Self-Organization of Complex Systems

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

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
Origin of attraction basins

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

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

\[
\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad i = 1, 2, \ldots N \tag{1a}
\]
\[
\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} - \alpha p_j \delta_{ji}, \quad i, j = 1, 2, \ldots, N \tag{1b}
\]

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 → dynamic instability

Variables $x = (x_1, x_2, ..., x_c)$ in complex systems don’t evolve deterministically from their initial states:

- Sensitivity to initial conditions
- Sensitivity to noise

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

Master equation:

$$\frac{dP(x, t)}{dt} = \sum_{x'} W(x, x') P(x', t) - P(x, t) \sum_{x' \neq x} W(x', x)$$  \hspace{1cm} (3)
From master to Fokker-Planck eqs

In many practical cases:

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

- $N \gg 1$ (almost a continuous set)

- transitions are always to neighbor states

- system has no memory

- $W$ and $p(x, t)$ are functions of $x$

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

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

(4)
where $C$ is the number of variables and:

$$K_i(x_0, t) = \frac{1}{N} \sum_k k_i w_{x+k \rightarrow x}(t) =$$

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

and the drift and fluctuations matrix:

$$Q_{ij}(x, t) = \sum_k k_i k_j w_{x+k \rightarrow x}(t) =$$

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

(6a)

(6b)

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

The drift is the mean instantaneous rate of change of states close to $(x, t)$.

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

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

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

$$p(z, t + \Delta t) = \int_x dx p(x, t) \sqrt{\frac{\text{det}[Q(y, t)]}{(2\pi)^N \Delta t}} \exp \left[ \frac{[z - y - K(y, t) \Delta t]^T [Q(y, t)]^{-1} [z - y - K(y, t) \Delta t]}{-2\Delta t} \right]$$

(7)
With b.c., it is easier to solve a set of Langevin stochastic equations, which are formally equivalent:

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

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

\[
\vdots
\]

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

where \( \zeta_i \) is a \( \delta \)-correlated Gaussian fluctuating (or random) perturbation in the variable \( i \).

Relationship between the two formulations:

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

\[
\frac{1}{N} Q_{ik}(x) = \sum_{j=1}^{C} g_{ij}(x) g_{kj}(x)
\]
P(q,t) when drift $\delta(q)$ derives from a potential $V(q)$

- The attractor is in the bottom of $V(q)$
- If parameters $\alpha$, $\gamma$, $\beta$ 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
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 synchronize 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 synchronization
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 awakes 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:
    \[ S + T \rightarrow ST \] catalized by STU
  • STU is replaced against degradation:
    \[ ST + U \rightarrow STU \] catalyzed by SU
  • SU is replaced by:
    \[ S + U \rightarrow SU \], catalyzed by STU
Self-maintaining metabolism (2)

\[ \frac{d[ST]}{dt} = k_3[STUST] - k_{-3}[STU][ST] \]

\[ -k_5[ST][SU] + k_{-5}[SUST] - k_{11}[ST] \]

\[ d[STU] / dt = \ldots \]

\[ d[SU] / dt = \ldots \]

\[ d[STUST] / dt = \ldots \]

\[ d[SUST] / dt = \ldots \]

- 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 diffusion 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:
  \[ n(t) = [n_I(t), n_A(t), n_{AS}(t), n_{AP}(t), n_b(t), n_s(t), n_p(t)] \]

- Time evolution of \( n \) is given by a Master eq:
  \[ \frac{dp(n, t)}{dt} = \sum_k \omega_{n \rightarrow n+k}(t) p(n+k, t) - \sum_k \omega_{n+k \rightarrow n}(t) p(n, t) \]

\[ \omega = h k / V, \] where \( k \) is a reaction rate, and \( h \) the combinations of collisions producing the change.
Models of metabolism (II)

• Simplified models of cell energy metabolism (CEM), where three energetic reservoirs are filled when its substrate in cell is high, or its level is too low

• One problem is the occurrence of *futile cycles*: the wasteful dissipation of energy that can take place in ATP-dependent cycles like those between $i$ and $Pi$ and between $i$ and $Di$ if right and left reactions are active

• 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 one of the three processes of storage-use of energy:
- PFKase is activated by its product FBP (fig. A) and FBPase is inhibited by FBP (fig. 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: **glycolitic dominance (A)** and **gluconeogenetic dominance (B)**
- 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](image)
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 appropriate biological features

- Cell differentiation would be a transition to a different attractor
- Natural selection would work on the permitted 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
Other fields of application

• Biological assemblage

- 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

Serial endosymbiosis of monera → eukaryote
Animal social behavior

- 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

![Graph 1](image1.png)  ![Graph 2](image2.png)

*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

![Diagram showing social emergence concepts and methodologies](image)

**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