FRONTIERS IN COMPLEX SYSTEMS RESEARCH

- Complexity leads to the reassessment of long-standing principles and practices.
- New issues.
- Multilevel approach, blending and cross-fertilization of ideas and tools originating from different disciplines.
- Complexity, a new scientific paradigm.

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

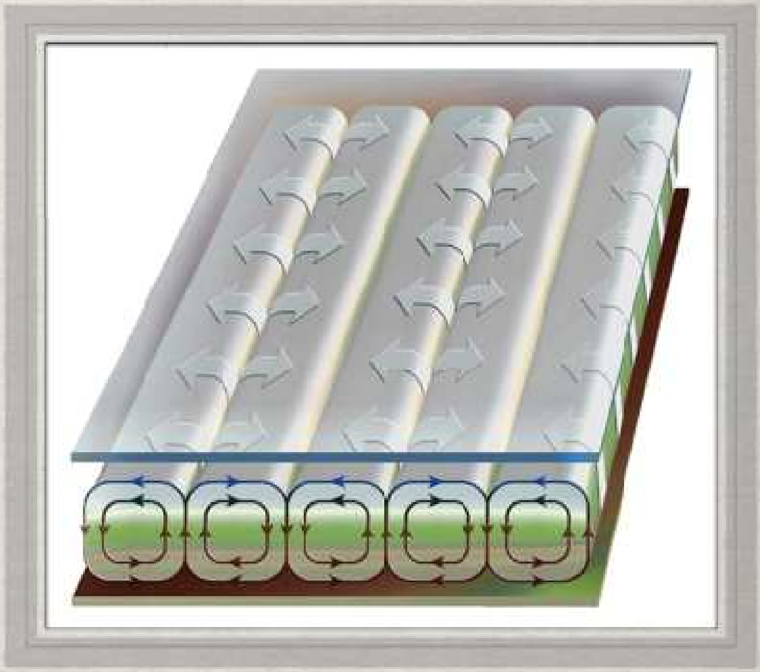
I. SURVEY OF KEY FEATURES OF COMPLEX SYSTEMS

A. COMPLEX SYSTEMS DISPLAY A PHENOMENOLOGY OF THEIR OWN

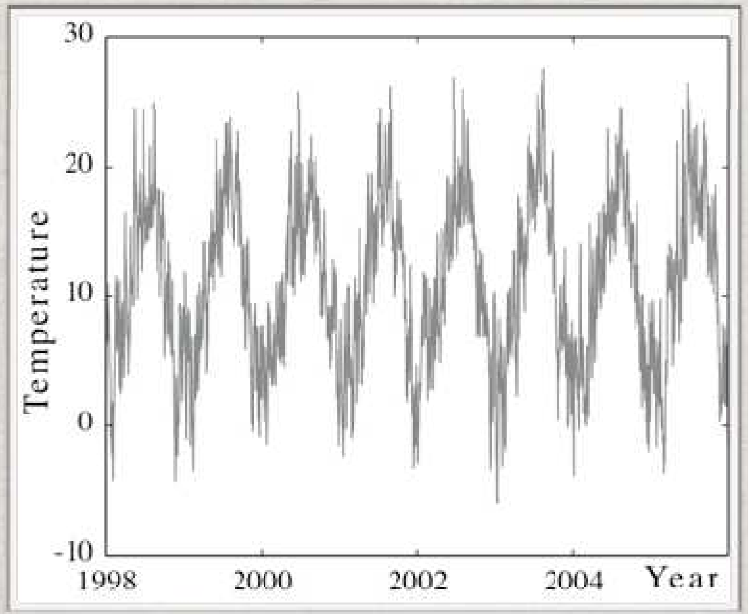
Principal signature of complex systems: multiplicity of possible outcomes.

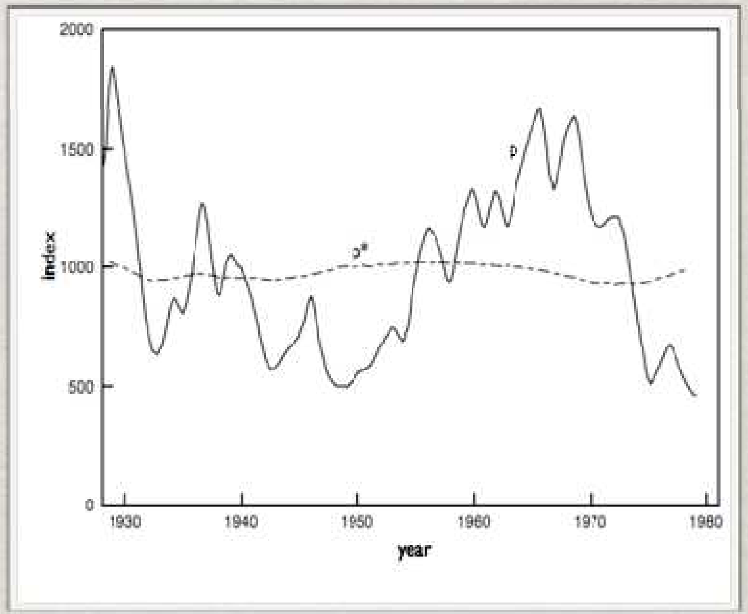
Two different manifestations:

- 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.

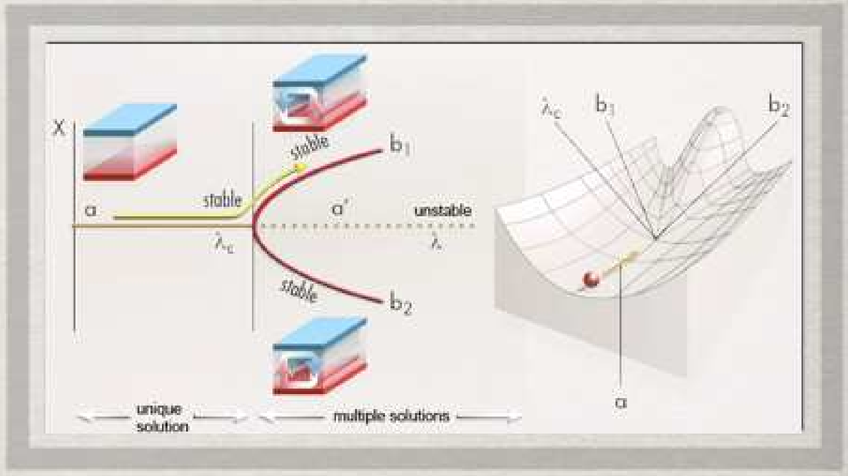


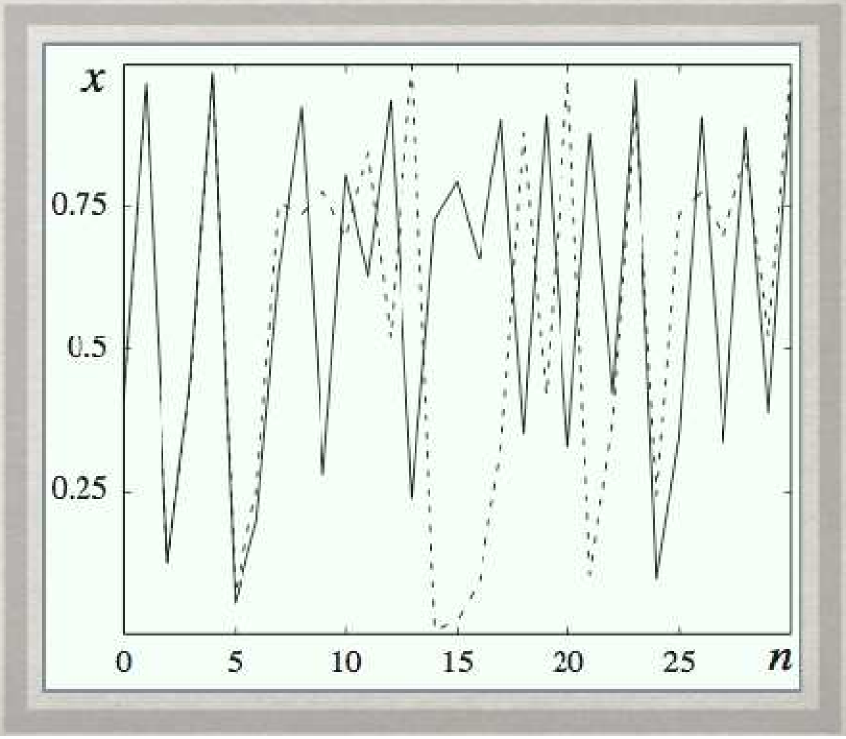
- Intertwining of order and disorder.





B. COMPLEX SYSTEMS POSSESS AN IRREDUCIBLE RANDOM ELEMENT





- 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 evolutionary scenarios.

C. EMERGENCE

- Complexity follows its own rules, yet since laws of nature are deterministic these rules are bound to be determined by the interactions between lower order hierarchical levels.

- Key to the resolution of the apparent paradox: existence of a closed description involving a limited number of variables.

SOME INSTANCES WHERE CLOSURE CAN BE REALIZED

- Macroscopic level (mean field) description

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

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

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

- 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.

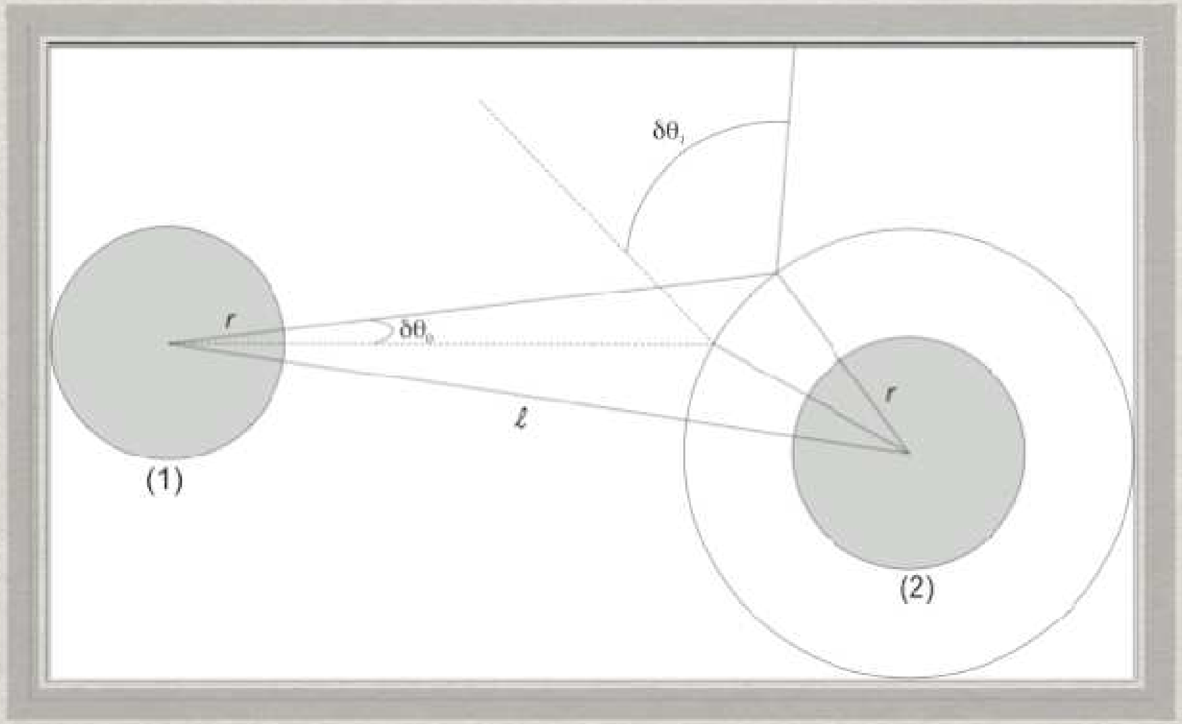
Limits of the hierarchical description : breakdown of the decoupling between levels of description.

- 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.

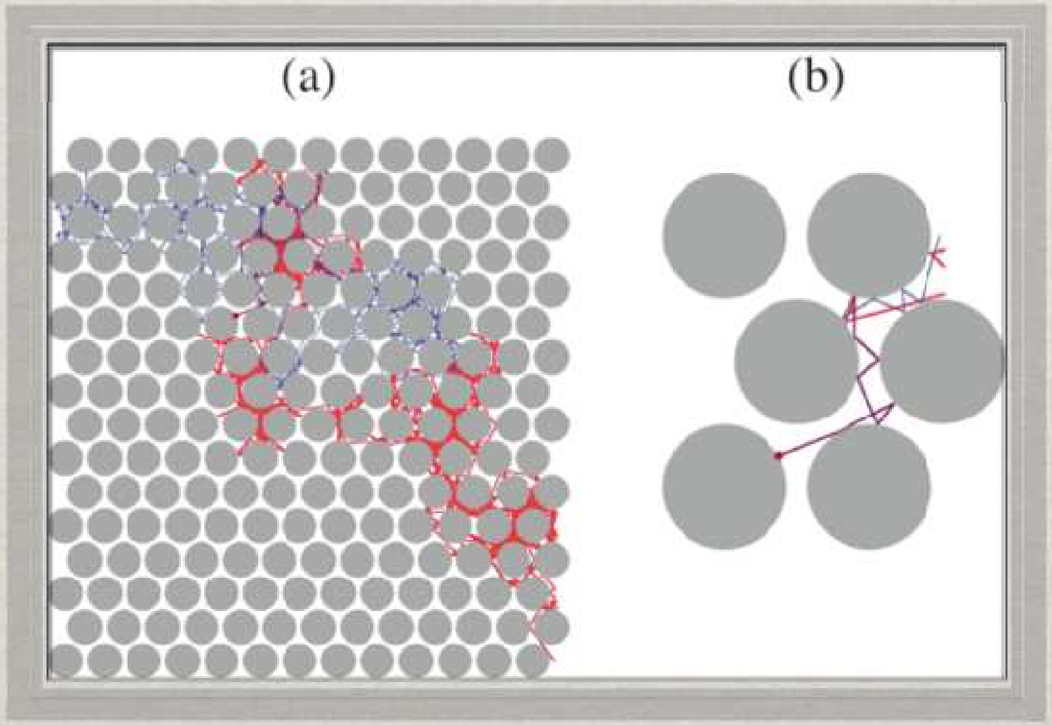
II. MICROSCOPIC LEVEL COMPLEXITY AND THE FOUNDATIONS OF IRREVERSIBILITY

- 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

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

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!

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

with

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

Irreversibility as an emergent property

III. EQUILIBRIUM VERSUS NONEQUILIBRIUM

Classic prototype of complexity: rhythms and patterns formed under nonequilibrium conditions.

- Characteristic time and space scales in the macrscopic range.
- Function determines structure.

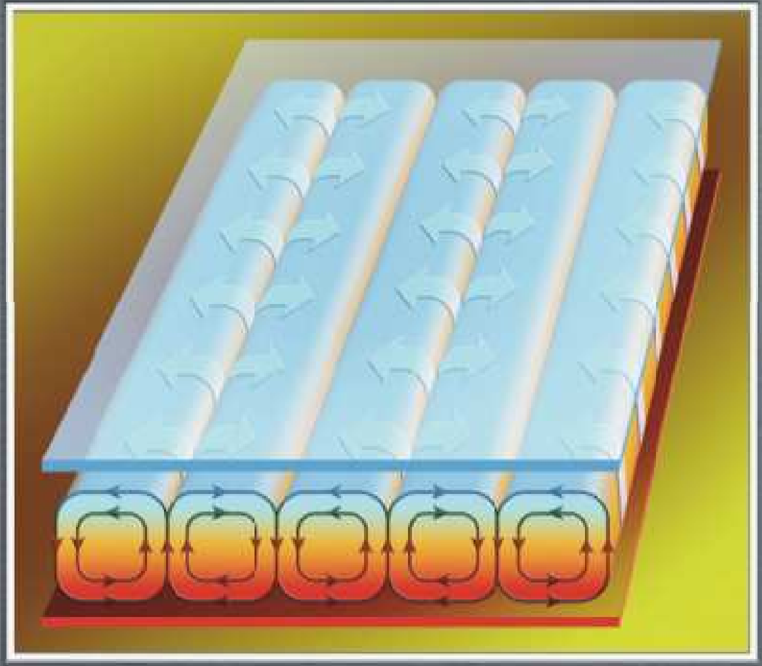
Is complexity basically a nonequilibrium phenomenon?

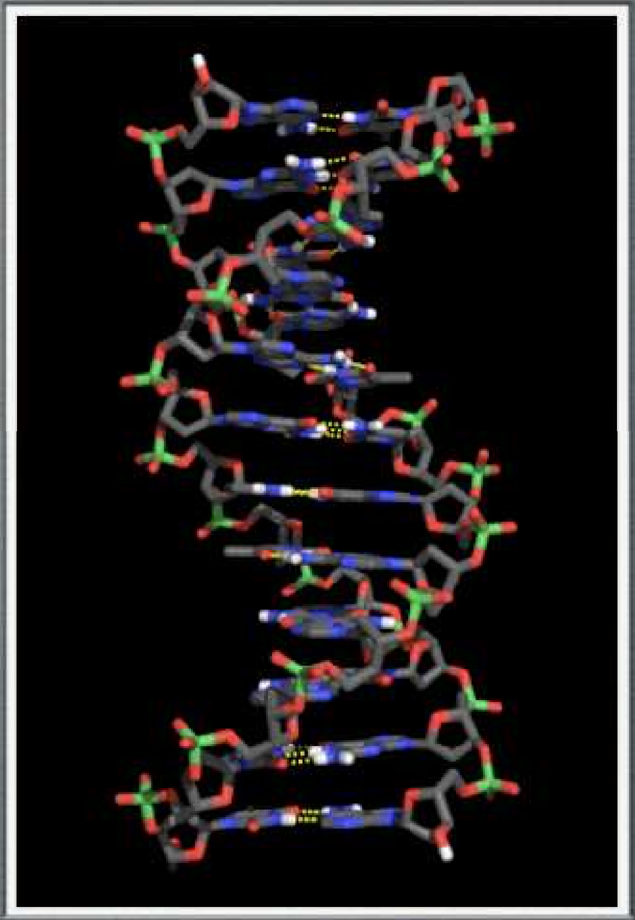
Self-assembly phenomena leading to macromolecular and supermolecular level structures in equilibrium with their environment, that can definitely be qualified as complex.

- Characteristic space scales in the microscopic or the mesoscopic range.
- Structure determines function.

The evolutionary perspective: structure (equilibrium) and function (nonequilibrium) intimately intertwined. Need to break detailed balance.

Nucleation: equilibrium and nonequilibrium meet in a natural way. Non standard scenarios.

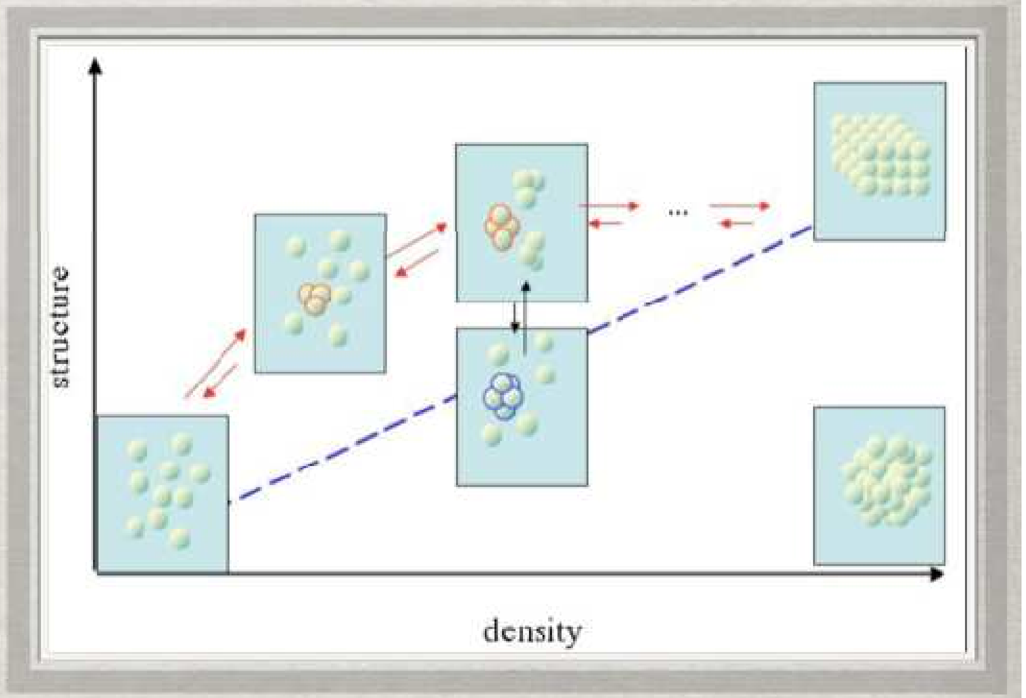




NON STANDARD NUCLEATION MECHANISMS WITH COMBINED STRUCTURAL AND DENSITY FLUCTUATIONS

- Importance of kinetic effects arising from the co-existence of competing mechanisms.

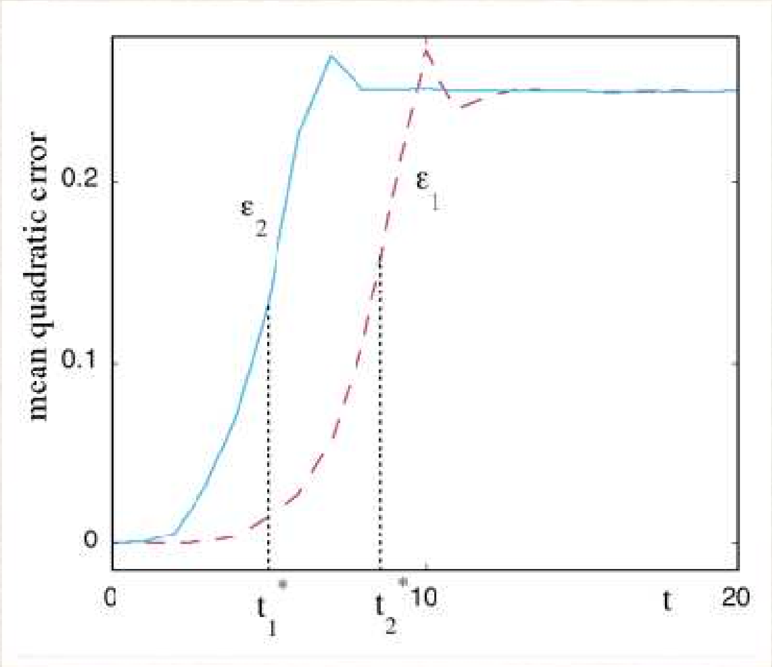
- Enhancement of nucleation rate under certain conditions via favorable pathways in the two order-parameter phase diagram.

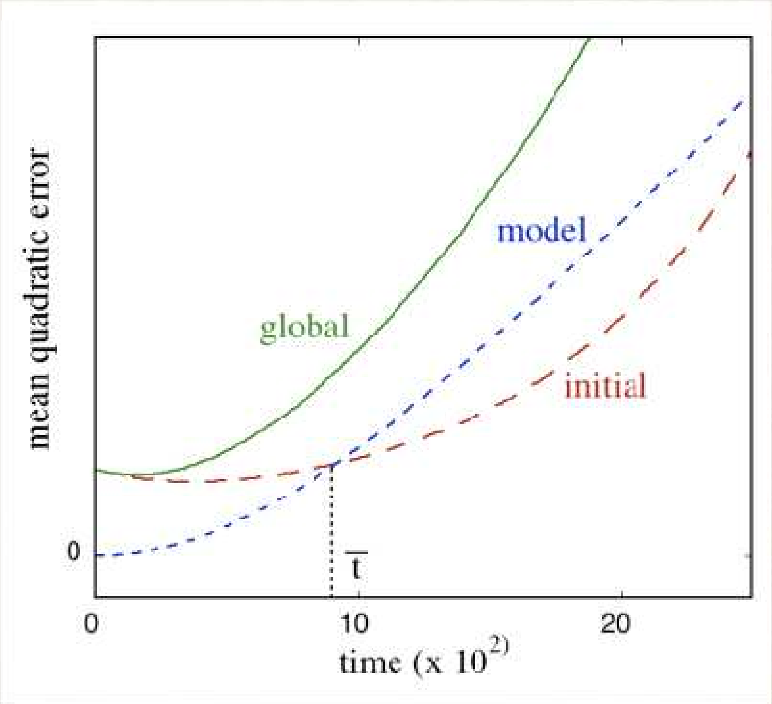


IV. PREDICTION

A. THE BUTTERFLY EFFECT

- Predicting under uncertainty: finite precision in the initial conditions, model and observational imperfections.
- Complexity: intricate ways events unfold in time and organize in space. Growth of inherent errors in time.
- Errors as “revelators” of complexity.





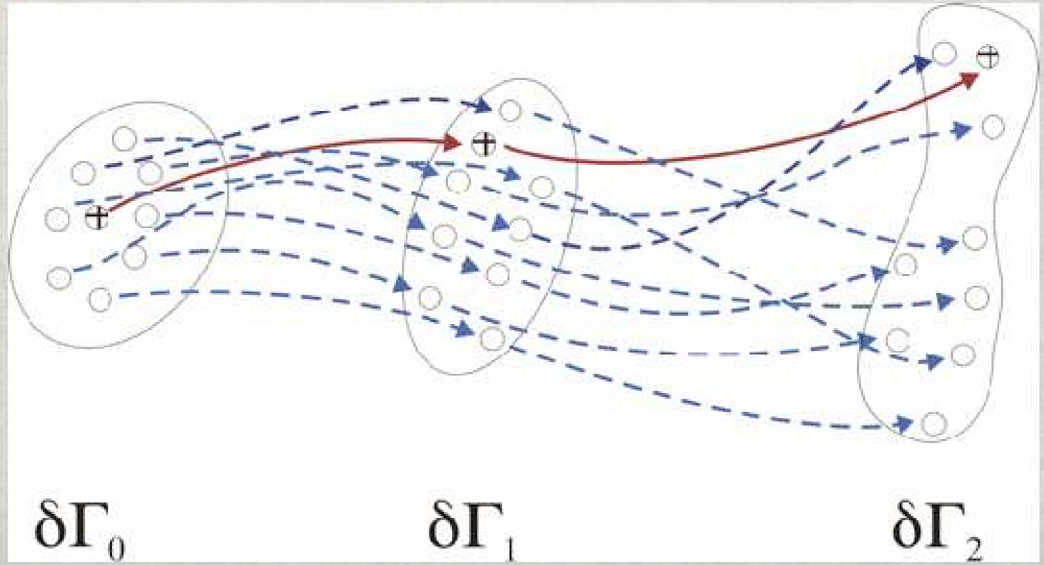
B. THE PROBABILISTIC APPROACH TO PREDICTION

- From the classical view of a world of unlimited predictability to the real world of limited predictability. Need for an alternative to the traditional deterministic description accounting for random-looking successions of events and an increasing delocalization in state space: the probabilistic approach

- Probabilities from dynamics: "deterministic randomness".

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

- Ensemble forecasts.

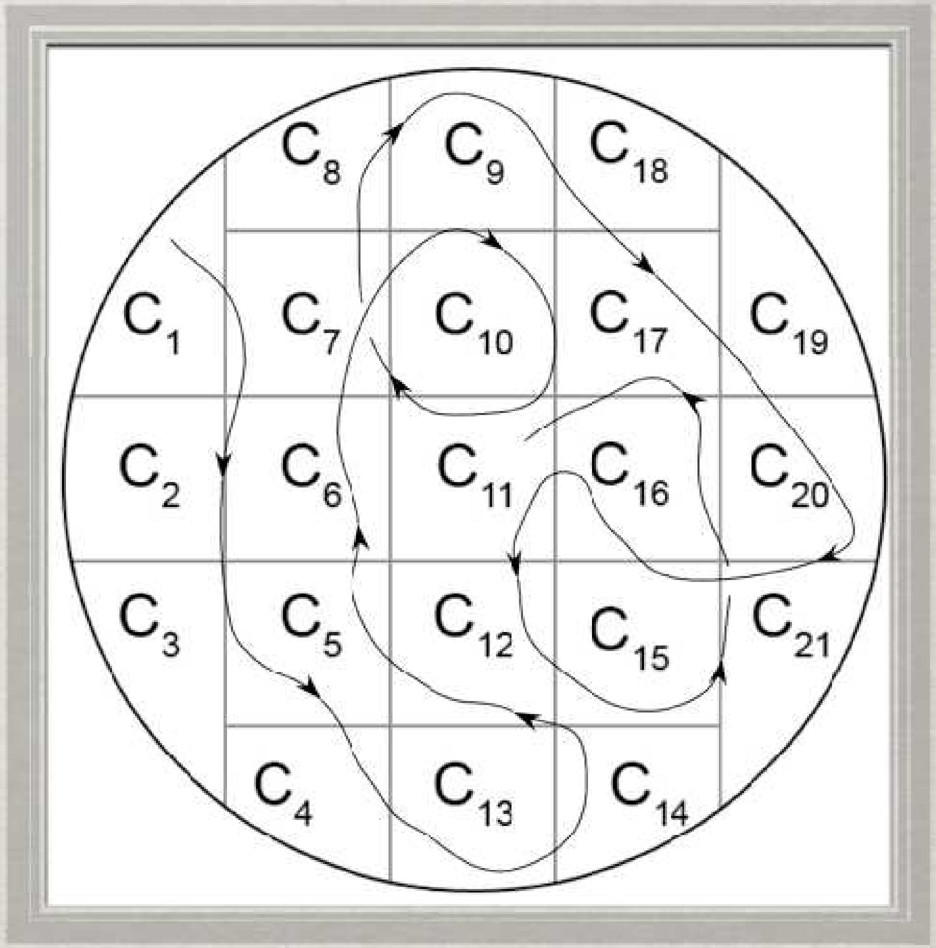


C. EXTREME EVENTS

- Ubiquity, deep impact.
- Where the validity of a closed description breaks down. Details (queues,…) begin to matter, yet remarkable statistical regularities.
- Classical statistical theory: Gumbel, Fréchet, Weibull universal distributions.
- Extreme events from deterministic dynamical systems. Differences from classical statistical theory.

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:

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

- Shannon-Mac Millan theorem

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

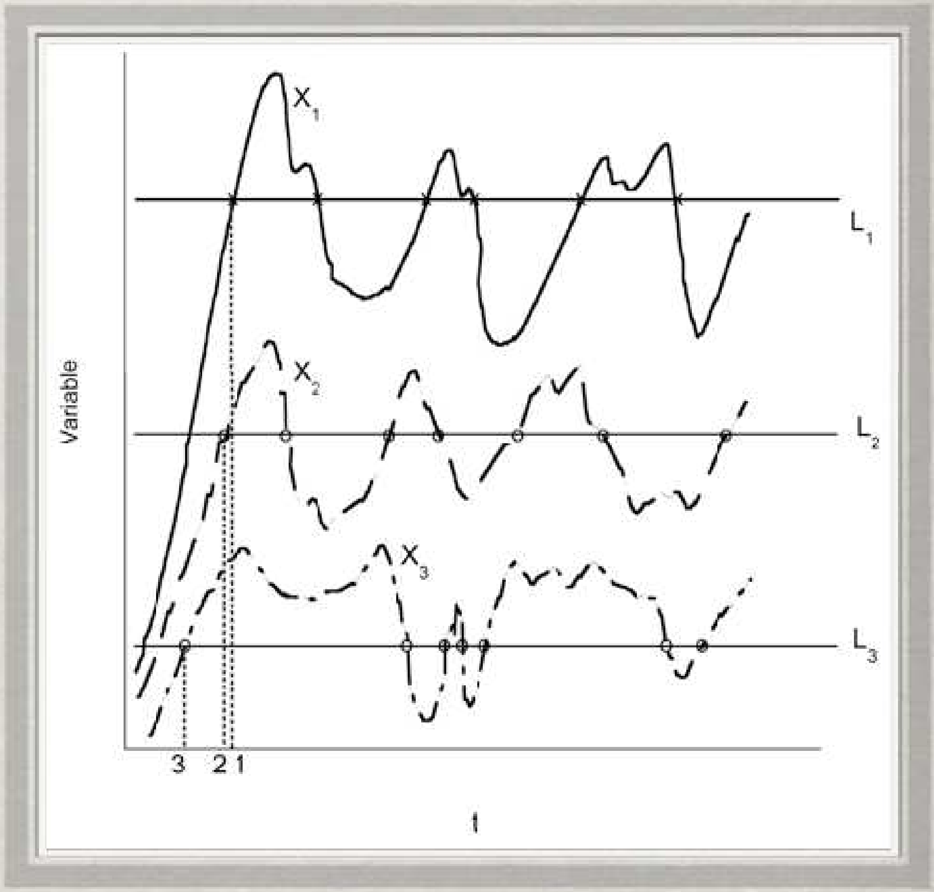
- the problem of combinatorial explosion.

- 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 !)

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

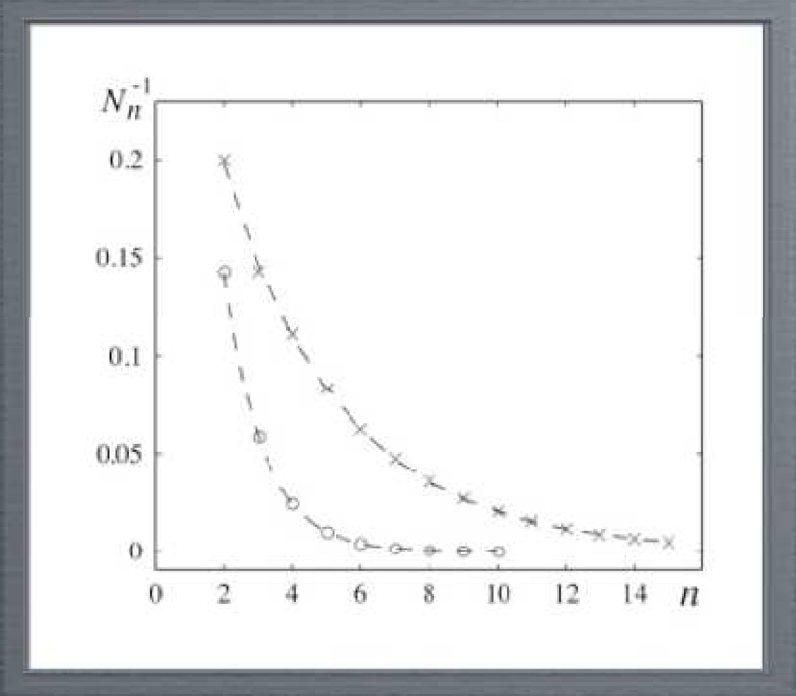
$$\alpha \quad \beta \quad \beta \quad \alpha \quad \beta \quad \alpha \quad \alpha \quad \gamma \quad \alpha \quad \ldots$$

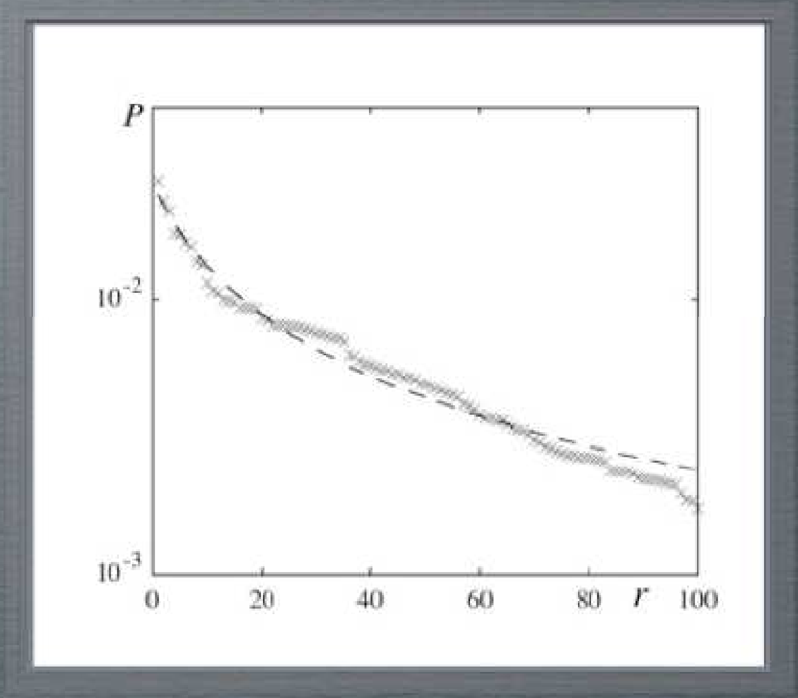
weakly correlated

- Selection, as measured by number of allowed sequences.

- Finite time ("fluctuating") information.

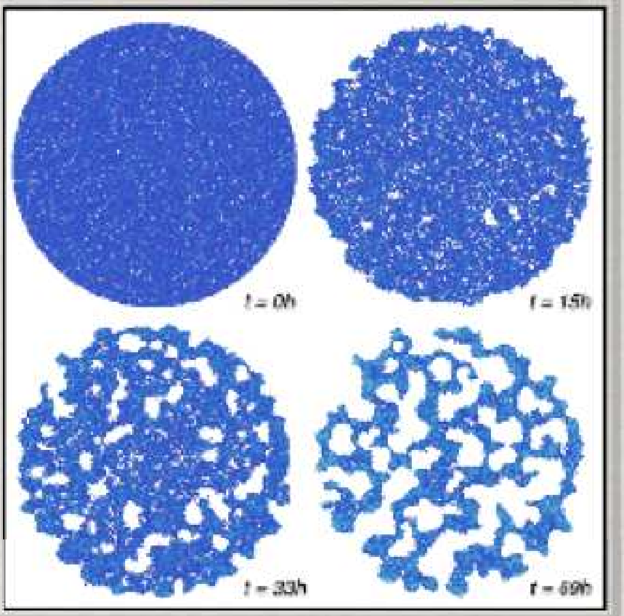
- Emergence of a Zipf type law.


N_n^{-1}
0.2
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.
- Nonlinear dynamics and self-organization at the biochemical, cellular and organismic levels.
- Group-living organisms. Biological superstructures.

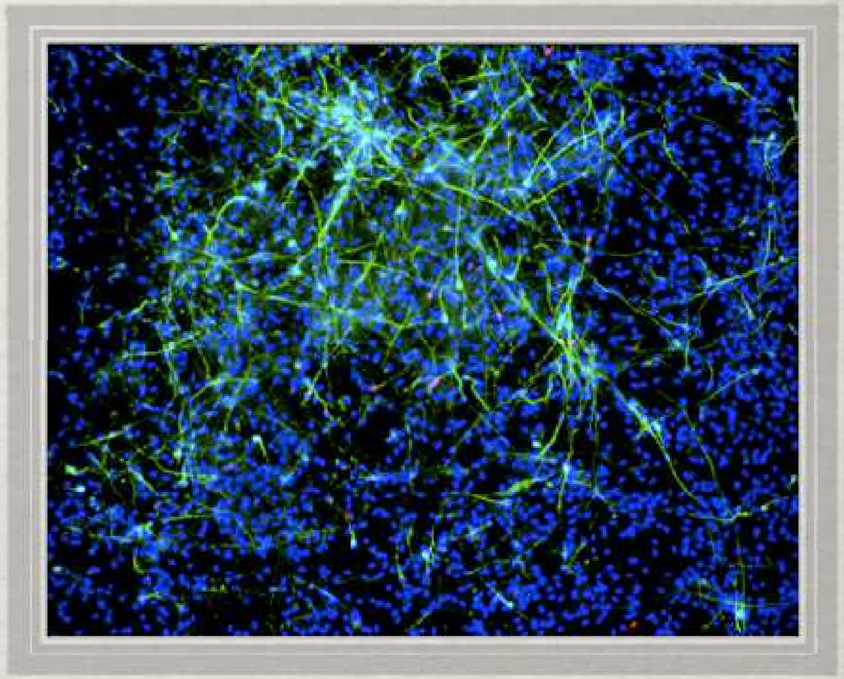


- Biological networks at the metabolic, genetic, immune and nervous system levels.

  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, incorporatiing explicitly the concept of selection and displaying the role of both the equilibrium and the nonequilibrium constraints.
- Vizualization in the sequence source. The concept of error threshold.
- Towards a molecular evolution engineering.

VII. CONCLUSIONS

- Complexity is an active, fast growing branch of science.
- Complexity research is a forum for the exchange of information and ideas of an unprecedented diversity cutting across scientific disciplines.
- 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.