Self-Organization of Complex Systems

Antonio García-Olivares
ICM-CSIC
agolivares@icm.csic.es

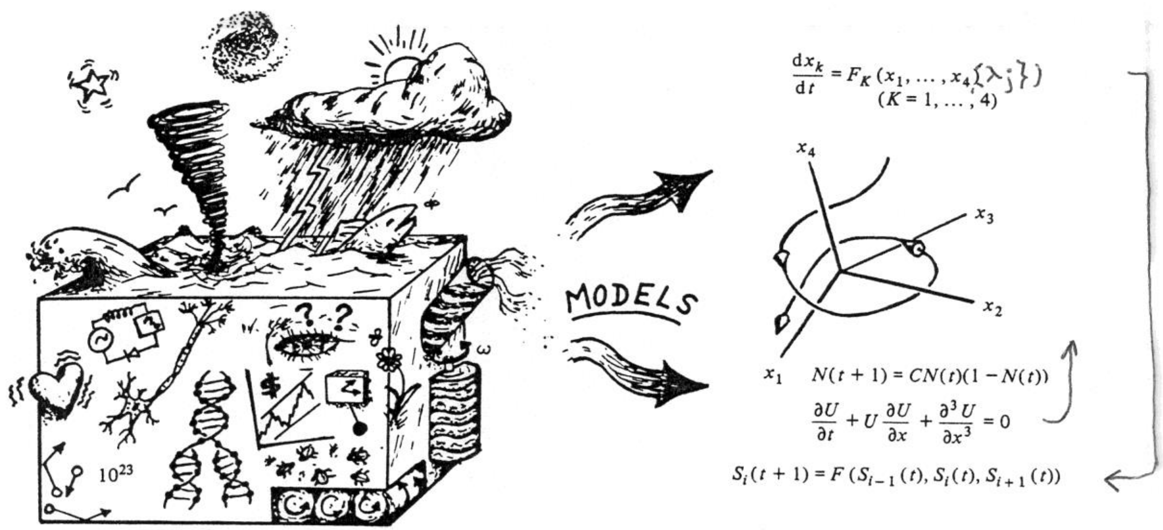
Ramon Margalef Summer Colloquia "What Ecology can learn from natural and human-induced disturbances – A cross-system view", July 2014.

Abstract

- The concept of self-organization is introduced in relation to its mathematical description and applications in biological sciences. The evolution of complex systems may be driven by synergetic changes and structural instability. related concepts such as biological assemblage, self-maintaining systems, and boolean networks are discussed. An example of modelling of enzymatic metabolism with master equation is shown. Some examples of modelling of co-evolution, cognitive emergences and social emergence are shown

Real world is complex

- Real phenomena precise complex models
- Complex models are simplified abstractions of real phenomena
- Which try to describe the most relevant qualitative features of them



Dynamics in the real world

This process contains the physical insight ('artistry') of the theorist in attempting to describe real phenomena

Nonlinear dynamics in the phase space of the physical variables

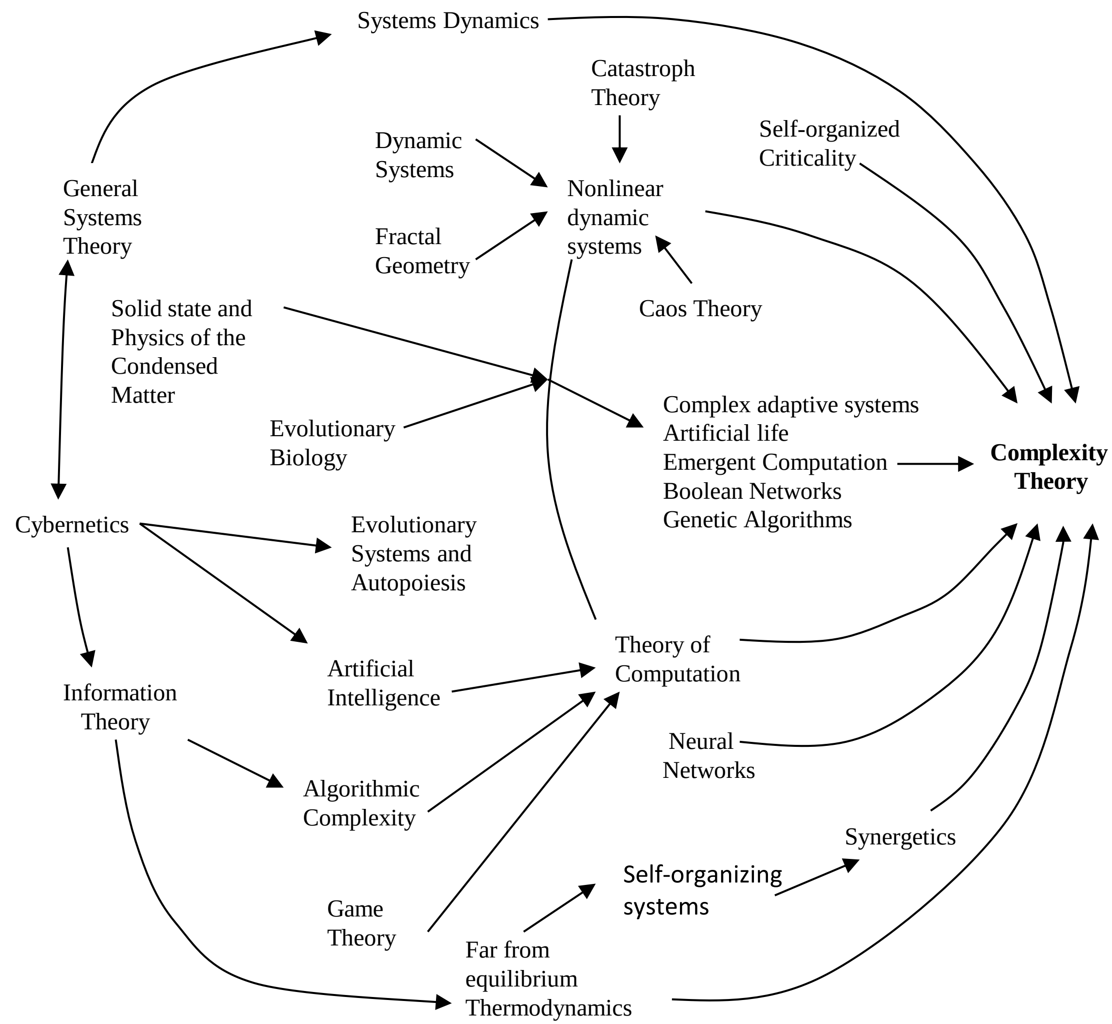
Nonlinear phenomena concern processes involving 'physical' variables, which are governed by nonlinear equations. These models have been obtained, by some approximate 'projection' rationale from presumably more fundamental microscopic dynamics of the system. (JACKSON, 1991).

Components of the complexity paradigm

➢ A set of contributions have converged in the attempt to model complex phenomena

- General systems (Bertalanfy): 1928
- Game theory (1928-1950's):
  von Neumann, Nash
- Cybernetics & Information: 1940's
- Systems dynamics (Forrester): 50's
- Far from eq thermo (Prigogine): 60's
- Self-organization & synergetics: 70's
- Complex adaptive systems
- Nonlinear dynamics
- Boolean networks

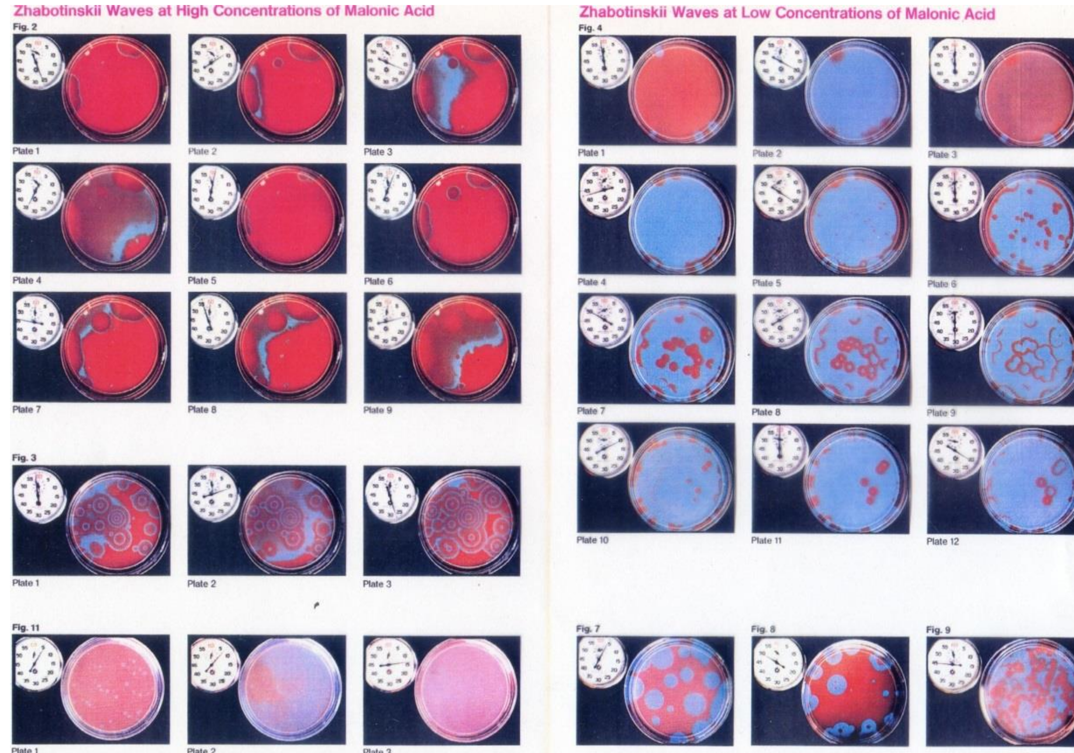
→ **Complexity paradigm**



Self-Organization

- One main feature of real phenomena is self-organization
- Ability of a system to spontaneously arrange its components or elements in a purposeful (non-random) manner, under appropriate conditions but without the help of an external agency
- It is as if the system knows how to 'do its own thing'
- Many natural systems show this property: galaxies, chemical compounds, cells, organisms, and even human communities

Physical and chemical patterns formation



- Belousov-Zhabotinsky reaction (Prigogine, Haken)

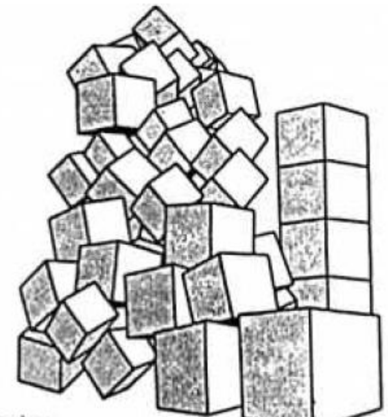
- Advective structures in a waste-water purification lagoon

Needed Ingredients of self-organization

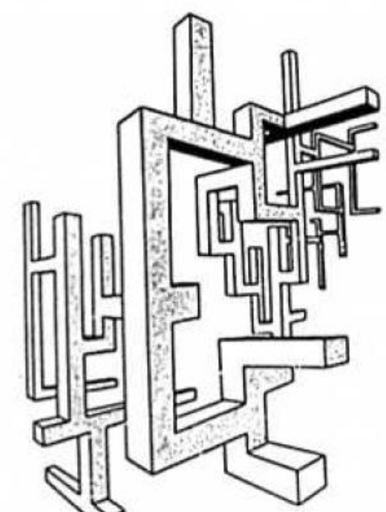
- A set of (many) elements
- Some interactive tendency (conatus):
  - Interaction probability between particles
  - Forces between molecules
  - Instincts, impulse in living beings
- It may depend on the state of the element and environment
- Random perturbations of the state of every element

Random perturbations and order from noise

- Von Foerster (1960): noise let the system explore its state space and find ‘attractors’
- Magnetic forces are stronger along certain directions
- Random perturbations permits to explore all the configurations and find the one with minimum energy



Antes de las agitaciones



Después de las agitaciones

Origin of attraction basins

A N-particles system can be described by the evolution of its state $(q_1, q_2, ...q_N, p_1, p_2...p_N)$

If there are frictions proport to velocity, the motion eqs:

$$dq_i/dt = \partial H/\partial p_i, \qquad i = 1, 2, ...N \tag{1a}$$

$$dp_i/dt = -\partial H/\partial q_i - \alpha p_j \delta_{ji}, \quad i, j = 1, 2, ..., N \tag{1b}$$

describe how the state goes through the phase space.

Any volume element in the phase space shrinks if the trajectory divergence is negative, which is our case:

$$\sum_{i=1}^{s} \left[\frac{\partial}{\partial q_i}\left(\frac{dq_i}{dt}\right) + \frac{\partial}{\partial p_i}\left(\frac{dp_i}{dt}\right) \right] = -\alpha \leq 0 \tag{2}$$

Any dissipative system satisfies this condition.

Open (to energy) dissipative systems have always attracting basins in their space of variables

Probabilistic evolution

Another feature of complex systems: many components $\rightarrow$ dynamic instability

Variables $\mathbf{x} = (x1, x2, ..., xc)$ in complex systems dont evolve deterministically from their initial states:

- Sensitivity to initial conditions
- Sensitivity to noise

They obey to transition probabilities per unit of time $W(\mathbf{x}, \mathbf{x}')$

Master equation:

$$\frac{dP(\mathbf{x},t)}{dt} = \sum_{\mathbf{x}'} W(\mathbf{x},\mathbf{x}')P(\mathbf{x}',t) - P(\mathbf{x},t)\sum_{\mathbf{x}'\neq\mathbf{x}} W(\mathbf{x}',\mathbf{x}) \qquad (3)$$

From master to Fokker-Planck eqs

In many practical cases:

-the N states (in every variable) are neighboring each other

- $N >> 1$ (almost a continuous set)

-transicions are always to neighbor states

- system has no memory

- W and $p(\mathbf{x}, t)$ are funtions of **x**

Making a Taylor expansion of the right side of (3) permits to obtain the Fokker-Planck eq:

$$\frac{\partial p(\mathrm{x}, t)}{\partial t} = -\sum_{i=1}^{C} \frac{\partial}{\partial x_i} \left[K_i(\mathrm{x}, t) p(\mathrm{x}, t)\right] + \frac{1}{2} \sum_{i,j=1}^{C} \frac{\partial^2 \left[Q_{ij}(\mathrm{x}, t) p(\mathrm{x}, t)\right]}{\partial x_i \partial x_j} \quad (4)$$

where C is the number of variables and:

$$K_i(\mathbf{x_0}, t) = \frac{1}{N} \sum_{\mathbf{k}} k_i w_{\mathbf{x+k \to x}}(t) =$$

$$\lim_{\tau \to 0} \frac{1}{\tau} \langle [x_i(t+\tau) - x_{0i}(t)] \rangle \qquad i, j = 1, 2, ..., C$$

and the *drift* and *fluctuations* matrix:

$$Q_{ij}(\mathbf{x}, t) = \sum_{\mathbf{k}} k_i k_j w_{\mathbf{x+k \to x}}(t) = \tag{6a}$$

$$\lim_{\tau \to 0} \frac{1}{\tau} N_0 \langle [x_i(t+\tau) - x_{0i}(t)] [x_i(t+\tau) - x_{0i}(t)] \rangle \tag{6b}$$

with $k_i, k_j \in \{0, \pm 1\}$, if $\mathbf{x}$ are occupation numbers.

The drift is the mean instantaneous rate of change of states close to $(\mathbf{x}, t)$

The fluctuation matrix is the local rate of change of the variances of these states. It tends to zero in deterministic processes

When transition probabilities are not known, Fokker-Planck eq is useful as an euristic tool:

- Drift of the mean state can be inferred from the mean observed trajectory

- $\mathbf{Q}$ can be modelled as a *noise* intensity coming from microscopic fluctuations and external perturbations

- Fokker-Planck eq without b.c. can be solved explicitly:

$$p(\mathbf{z}, t+\Delta t) = \int_{\mathbf{x}} d\mathbf{x} p(\mathbf{x}, t) \sqrt{\frac{det[Q(\mathbf{y}, t)]}{(2\pi)^N \Delta t}} \exp \left[\frac{[\mathbf{z} - \mathbf{y} - \mathbf{K}(\mathbf{y}, t)\Delta t]^T [Q(\mathbf{y}, t)]^{-1} [\mathbf{z} - \mathbf{y} - \mathbf{K}(\mathbf{y}, t)\Delta t}{-2\Delta t} \right. \tag{7}$$

With b.c., it is easier to solve a set of Langevin stochastic equations, which are formally equivalent:

$$\frac{dx_1}{dt} = f_1(x_1, \{x_j\}, t\}) + \sum_{j=1}^{C} g_{1j}\zeta_1(t)$$

$$\frac{dx_2}{dt} = f_2(x_2, \{x_j\}, t\}) + \sum_{j=1}^{C} g_{2j}\zeta_2(t)$$

$$\cdots$$

$$\frac{dx_C}{dt} = f_N(x_N, \{x_j\}, t\}) + \sum_{j=1}^{C} g_{Cj}\zeta_C(t)$$

where ζ_i is a δ-correlated Gaussian fluctuating (or random) perturbation in the variable i.

Relationship between the two formulations:

$$K_i(\mathrm{x}) = f_i(\mathrm{x}) + \frac{1}{2}\sum_{\mathbf{k,j=1}}^{C} \left[\partial_k g_{ij}(\mathrm{x})\right] g_{kj}(\mathrm{x}) \qquad and:$$

$$\frac{1}{N}Q_{ik}(\mathrm{x}) = \sum_{j=1}^{C} g_{ij}(\mathrm{x}) g_{kj}(\mathrm{x})$$

P(q,t) when drift $\delta(q)$ derives from a potential V(q)

- The attractor is in the bottom of V(q)

- If parameters α, γ, β change and V(q) bifurcates, the Fokker-Planck eq tells us how P(q) adapts to the new attraction basin

- This is a way to model qualitative change of a system that losses stability due to environmental change

- Qualitative changes correspond to topo-logical changes in the attraction basin

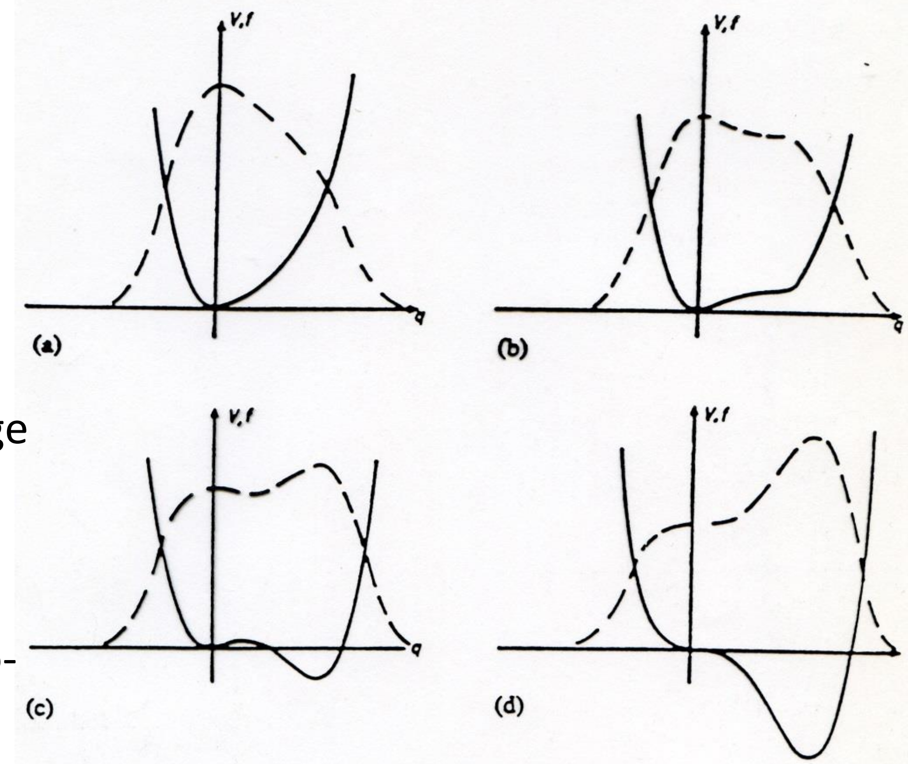
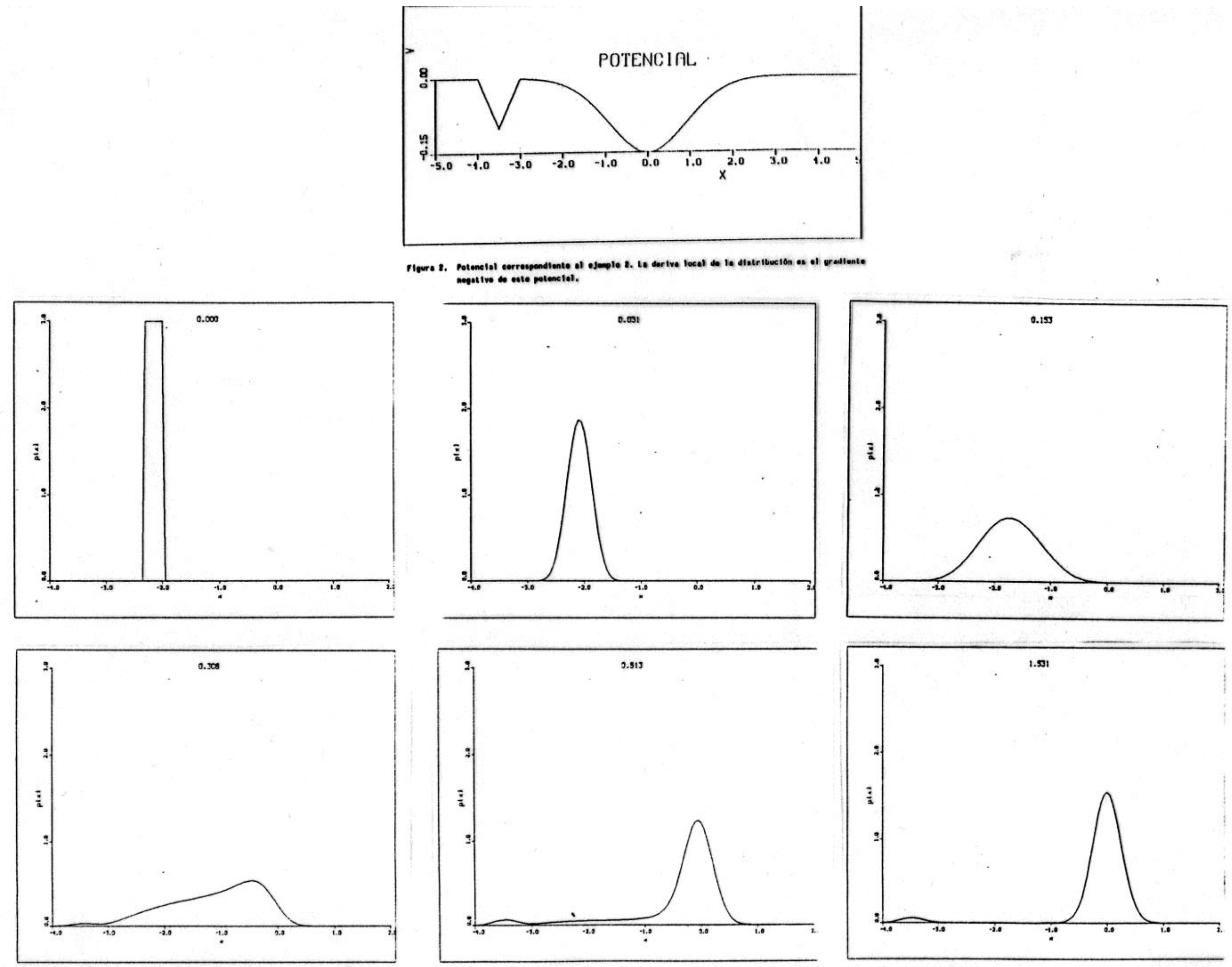


Fig.9.12 Bifurcación no-simétrica de una cuenca atractora y probabilidad asociada de la variable macro q en presencia de ruído. La evolución del sistema viene dada por $dq/dt = \underbrace{-\alpha q - \gamma q^2 - \beta q^3}_{\delta(q) = -\tilde{\nabla} U(q)} + f(t)$ siendo f(t) el ruido.

Su covariancia es la $\hat{Q}(q)$

Evolution of P(x) with a two-minima V(x)



Self-organization and qualitative change

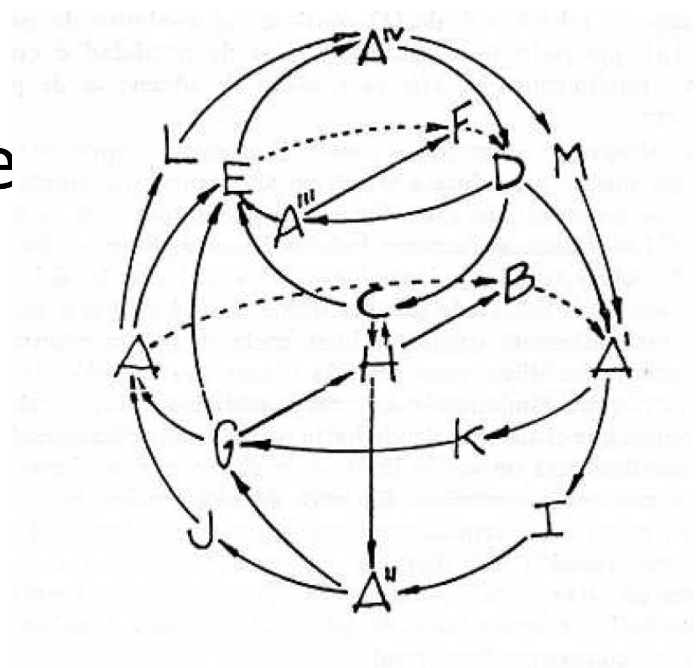
- In many of the most complex self-organizing processes we find that:
  1. The process involves many interactive components
  2. Eventually, the component interactions syncronize each other by chance and it makes emerge some mesoscopic (middle size) regularity (fluctuation)
  3. In some cases, the macro pattern so obtained probabilistically favors the growth of the initially random syncronization
  4. The macro pattern grows until it uses all the energy flowing through the systems, or it is inhibited by the boundaries (resulting in an *emergent* macroscopic pattern)

- Qualitative change in the self-organizing pattern:
  A. Synergetic change: parameters which control flows, thermodynamic forces, interactions between components change; it weakens the system attractor; it makes the system specially sensitive to new fluctuations
  B. Structural instability due to new variables: New interactions with external components (or systems) appear; it adds new dynamic variables; it provokes instability in the old attractors and a new topology of attractors in the new (higher dimension) phase-space

- Biological assemblage of self-maintaining systems can be described with B.

Self-maintaining systems

- Hejl: a series of systems in which self-organizing components produce each other in an operationally closed way
- Are the consequence of a constructive feed-back loop (organization) which permits the continuous regeneration of the components (Varela 1974)



Self-maintaining metabolism

- ✓ In living cells all of the catalysts essential for survival of the cell are internally produced
- ✓ Rosen: metabolism-replacement systems
- ✓ Piedrafita et al. (2010) example of 8 eqs. model:
- Metabolic process from external molecules S,T,U:

S + T→ ST catalized by STU

- STU is replaced against degradation:

ST + U→STU catalyzed by SU

- SU is replaced by:

S + U → SU, catalyzed by STU

Self-maintaining metabolism (2)

$$\frac{d[\mathrm{ST}]}{dt} = k_3[\mathrm{STUST}] - k_{-3}[\mathrm{STU}][\mathrm{ST}] - k_5[\mathrm{ST}][\mathrm{SU}] + k_{-5}[\mathrm{SUST}] - k_{11}[\mathrm{ST}]$$

Rate of production of ST as a function of several reaction rates

d[STU] / dt = …

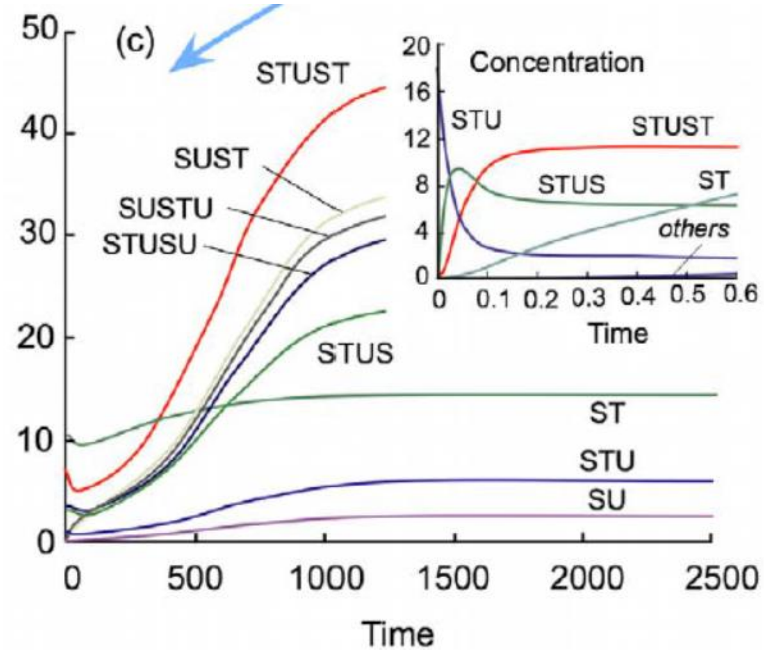
d[SU] / dt = …

d[STUST] /dt = …

d[SUST] /dt = …

- Steady state attractors are obtained which are stable to molecular fluctuations:

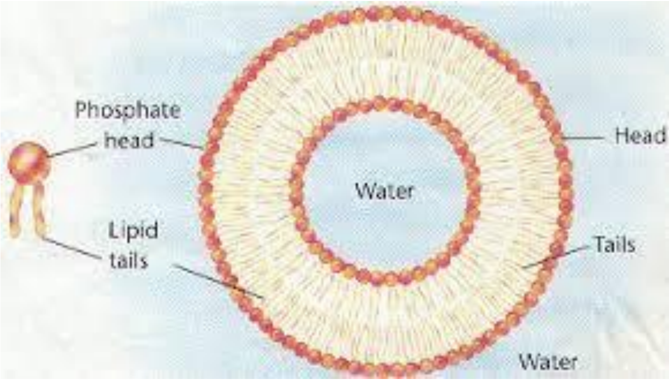
- Candidate to represent the prebiotic precursor of modern cell metabolism

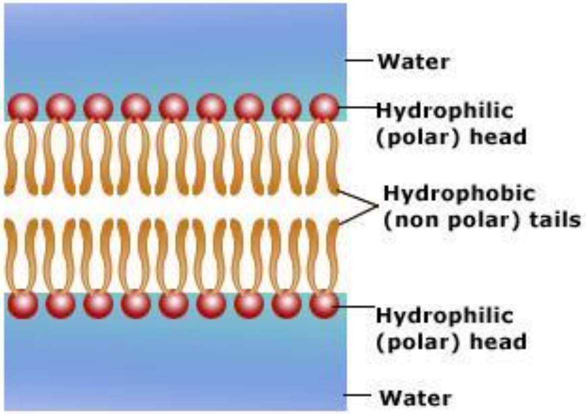


Cell membrane

- Those metabolic reactions would not be self-maintaining if molecular diffussion were included

- Neighborhood of reactants is difficult to maintain
- Cells have solved this problem by circumscribing metabolism inside lipid bilayers
- Bilayers are quite stable but they may suffer damage and need metabolic repairing





Enzymatic metabolism

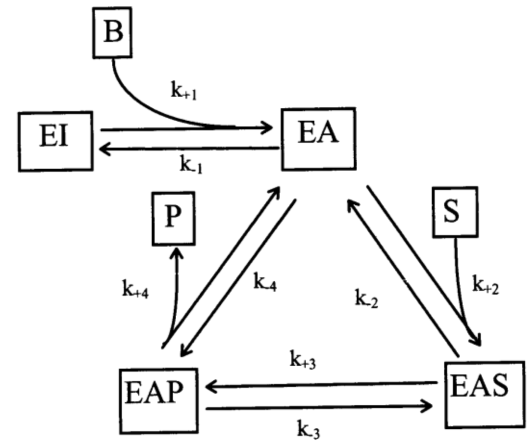
- In modern cell metabolism, catalysts are complex molecules called enzymes
- Enzymes can be modelled as stochastic automata
- Regulation by activator: A specific molecule B ensambles with the Inactive Enzyme (EI) which become active (EA)
- EA, with a certain probability, reacts with a substrate S and produce a product P
- The process is probabilistic
- The state of the enzyme and its reactants in the cell can be described by the vector **n**(t) with the occupation numbers of all the reactants

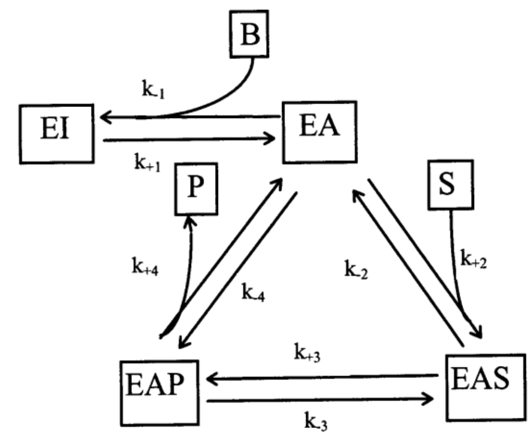
  $\mathbf{n}(t) = [n_I(t), n_A(t), n_{AS}(t), n_{AP}(t), n_b(t), n_s(t), n_p(t)]$

- Time evolution of **n** is given by a Master eq:

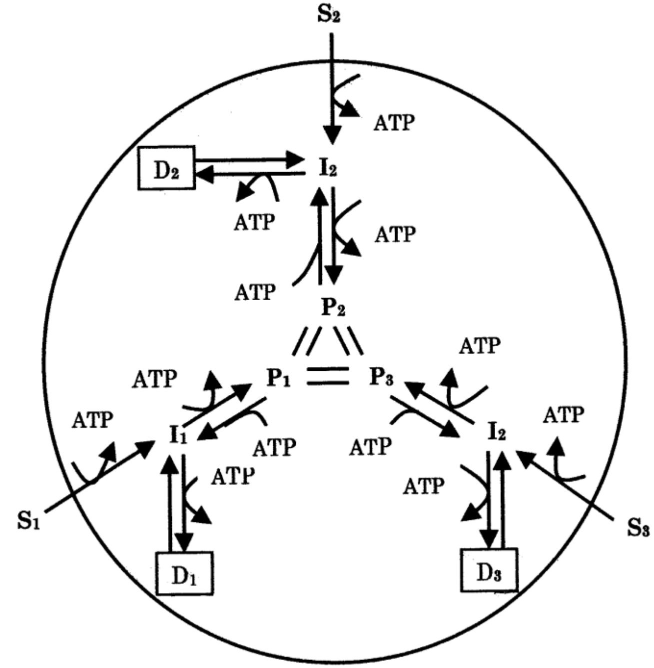
$$dp(\mathbf{n}, t)/dt = \Sigma_{\mathbf{k}}\, \omega_{\mathbf{n+k}\rightarrow\mathbf{n}}(t)\, p(\mathbf{n}+\mathbf{k}, t) - \Sigma_{\mathbf{k}}\, \omega_{\mathbf{n}\rightarrow\mathbf{n+k}}(t)\, p(\mathbf{n}, t)$$

$\omega = h\, k / V$, where k is a reaction rate, and h the combinations of collisions producing the change



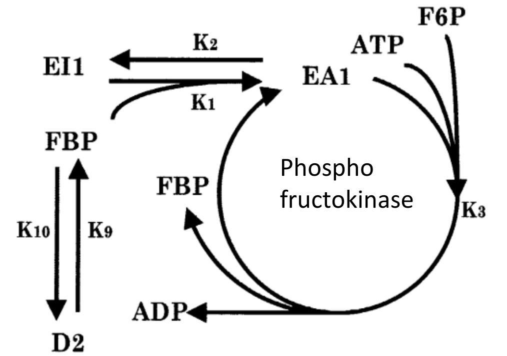


Models of metabolism (II)

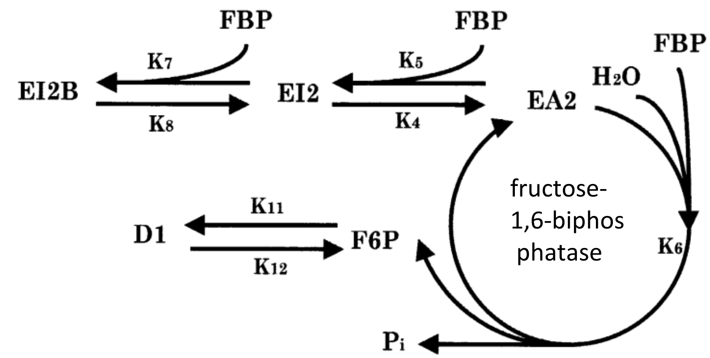


- Simulation of cell energy metabolism (CEM)
- Three reservoirs with energetic molecules that are produced from external substrates S_1, S_2, S_3
- A depot is filled when its substrate in cell is high, or its level is too low
- A difficulty appears in double-direction branches that use ATP (like those between *Ii* and *Pi* and between *Ii* and *Di*)
- If the right and left reactions are active → wasteful dissipation of energy (ATP)
- Futile cycles can be controlled if the opposing reactions are reciprocally controlled by some regulator, such as the reaction product itself, *Pi*

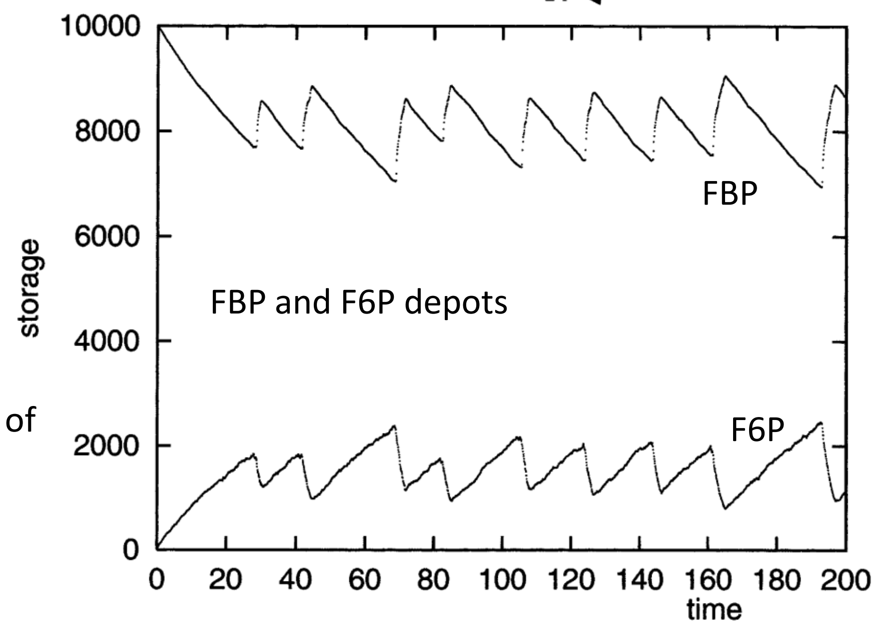
- This occurs in the carbohydrate branch of CEM, where the forward reaction enzyme, phosphofructokinase, is activated by its product fructose-1,6-P2 (FBP), while the antagonist enzyme, fructose-1,6-biphosphatase, is inhibited by FBP.
- A simple two enzymes model to simulate the two directions of the reaction: **glycolysis (A) and gluconeogenesis (B)**
- Futile cycle (simultaneous storage and use of energy) is impeded by the **alternating dominance of one of the two processes**



- Self-oscillatory glycolitic cycles:



- Randomness is crucial when F6P is high and FBP is low to produce the small threshold conc of FBP which self-catalyzes
- Allosteric regulation of enzyme activity is the key to create networking controls (Monod: “j’ai decouvert le deuxieme secret de la vie»)



Stochastic simulation of the master equation by using the Gillespie method

Boolean networks

Kaufmann (2004) genetic regulatory networks

- Cells as networks of N genes which activate/inhibit in a specific circular sequence
- Every gene receive K inputs from other genes and has an internal code to decide if it inhibits or activates at the next time step
- The state of the network is an array of N bits [0011010001011…0101] (0: OFF, 1: ON)
- The network state changes at every step until reaching a previous state; then it cycles in a permanent cycle (attractor)
- These attractors could represent the metabolism of the 256 types of cells
- For this, the attractor must be stable to perturbations, period of hours, etc.
- K = 2 seems to have the apropriate biological features

- Cell diferentiation would be a transition to a different attractor
- Natural selection would work on the permited transitions emerged from self-organization
- Three sources of biological order:
    1. Metabolic self-organization
    2. Selection of adapted cells/colonies
    3. Symbiosis of self-maintaining cells or colonies

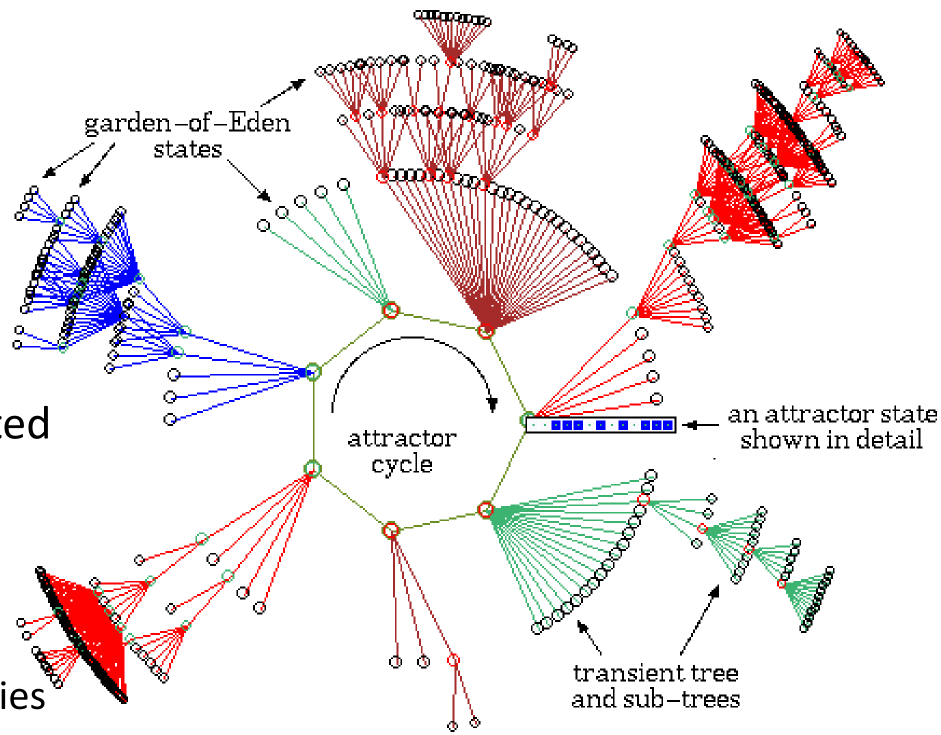
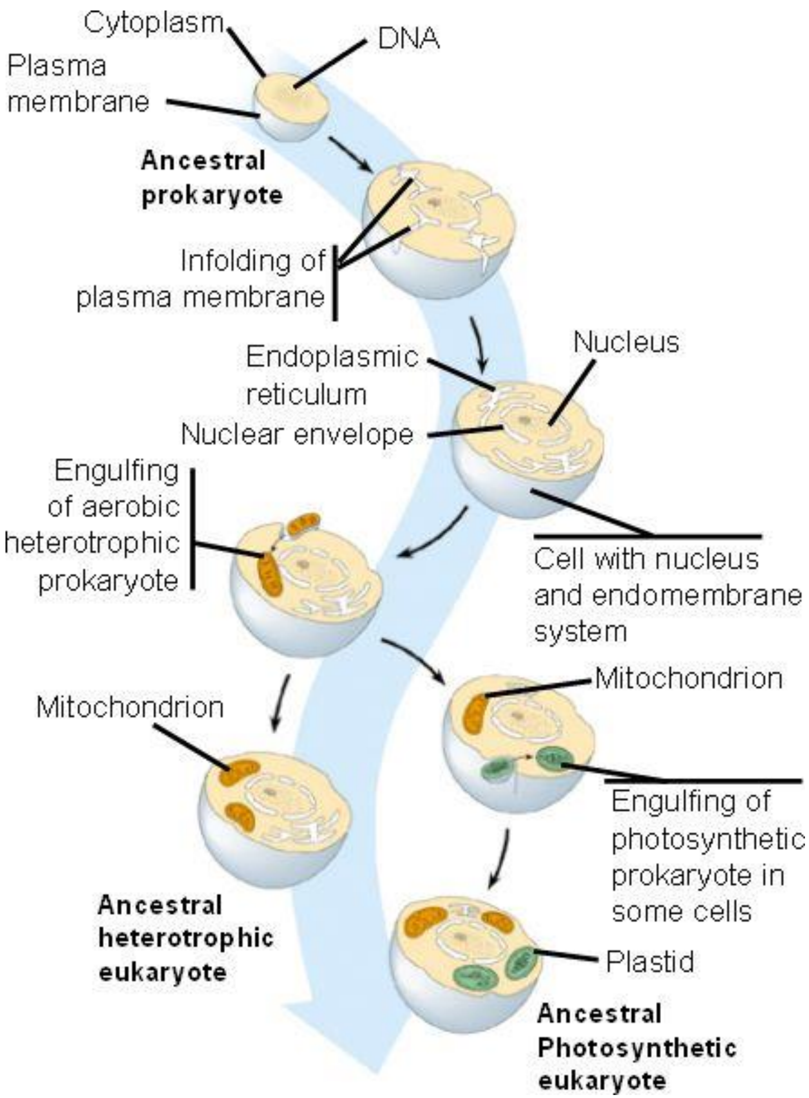


Fig.- Network attractor and its basin

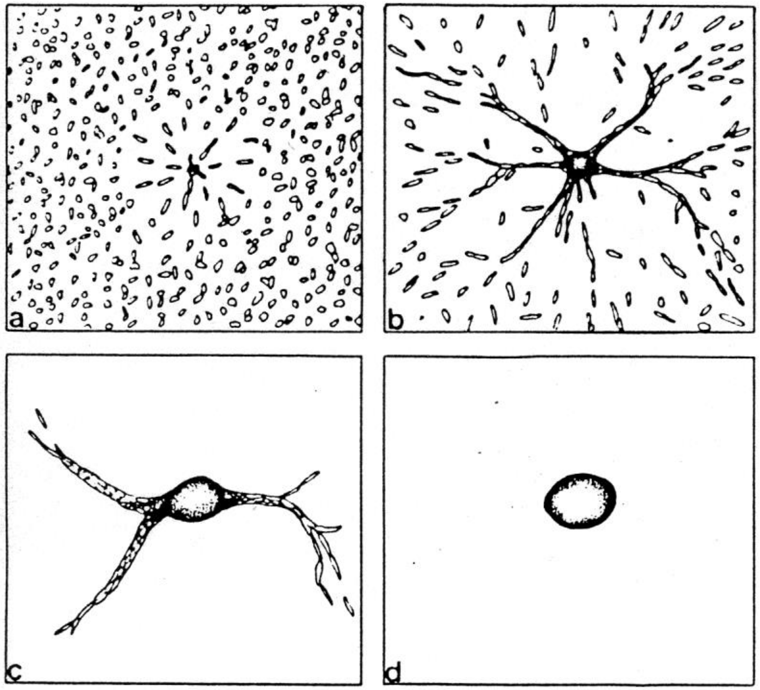
Biological assemblage

Lynn Margulis
Endosymbiotic
assemblage



Simple monera cells → eukaryote cell

- Cooperative self-organization of cells to form a pluricellular being
- Sawai, 2005; Höfer et al. 2006



Aggregation of cells of Dictyostelium Discoideum (a) and (b) to produce a plasmodium (c) which migrates and grows vertically (d) and reproduces

Animal social behavior

1. The ants emit a quantity α of pheromone per unit of time.
2. H decomposes at a rate proportional to its density: $-\beta H$.
3. Its propagation in the medium obeys Fick's law where D_H is the diffusion coefficient.

Random depositing persists as long as the number of insects participating in nest building is small.

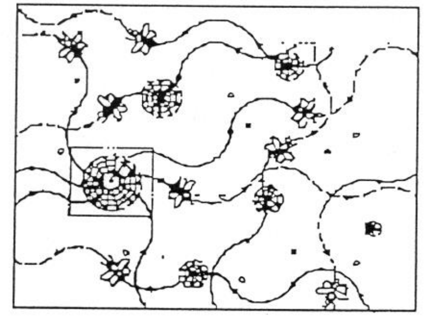


Figure 9: Termite Zeroing in on Random Deposit Sites

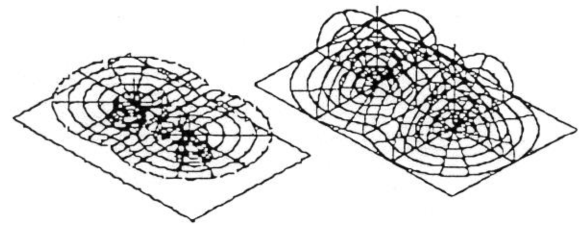


Figure 10: Pheromone Diffusion Gradient Surrounding Two Pillars. Because the two pillars act as competing attractors for the termites, a *saddle-point* is created between them. Here we see a 2-D (left) and 3-D field of equipotential curves radiating out from the deposit sites soon to become pillars.

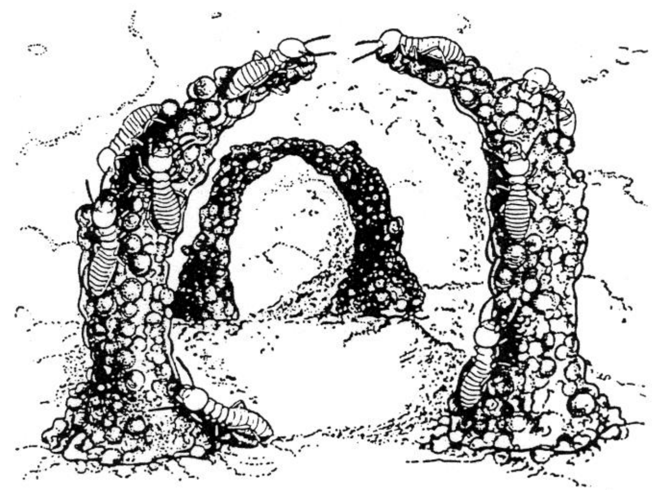
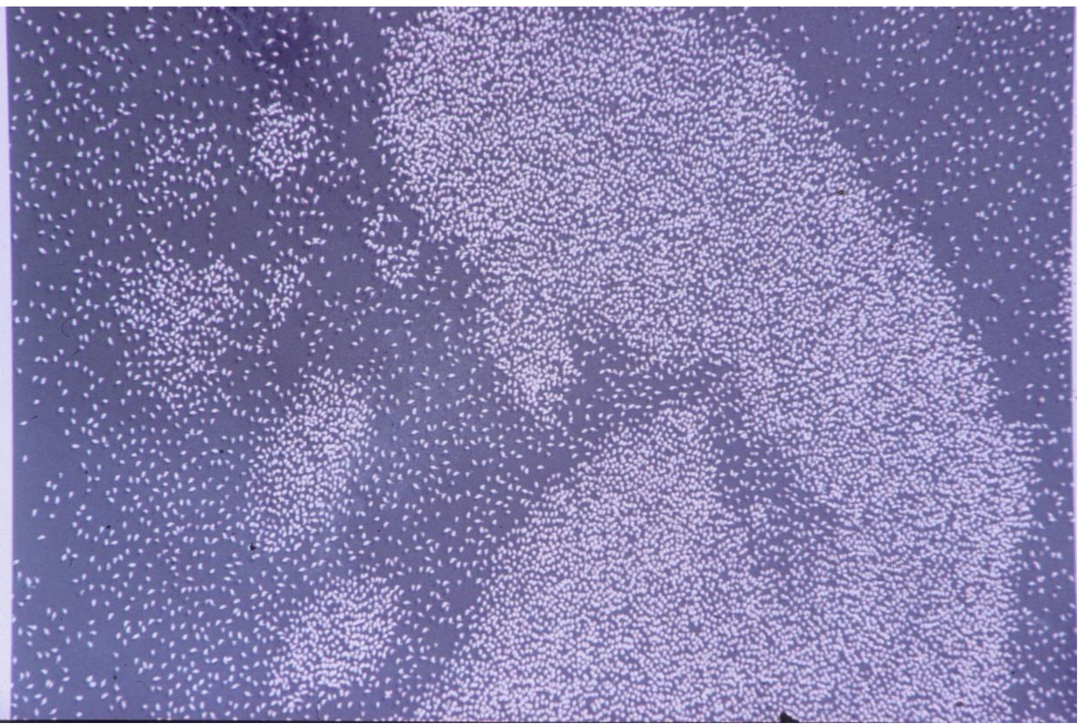


FIGURE 5.10. The construction of pillars and arches by a group of termites (drawing by Turid Holldobler, see Wilson, 1971).



- Flamingos just arrived on Lake Bogoria, Kenya
- Darwin said that a bird is able to leave her calf before disobeying the call to migration

Co-evolution of ecological communities

De Angelis et al (1981):

- Systems rich in all **types of resources**, which are widely distributed, tend to favor the evolution of "specialists" (such as lynx)
- Systems in which each resource is not widespread, encourage evolution of "generalists" (such as Fox)
- The higher the fluctuation of environmental resources, the greater the separation from the niches and less overlap of several species in each niche
- Resource rich ecosystems that don’t experience large fluctuations will have more species (tropical forests)
- Environmental fluctuations will reduce this number
- A system with dispersed limited resources:
  - if their densities do not fluctuate greatly: many generalists with a large niche overlap
  - if the fluctuations are large: a few generalist species

Prof. Levin have many things to say on it

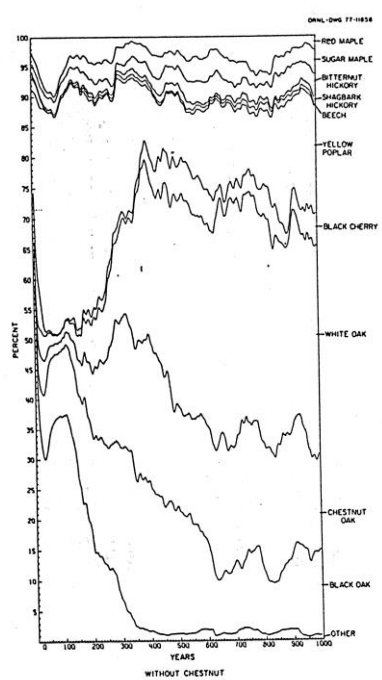


Fig. 3.: Changes in species composition through time predicted by the stochastic tree stand model. (From Shugart and West 1977, with permission of J. of Envir. Manage. Copyright by Academic Press, Inc. (London) Ltd.

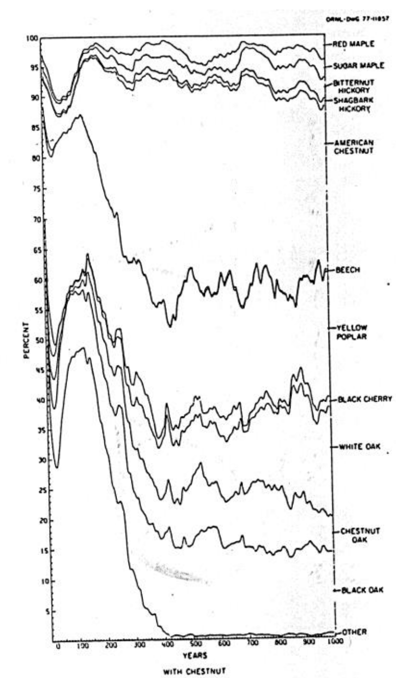


Fig. 4.: Changes in species composition through time predicted by the stochastic tree stand model when American chestnut is included. (From Shugart and West 1977, courtesy of Academic Press).

Cognitive emergences from neural syncronization

K. Mainzer, 2007
Thinking in Complexity

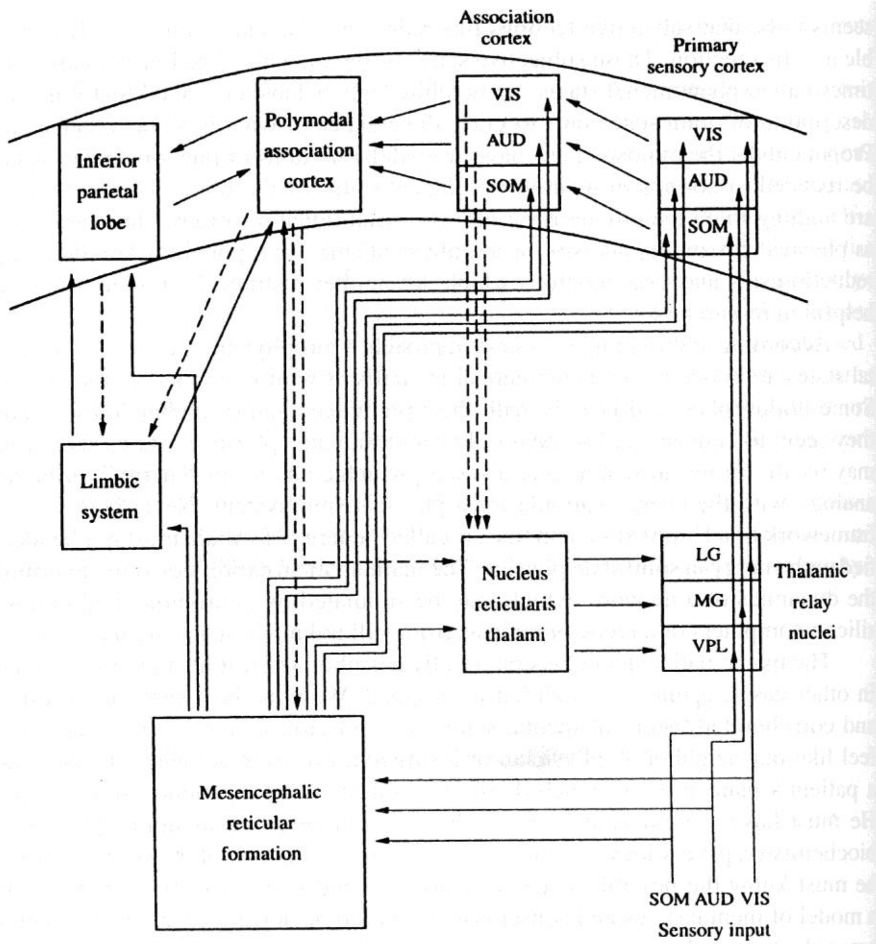


Fig. 4.19. Inputs to the cerebral cortex with somasensory pathways (SOM), auditory pathways (AUD), visual pathways (VIS), lateral geniculate (LG), medial geniculate (MG), nucleus ventralis posterolateralis (VPL) [4.46]

Social emergence

- Emergence of macroscopic patterns from micro-components interactions
- Prigogine, Haken, Weidlich, Haag, Hejl, Allen, Sawyer, Schweitzer, Levin

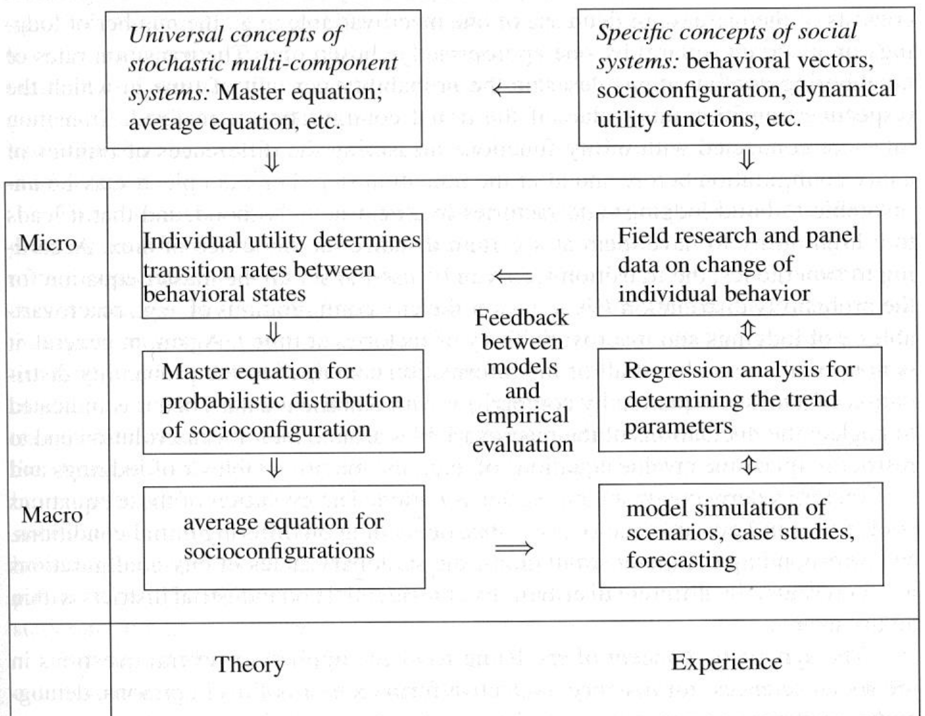


Fig. 8.5. Synergetic methodology for modeling social dynamics [8.16]

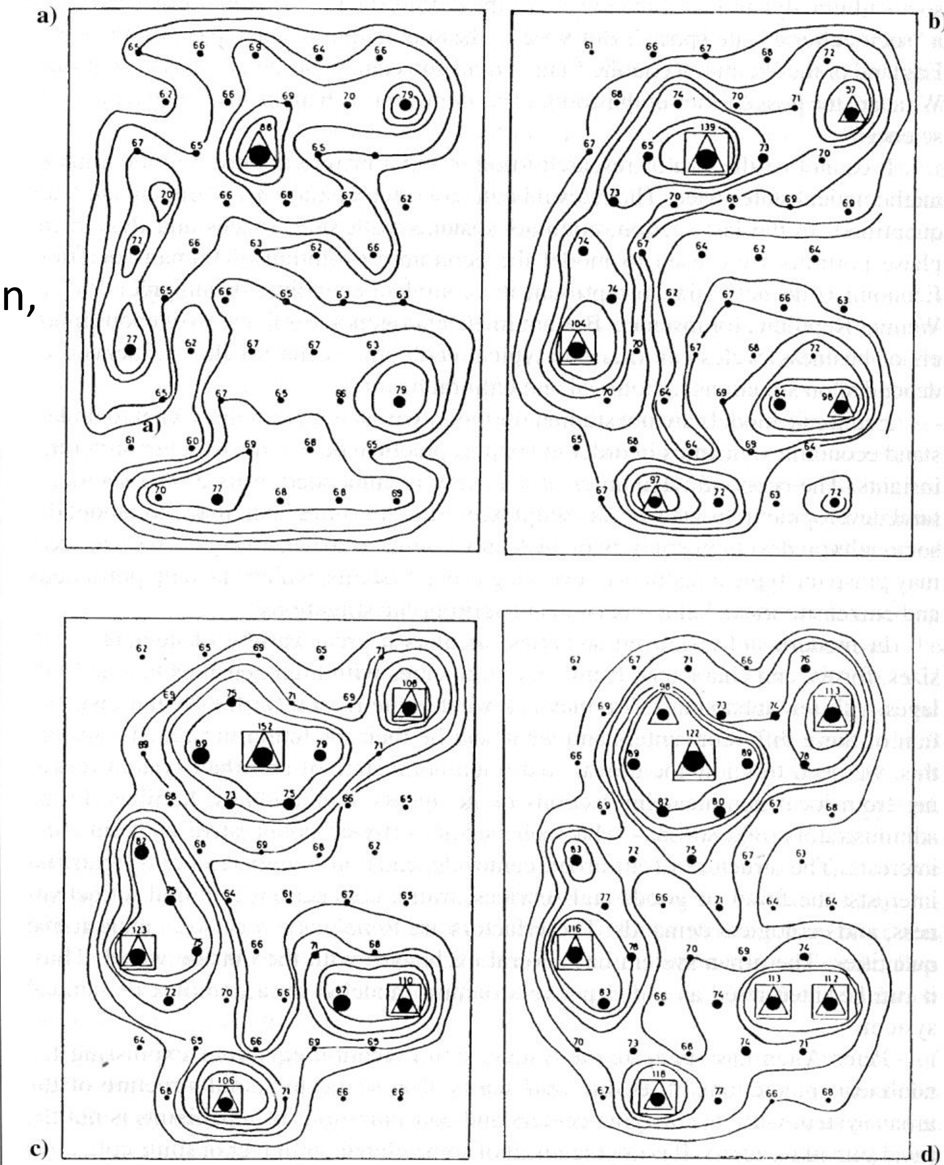
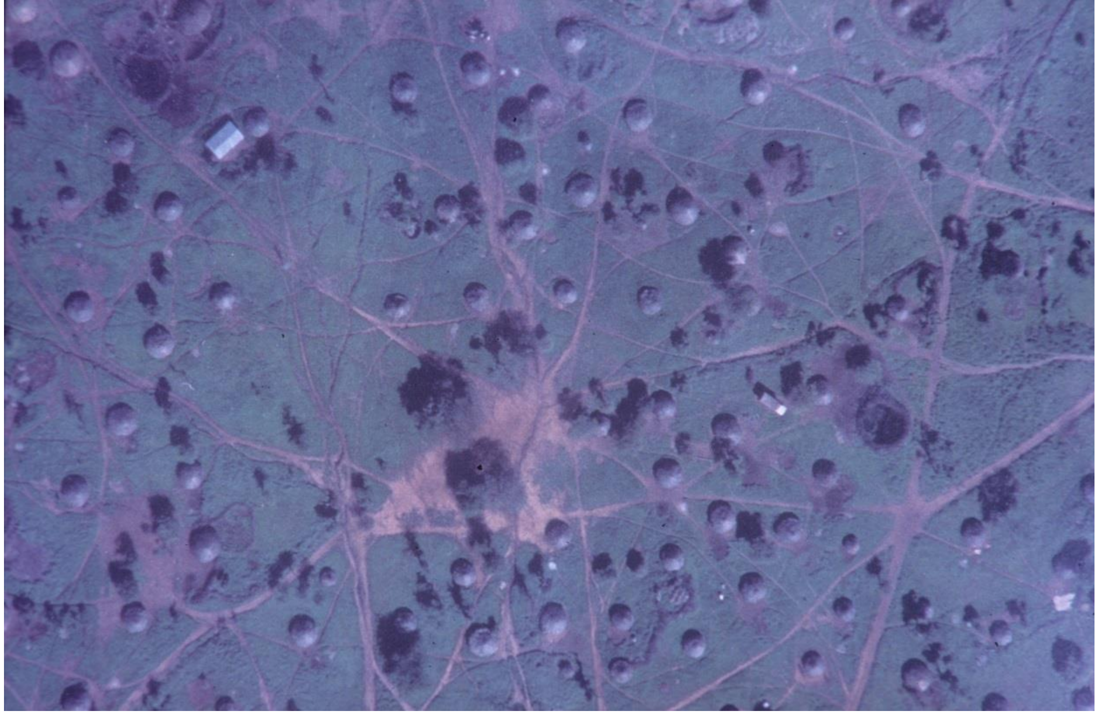


Fig. 8.4a–e. Computer-assisted model of urban evolution at time (**a**) $t = 4$, (**b**) $t = 12$, (**c**) $t = 20$, (**d**) $t = 34$, (**e**) $t = 46$ [8.14]

Trails, networks and drainage patterns formation

F. Schweitzer, Cellular automata, Brownian Agents, and active particles



Village in Serengueti, Tanzania

Saline mud of Lake Natron, Tanzania