Frontiers of complex systems research: a view from the foundations

COMPLEXITY AS A PHENOMENON ROOTED INTO THE LAWS OF NATURE

- Complexity as a new, post-Newtonian scientific paradigm.
- Complexity in a fundamental science perspective. Multilevel approach, blending of ideas and tools, interdisciplinary dimension, reconceptualization of long standing ideas and practices, new issues.
- Beyond the standard conception where "fundamental" is tantamount to the exploration of the very small and the very large.

Outline

I. Survey of key features of complex systems

II. Microscopic level complexity and the foundations of irreversibility

III. Equilibrium versus nonequilibrium

IV. Prediction

V. Complexity and information

VI. Perspectives on biological complexity

VII. Conclusions

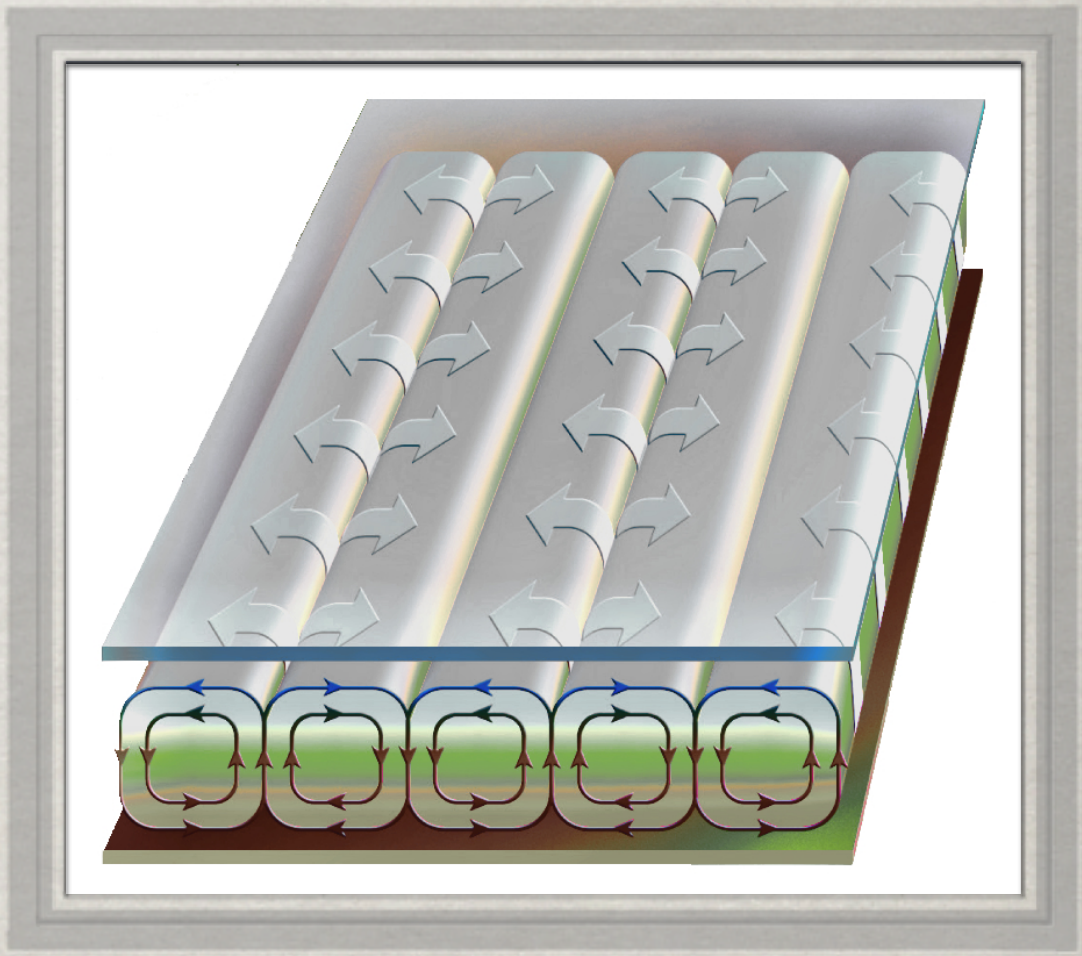
I. Survey of key features of complex systems

A. Complex systems display a phenomenology of their own

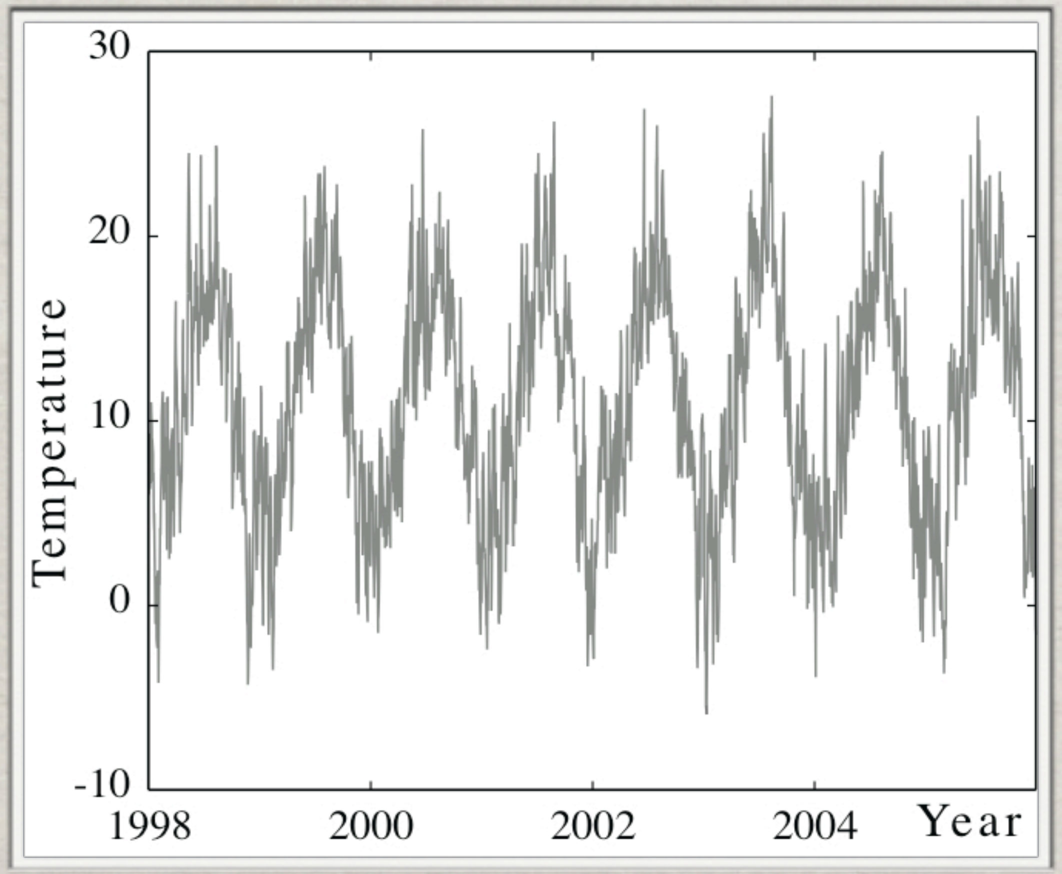
Principal signature of complex systems: multiplicity of possible outcomes.

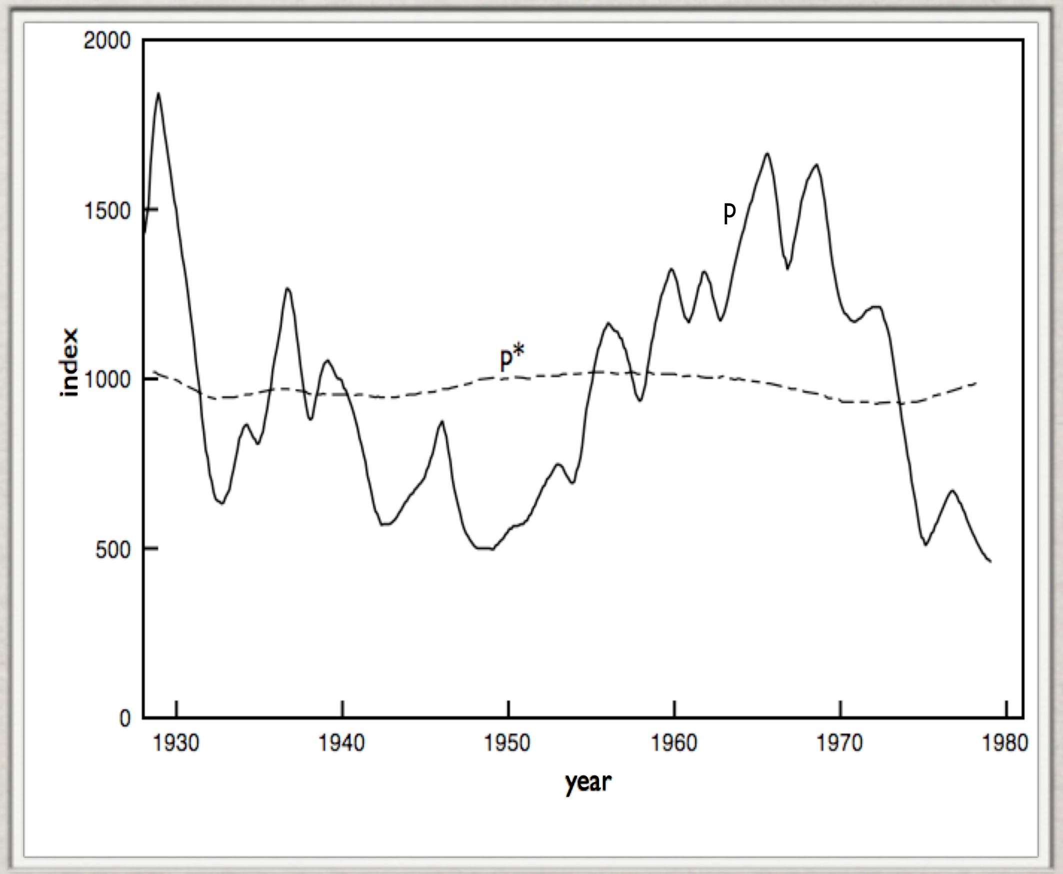
Two different manifestations:

- Emergence of global traits non-reducible to the properties of the constituent parts. Creation of self-organized states of hierarchical and modular type by a bottom-up mechanism rather than through a top-down design and control, from fluid mechanics to chemistry to biology.



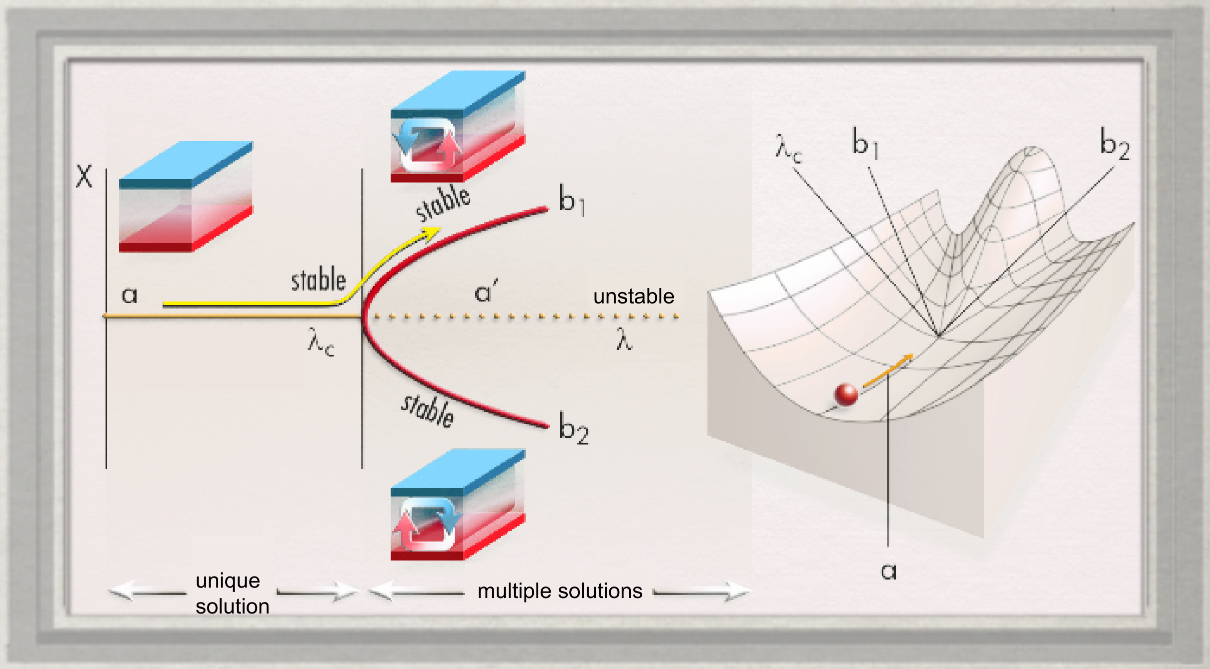
- Intertwining of order and disorder: the issue of prediction, from the atmosphere to the stock market.

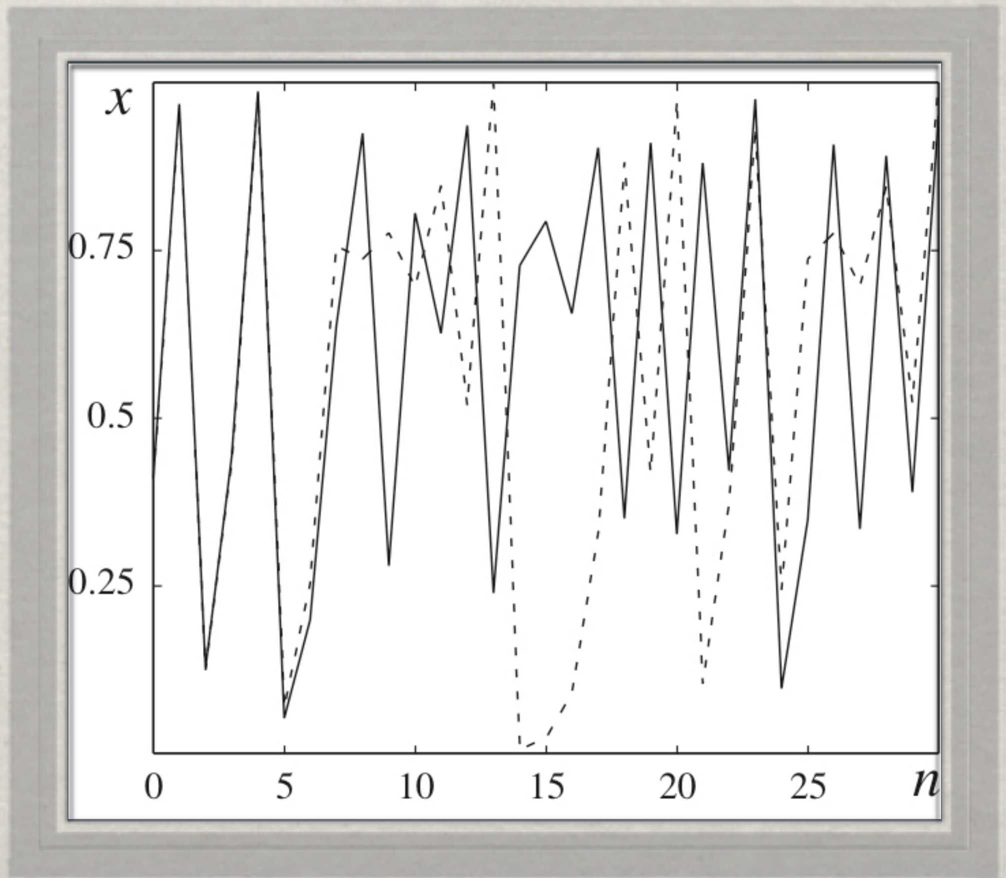




B. Complex systems: at the crossroads of the deterministic and probabilistic views of nature

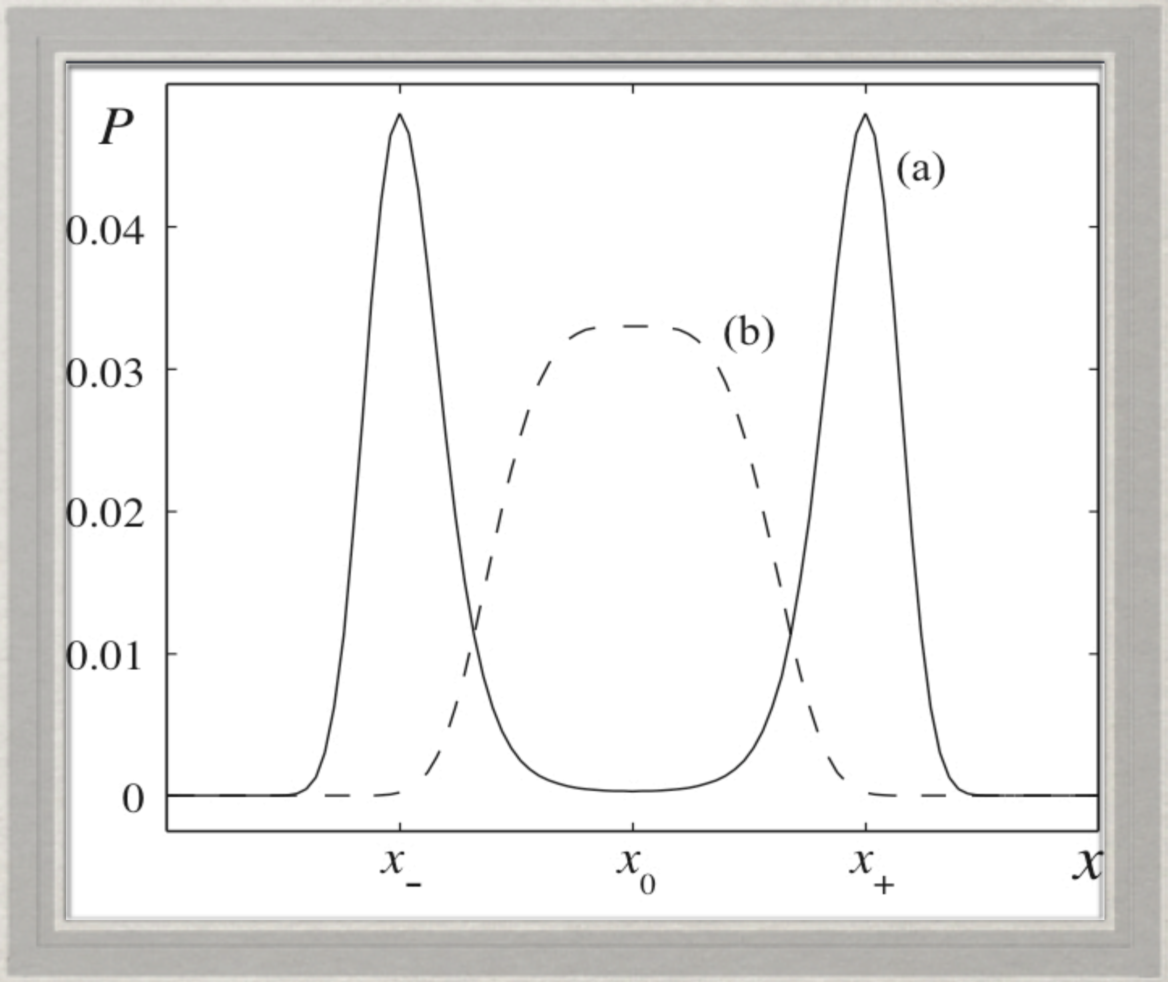
- The conjunction of nonlinearity and of nonequilibrium constraints.
- Sensitivity to the parameters: qualitative changes near criticalities associated to instabilities and bifurcations.
- Sensitivity to the initial conditions: coexisting attractors, deterministic chaos.
- Unlimited numbers of scenarios.





- Need for an alternative to the traditional deterministic description: probabilistic approach.

- Linearity and stability of the probabilistic description versus the nonlinearity and instability underlying the deterministic description.



C. Complex systems imply the emergence of levels of description obeying to their own laws

- Macroscopic level (mean field) description

$$\frac{dX_i}{dt} = F_i\,(X_j\ ,\lambda)$$

Drastic reduction of description near criticalities of certain kinds.
Order parameters, normal forms as e.g.

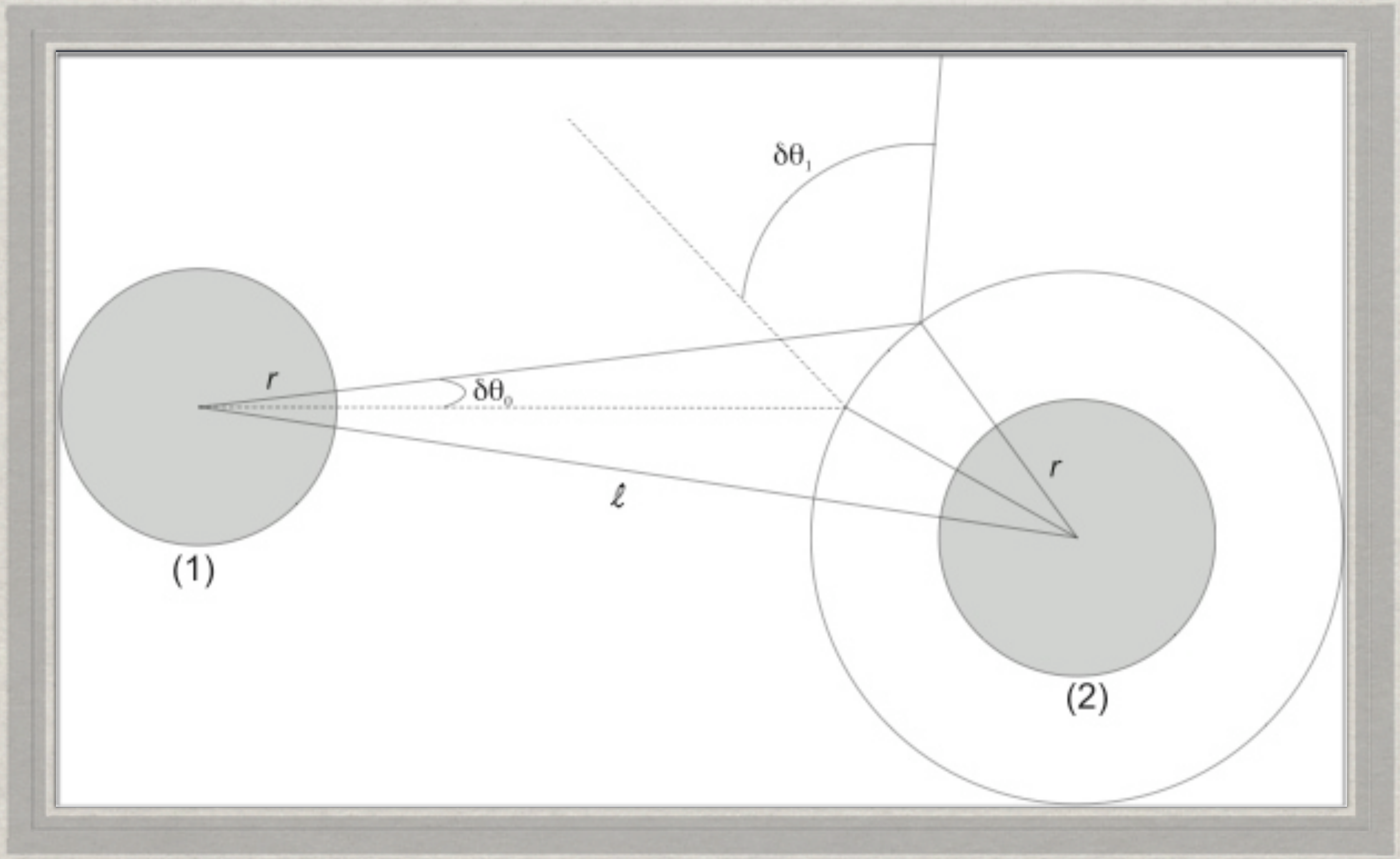
$$\frac{\partial z}{\partial t} = (\lambda - \lambda_c)\,z - u|z|^2 z + D\nabla^2 z$$

- The mean field description as an emergent property starting from a probabilistic description.
    - Closing the hierarchy of moment equations. Conditions on the spectrum of the associated evolution operators.
    - Projection operators.
- The probabilistic description as an emergent property starting from a full-scale deterministic description at the microscopic level, free of heuristic approximations. Role of the instability of the underlying dynamics.

- Limits of the hierarchical description : breakdown of the decoupling between levels of description.
  - Nanoscale systems: nonequilibrium constraints and asymmetric interactions lead to unexpected modes of energy transduction.
  - Strong geometric constraints: anomalous fluctuations, segregation.
  - Coexistence of a continuum of scales: turbulence, finance.
  - Extreme events.
- Full scale description becomes necessary. Fine details of probability distributions begin to matter. Large deviations, fluctuation theorems, role of the reverse process, unexpected connections with thermodynamics.

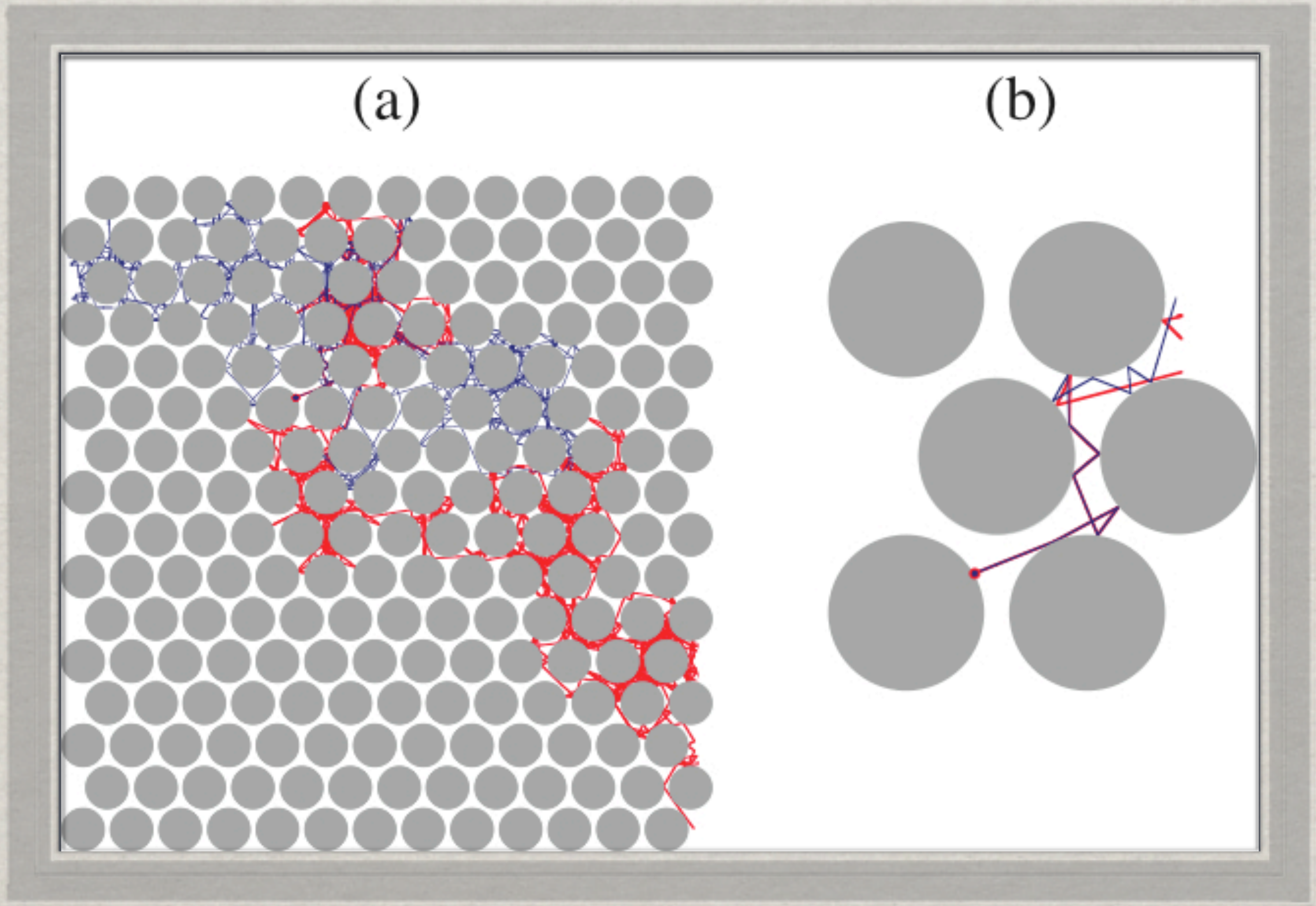
II. Microscopic level complexity and the foundations of irreversibility

- Ubiquity of complexity at the microscopic level.
- Defocusing character of the collisions: dynamical chaos.



- The Lorentz gas paradigm.

Onset of deterministic diffusion: bridging the gap between time reversal invariance of the evolution laws at the microscopic level and macroscopic level irreversibility.



- Principal quantifiers of microscopic level complexity:
    - Lyapunov exponents σ_i (dynamical instability).
    - Kolmogorov-Sinai entropy h (dynamical randomness).

      Multiple time probability $P(X_1 \ldots X_n)$ to observe the system in successive coarse-grained states $X_1 \ldots X_n$ at regular time intervals.

      h: mean decay rate of $P(X_1 \ldots X_n)$

$$h(P) = \lim_{n\to\infty} \frac{-1}{n\tau} \sum_{X_1, \ldots X_n} P(X_1, \ldots X_n) \ln P(X_1, \ldots X_n)$$

* Transport viewed as escape from a fractal repellor F

Escape rate: $$\gamma \approx D / L^2$$

with

$$\gamma = \sum_{\sigma_i > 0} \sigma_i(F) - h_{KS}(F)$$

Fractal character of the associated modes.

* Rate of entropy production related to the difference between the time-reversed and forward Kolmogorov-Sinai entropies: time symmetry breaking!

$$\frac{1}{\tau}\Delta_i S = h_R(P) - h(P) \geq 0$$

with

$$h(P) = \lim_{n \to \infty} \frac{-1}{n\tau} \sum_{X_1, \ldots X_n} P(X_1, \ldots X_n) \ln P(X_n, \ldots X_1)$$

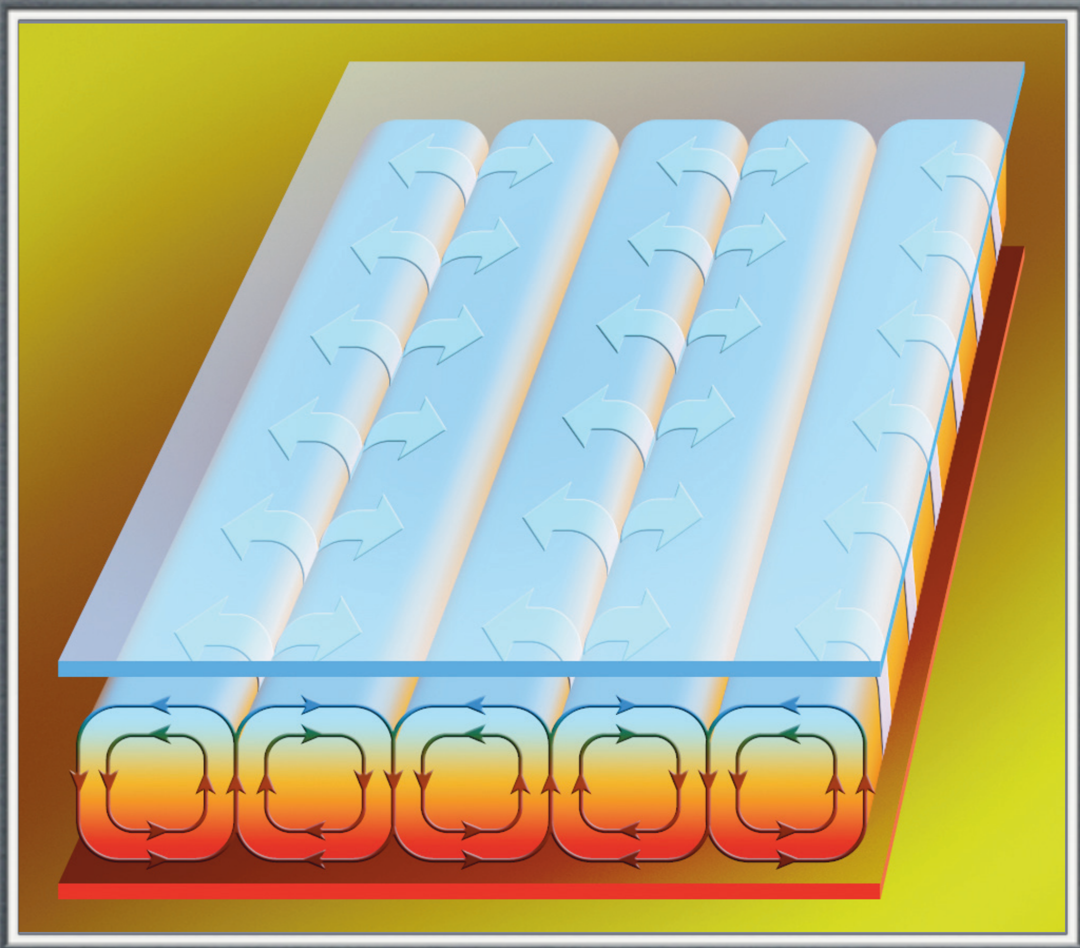
Irreversibility as an emergent property

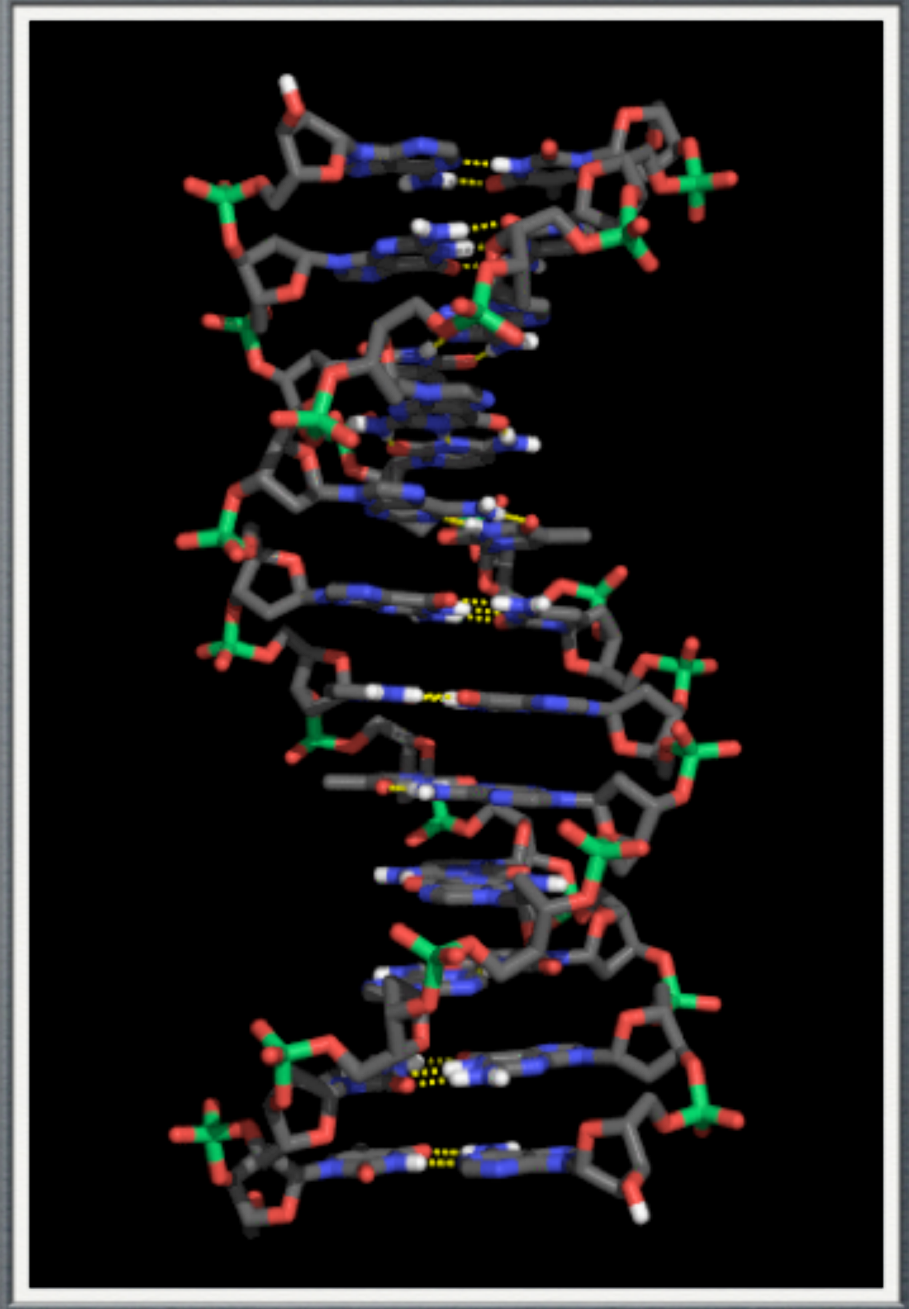
III. Equilibrium versus nonequilibrium

Originally, complexity and self-organization contrasted with equilibrium mediated ordering phenomena (self-assembly…).

The distinction is at present less clearcut: structure (equilibrium) and function (nonequilibrium) are intimately intertwined.

Macroscopic structures:	**Macromolecular and supramolecular structures:**	**Nucleation:**
Characteristic space scales in the macroscopic range.	Characteristic space scales in the microscopic or mesoscopic range.	Thermodynamics meets kinetics in a natural way.
Non-trivial behaviors in time.	No permanent time activity.	Non standard scenarios.
Function determines structure.	Structure determines function.	
	The evolutionary dimension.	





Self-organization phenomena involving nanosize materials (protein solutions, zeolites, etc ...)

Common features :

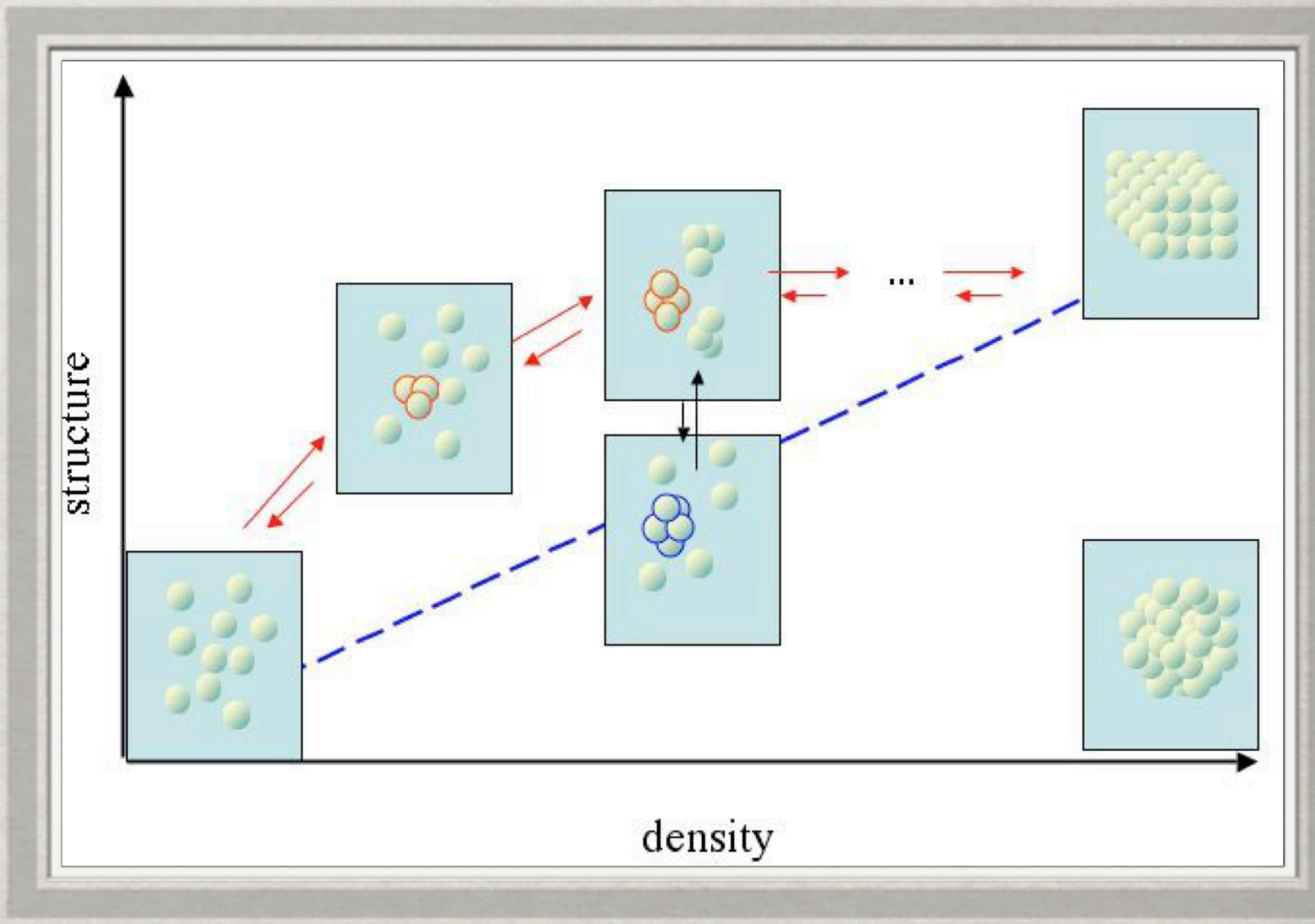
- weak and short ranged attractive interactions compared to simple atomic fluids.

- spontaneous self-assembly towards ordered phases compromized by the presence of high nucleation barriers (≈100 $k_B T$ for the crystallization of protein solutions in ordinary conditions).

Increasing evidence of presence, in such materials, of metastable phases (high concentration protein solutions, etc...) and of their interference with the above phenomena.

Non standard nucleation mechanisms with combined structural and density fluctuations

- Importance of kinetic effects arising from the co-existence of competing mechanisms.
- Enhancement of nucleation rate under certain conditions via favorable pathways in the two order-parameter phase diagram.



IV. Prediction

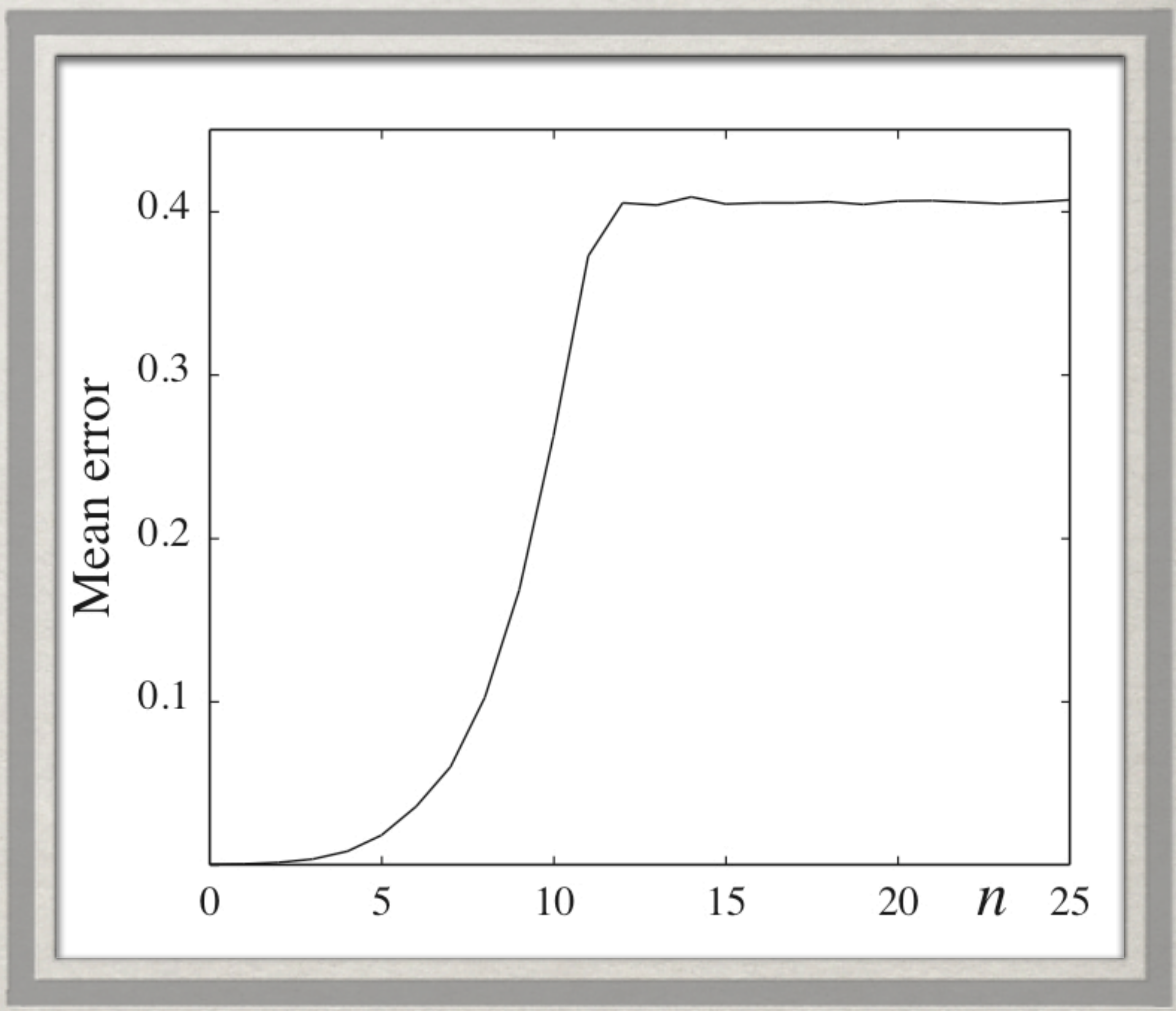
- Prediction for the future : a major objective of science and a built-in human need. Deep societal impact (environment, finance,…).
- Intricate way events unfold in time and organize in space in a complex system.
- How to observe, to analyze and to predict under these conditions in a way that does not miss essential features of the system at hand.
- Conversely, on the basis of this knowledge how to gain access to key indicators of complexity and how to use them for the purposes of decision making.

- Standard and nonlinear data analyses, dynamical reconstruction.

- Modeling:

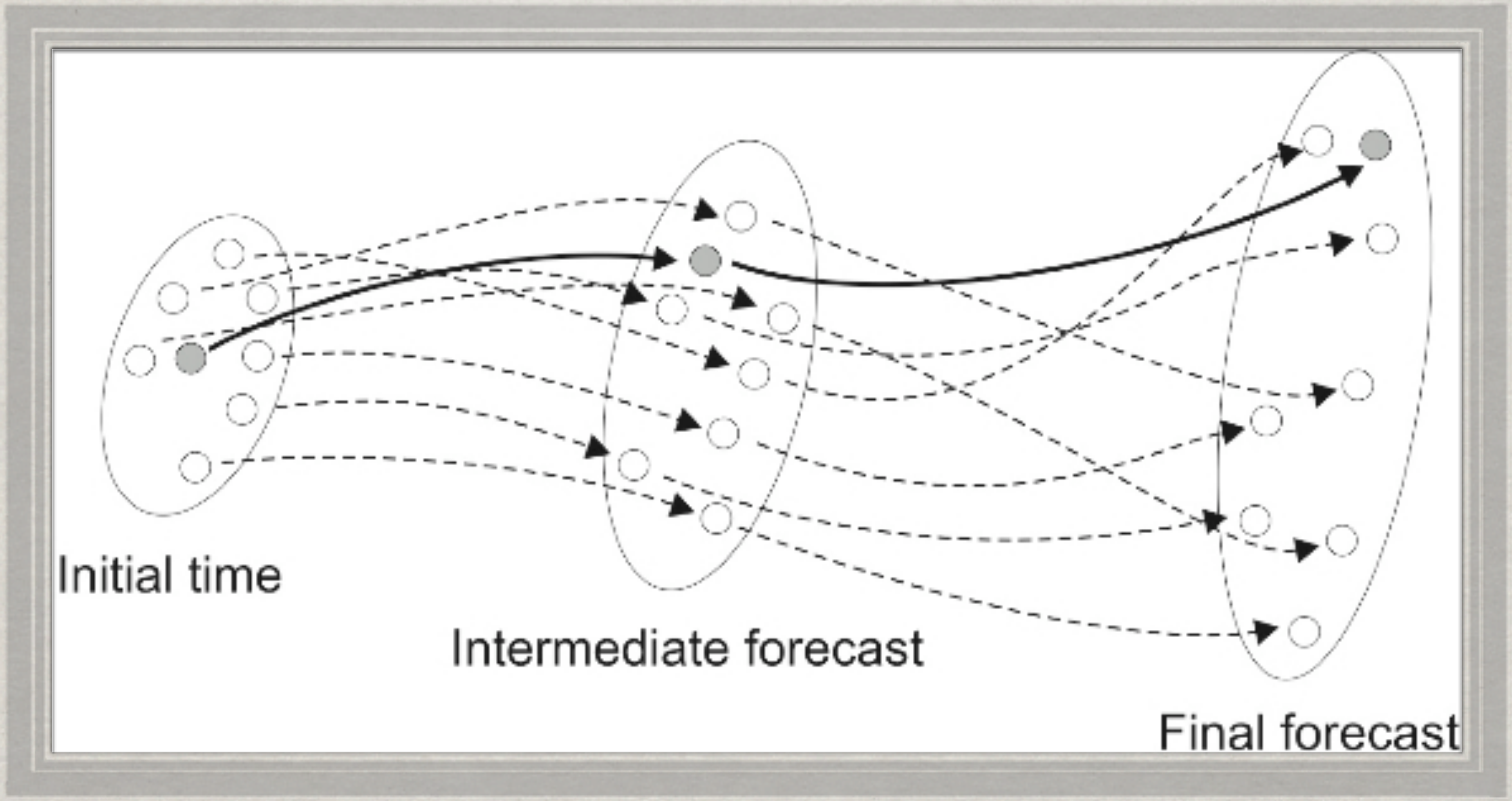
    - Uncertainties in the initial conditions, model imperfections.

    - Signature of complexity: initial condition and model errors are increasing in time. “Butterfly effect”.



- From the classical view of a world of unlimited predictability to the real world of limited predictability. Predicting under uncertainty.

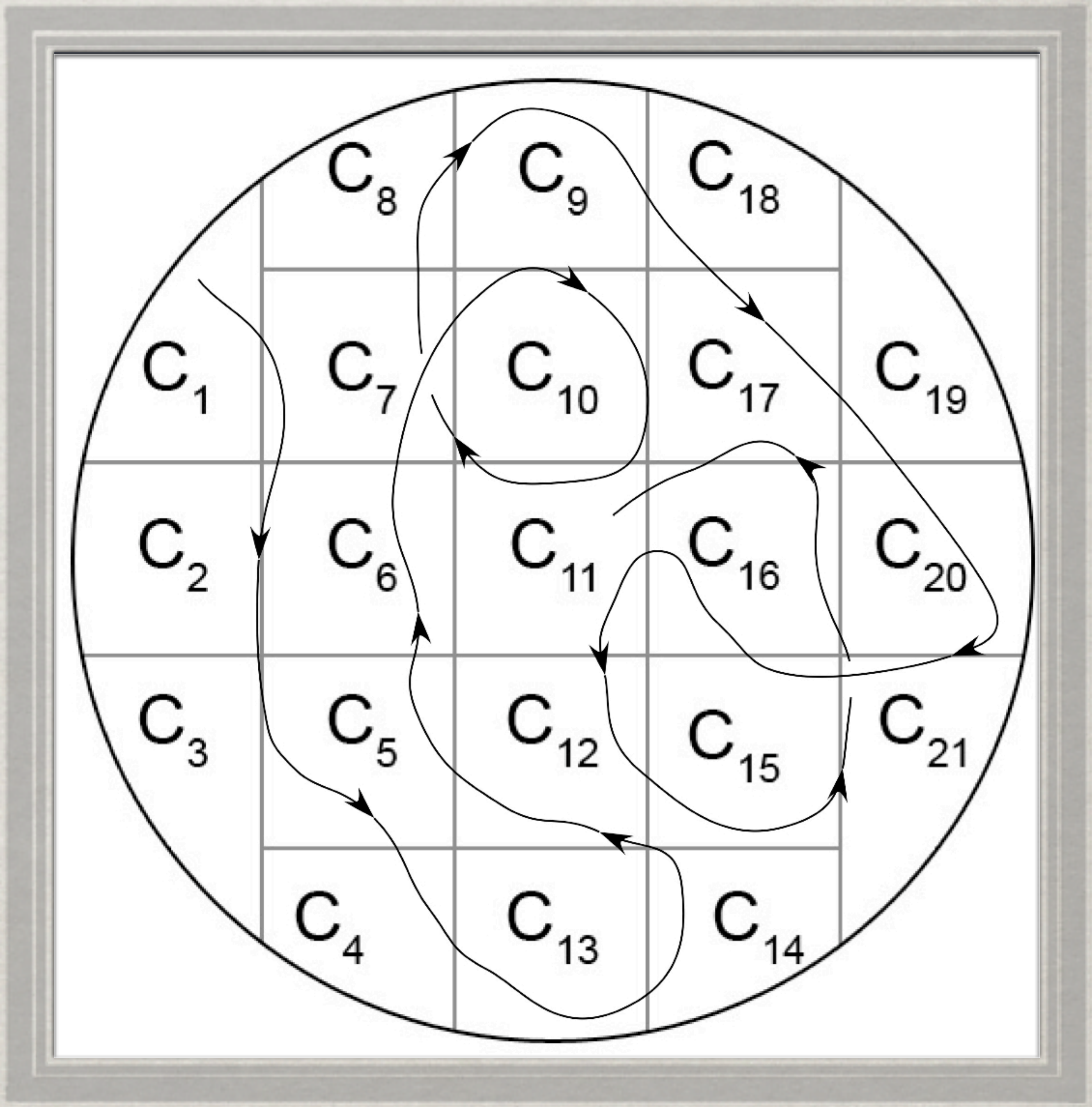
- Probabilistic prediction as the natural way to cope with this fundamental limitation. Ubiquity of randomness!



- Climatic change in the light of complex systems research.

V. Complexity and information

- Dynamics as generator of symbolic sequences.
- Algorithmic and information theory views of complexity.



Characterization through Shannon entropy S_I, block entropies S_k.

- Scaling of S_k with length k:

$$S_k \approx e + hk + gk^{m_1} (\ln k)^{m_2}$$

- Shannon-Mac Millan theorem

$$P(X_1, ...X_k) \approx \exp(-S_k)$$

- The problem of combinatorial explosion.

- Common features and fundamental differences between algorithmic complexity and physical complexity.

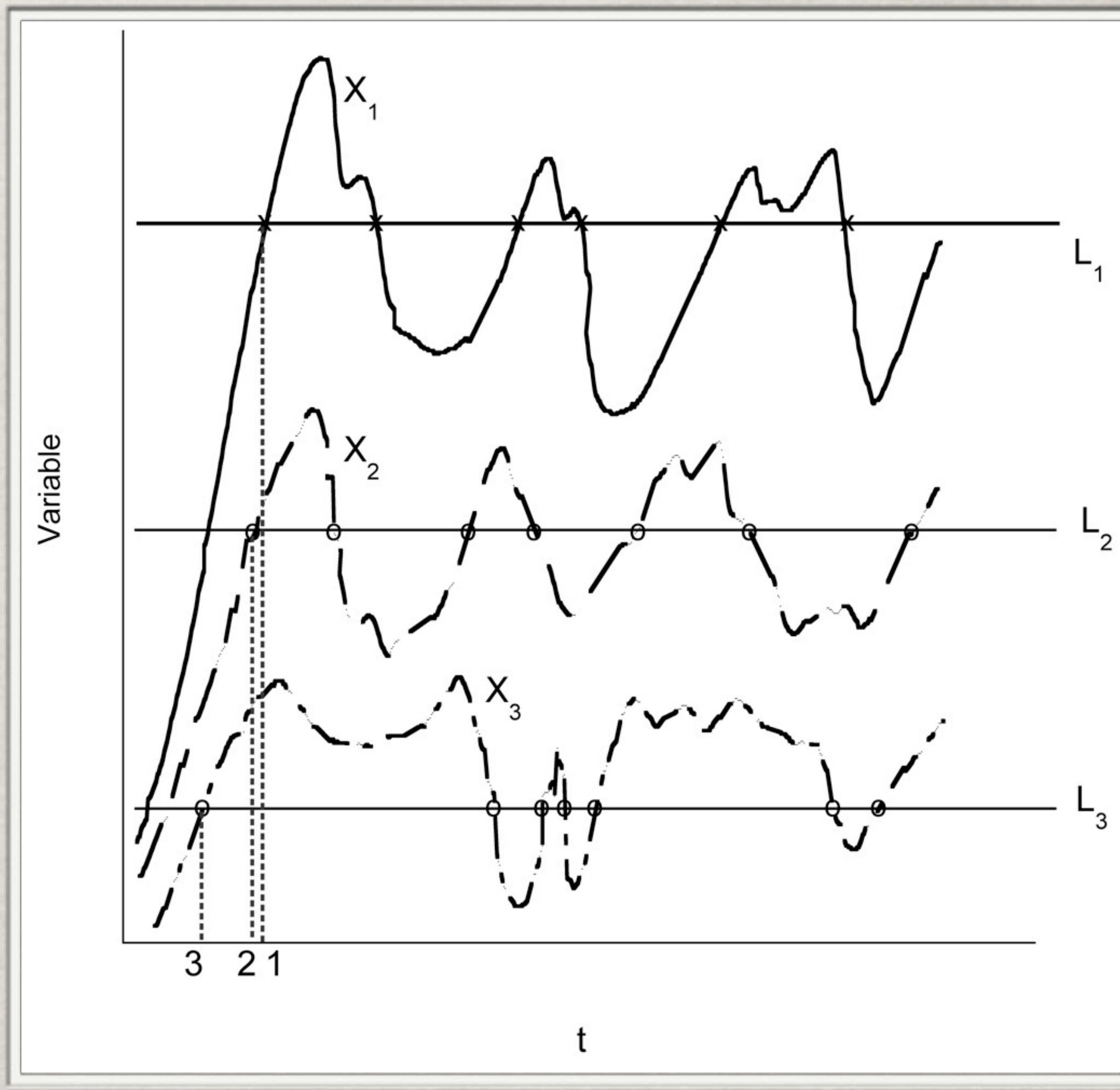
- Information theory revisited in the light of dynamical systems theory and nonequilibrium physics ? Rehabilitation of time. Source, channel and receiver as a single dynamical system under constraint.

- New feature: nonequilibrium constraints and dynamics select, within a finite time span, structures (sequences) whose a priori probabilities would be insignificant.

Chaotic attractors as information sources and processors

- A case study: generation of asymmetric strings of symbols by the Rössler model through a level-crossing mechanism.

$$\begin{aligned}\dot{x} &= -y - z\\ \dot{y} &= x + ay\\ \dot{z} &= bx - cz + xz\end{aligned}$$



- Typical symbol sequence

$$zyx \quad zxyx \quad zxyx \quad zyx \quad zxyx \quad zyx \quad zyx \quad zx \quad zyx \quad \ldots$$

strongly correlated

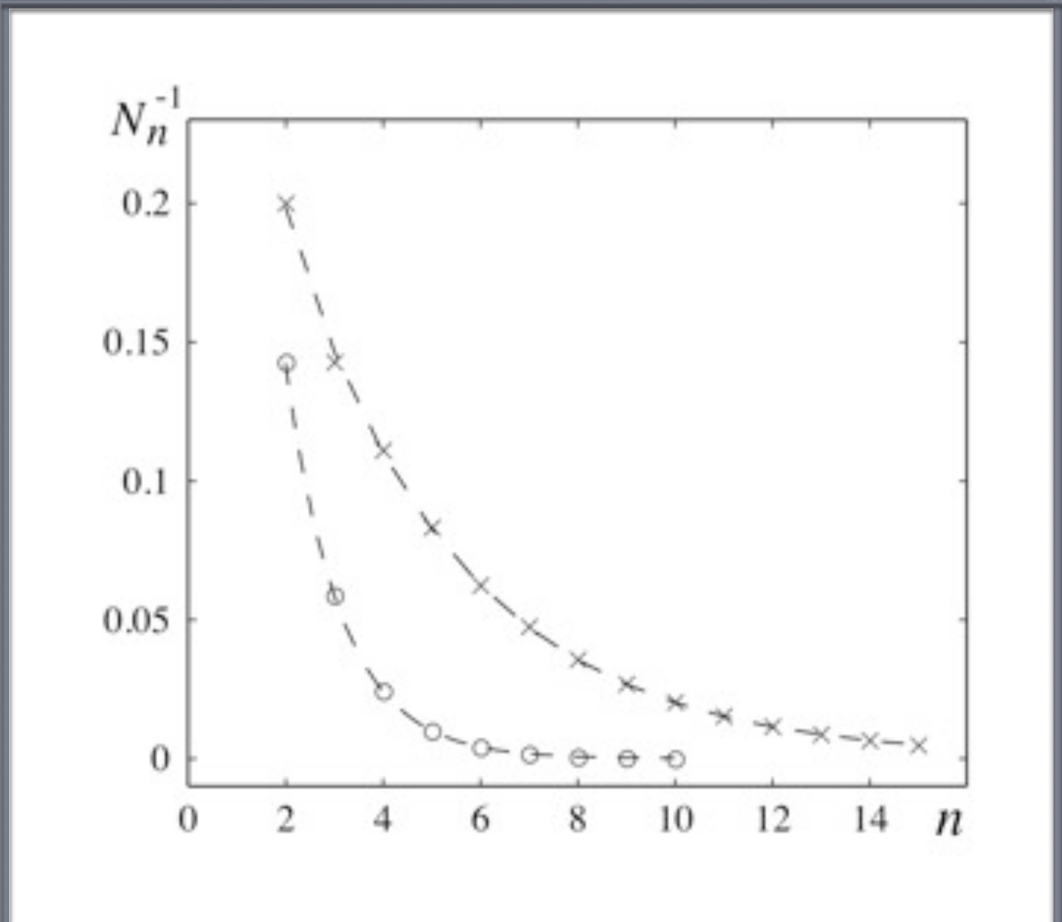
- Reformulation in terms of the hypersymbols (grammatical rules !)

$$\alpha = zyx \quad \beta = zxyx \quad \gamma = zx$$

$$\alpha \quad \beta \quad \beta \quad \alpha \quad \beta \quad \alpha \quad \alpha \quad \gamma \quad \alpha \quad \ldots$$

weakly correlated

- Selection, as measured by number of allowed sequences.
- Finite time (“fluctuating”) information.
- Emergence of a Zipf type law.


N_n^{-1}
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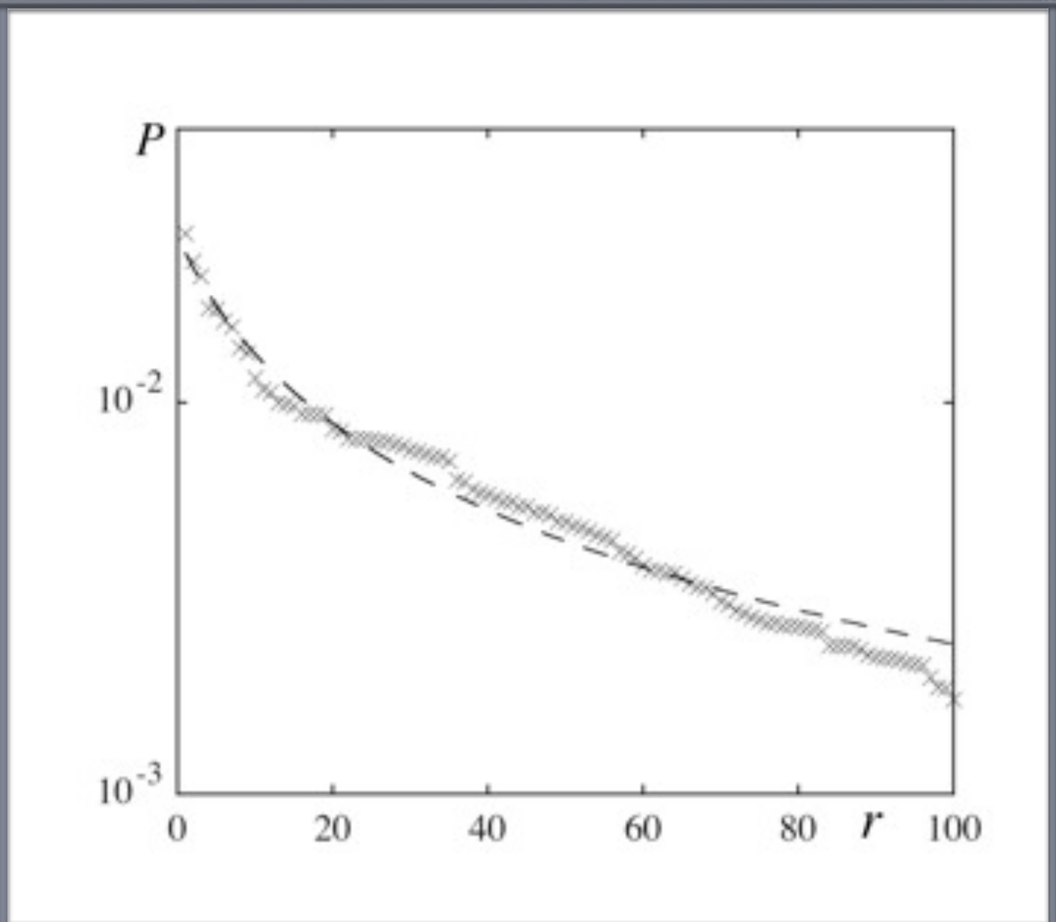
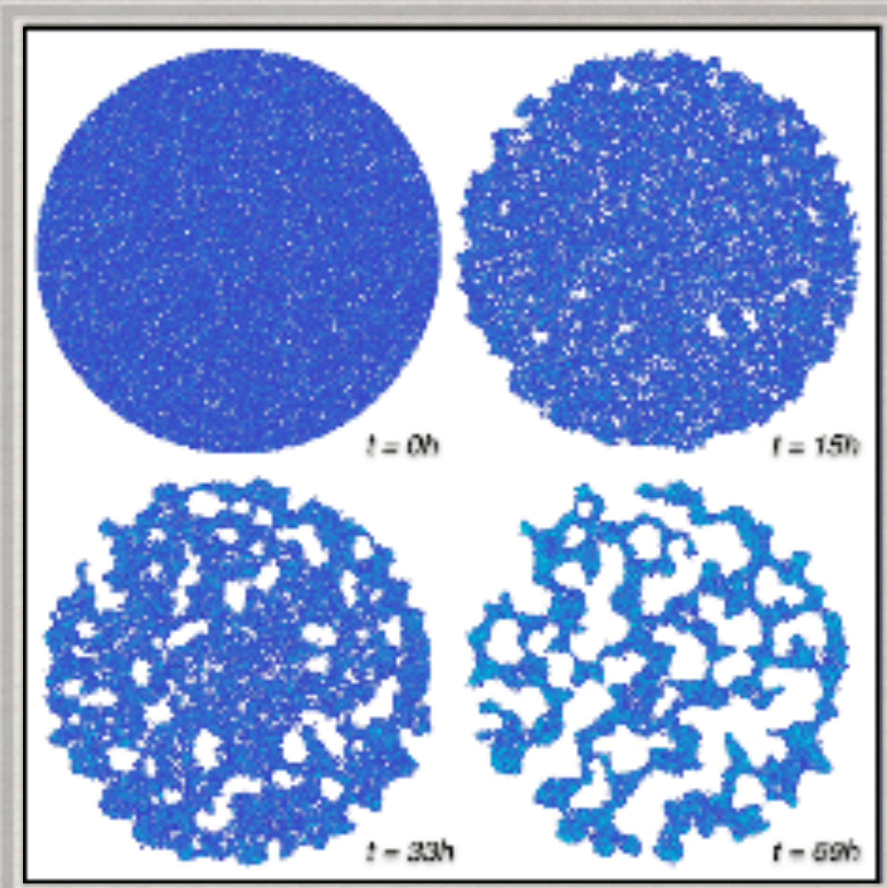
0.15
0.1
0.05
0
0
2
4
6
8
10
12
14
n

P
10^{-2}
10^{-3}
0
20
40
60
80
r
100

VI. Perspectives on biological complexity

- Understanding biology at the system level.
- Need to account for the specificities differentiating life from phenomena occurring in ordinary matter when addressing biology in the perspective of complex systems research. Ernst Mayer's **double-causality** concept.
  - Nonlinear dynamics and self-organization at the biochemical, cellular and organismic levels.
  - Biological superstructures.

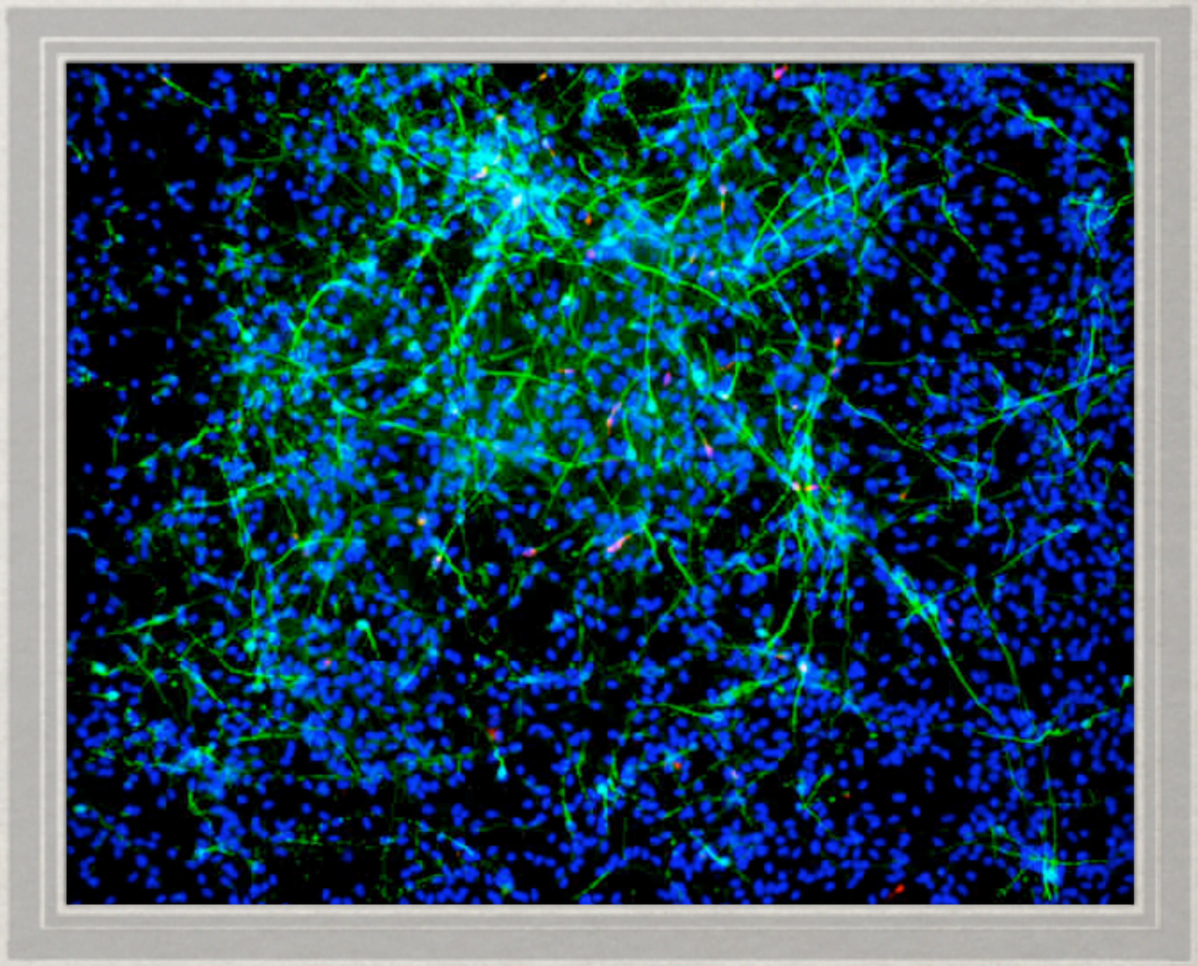


- Biological networks at the metabolic, genetic, immune and nervous system levels.

  Logical structure of the underlyning regulatory interactions, role of connectivity.

- Complexity and the genome organization.

  Coding versus non-coding regions



- Molecular evolution: self-organization in the information space.
- Replication-mutation dynamics in the language of chemical kinetics, incorporating explicitly the concept of selection and displaying the role of both the equilibrium and the nonequilibrium constraints.
- Vizualization in the sequence space. The concept of error threshold.
- Towards a molecular evolution engineering.

VII. Conclusions

- The evolution of complex systems is an open-ended process.
- The concept of emergence can be quantified.
- Complex systems possess an irreducible random element.
- The concepts and strategies of prediction and of monitoring need to be redefined.
- Natural large scale systems in the light of complex systems research. Conversely, natural complexity as a source of inspiration for progress at the fundamental and applied levels.
- A “nonequilibrium” extension of information and computation theories. Towards a thermodynamics of complex systems.
- Complexity: from fundamental science to everyday practice. Need for new theoretical and computational approaches. Unification and respect for specificities.
- Building-up a recognizable complexity community. Need for novel training schemes.