that coexist in the brains of higher vertebrates:

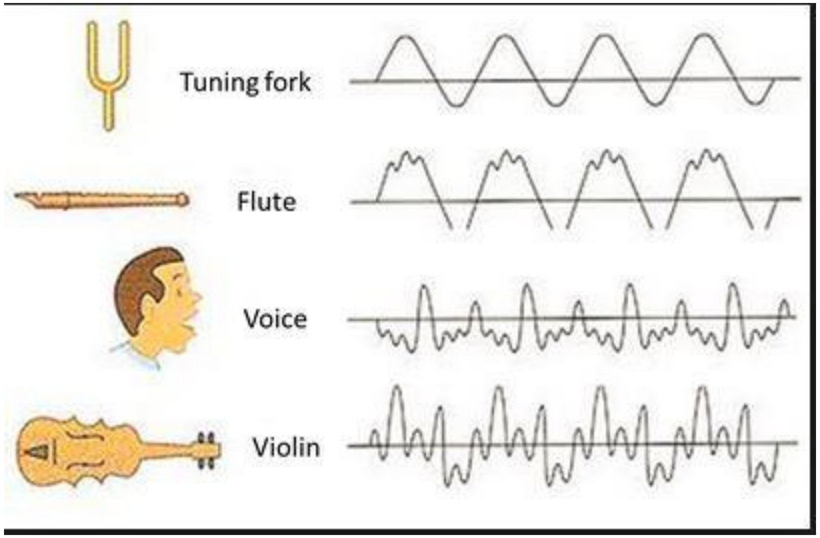
- the functional segregation of different brain regions
- their integration in perception and behavior.

The understanding of these two aspects of brain organization is central to any theoretical description of brain function.

Complexity should be low if the components of a system are completely independent or uniformly dependent, and complexity should be high if there is evidence of various degrees of dependence and independence: ***brain is supercomplex!***

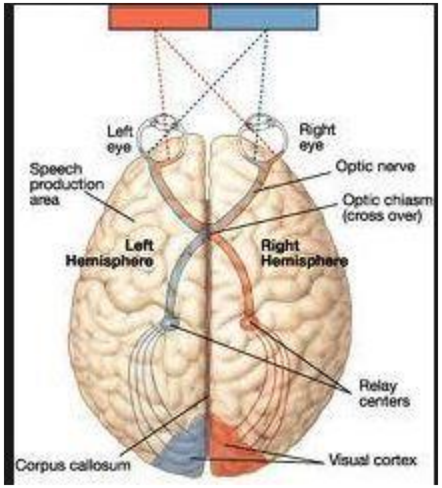
Sound and timbre

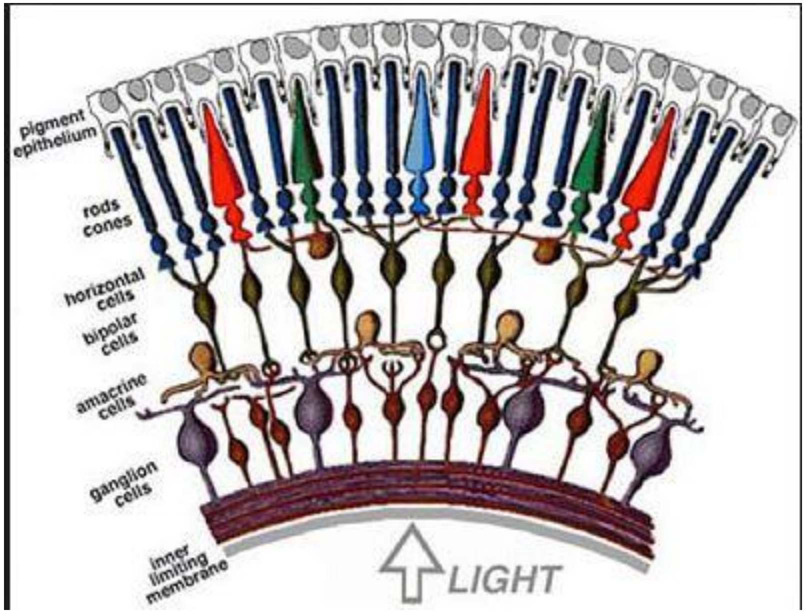




The Corti's organ is the ear transducer

Vision and colors





The chromophores present on the retina are able to transform the electromagnetic waves into signals that are propagated up to the cortex to give us the color sensations. The colors do not exist in nature! To see an object is a emergence of many different processes at the level of areas or subdivisions of areas; there is functional segregation for different stimulus attributes such as color, motion, and form: emergence is widespread patterns of correlations among neuronal groups as a temporal synchronization!

Tononi, 1994

Ecosystems

We have seen how a complex system is a group or organization which is made up of many Interacting parts. Archetypal complex system is an Ecosystem

Depending on one's point of view, one may regard either individual organisms, or entire species, as being the agents from which an ecosystem is built, Interactions among these agents take a variety of forms:

- predator-prey
- host-parasite interactions.

These interactions are asymmetric, the two agents involved playing different roles.
There are also symmetric interactions: competition among agents for resources like food or space.

Competition may be among members of different species or among members of the same species. Competition for mates: only among members of the same species.
Symbiotic relationships between individuals or species are another form of symmetric interaction, in this case beneficial to both partners.

Mitchell, 2002

What is the emergent behavior of an ecosystem?

There are many emergent behaviors, in fact. The very structure of an ecosystem is itself an emergent property: the fact that we have many competing species rather than only a single one is a result of species interactions.

Competition and cooperation between species makes it advantageous for species to inhabit restricted “niches," feeding on specific resources, or living in particular environments.
The many different forms of life seen on the Earth today are as much the result of interactions between organisms as they are the result of the influence of the external physical environment. Animal and plant behaviors are also substantially the result of interactions.

Emergent behavior of an ecosystem is evolution, and in fact the other behaviors above can themselves be regarded as merely one aspect of the evolution.

Evolution, the compounded result over long time periods of variation and selection, is responsible for every feature of ecosystem diversity that we see today. But conversely, ecosystem diversity is itself responsible for evolution.

Mitchell, 2002