6th Ph.D. School/Conference on
Mathematical Modeling of Complex Systems
Università “G. d’Annunzio”, Pescara. Italy, July 3 – 11, 2019

Founding Complexity Science: the work of Gregoire Nicolis

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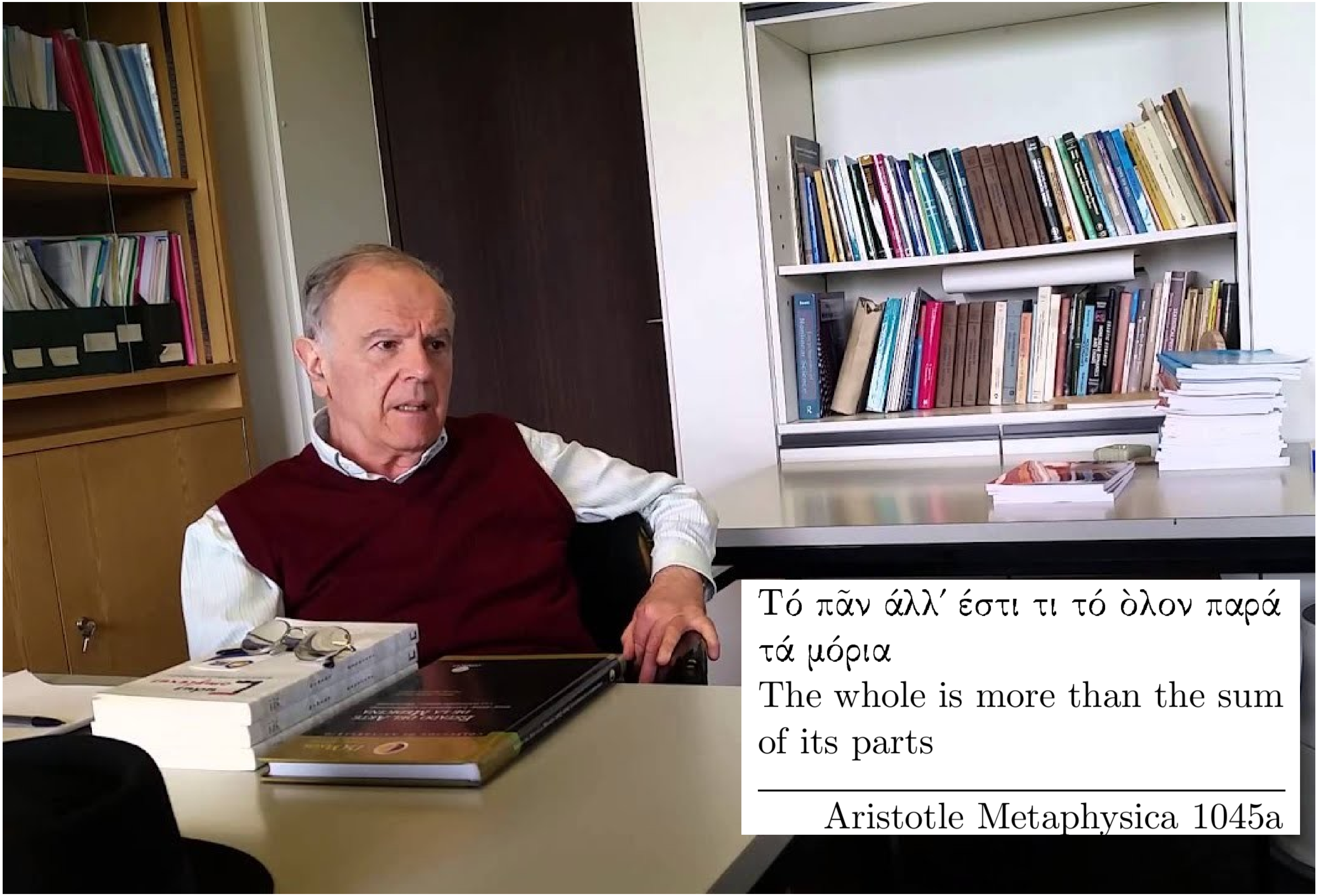
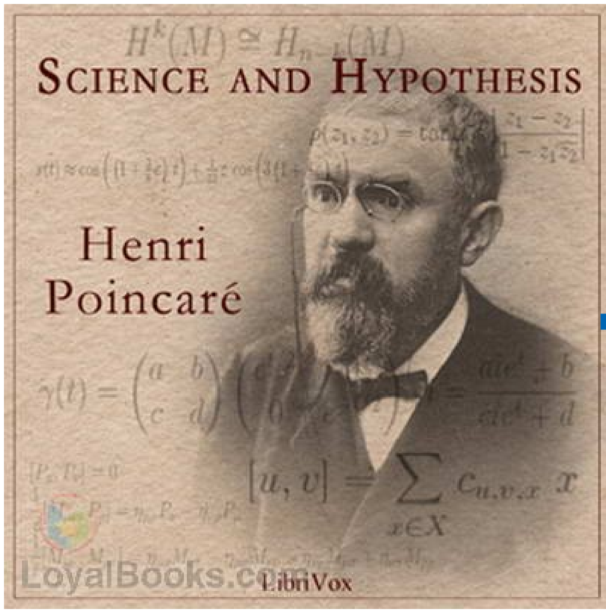
Interdisciplinary Centre for Nonlinear Phenomena & Complex Systems (Cenoli-ULB)
&
Département de Physique des Systèmes Complexes et Mécanique Statistique,
University of Brussels (ULB), Brussels.



Gregoire Nicolis (1929-2018) in his study room at *ULB – CeNoLi* circa 2015

Gregoire's Nicolis Academic 'Family' Tree



Poincaré, Henri
(1854 – 1912)
Chaos
Relativity
3-Body-Problem
Philosophy of Science
…
…

De Donder, Théophile Ernest (1872-1957)
'Brussels School of Thermodynamics'
Chemical Affinity,
Irreversibility ...

Ilya Prigogine
(1917-2004)
'Brussels School of Thermodynamics'
Chemical Affinity,
Irreversibility ...

Gregoire Nicolis’ Enconium & Heritage:

Open Systems & the 2nd Law of Thermodynamics

Dissipative Structures

Bifurcations & Chaos

Self-Organization & Pattern Formation

Constructive Role of Fluctuations & Chaos
(+ Stochastic Resonance)

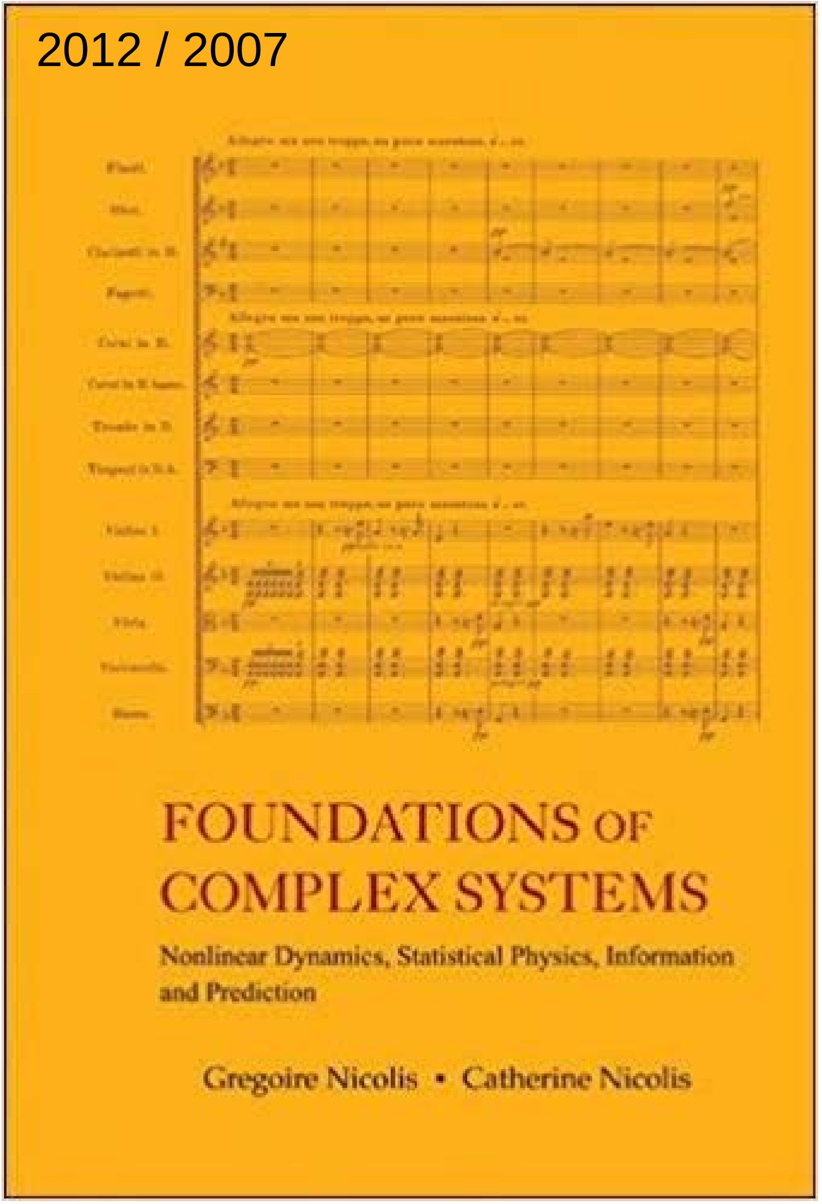
Self-reference & Nonlinear Feedback

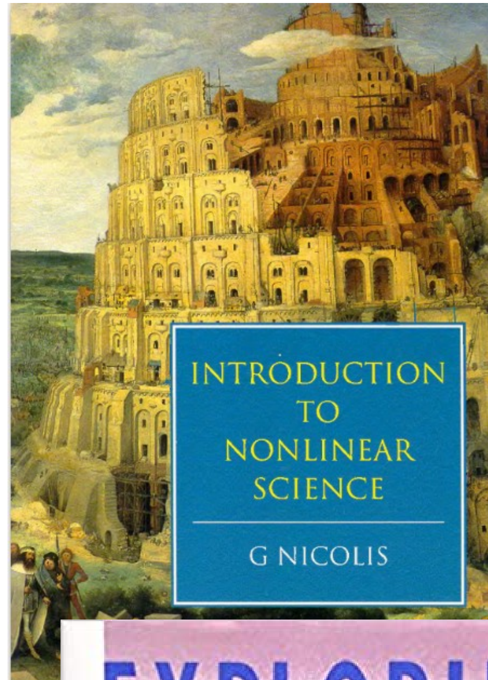
Information Dynamics
(+ Entropy & Symbolic Dynamics + Prediction)

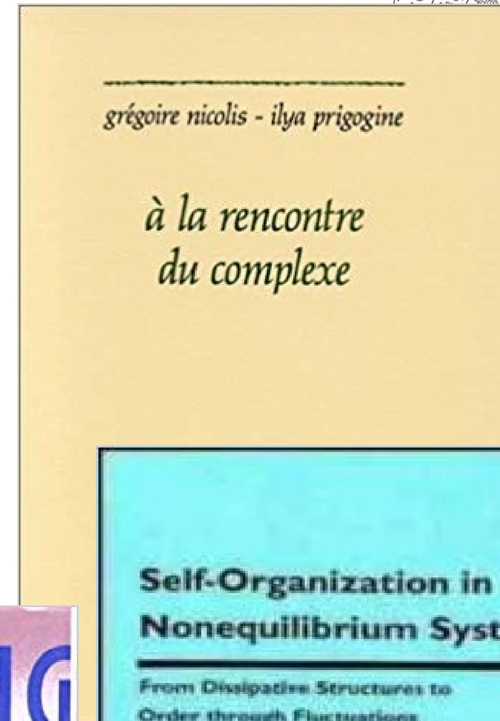
Emergence & Irreversibility

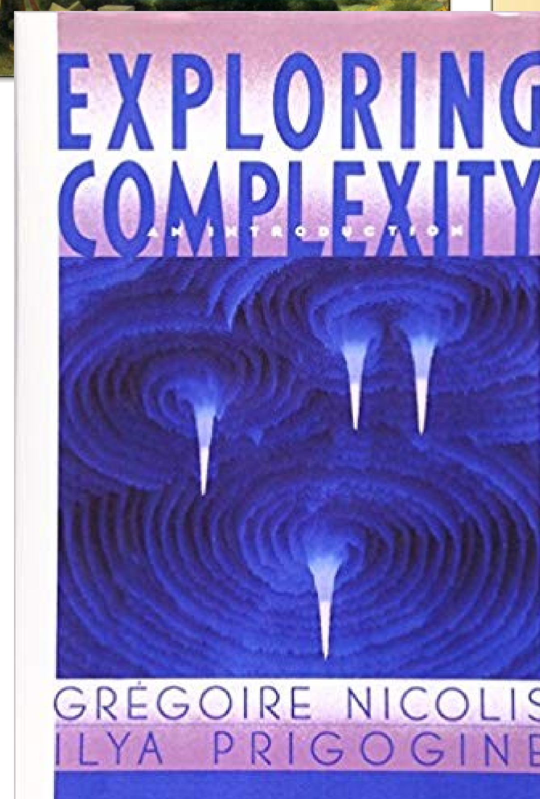
Complexity Science bookshelf

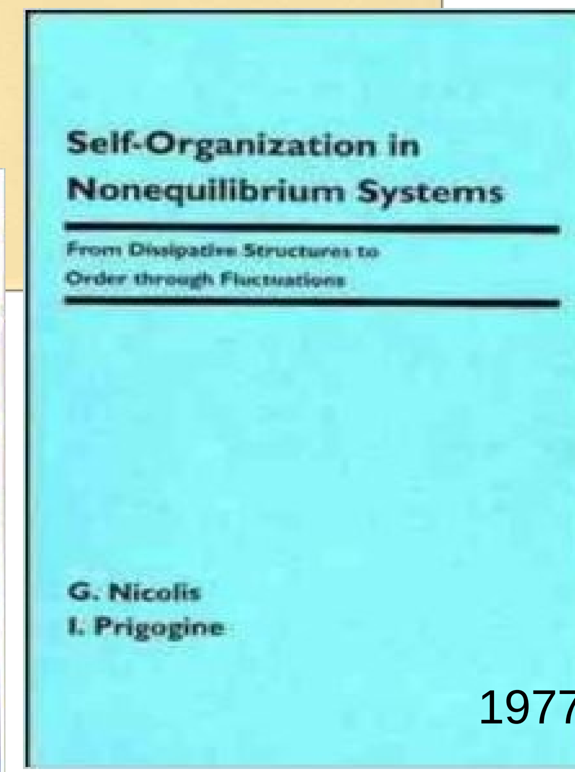
2012 / 2007







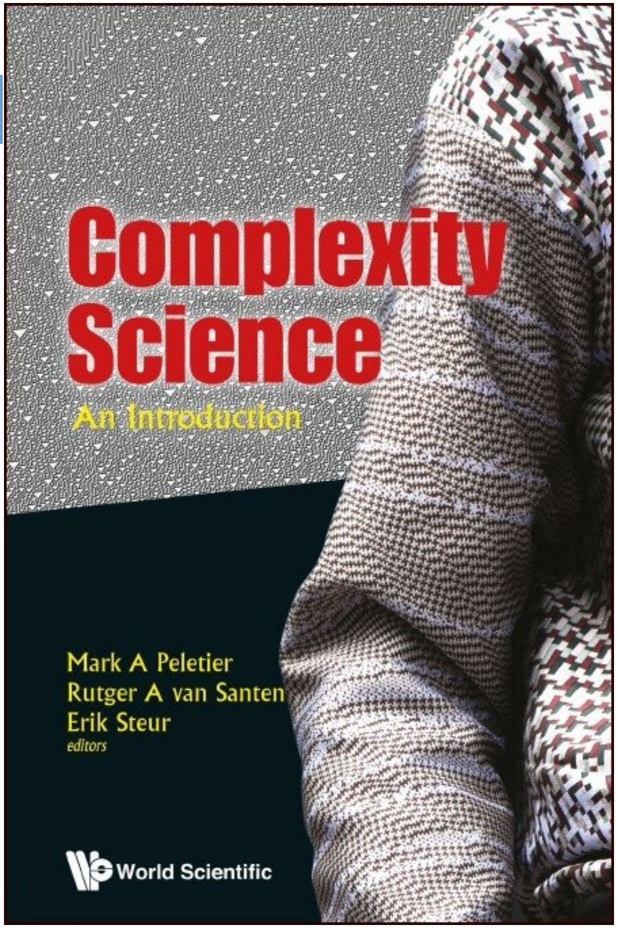




1977

Complex =
many parts + nonlinear relations

Chapter 1:
“The many facets of complexity”
by Grégoire Nicolis



Τό πᾶν άλλ΄ έστι τι τό ὀλον παρά τά μόρια
The whole is more than the sum of its parts

Aristotle Metaphysica 1045a

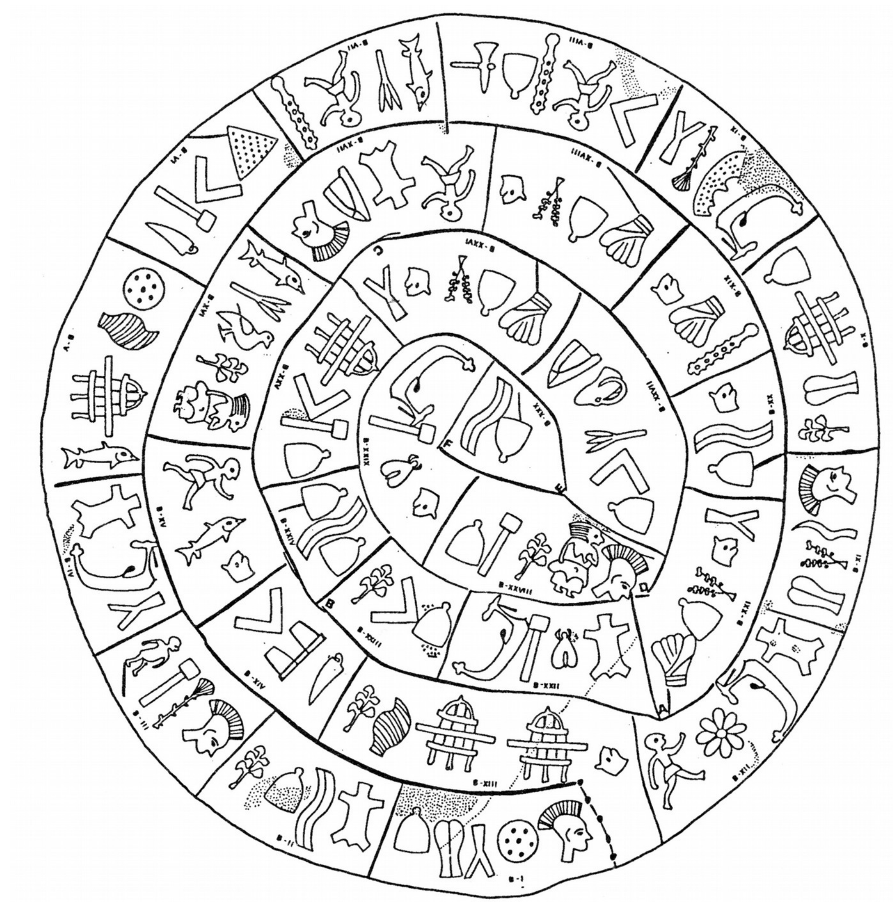
Complexity Science

Nonlinear dynamics and chaos theory,

Thermodynamics and statistical physics,

Information and probability theories,

Numerical simulation and techniques from data analysis.

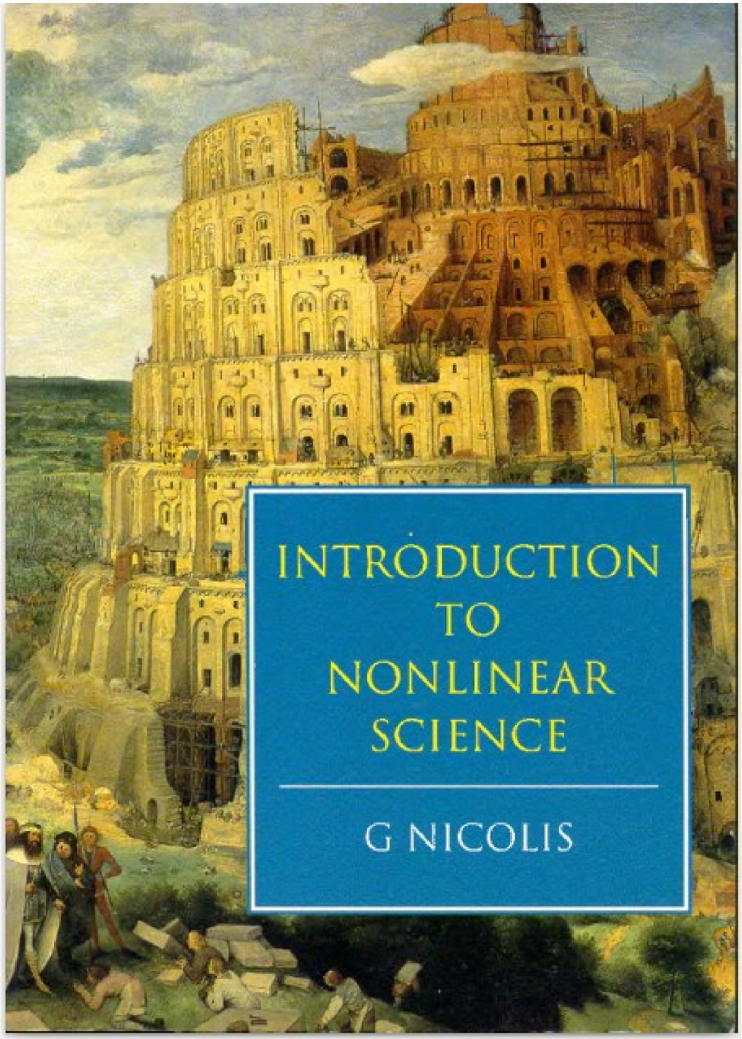


“Nonlinear science introduces **a new way of thinking** based on a subtle interplay between qualitative and quantitative techniques, between **topological, geometric and metric** considerations, between deterministic and statistical aspects.

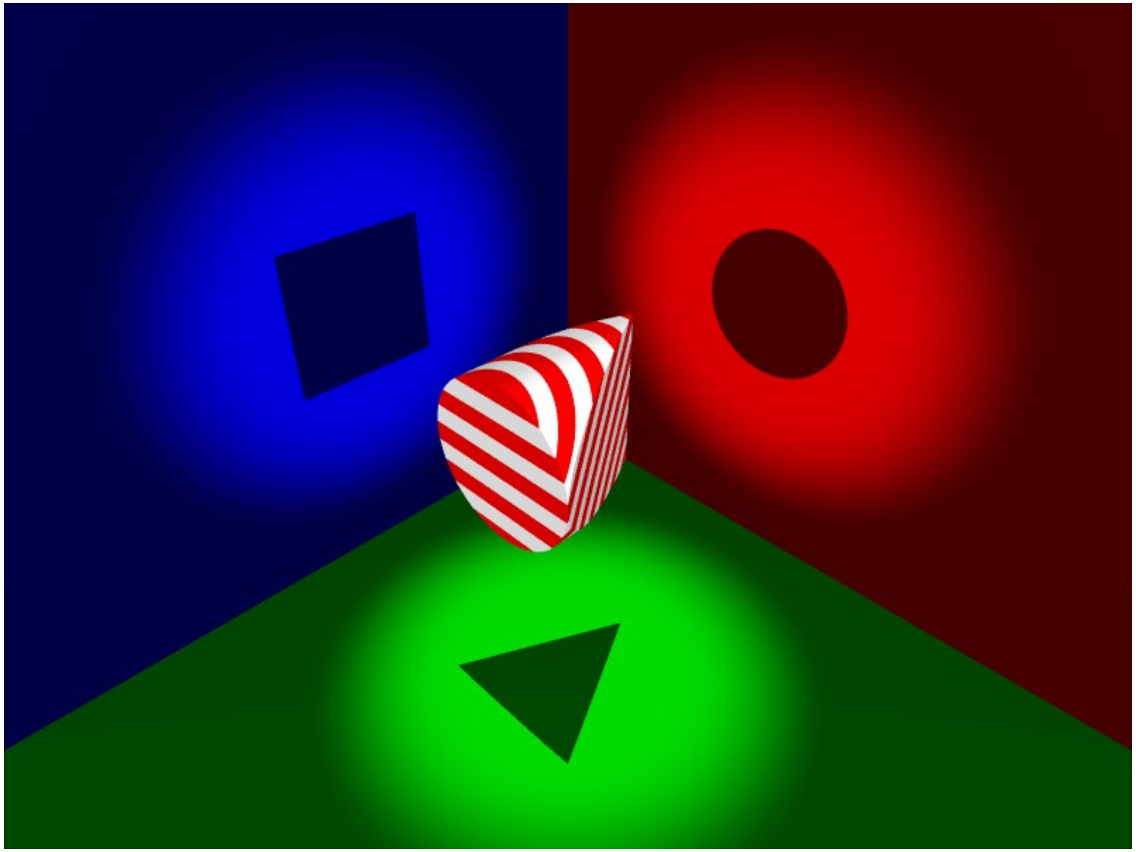
It uses an **extremely large variety of methods from very diverse disciplines**, but through the process of continual **switching between different views of the same reality** these methods are cross-fertilized and blended into a unique combination that gives them a marked added value.

Most important of all, **nonlinear science helps to identify the appropriate level of description in which unification and universality can be expected.**”

“Introduction to Nonlinear Science”
by Gregoire Nicolis
(Cambridge Univ. Press, 1995)



"...appropriate level of description ..."



"...topological, geometric, metric ..."

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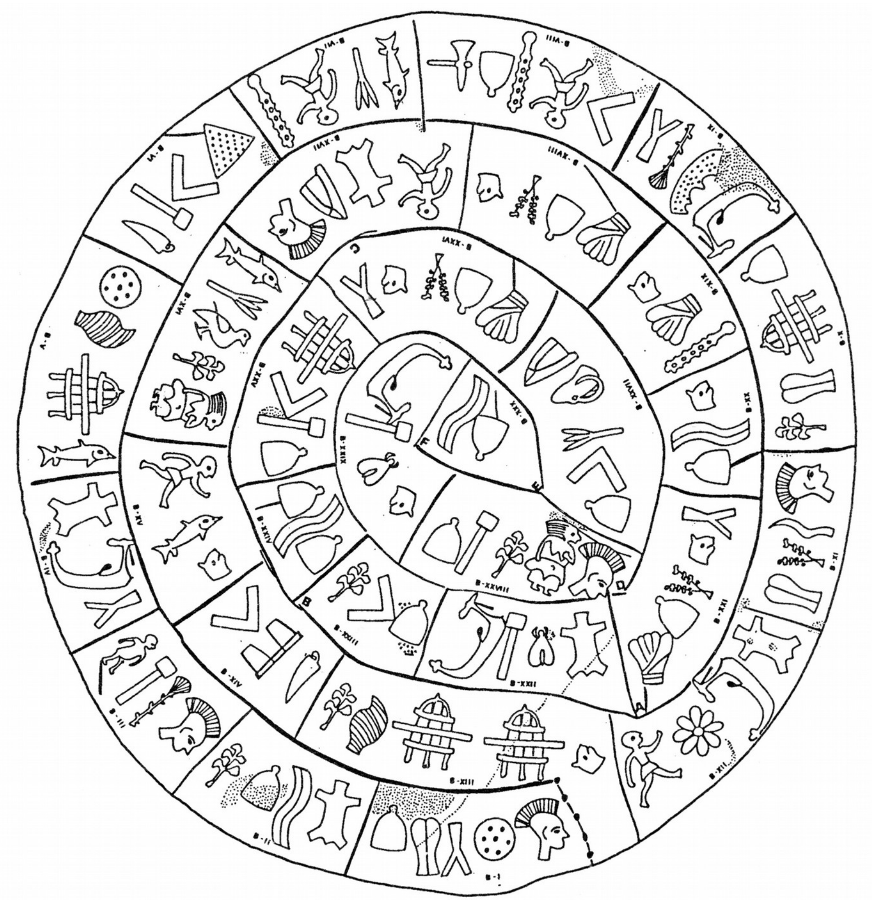
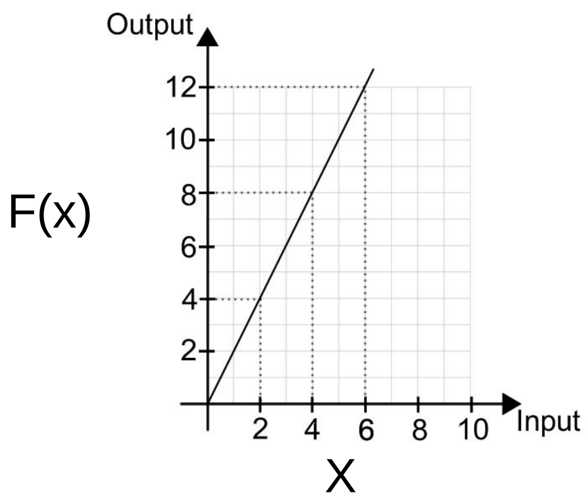


The Importance of Being Nonlinear

LINEAR

$F(x_1+x_2) = F(x_1) + F(x_2)$

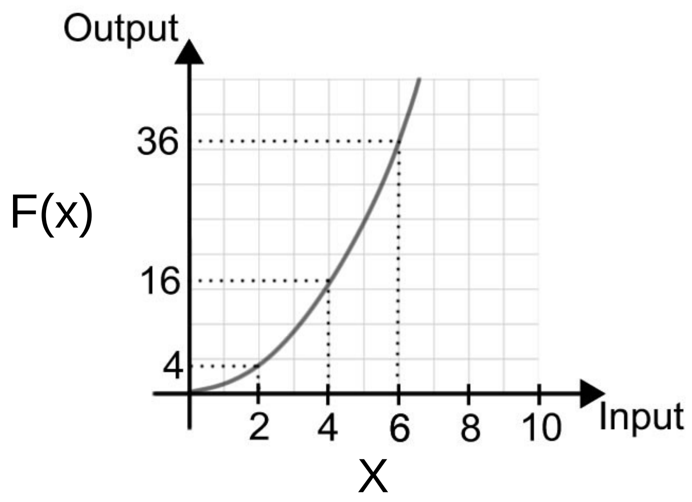
The whole IS
the sum of its parts



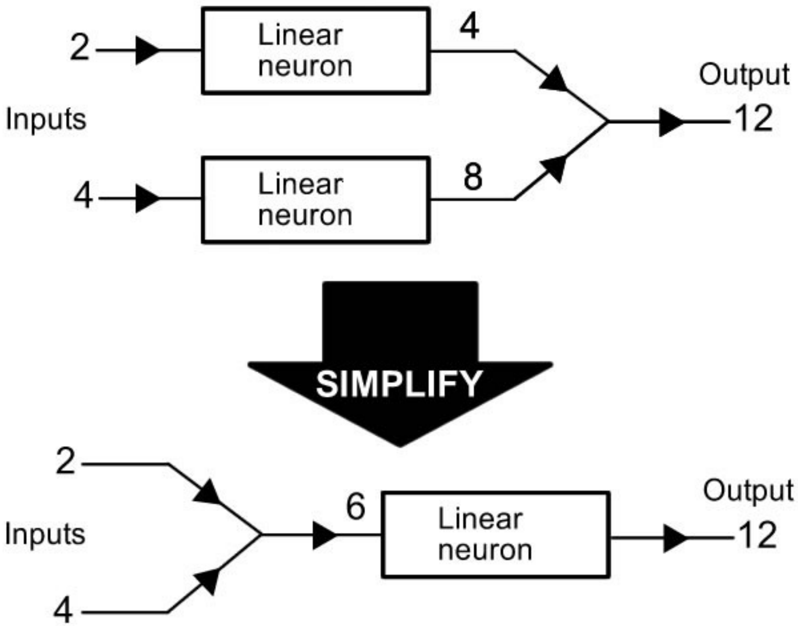
NONLINEAR

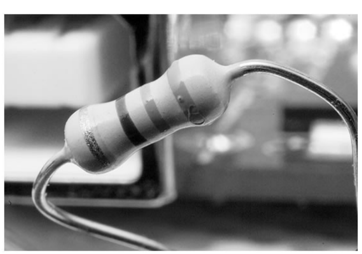
$F(x_1+x_2) =/= F(x_1) + F(x_2)$

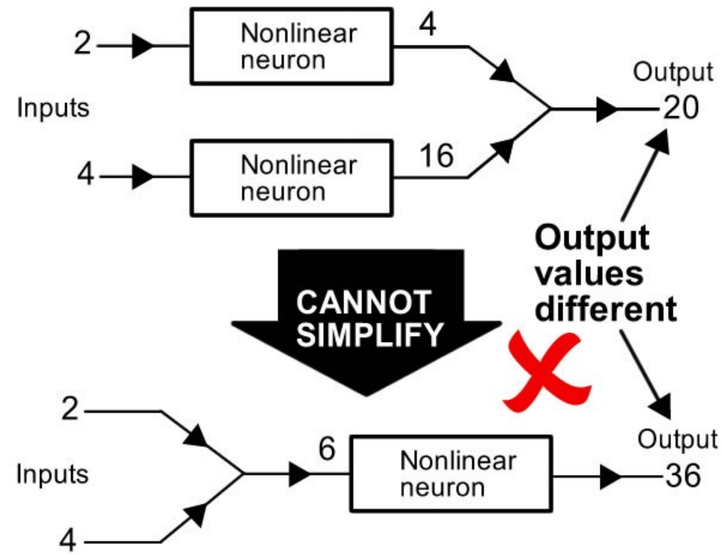
The whole IS NOT
the sum of its parts

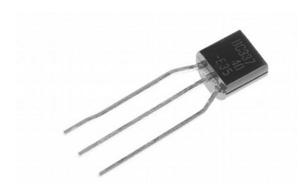


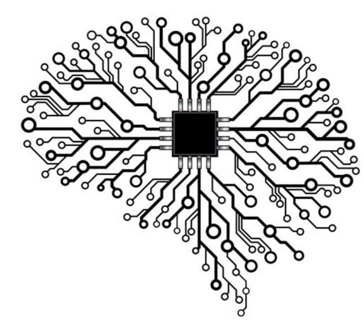
The Importance of Being Nonlinear: Information flow





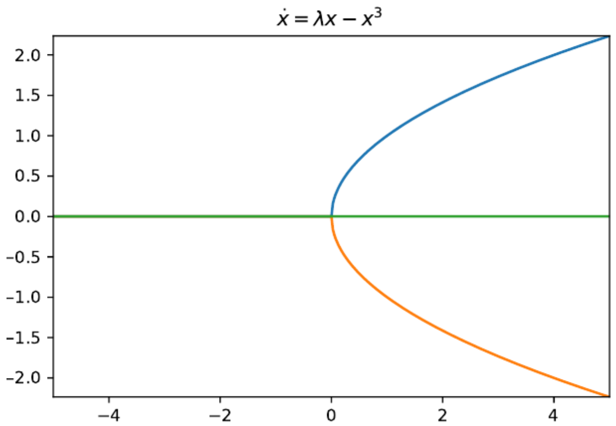


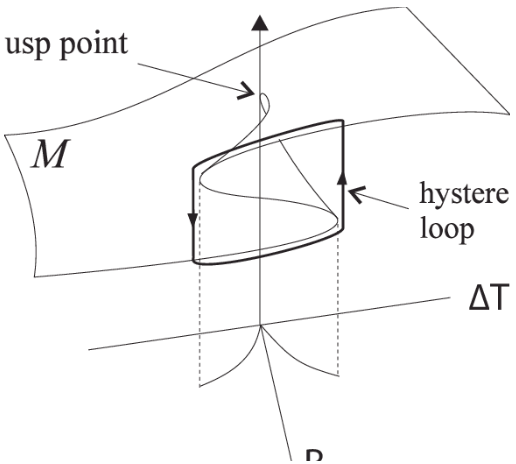




Only Nonlinear Elements can process information, i.e … compute !!!

The Importance of Being Nonlinear: Bifurcations & Multistability





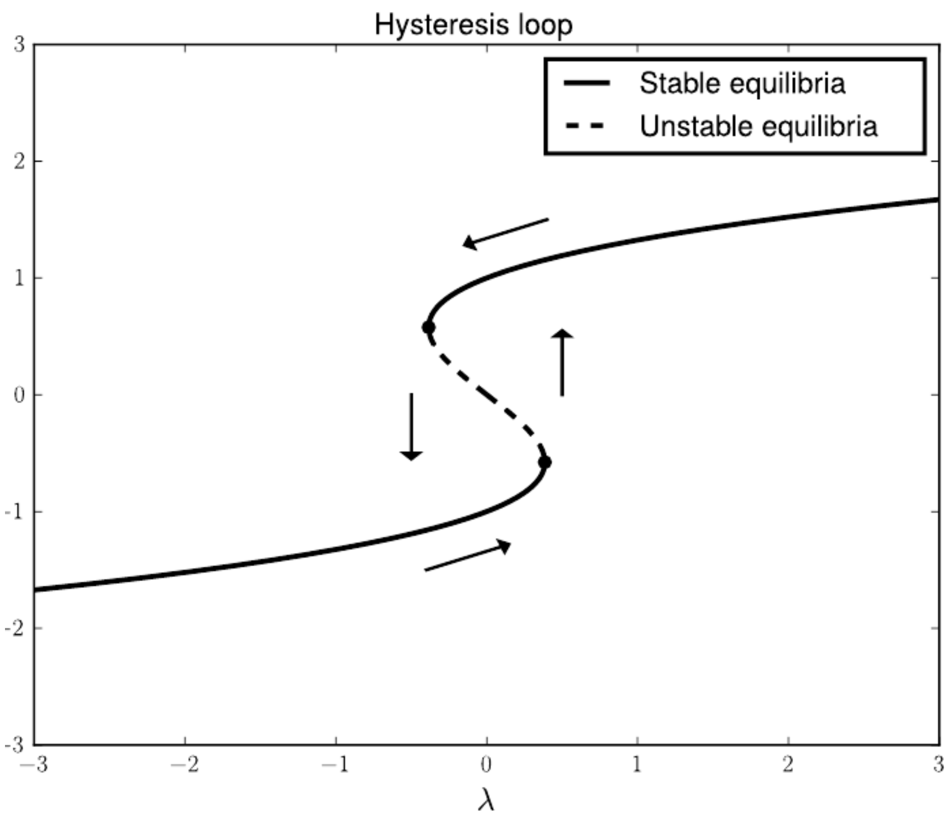


Figure 6.5: Bifurcation diagram for the ODE $x' = \lambda + x - x^3$.

Only Nonlinear Elements can have dynamic memory !!! (Hysteresis)

The Brusselator (1970s)
Prigogine, Nicolis, Lefever

$$A \to X$$
$$2X + Y \to 3X$$
$$B + X \to Y + D$$
$$X \to E$$

$$\frac{dX}{dt} = A + X^2Y - (B+1)X$$

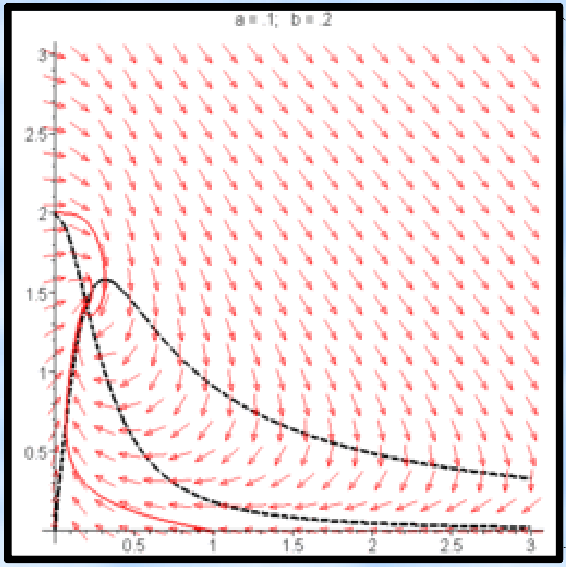
$$\frac{dY}{dt} = BX - X^2Y.$$

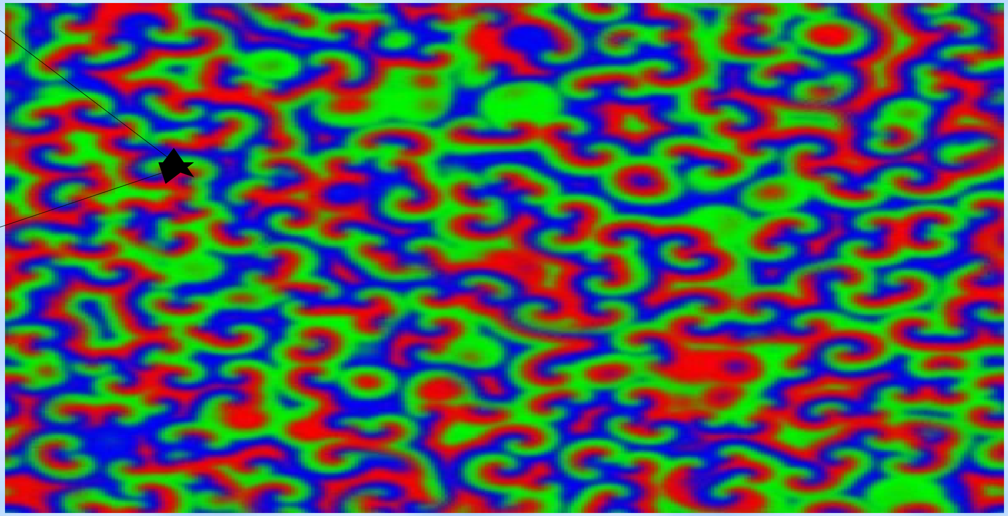
Dissipative Structures

Constructive Role of Fluctuations & Chaos

Self-reference & Nonlinear Feedback

Auto-catalytic reactions Pattern Formation





Feedback Circuits, Cycles, Chaos & Logic

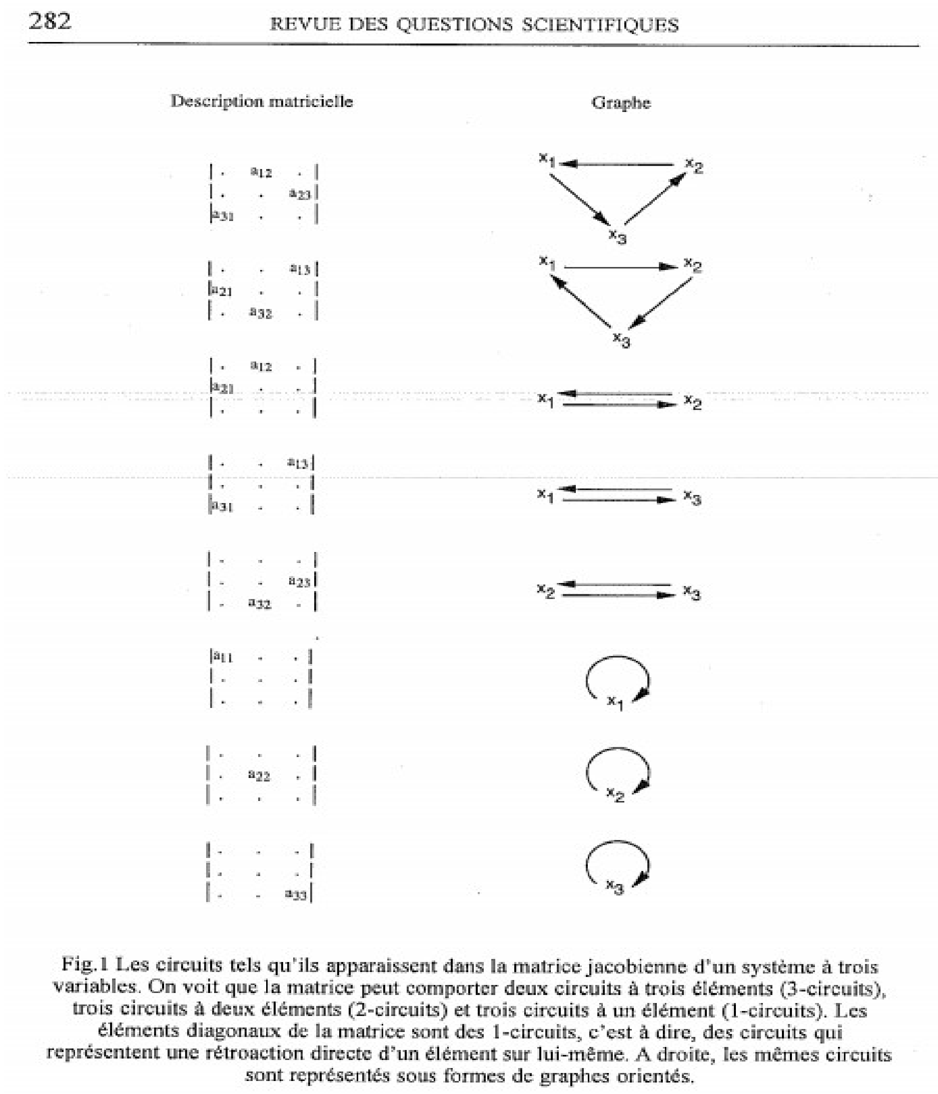
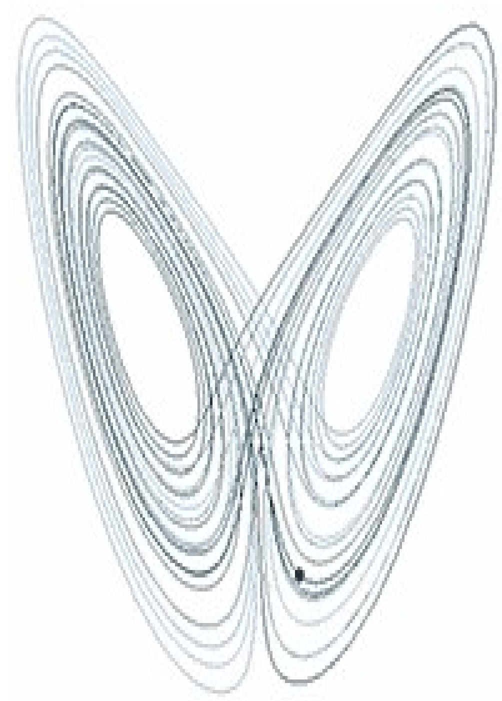
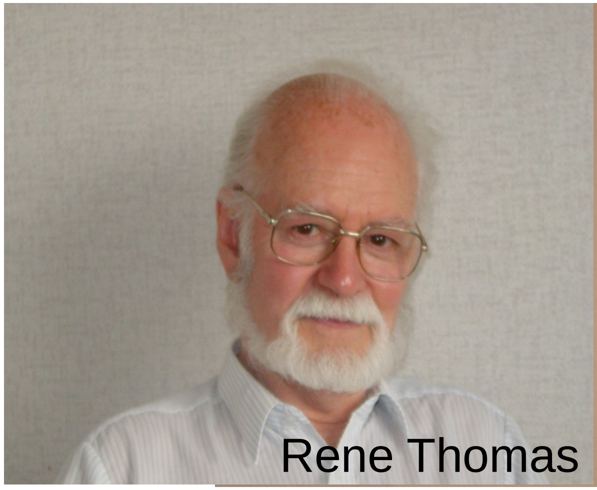


Fig. 1 Les circuits tels qu'ils apparaissent dans la matrice jacobienne d'un système à trois variables. On voit que la matrice peut comporter deux circuits à trois éléments (3-circuits), trois circuits à deux éléments (2-circuits) et trois circuits à un élément (1-circuits). Les éléments diagonaux de la matrice sont des 1-circuits, c'est à dire, des circuits qui représentent une rétroaction directe d'un élément sur lui-même. A droite, les mêmes circuits sont représentés sous formes de graphes orientés.

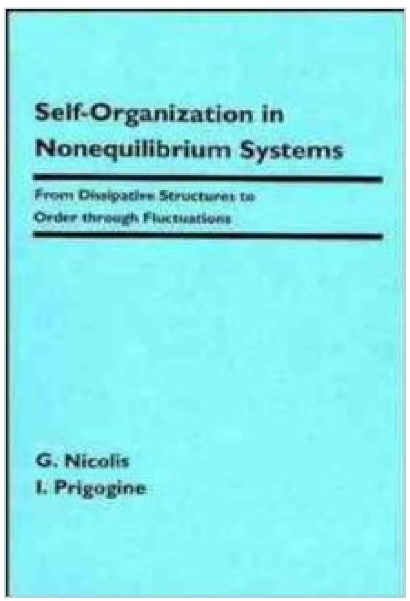


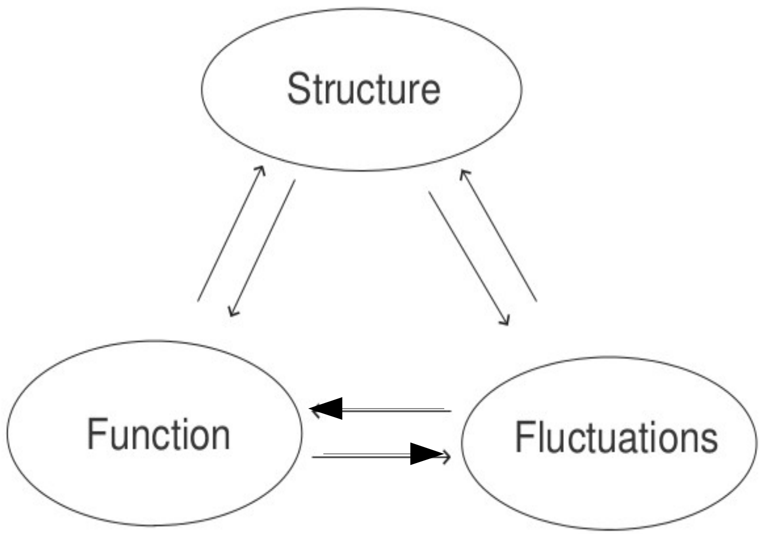


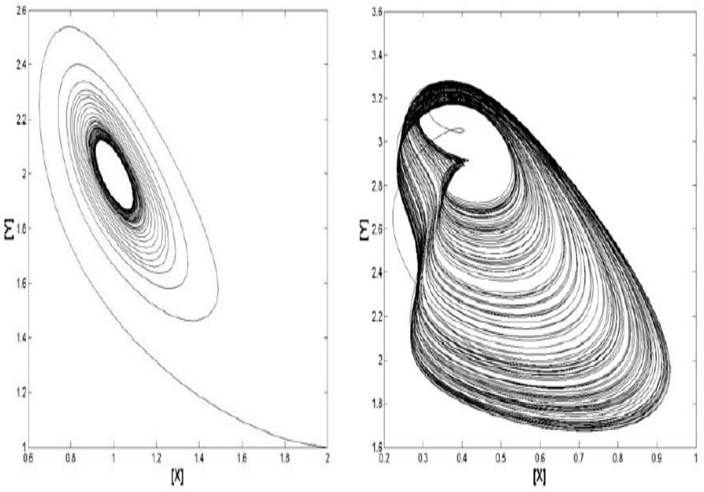
Int. J. of Bifurcation and Chaos **23**:09.(2013)

“...The fluctuations involved are not fluctuations in concentrations or other macroscopic parameters but fluctuations in the mechanisms leading to modifications of the [kinetic] equations...”

G. Nicolis and I. Prigogine







in: **“Self-Organization in Nonequilibrium Systems:**
From Dissipative Structures to Order through Fluctuations”
discussing auto-catalytic reactions and Manfred Eigen's “hypercycles”

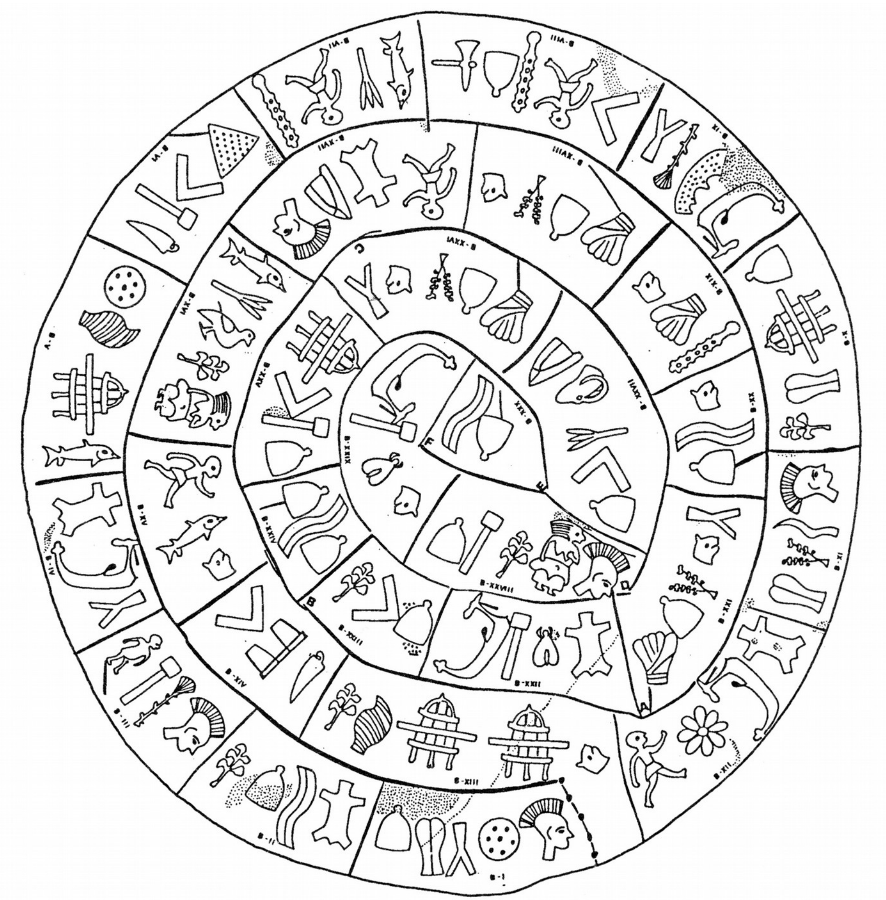
Complexity Science

Nonlinear dynamics and chaos theory,

Thermodynamics and statistical physics,

Information and probability theories,

Numerical simulation and techniques from data analysis.



Non (-) equilibrium or Nonequilibrium?

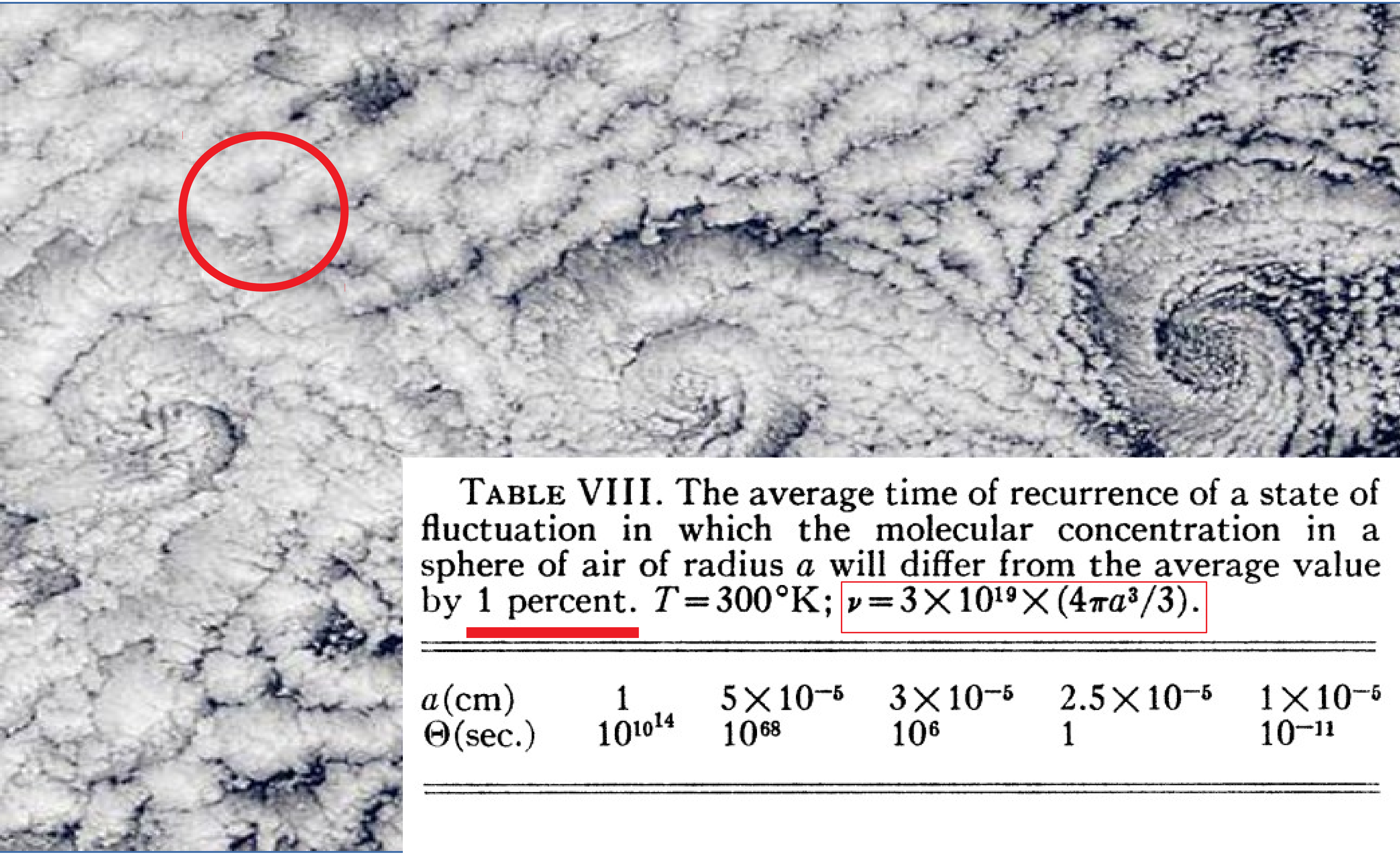


TABLE VIII. The average time of recurrence of a state of fluctuation in which the molecular concentration in a sphere of air of radius a will differ from the average value by 1 percent. $T=300°K$; $\nu=3\times10^{19}\times(4\pi a^3/3)$.

a(cm)	1	5×10^{-5}	3×10^{-5}	2.5×10^{-5}	1×10^{-5}
Θ(sec.)	$10^{10^{14}}$	10^{68}	10^{6}	1	10^{-11}

sider, following Smoluchowski, the average time

Matter is Active: self-organization, rhythms and dynamics

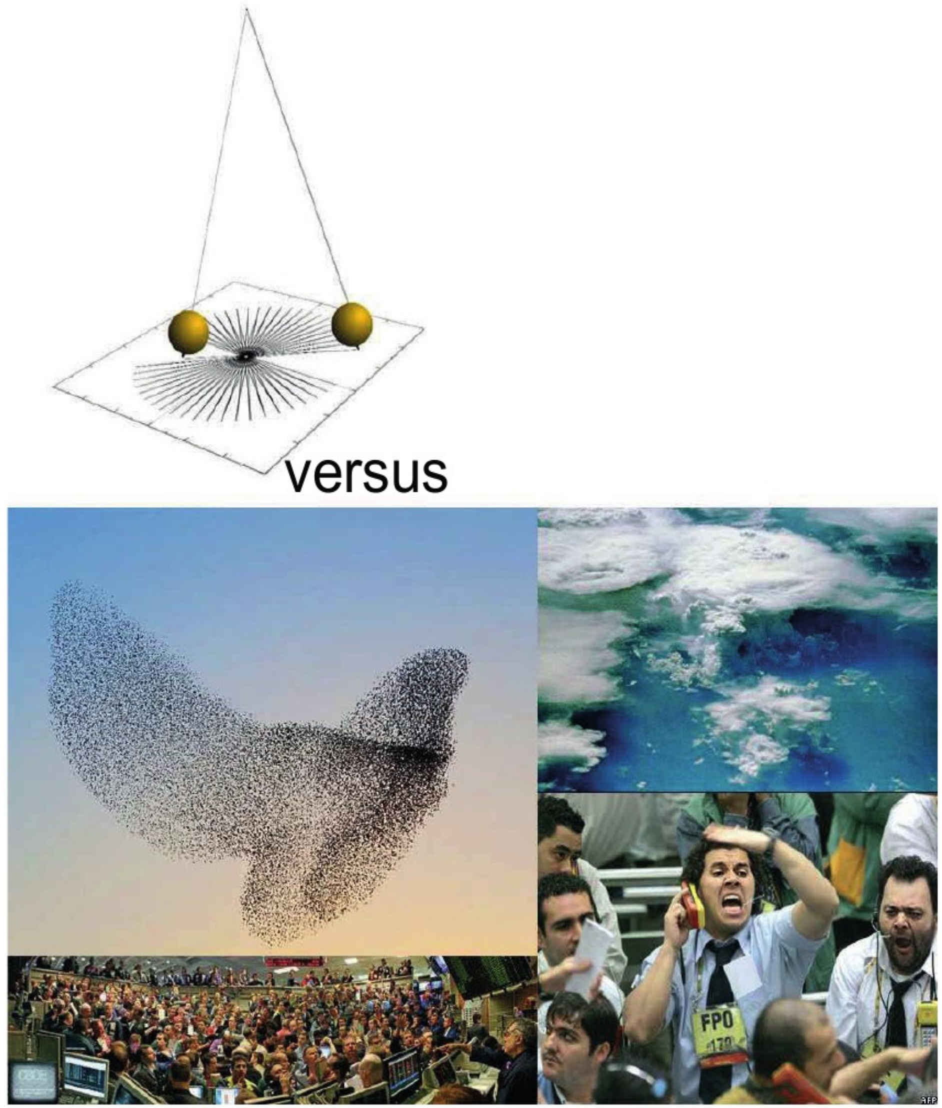
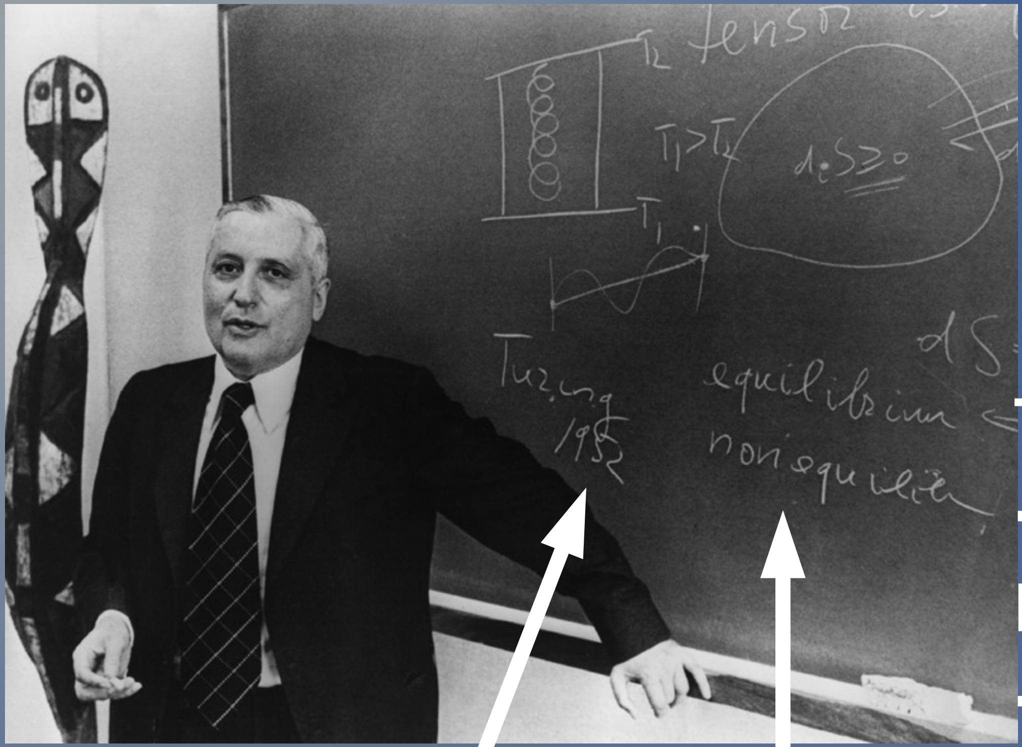
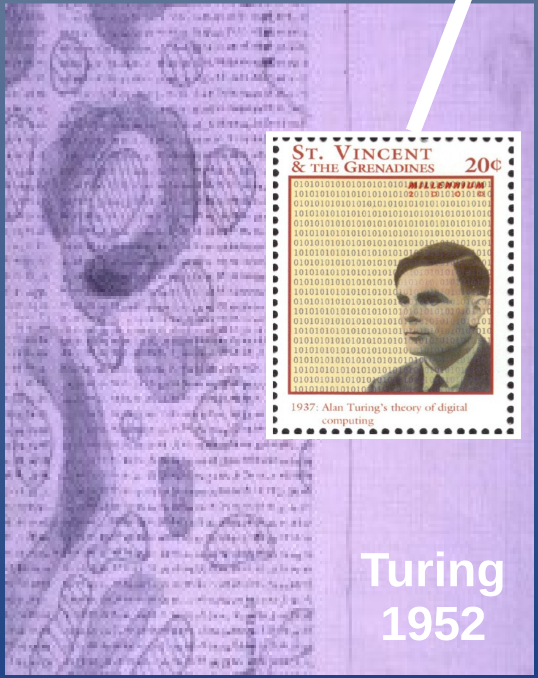


Fig. 1. Upper part: Simple pendulum. Lower part: Three manifestations of Complexity in everyday experience. Clockwise Bird flocking, the earth-atmosphere system, trading in the stock market.





!

Prigogine Nicolis & Lefever (Nobel 1979)

Turing's Morphogenesis

+

Entropy Production Theorem

+

Fluctuation Dissipation Theorem

=

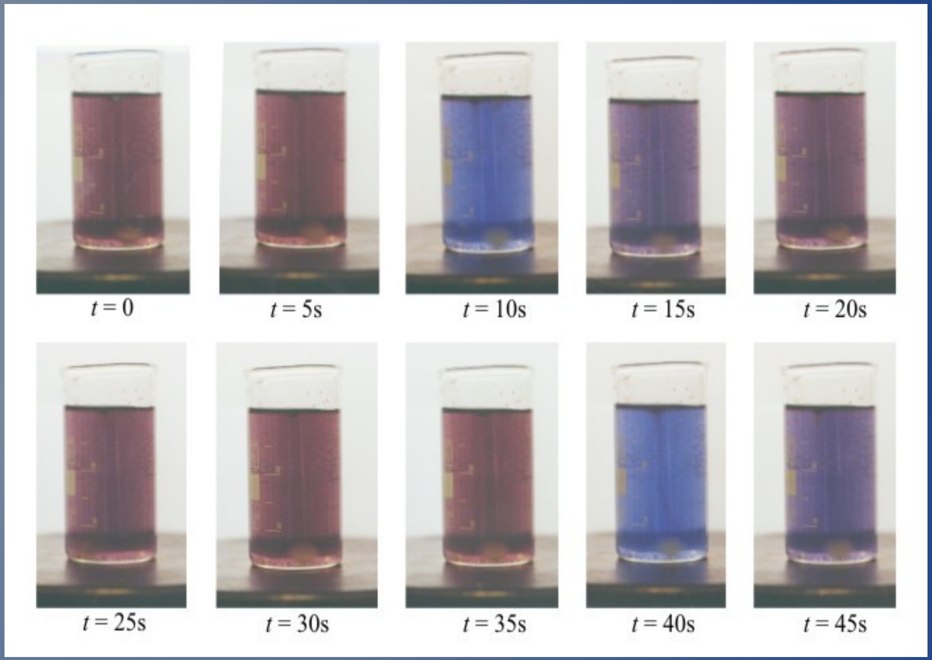
Dissipative Structures

+

Self-Organization & Pattern Formation

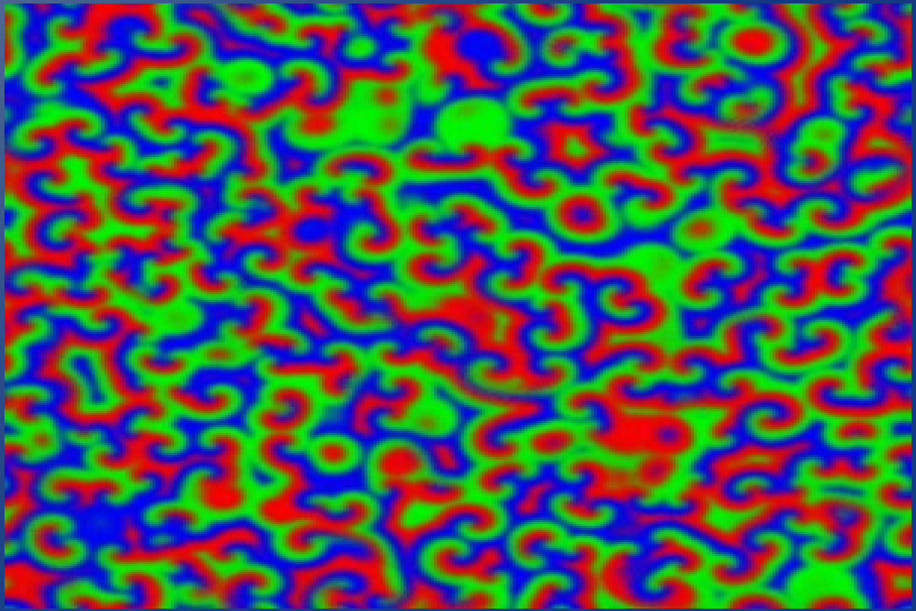
Boris Pavlovich Belousov

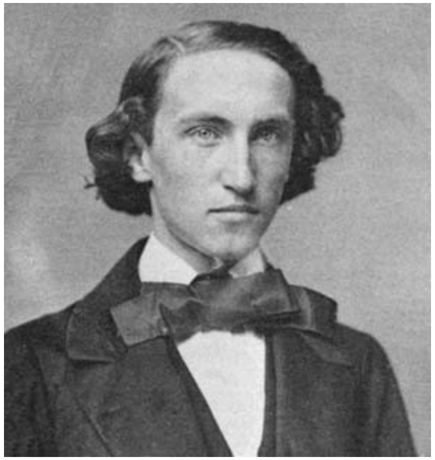
1893 – 1970



Anatol Markovich Zhabotinsky

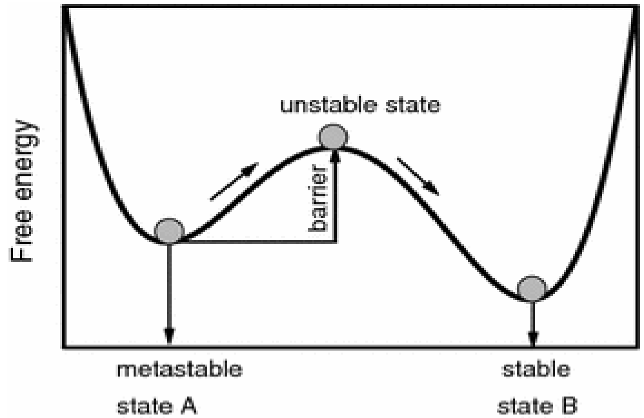
1938 – 2008





Josiah Willard Gibbs (1839 - 1903)

stealing an idea from Gibbs to understand nucleation:



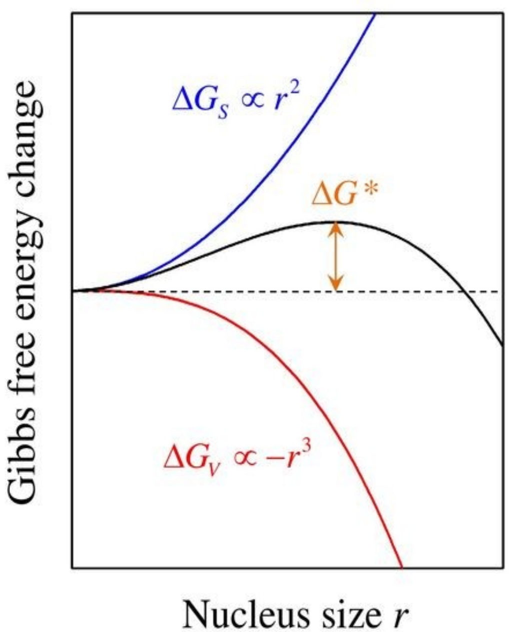
$\Delta G = r(i)\,\Delta G(i) - T\Delta S(r(i))$

$[\, d\Delta G / dr(i) \,] = 0$, at $r = r^*(i)$

Equilibrium Assumption

$N \rightleftharpoons N^* \longrightarrow S$

a)



- Gibbs free energy change of nucleation

$$\Delta G = -\frac{\Delta H_m \Delta T}{T_m}\cdot\frac{4\pi r^3}{3} + 4\pi\gamma r^2$$

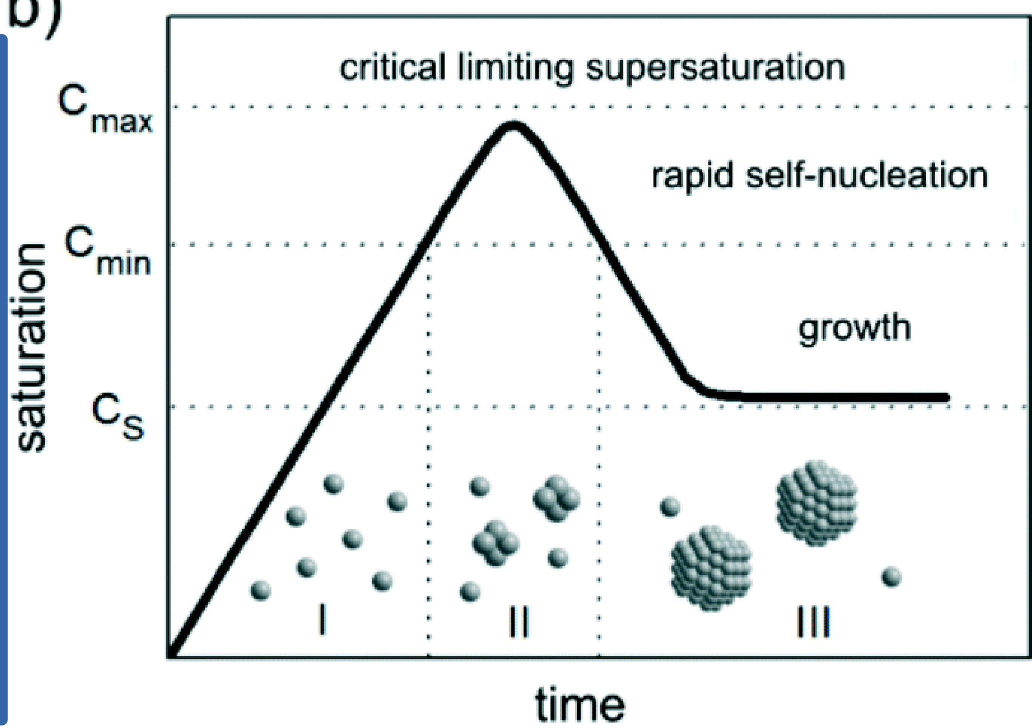
- Critical nucleus size

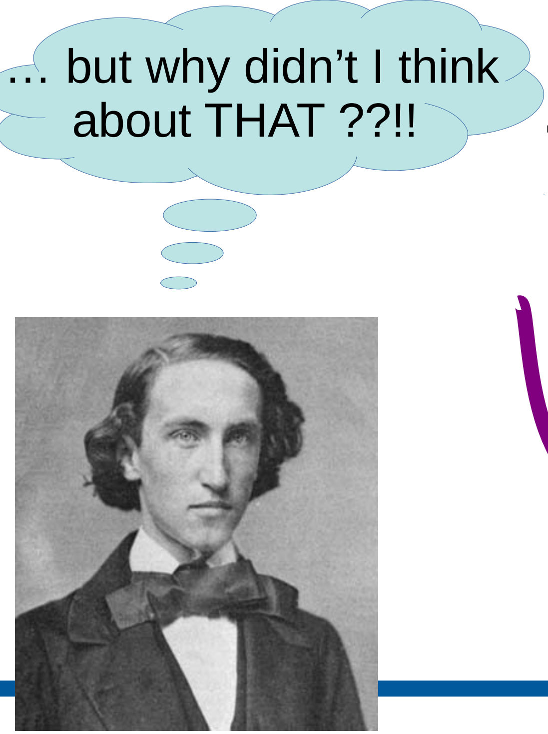
$$r^* = \frac{2\gamma T_m}{\Delta H_m \Delta T}$$

- Energy barrier towards nucleation

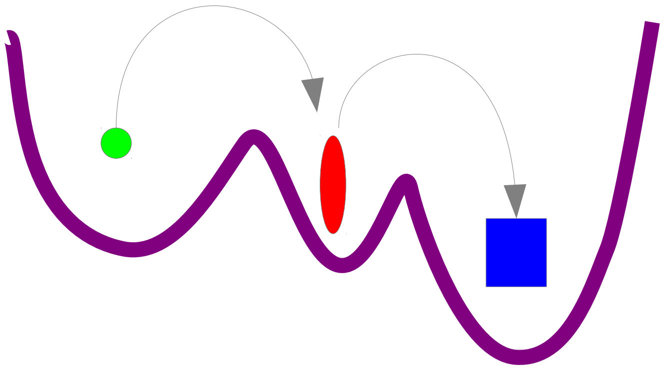
$$\Delta G^* = \frac{16\pi}{3}\cdot\frac{\gamma^3 T_m^2}{\Delta H_m^2 \Delta T^2}$$

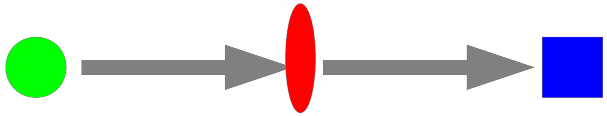
b)



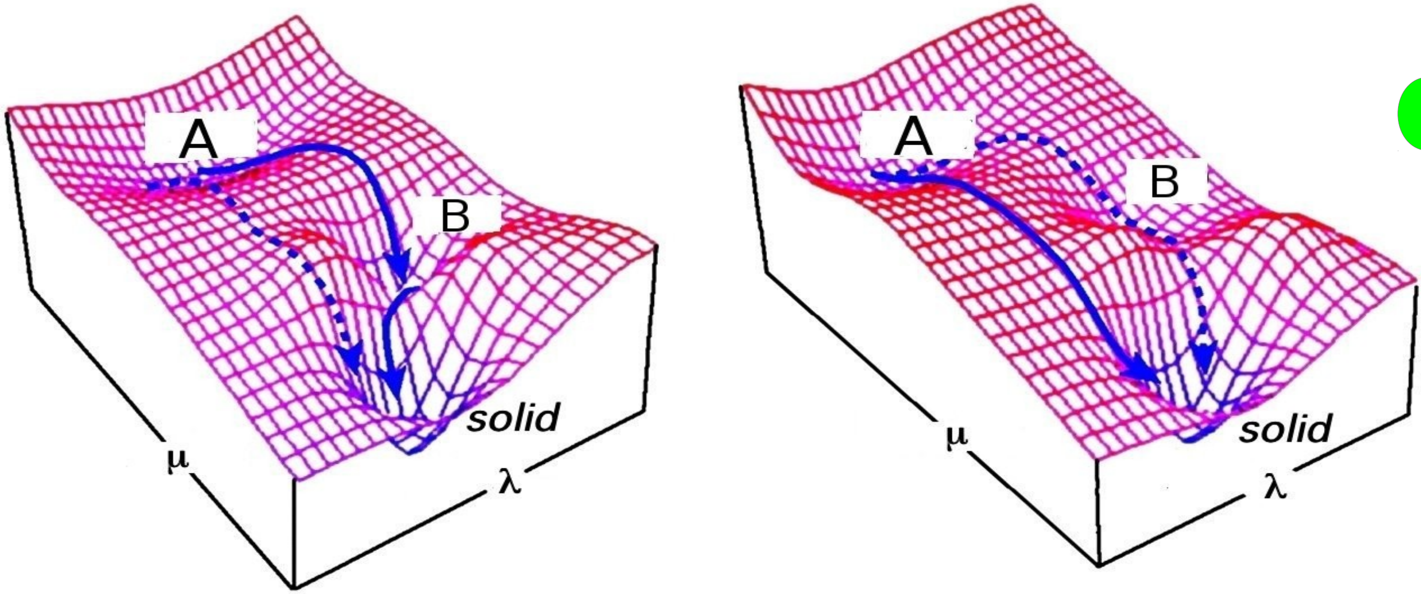


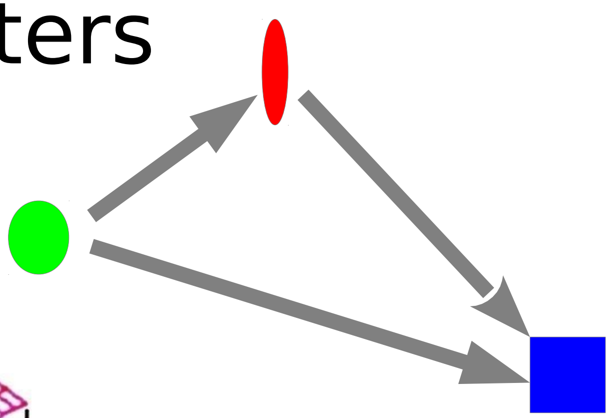
TWO-steps, ONE order-parameter





TWO-steps, TWO order-parameters

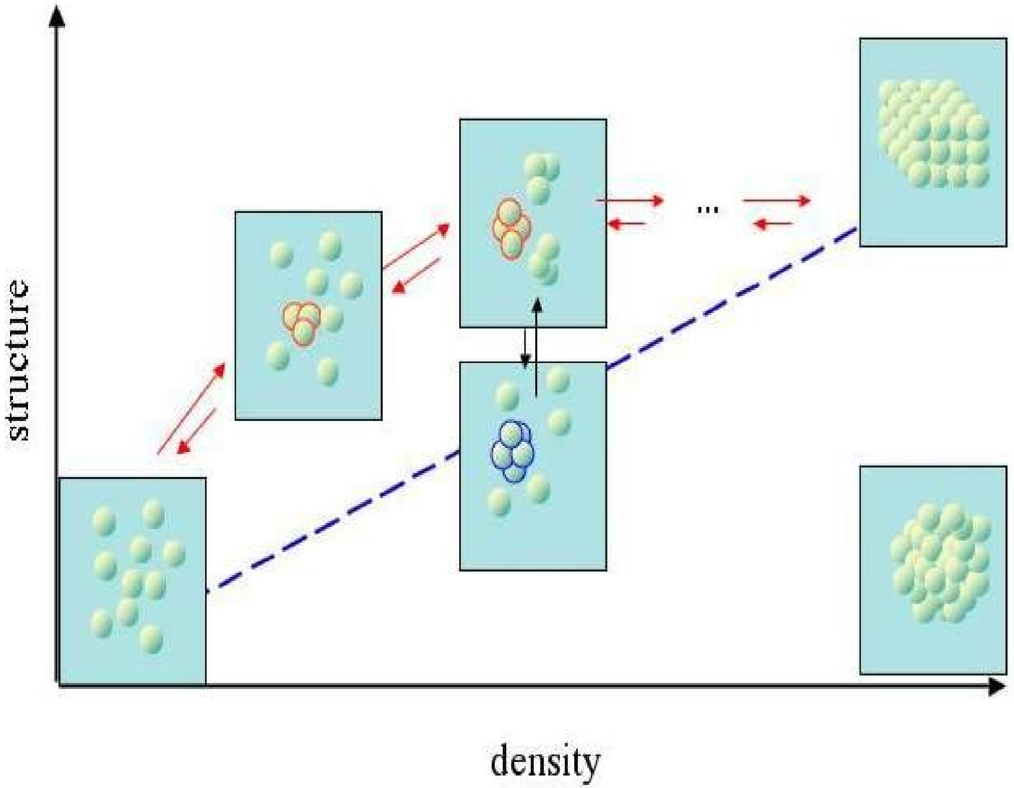




Non standard nucleation mechanisms with combined structural and density fluctuations

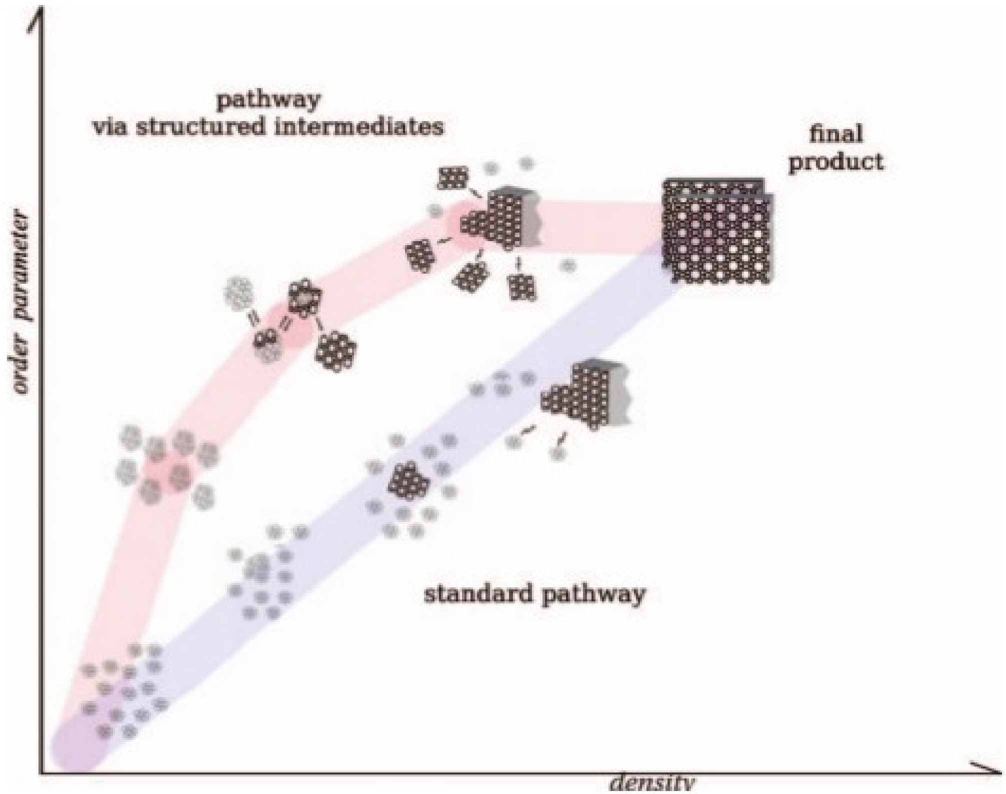
- Importance of kinetic effects arising from the co-existence of competing mechanisms

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



"Nonlinear Dynamics and Self-organization in the Presence of Metastable Phases"
G. Nicolis & C. Nicolis

Hierarchical aggregation of Zeolites:
2nd order parameter = Q4 number of Si bonds



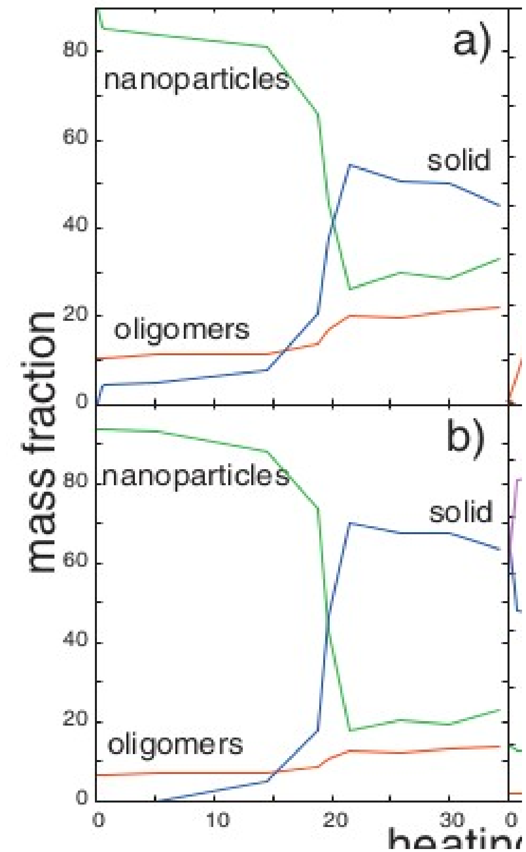
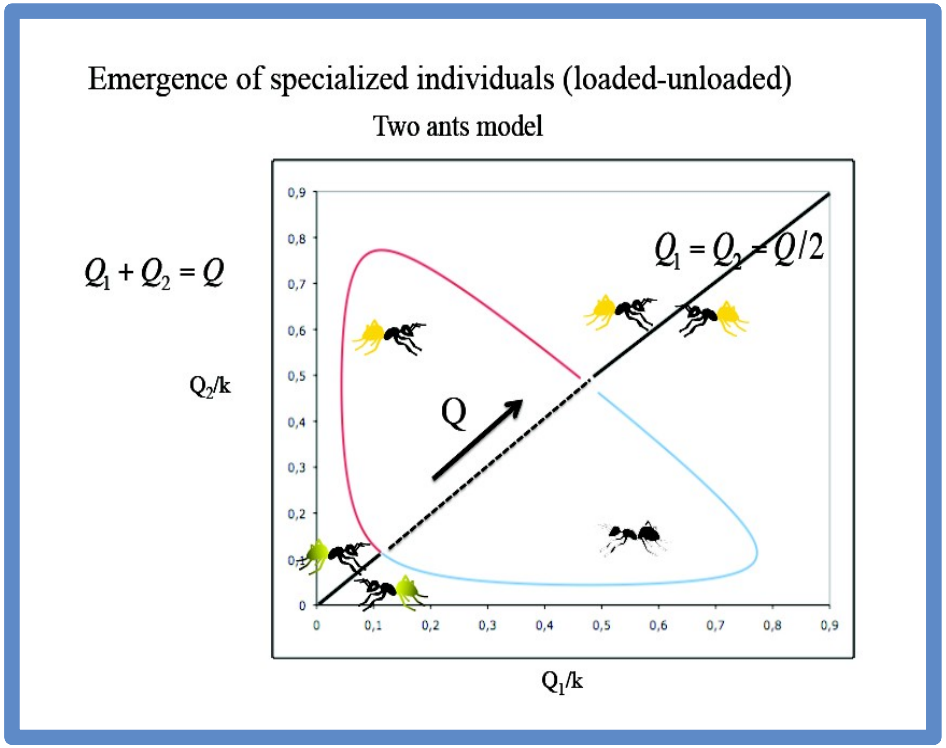
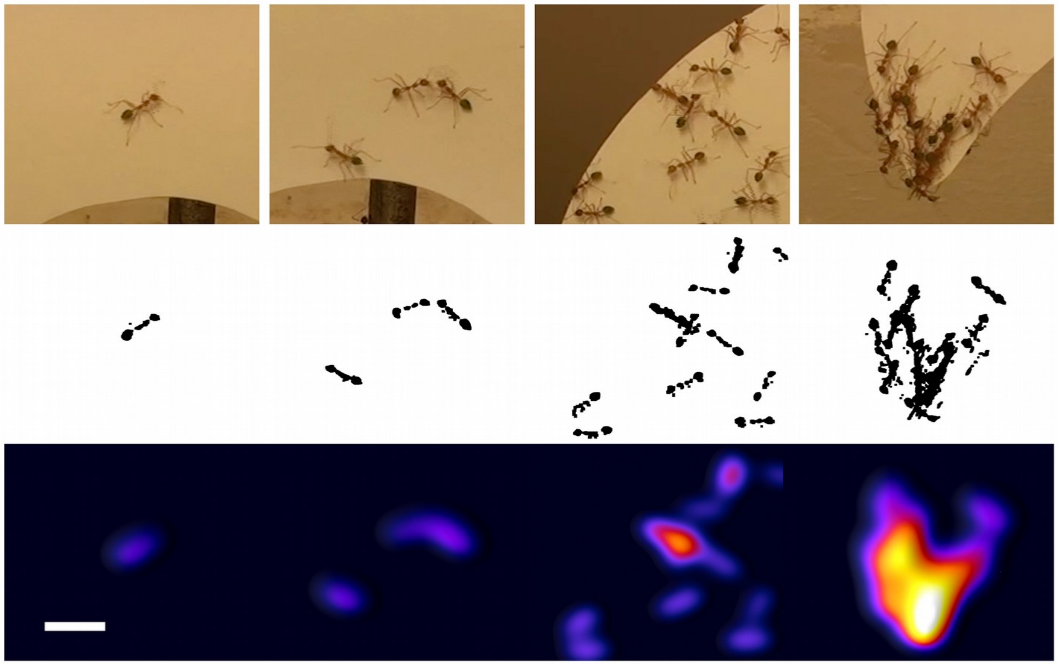


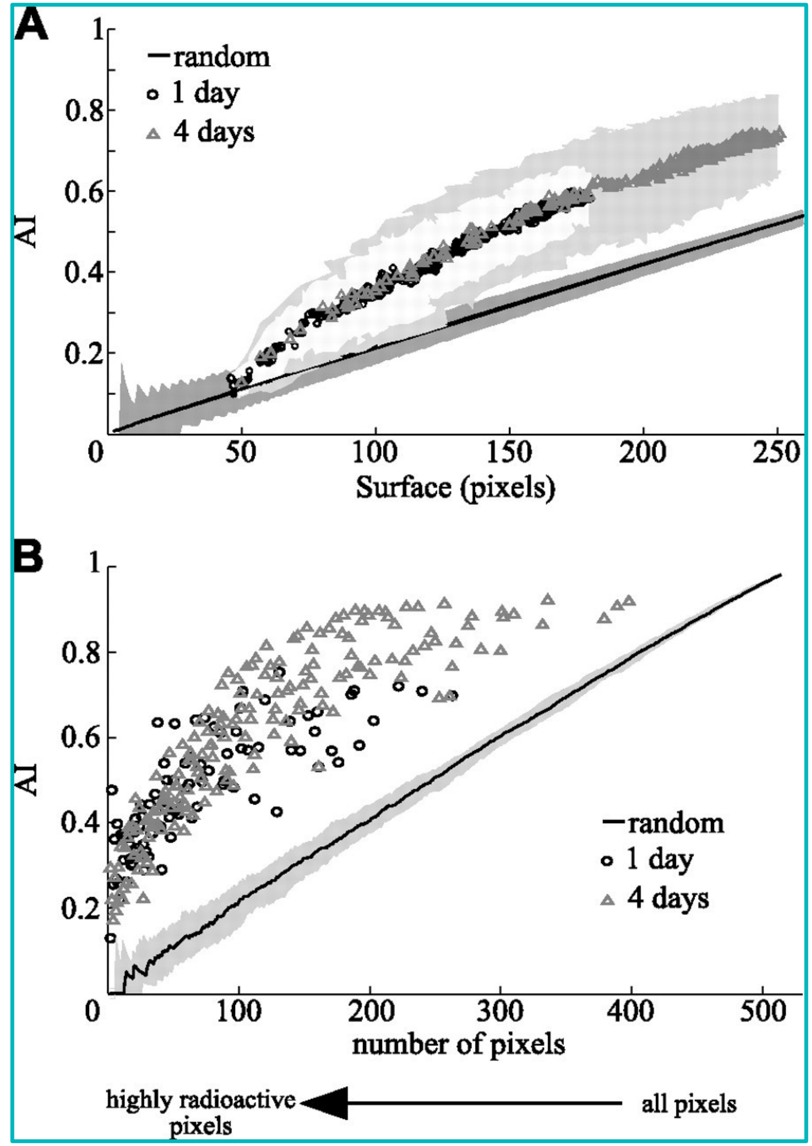
FIG. 1. A schematic demonstration of multistep versus standard synthetic

Trophallaxis Colony's Social Stomach filling up



Hierachical Self-assembly and Phoresis in Biological Communities
(what if … molecules were ants ??? ;-)





Two Step Aggregation: Phoretic Synergetic Carriers as Auto-catalytic Self-replicators

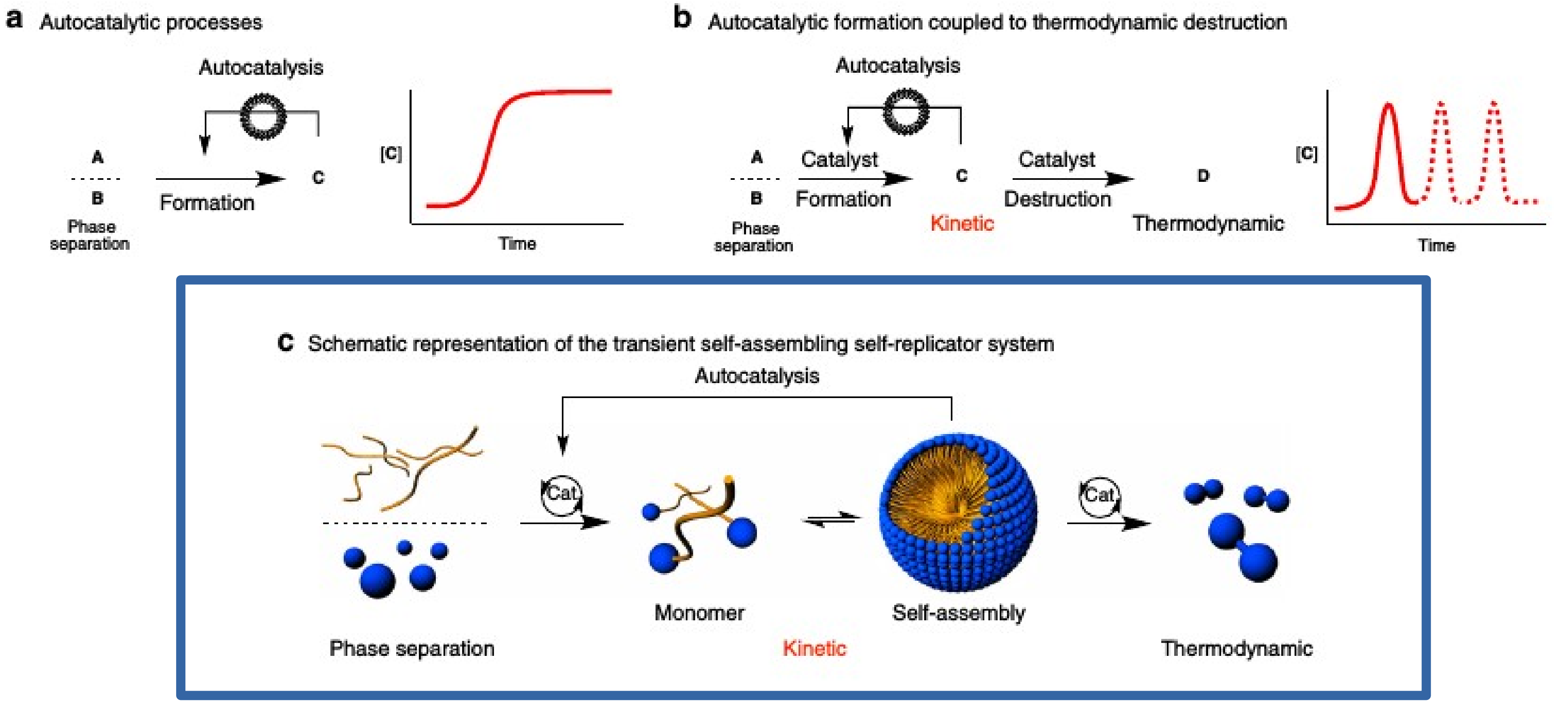
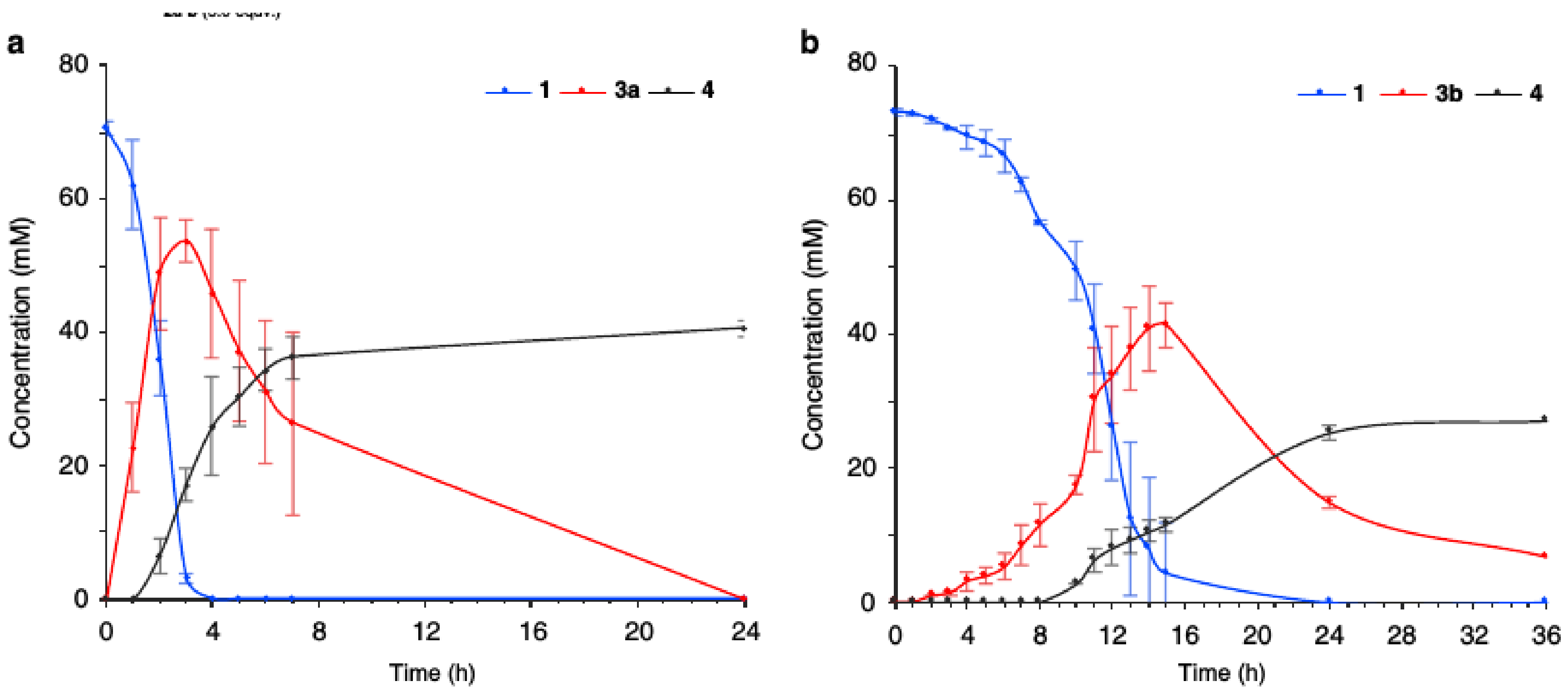


Fig. 1 Examples of autocatalysis. **a** An autocatalytic system based on phase separation. **b** An autocatalytic system based on phase separation, coupled to thermodynamic destruction, that in a closed set-up experiment will evolve towards thermodynamic equilibrium. **c** Schematic representation of a transient self-assembling self-replicator system

Two Step Aggregation: Phoretic Synergetic Carriers as Auto-catalytic Self-replicators



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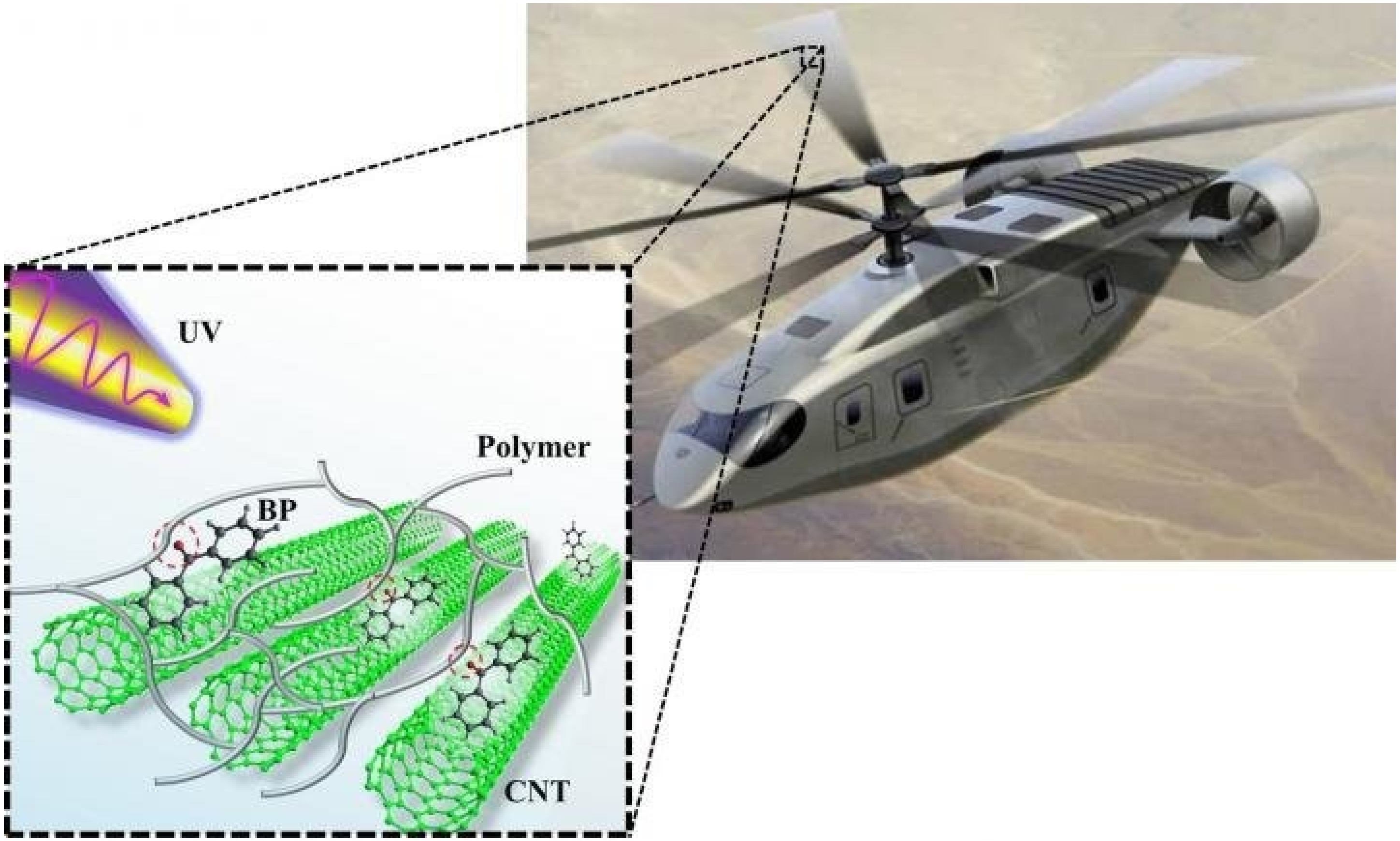
STEM MATERIALS

MISSION

In nature, living organisms consist of a limited number of primary components and chemical bonds, organized in complex systems capable to adapt to diversified environmental conditions. Materials are very rarely adaptable, and often require a large number of components to achieve high performances in specific functions. A comparison between organisms and materials

Matter is Active: self-organizated, adaptive, 'smart', information-rich, materials



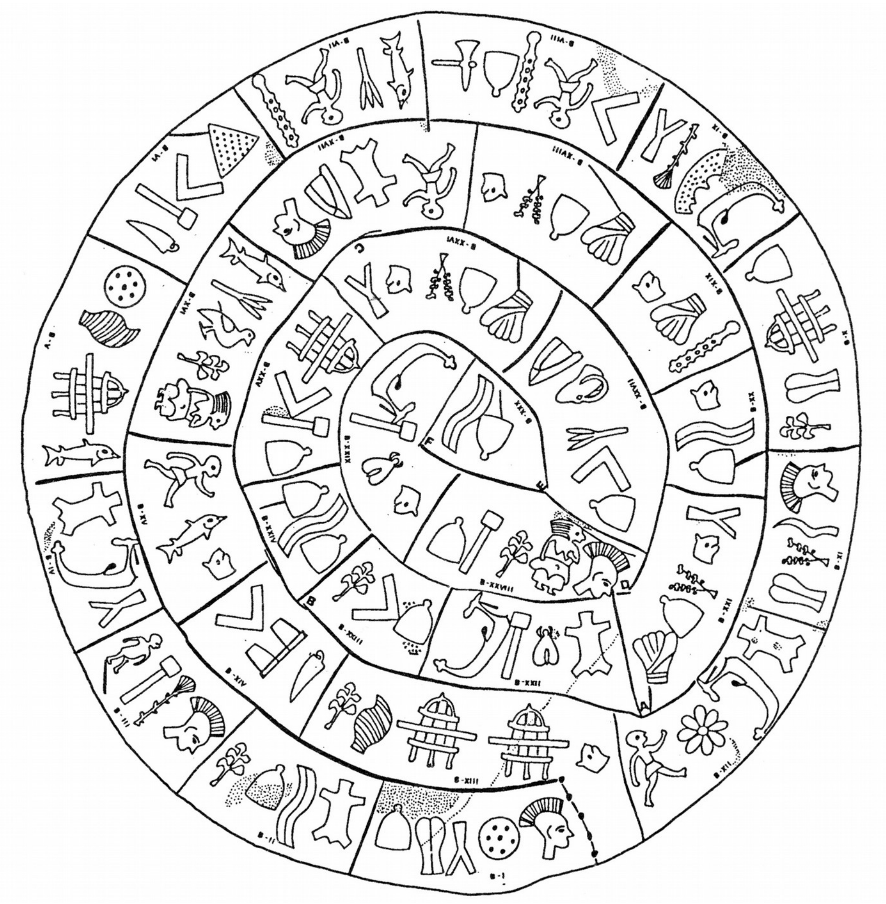
Complexity Science

Nonlinear dynamics and chaos theory,

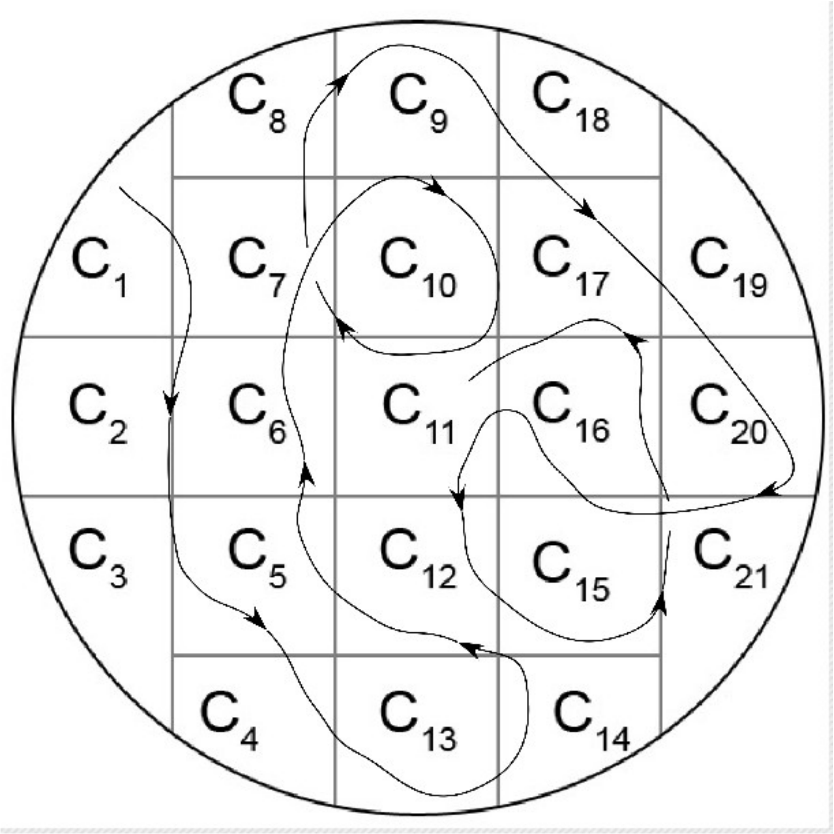
Thermodynamics and statistical physics,

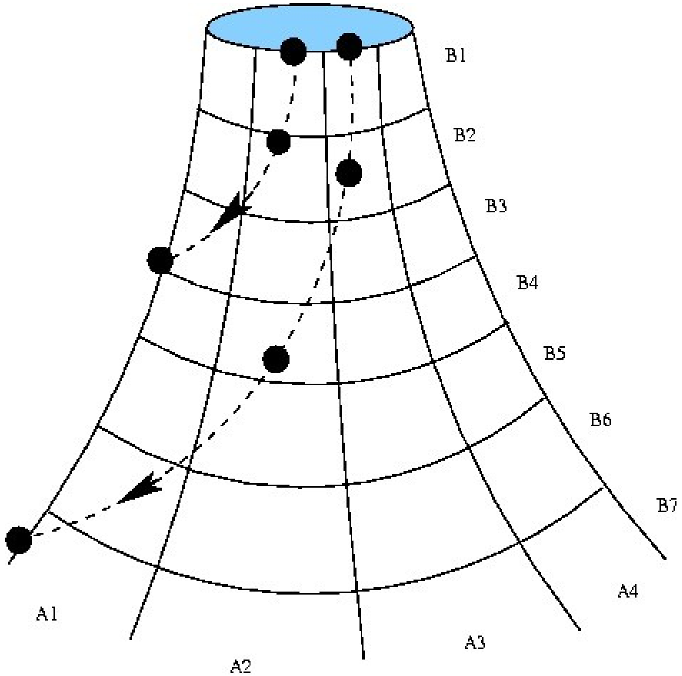
Information and probability theories,

Numerical simulation and techniques from data analysis.



“Coarse Graining”
“Symbolic Dynamics”





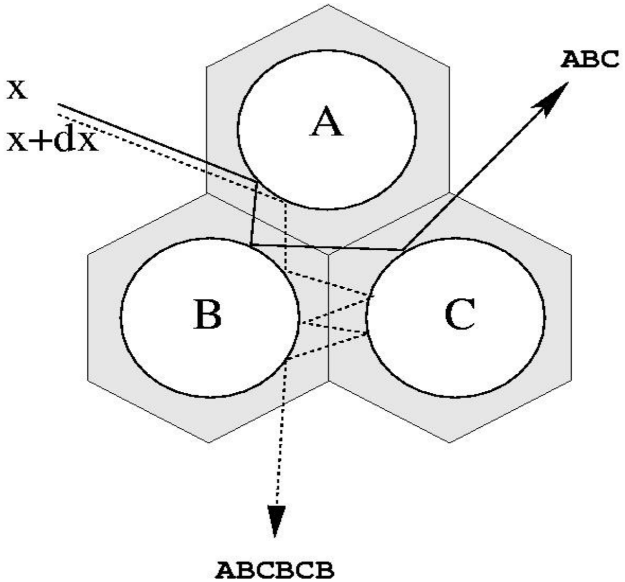
Poincaré (1890s) & Maxwell:
Nonlinear dynamical systems can exhibit sensitive dependence on initial conditions

Hadamard (1898):
motion on negative curvature is sensitive to initial conditions

Artin, Heldund and Hopf: the motion on a surface of constant negative curvature is ergodic.

Krylov: A physical billiard is a system with negative curvature, along the lines of collision

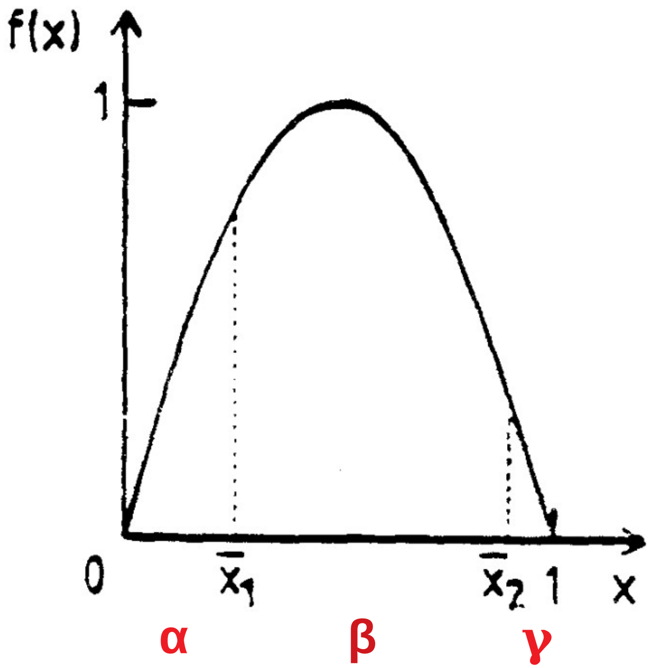
Sinai: a physical billiard can be ergodic.



J. Stat. Phys. 54,3/4, **1989**

"Chaotic Dynamics, Markov Partitions,& Zipf's Law"

G. Nicolis, C. Nicolis, J.S. Nicolis



$$x_{n+1} = 4x_n(1 - x_n), \qquad 0 \leqslant x \leqslant 1$$

period-two orbit $\bar{x}_1 \simeq 0.345$, $\bar{x}_2 \simeq 0.905$

$$W = \begin{pmatrix} 1/2 & 1/2 & 0 \\ 0 & 1/2 & 1/2 \\ 1 & 0 & 0 \end{pmatrix}$$

W_{21} **=** P(α → β)
… &c.

$$P_{n+1}(i) = \sum_{j=1}^{N} W_{ji} P_n(j), \qquad i = 1,\ldots, N$$

ααβγαββααγβαββγβαββαααββαβααβββαγααββγγβαβγ … &c.

The **Shannon Block Entropy** of the partition is :

$$H(m) = - \sum_{\text{all } m\text{-words}} P(w) \ln P(w)$$

where $P(w)$ is the probability of occurrence of each word, w, of length m

"The key is to realize that uncertainty represents potential information"
(David Applebaum)

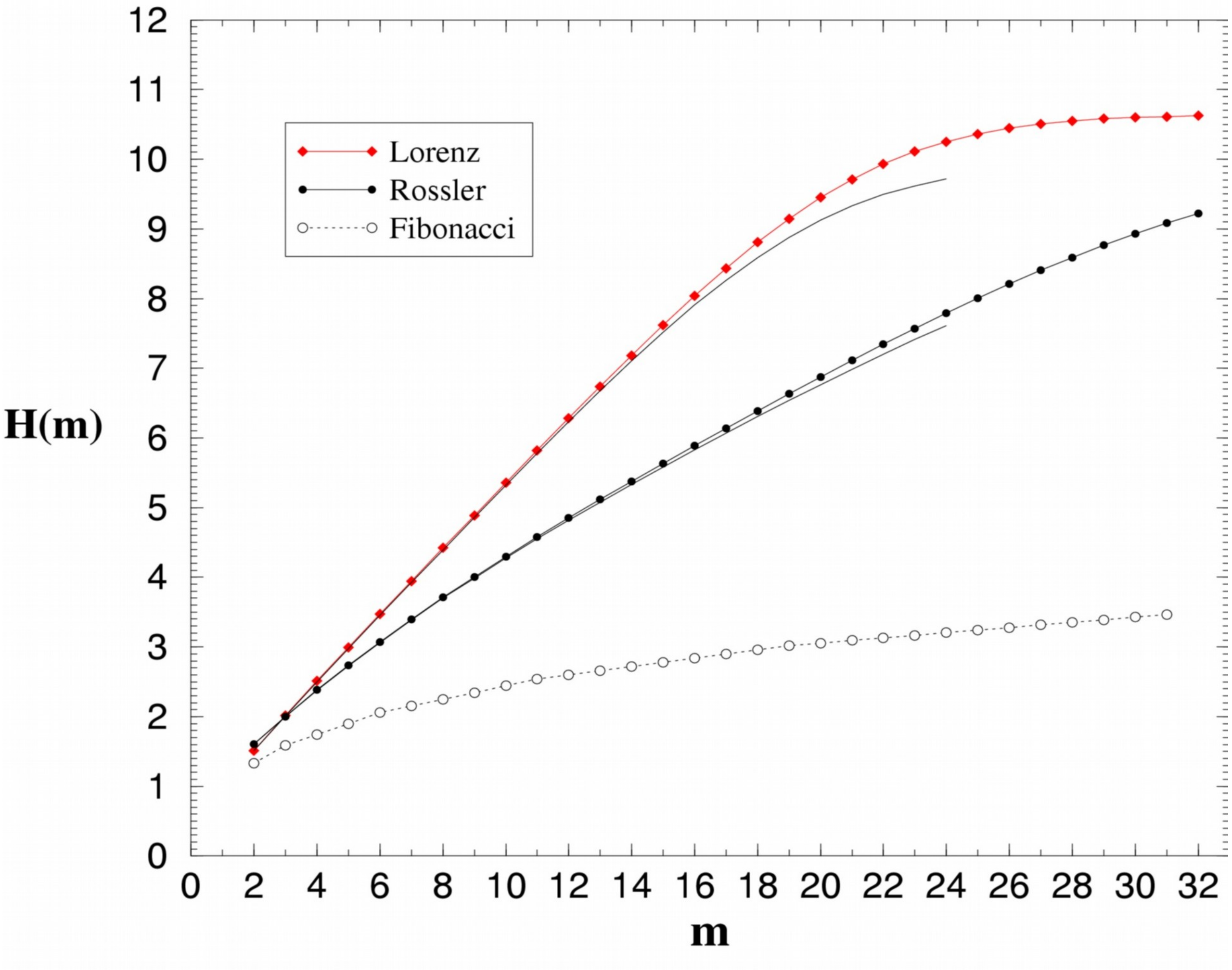
Shannon-McMillan Theorem :
The probability of a word of length m to appear
is "penalized" according to Entropy scaling w.r.t. its length

$$P[w(n)] \approx e^{-H(m)}$$

A Conjecture by Ebeling and Nicolis

In the course of their analysis of symbol sequences they proposed a general scaling law for the block entropy.

$$H_m = mh + gm^{\mu}\left(\log m\right)^{\nu} + e$$



$$H = hm$$

$$H = gm^{\mu}$$

$$H = \log(m)$$

- A. Provata and Y. Almirantis, **Statistical dynamics of clustering in the genome structure,** J. Stat. Phys. 106, 23-56 (2002).

- Y. Almirantis and A. Provata, **Long- and Short-Range Correlations in Genome Organization**, Journal of Statistical Physics, Vol. 97, Nos. 12, 1999

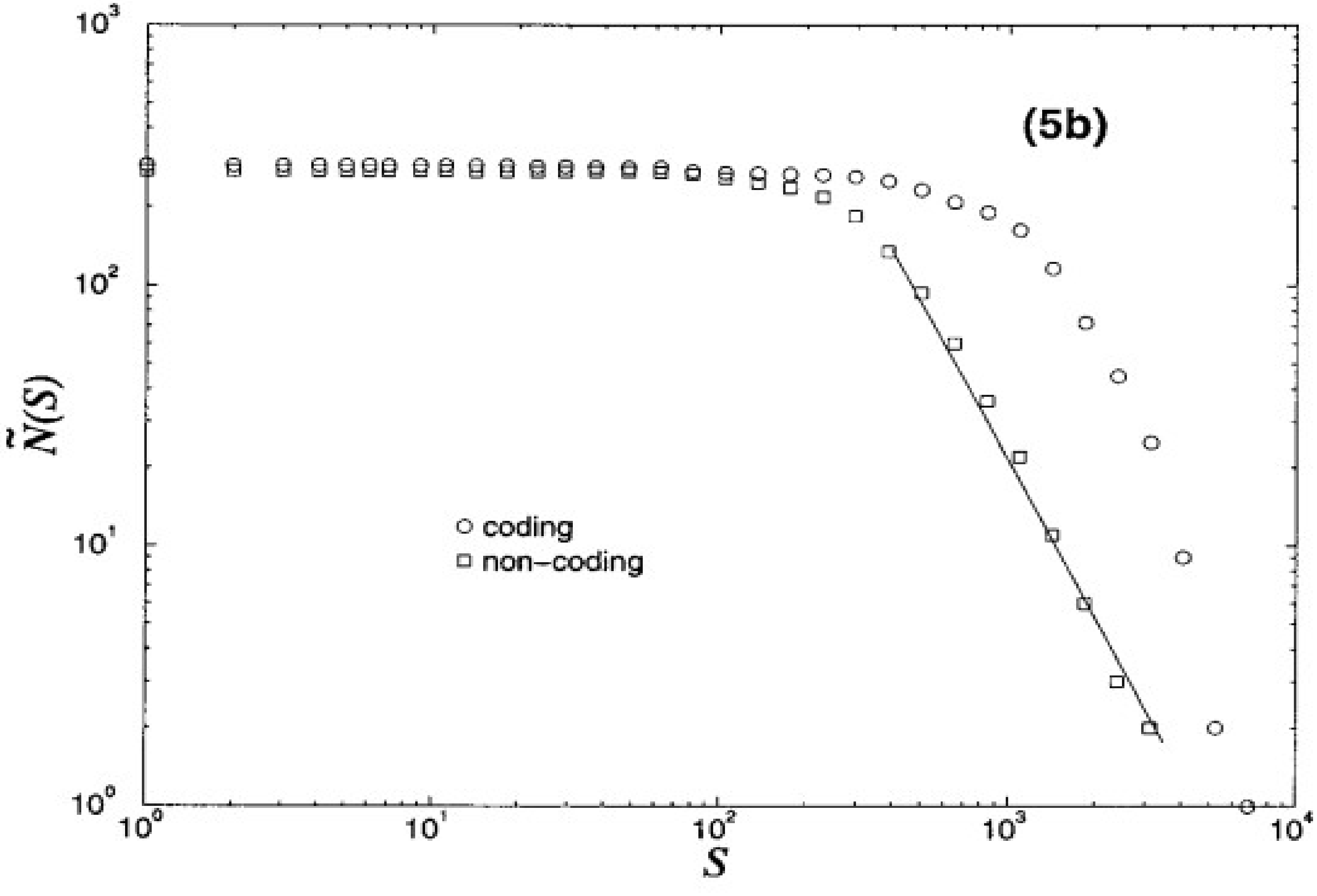
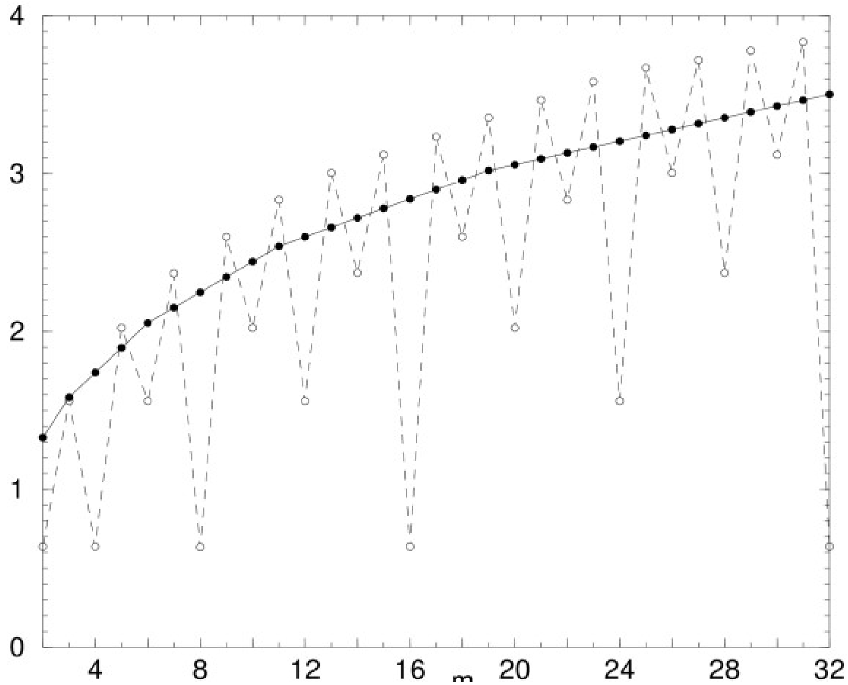


Fig. 5. The number of coding and non-coding regions of size $\geqslant S$, $\tilde{N}(S)$, for three fungal DNA sequences. The straight lines have the following slopes: (5a) $-\mu = -0.8$, (5b) $-\mu = -1.8$ and (5c) $-\mu = -1.3$.



META-SELECTION RULES:

Syntax, Context & Semantics

“We are no where”

“We are now here”

AUTOMATICITY & context:
K. Karamanos and G. Nicolis,
"Symbolic dynamics and entropy analysis of Feigenbaum limit sets",
Chaos, Solitons & Fractals 10(7), 1135-1150 (1999).

META-SELECTION RULES, context & the 'Nicolis-Ebeling Conjecture':

Vasileios Basios, Gian-Luigi Forti qnd Gregoire Nicolis
“Symbolic Dynamics Generated By A Combination Of Graphs”
Int. J. of Bifurcation and Chaos vol. 18, no. 08, pp. 2265-2274 (2008)

Complexity Science

Nonlinear dynamics and chaos theory,

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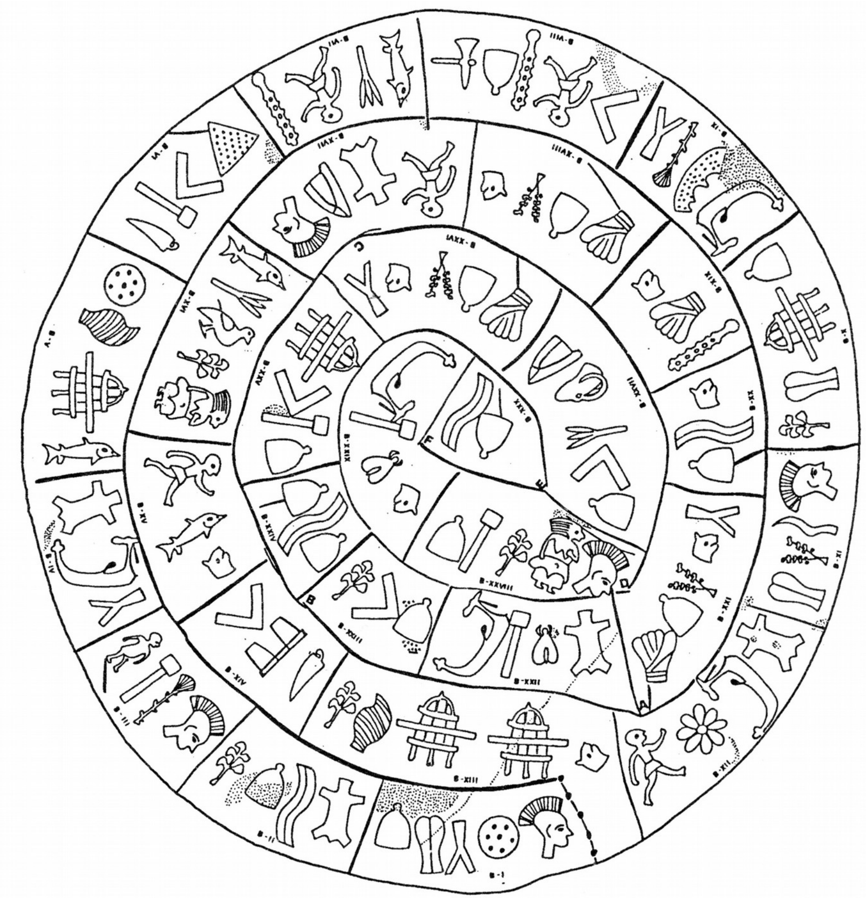
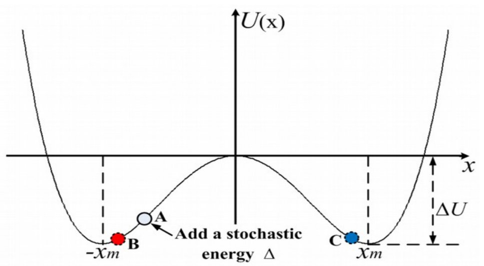


Stochastic Resonance
'Scholarpedia.org' by G. & C. Nicolis

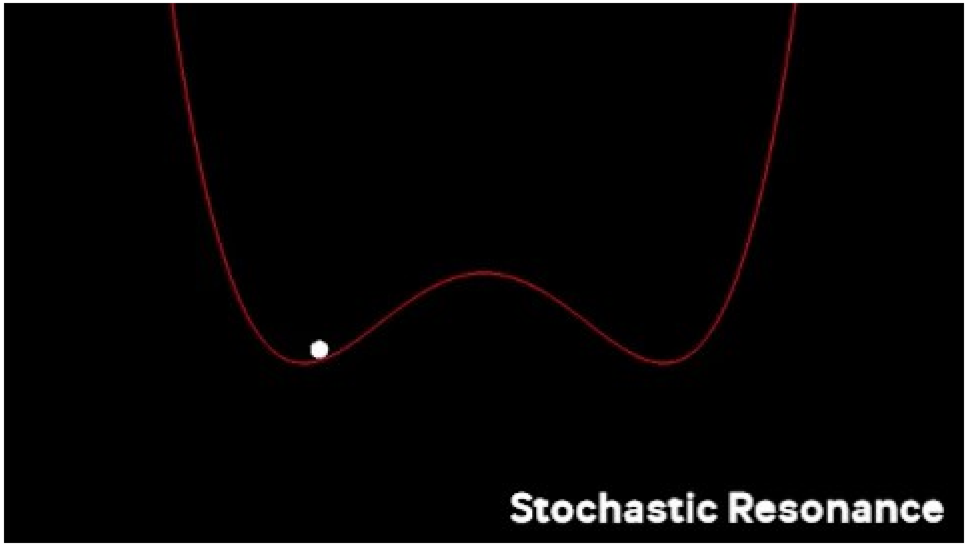
$$\frac{dx}{dt} = -\frac{\partial U}{\partial x} + F(t) + \epsilon h(x)\cos(\omega_0 t + \phi)$$

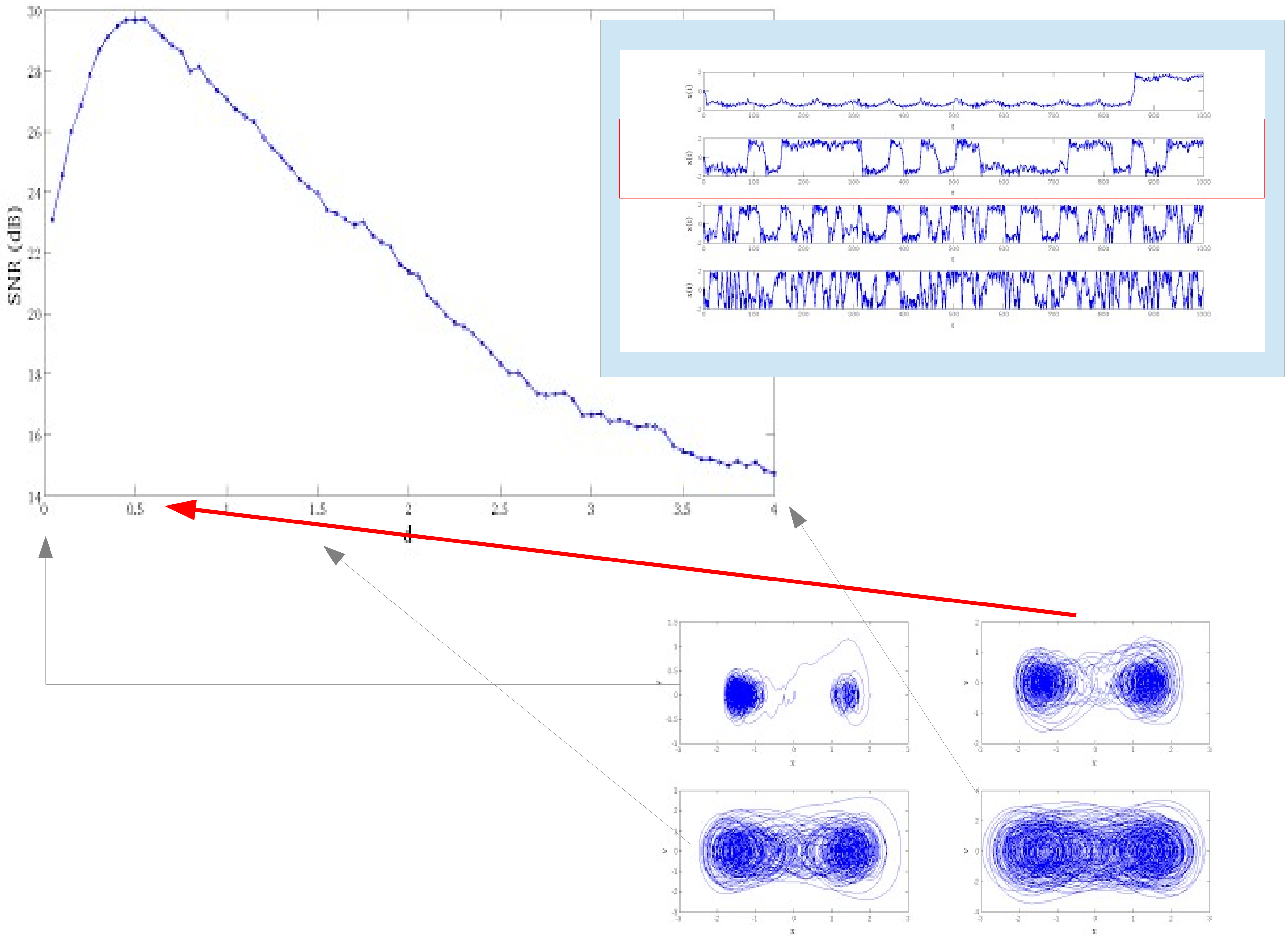
$$U(x) = -\lambda \frac{x^2}{2} + \frac{x^4}{4} \qquad (\lambda > 0)$$



$$W(x,t) = U(x) - \epsilon g(x)\cos(\omega_0 t + \phi)$$

with $dg(x)/dx = h(x)$.

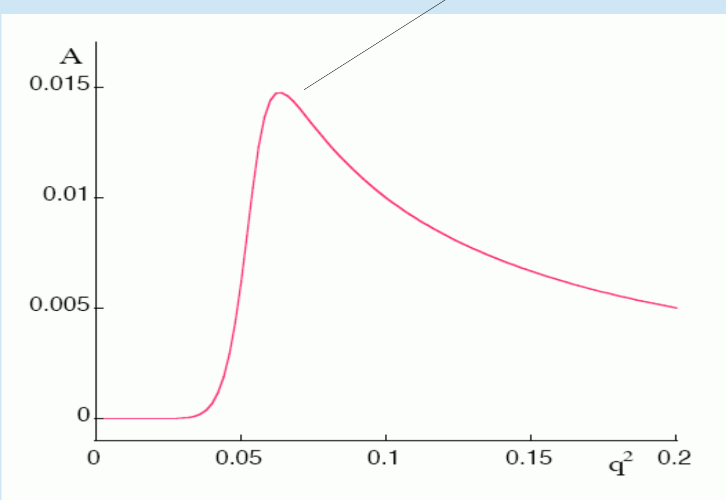




SNR (dB)
d

Stochastic Resonance

… when noise does not destroy but enhances the signal !



Extremely important for

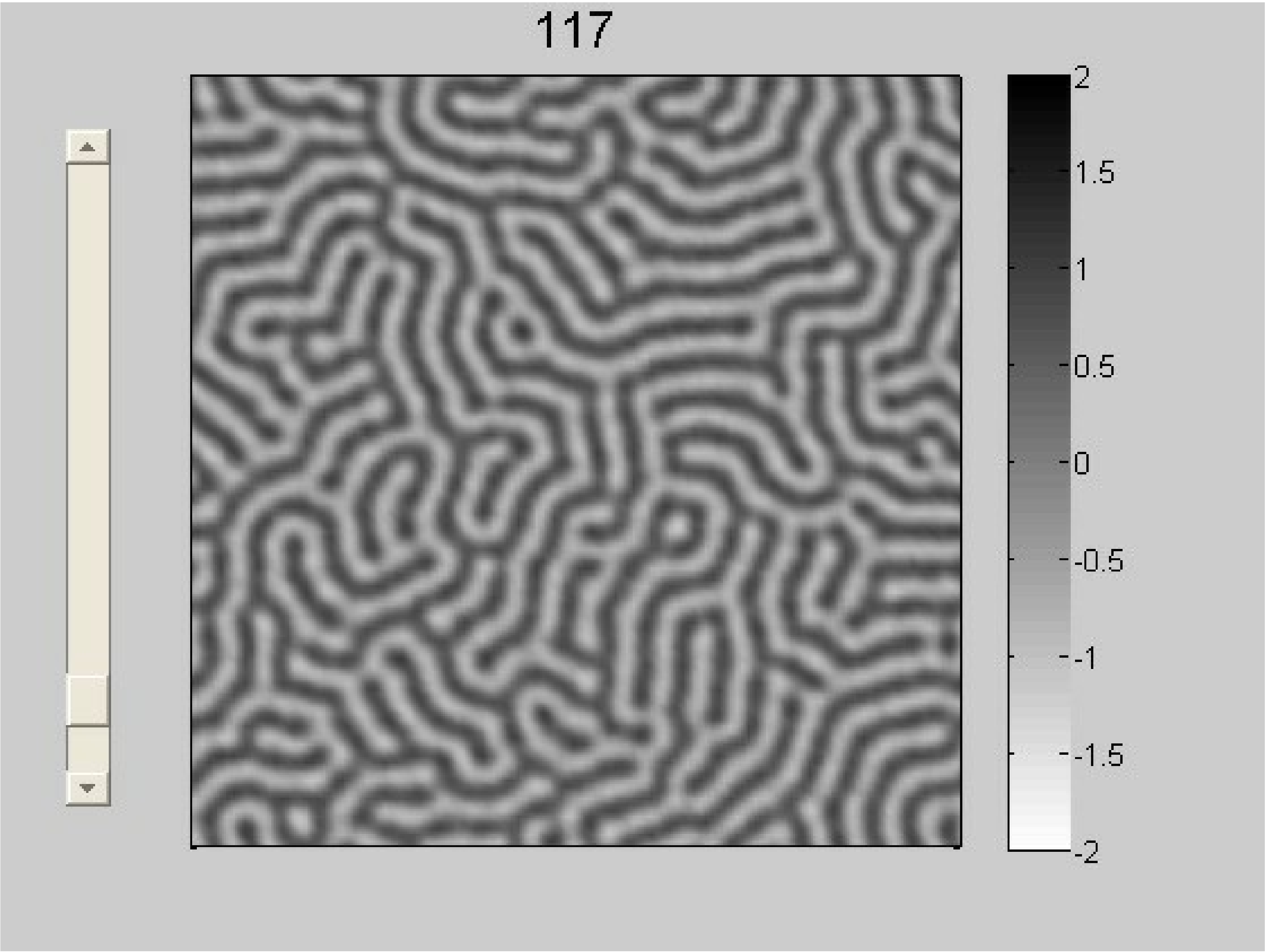
Image Processing,

Sensory Information Processing,

Decision Making,

Pattern Formation

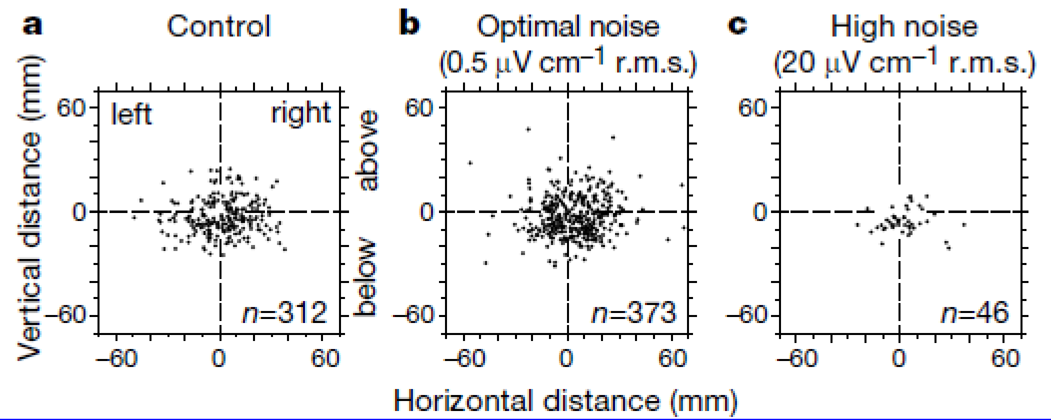
Stochastic Switching …

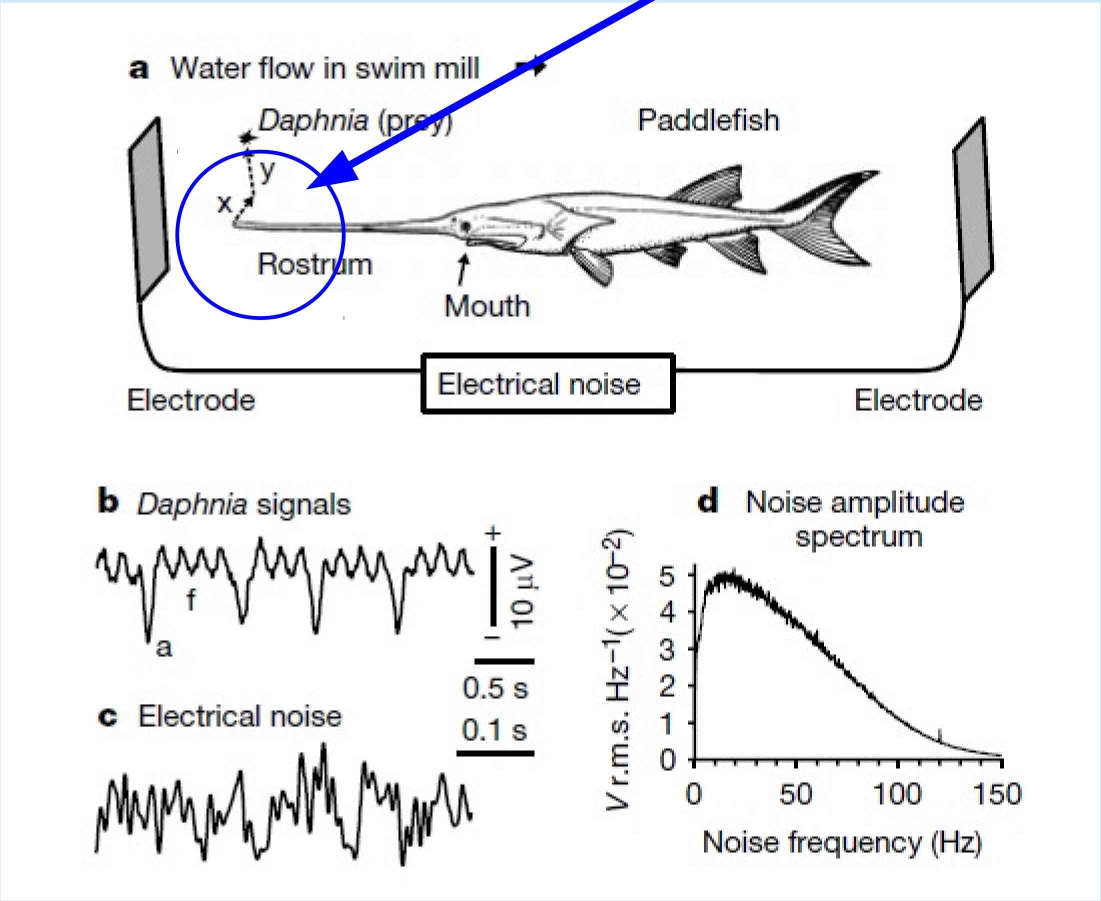


117
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2

Stochastic Resonance in Biology ...

“a beneficial adaptation”

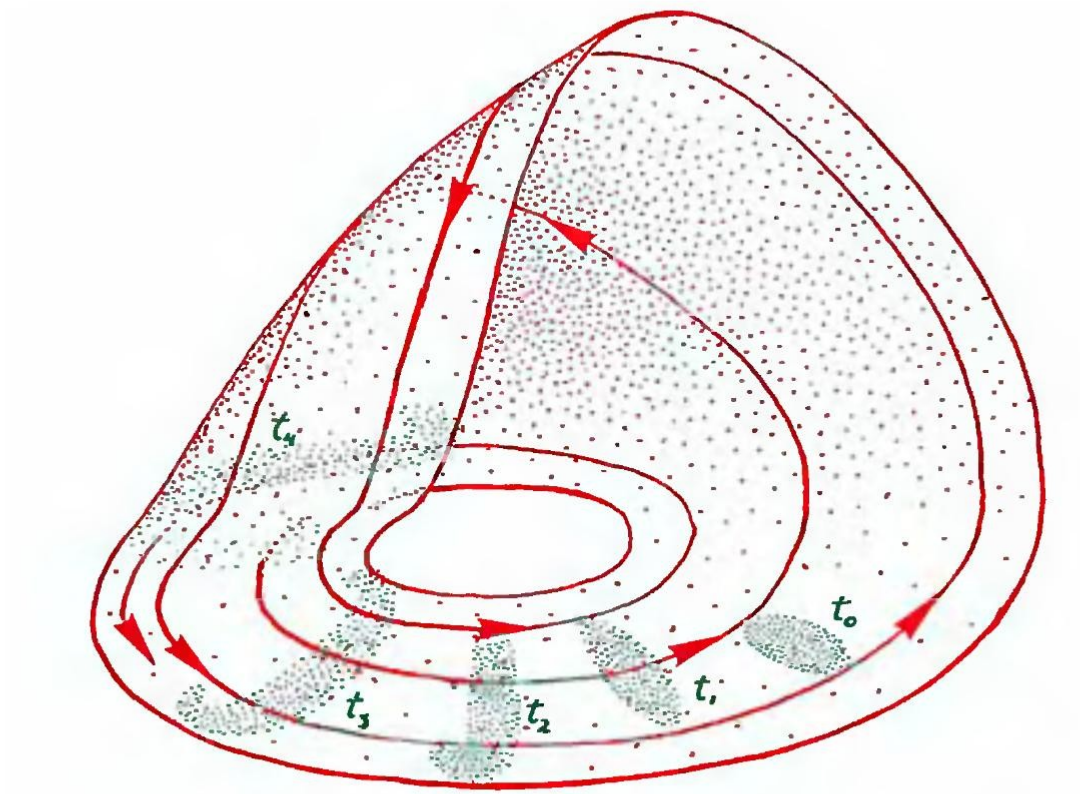




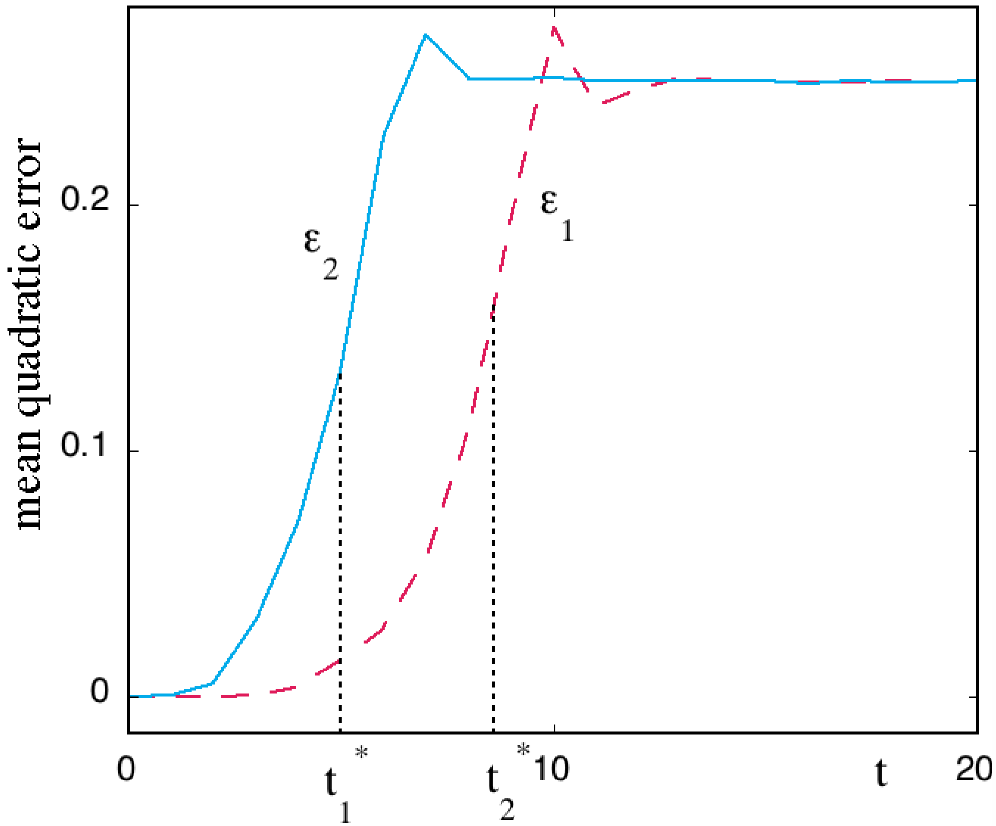
“Use of behavioural Stochastic resonance by paddle fish for feeding”

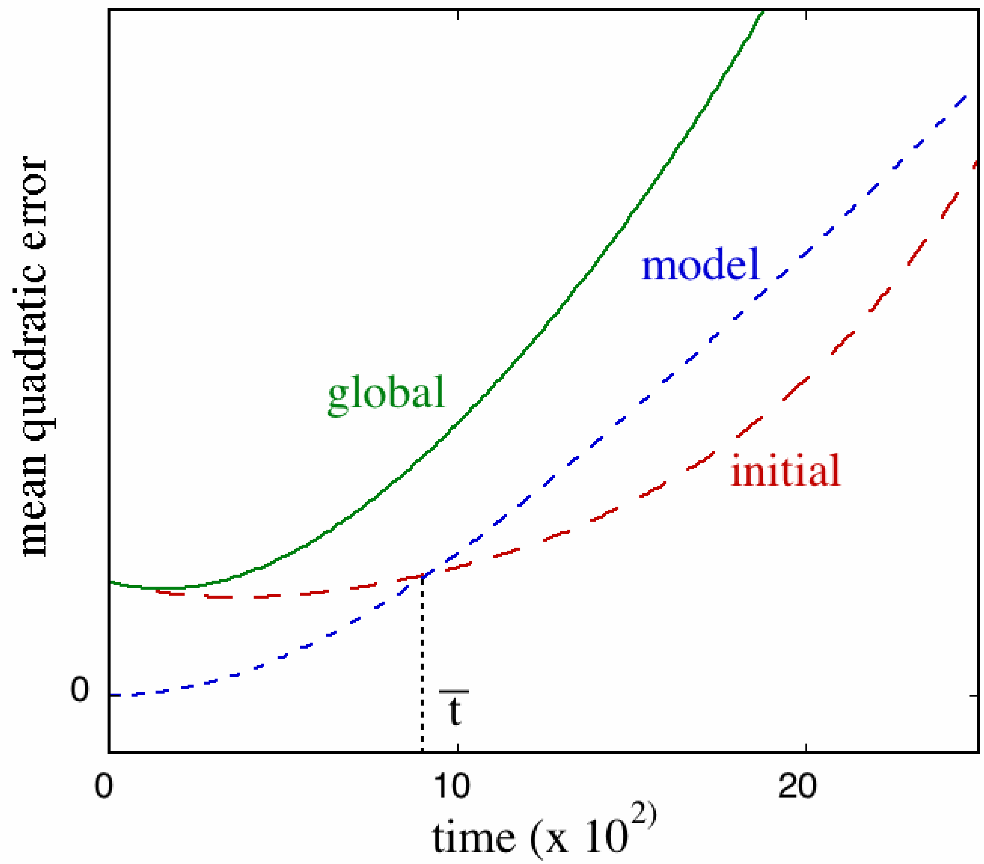
Letters to Nature (1999)

Frank Moss



Αύξηση με το με τον χρόνο των διαφόρων ειδών αβεβαιότητας ("λάθη") που προέρχονται από τις ατέλειες αυτές αναδεικνύοντας την Πολυπλοκότητα του συστήματος.





Από την κλασική αντίληψη απεριόριστης προβλεψιμότητας στην πραγματικότητα μίας περιωρισμένης προβλεψιμότητας: το φαινόμενο της πεταλούδας.

Αναθεώρηση της έννοιας της αιτιοκρατίας και άλλων βαθειά ριζωμένων ιδεών και πρακτικών, από την κλιματική αλλαγή στην οικονομία και την κοινωνιολογία.

Matter is Active: self-organization, collective motion, decision making and dynamics

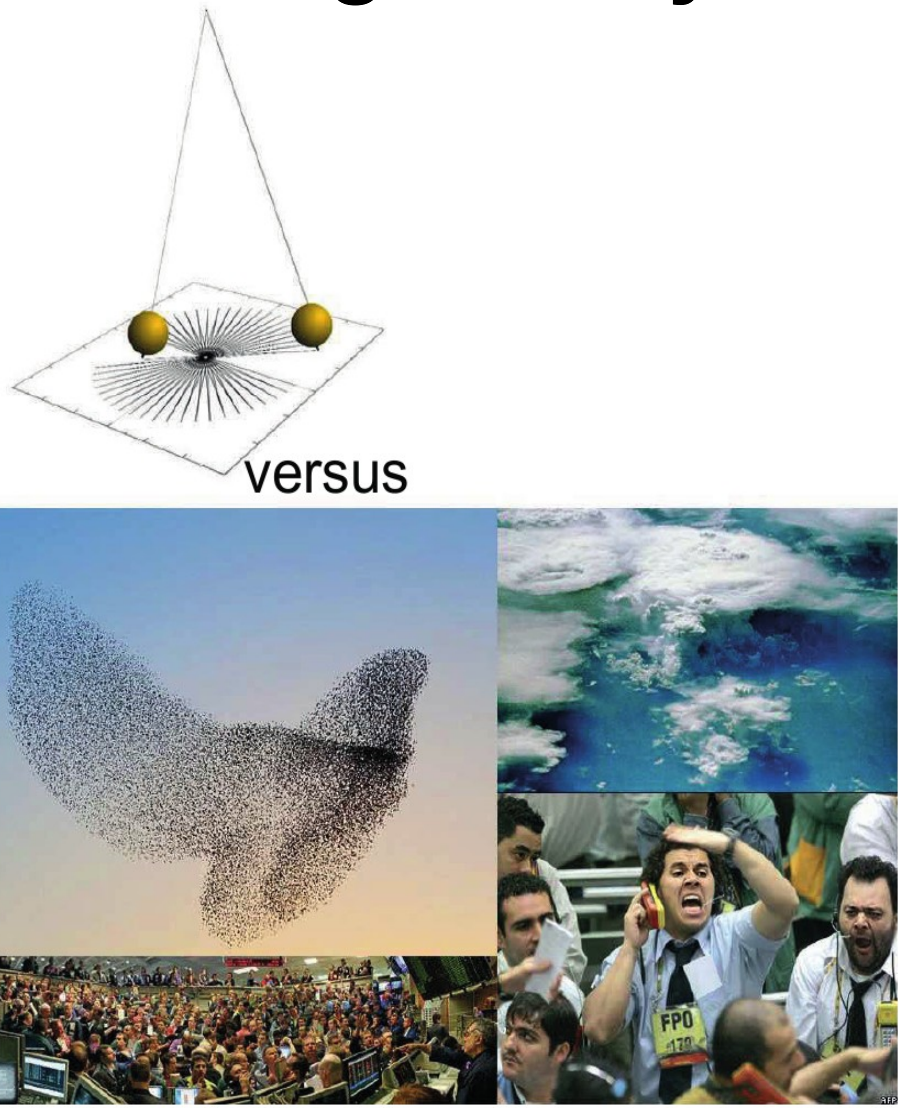
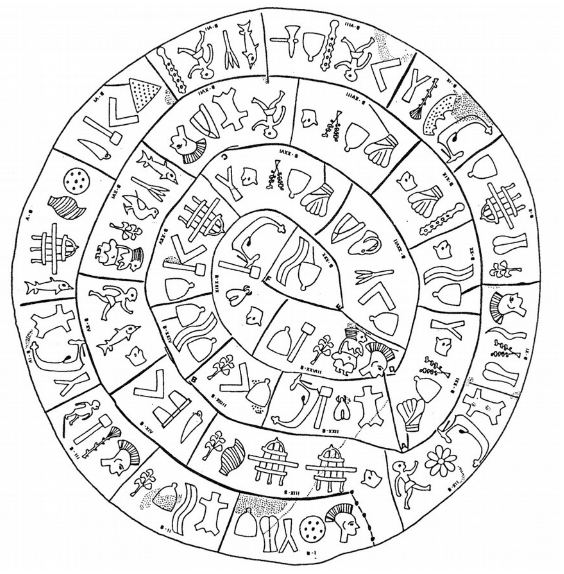
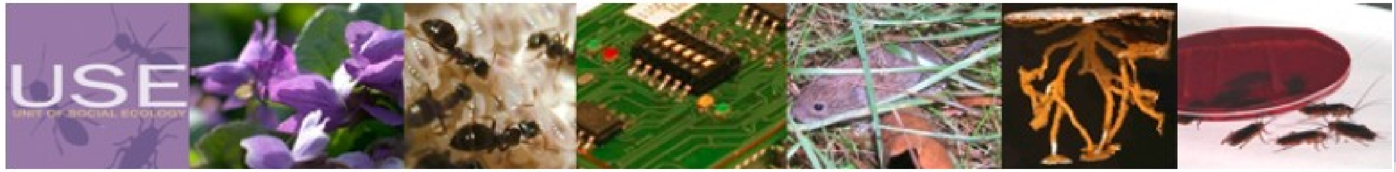


Fig. 1. Upper part: Simple pendulum. Lower part: Three manifestations of Complexity in everyday experience. Clockwise Bird flocking, the earth-atmosphere system, trading in the stock market.



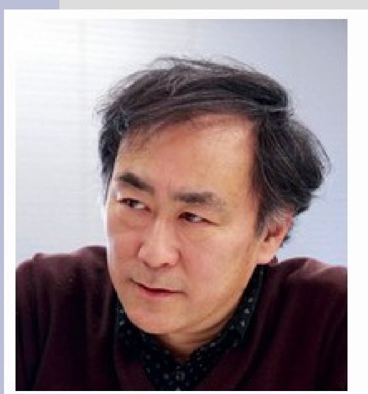
New Inspirations from the heritage of Gregoire Nicolis

Coordinated Aggregation: History & Hysteresis



▪ USE equipe ▪ USE index

Jean-Louis DENEUBOURG
Professeur ULB - Maître de recherches au F.R.S-F.N.R.S/ *Professor ULB - Senior research Associate from the F.R.S.- F.N.R.S.*



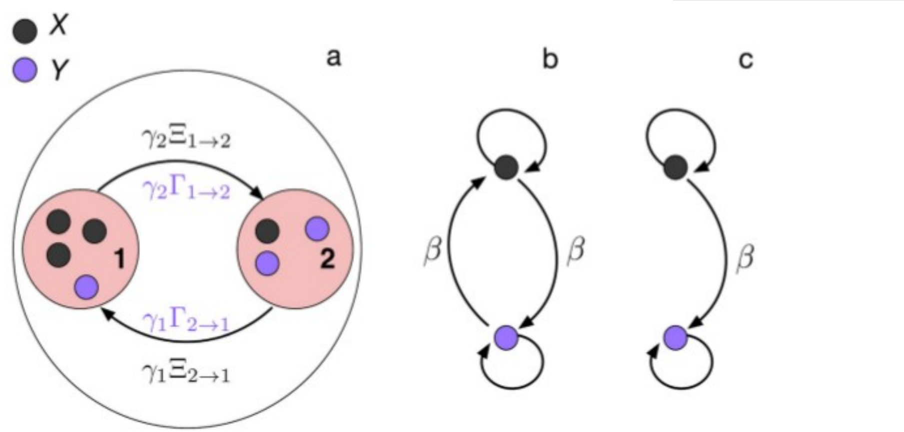


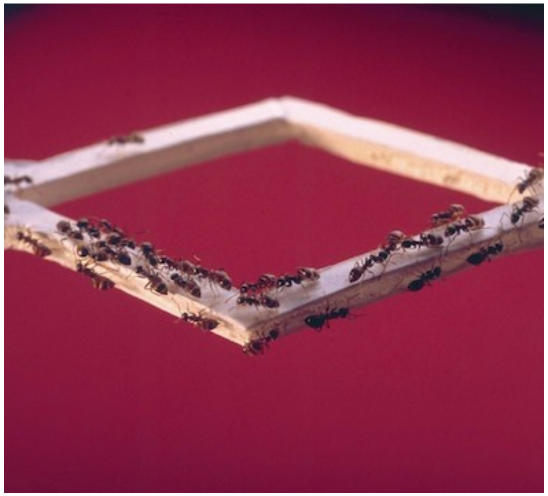
Figure 1. Experimental setup for the study of aggregation/segregation dynamics in an environment containing two equal patches and its relationship with the model defined by eq. (4) (**a**). Positive feedback networks of conspecific and heterospecific interactions : symmetrical (**b**) and asymmetrical (**c**) case.

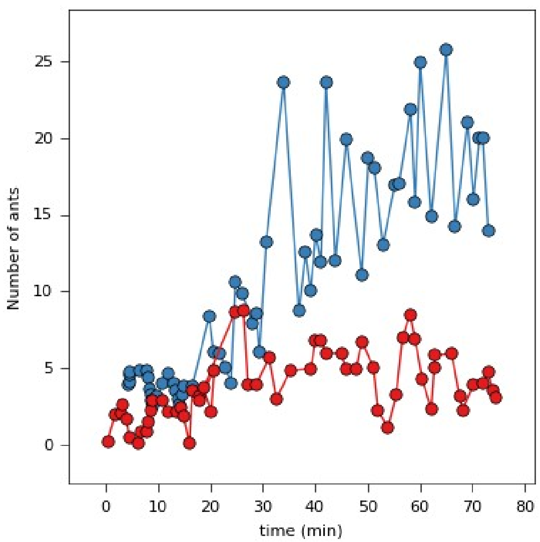
Eur. Phys. J. Special Topics 225, 1143-7 (2016)
DOI: 10.1140/epjst/e2016-02660-5

"Coordinated aggregation in complex systems: an interdisciplinary approach"

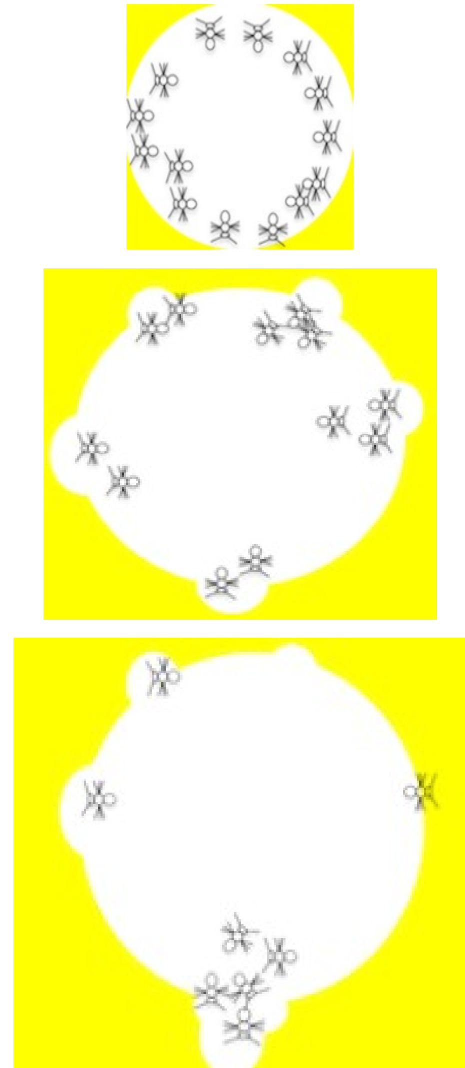
V. Basios, S. Nicolis, J.L. Deneubourg

Collective exploitation of their environment by ‘simple’ organisms in Complex Systems



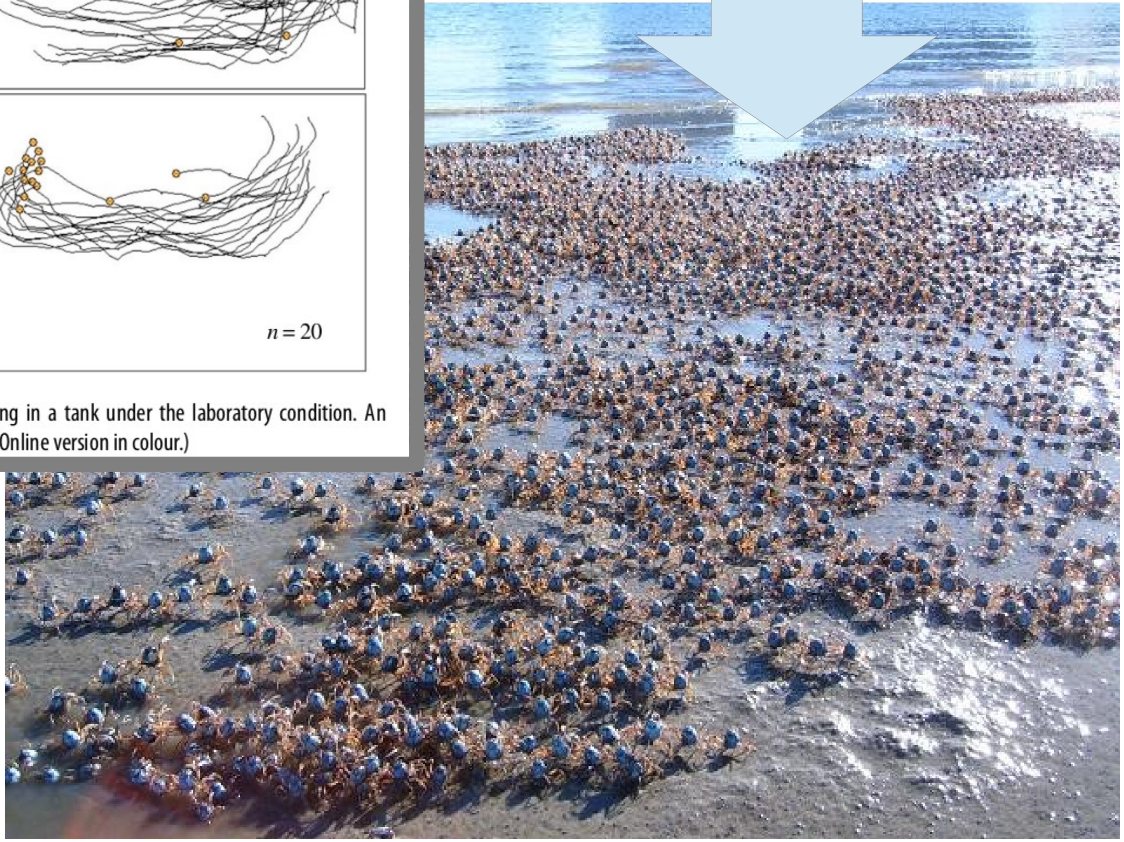


Pitchfork Bifurcation



Spatio-temporal Pattern Formation

Real Soldier-Crab decision making monitoring & data



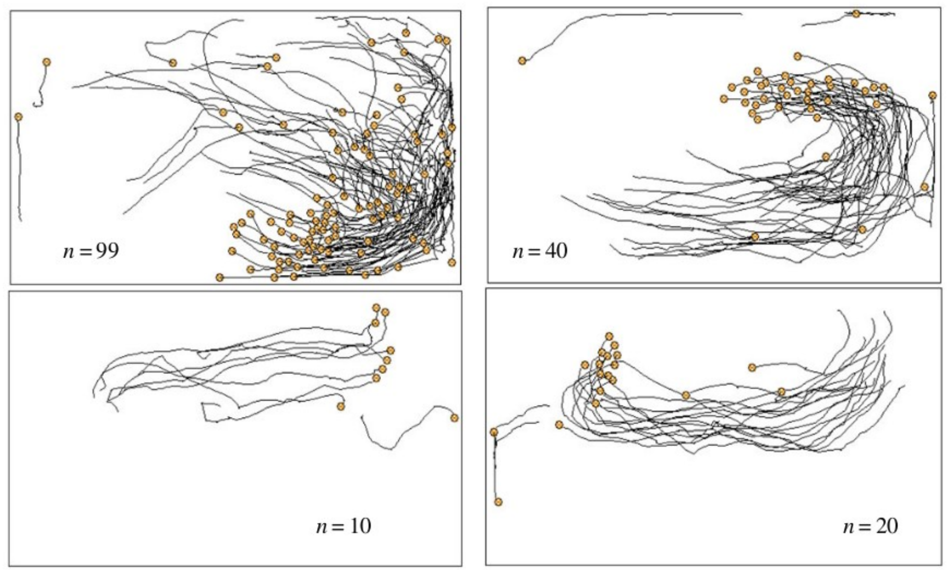


Figure 3. Snapshots of the real soldier crabs, *Mictyris guinotae*, wandering in a tank under the laboratory condition. An individual is represented by a circle accompanied by its previous trajectory. (Online version in colour.)

Modified Vicsek Model
With BIB as internal steering

BIB = Bayesian and Inverse Bayesian Inference Process

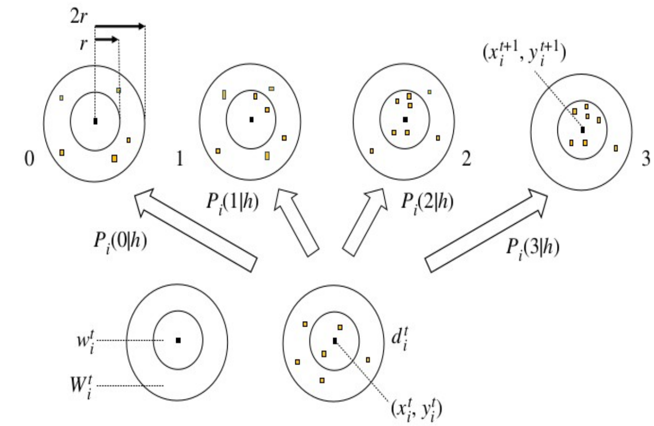


Figure 5. Schematic diagram of data and hypothesis adopted by a time series of real soldier crabs. (Online version in colour.)

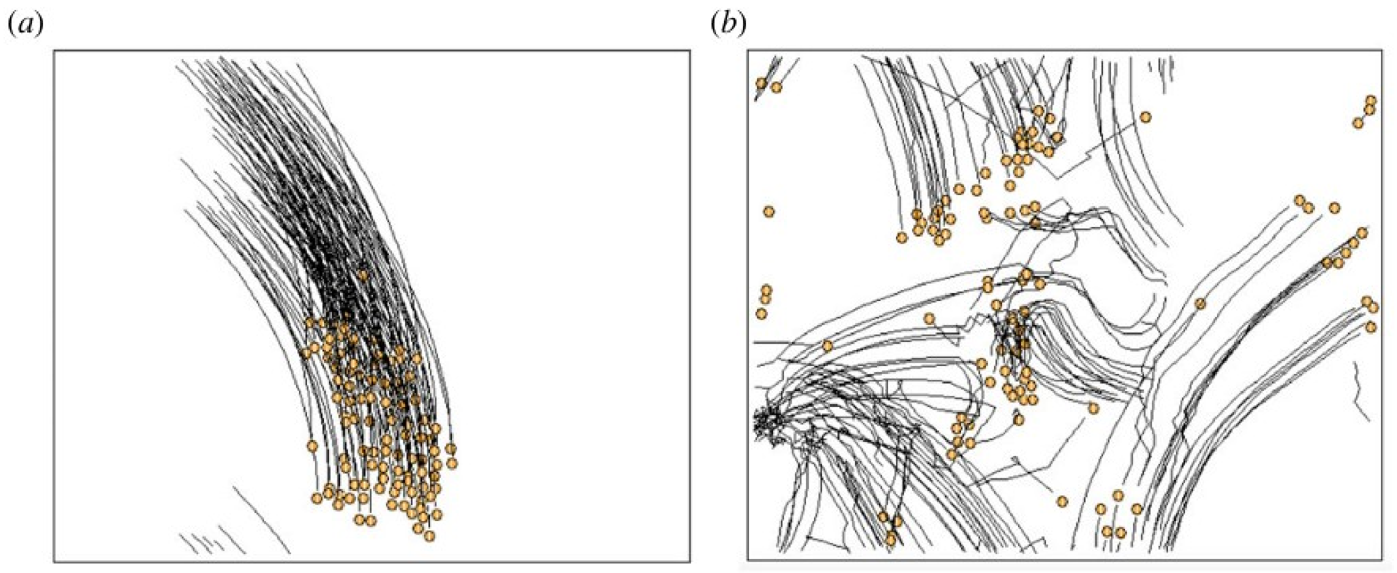


Figure 10. Snapshots of the swarm model based on BIB inference. Swarming phase (*a*) and dispersing phase (*b*). (Online version

Medical Test for disease A by test B

- **1%** of persons in the population have a disease called A.
  - **P(A)=0.01**
- **80%** of those with disease A get positive result to test B:

  P(B|A)=0.8
- But also **9.6%** of the persons without disease A

get a positive test B:

P(B) = 0.8***P(A)**+0.096*(**1−P(A)**)***P(B)**

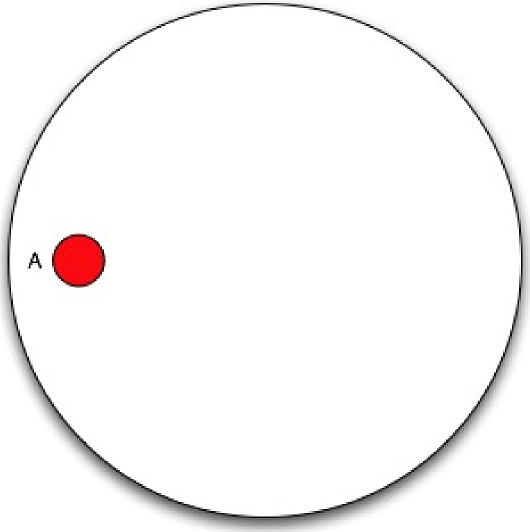
= 0.008+0.09504***P(B)** = **0.10304**

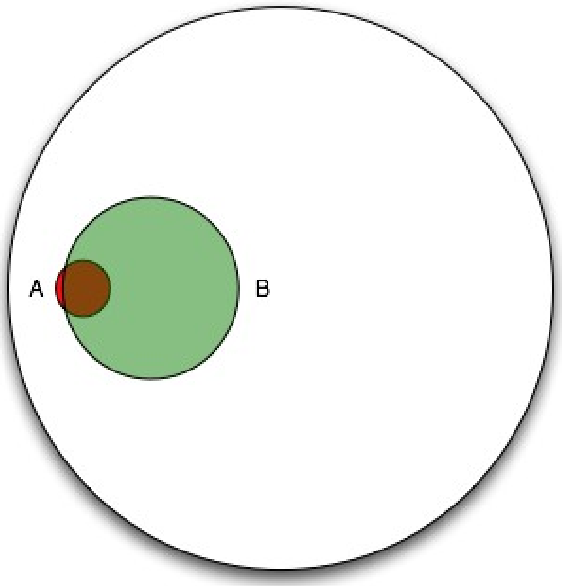
- Now let's plug those values into Bayes' theorem

P(A|B)=0.8∗0.010.10304 = **0.0776**

So about a 7.8% chance of **actually having**

disease A having tested positive by test B



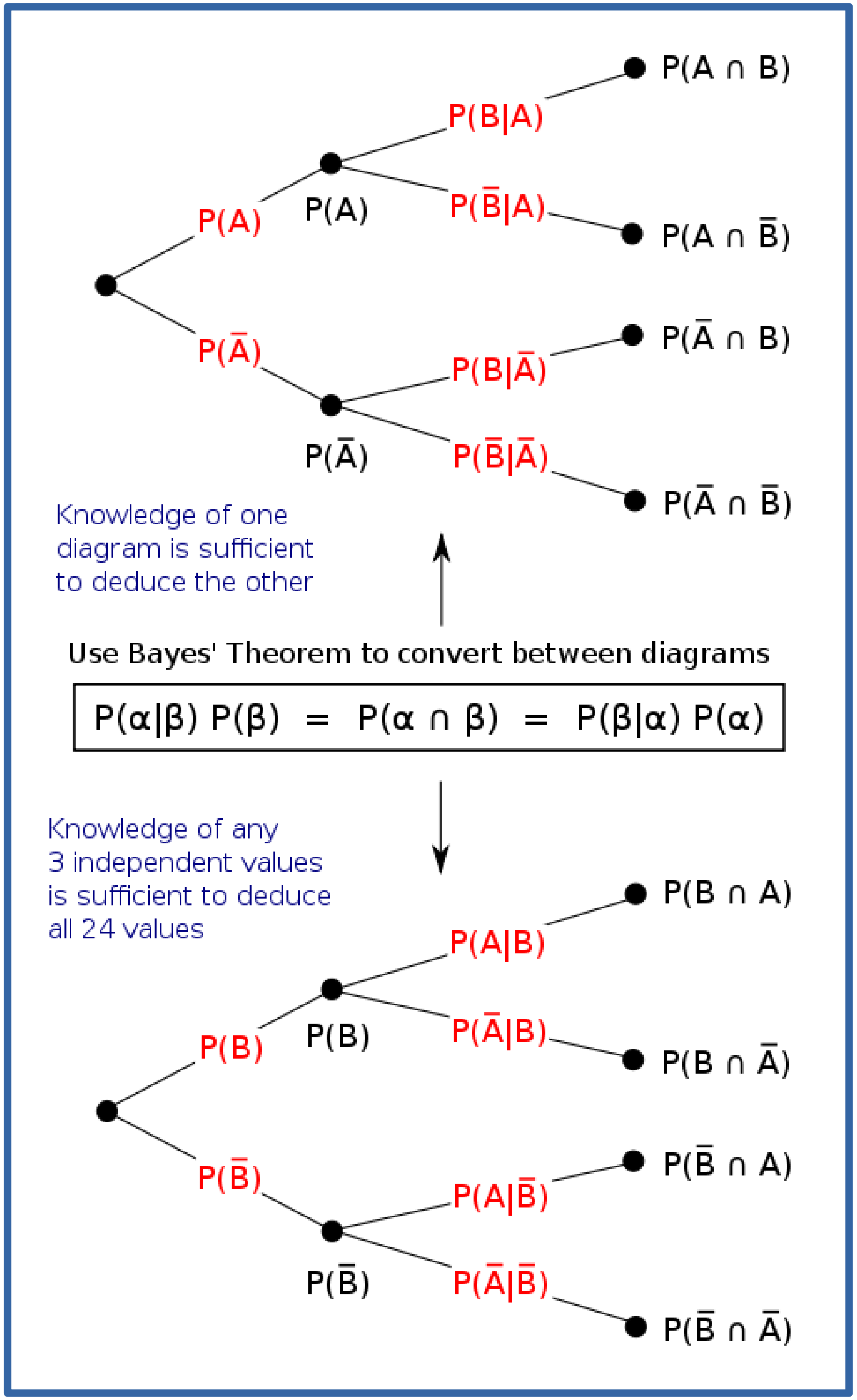


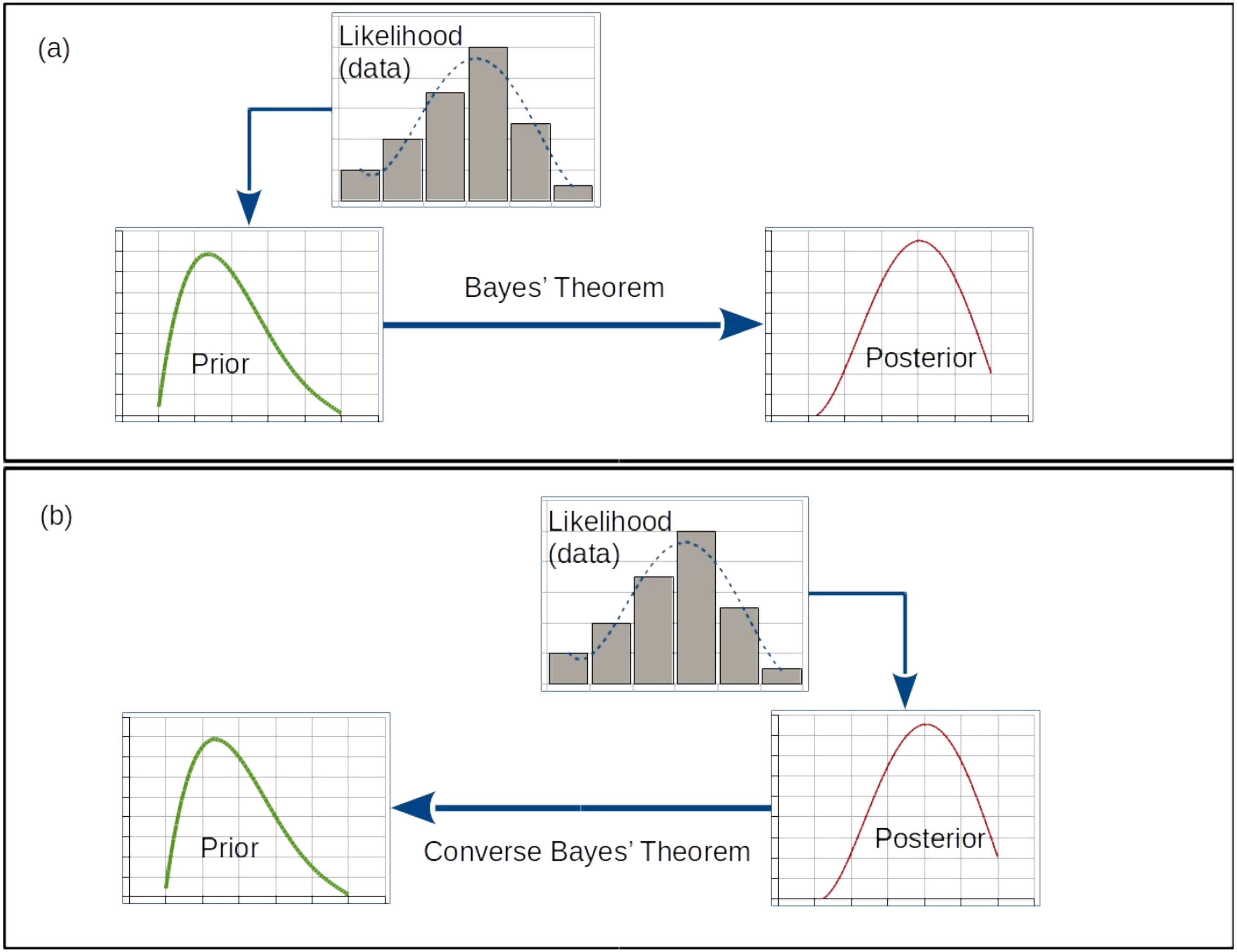
Bayes Inference: Rescaling Chance due to Bayes Theorem

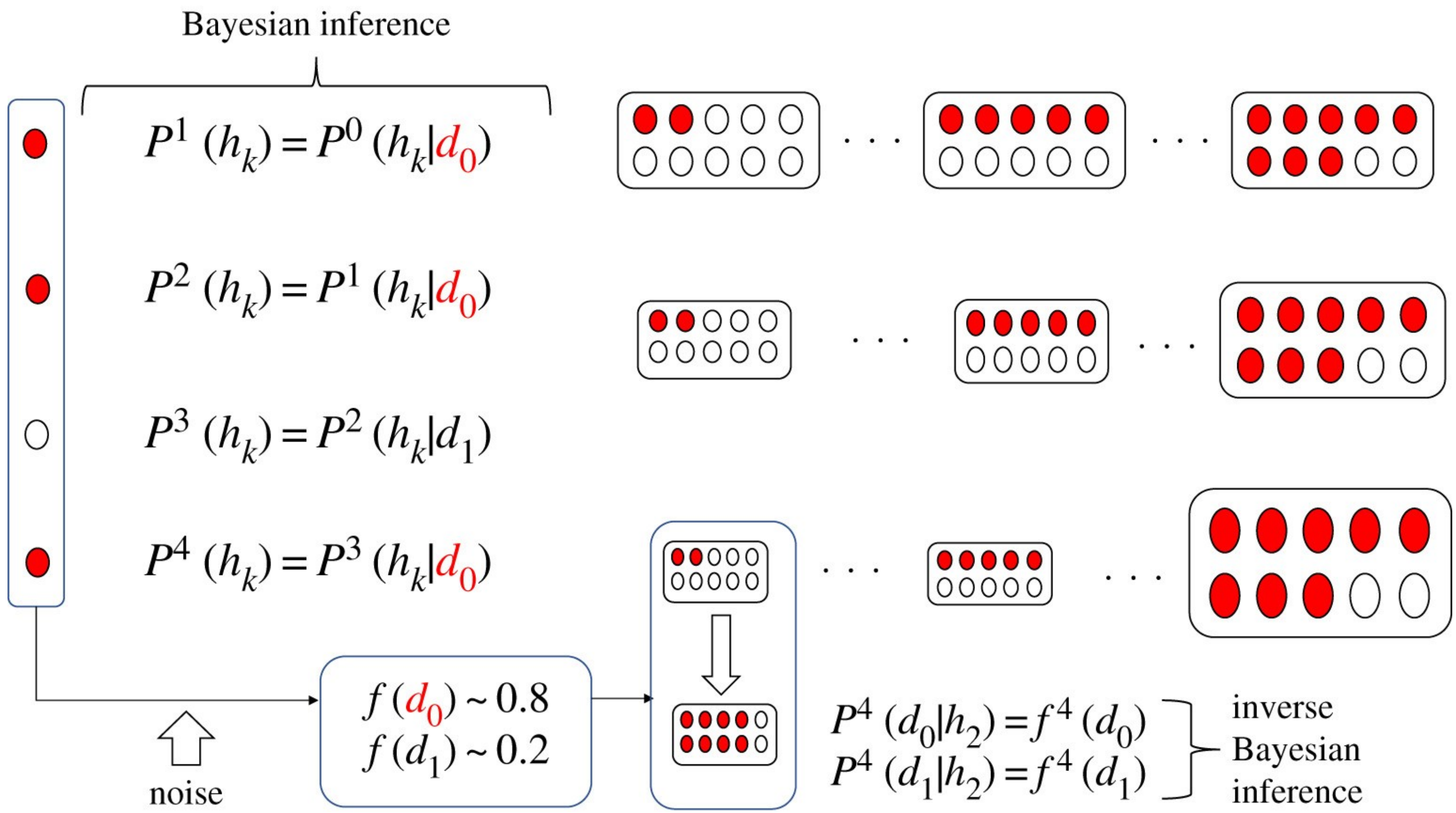
$$P(A \mid B) = \frac{P(B \mid A)P(A)}{P(B)}$$

where A and B are events and $P(B) \neq 0$.

- $P(A \mid B)$ is a conditional probability: the likelihood of event A occurring given that B is true.
- $P(B \mid A)$ is also a conditional probability: the likelihood of event B occurring given that A is true.
- $P(A)$ and $P(B)$ are the probabilities of observing A and B independently of each other; this is known as the marginal probability.




(a)
Likelihood
(data)
Prior
Bayes' Theorem
Posterior
(b)
Likelihood
(data)
Prior
Converse Bayes' Theorem
Posterior



Bayesian inference
$P^1(h_k) = P^0(h_k|d_0)$
$P^2(h_k) = P^1(h_k|d_0)$
$P^3(h_k) = P^2(h_k|d_1)$
$P^4(h_k) = P^3(h_k|d_0)$
. . .
noise
$f(d_0) \sim 0.8$
$f(d_1) \sim 0.2$
$P^4(d_0|h_2) = f^4(d_0)$
$P^4(d_1|h_2) = f^4(d_1)$
inverse Bayesian inference

PHILOSOPHICAL
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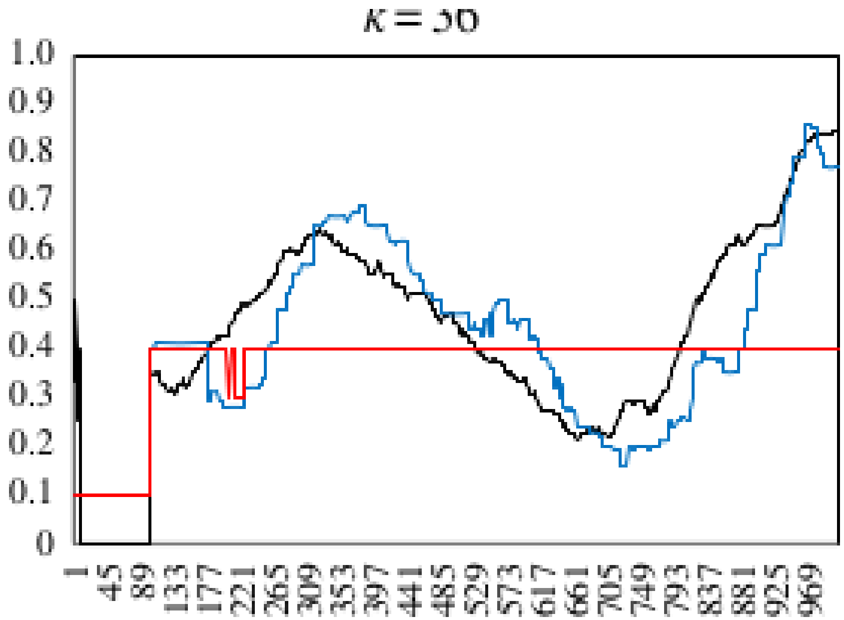
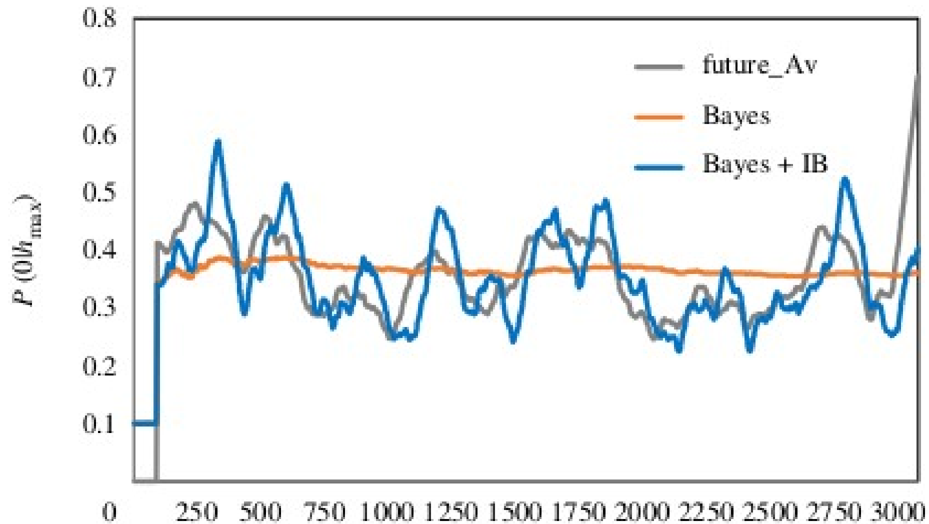
Inverse Bayesian inference in swarming behaviour of soldier crabs

Yukio-Pegio Gunji[1], Hisashi Murakami[2], Takenori Tomaru[3] and Vasileios Basios[4]





Scores of Prediction
of the next move

Bayesian
vs
Bayesian Inverse-Bayesian
inferences

individual crab (up)
average of a collective (down)

Philosophical Transactions of the Royal Society A Phys.& Math. 376: 20170370.
http://dx.doi.org/10.1098/rsta.2017.0370

accepted August 2018

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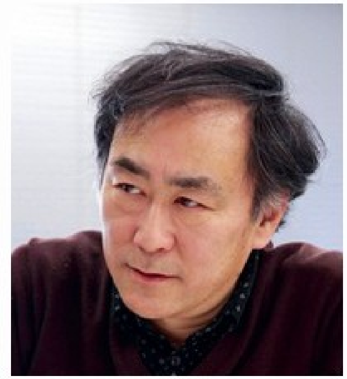
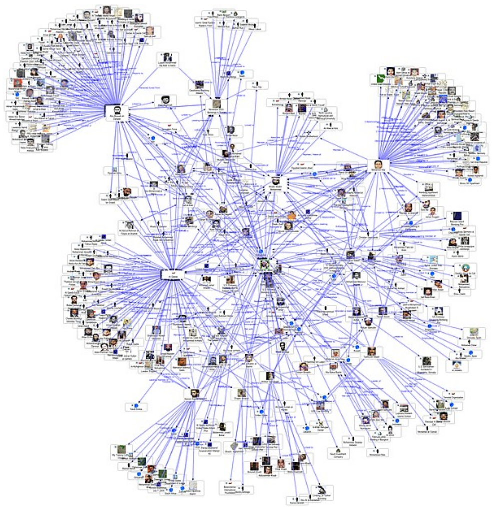
WASEDA University

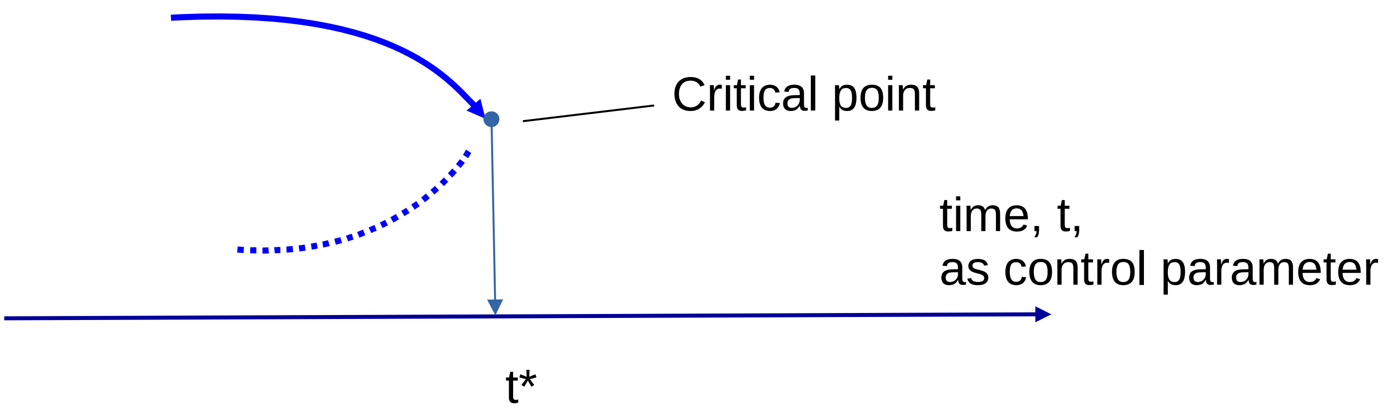


Complexity Science in Sociology & Economics

- Networks (internet, …). Optimization.



- Prediction of potentially disastrous state transitions.



Complex Systems', nonlinear, Data Analysis ("big data")

- Determination of characteristic dynamical aspects (number of variables, dimension of attractor(s), stability and Lyapunov exponents ,etc) based on data without initial model.

- Correlation Identification and of other collective (statistical) properties. Self-similarity, scaling laws, feedbacks.

- The role of dynamical Entropies:

$\mathbf{S_n \approx hn}$, random process or fully developed chaos

$\mathbf{S_n \approx n^{\alpha}}$, (α<1), n ≈ ln(n), long range correlations

“Nonlinear science introduces a new way of thinking based on a subtle interplay between qualitative and quantitative techniques, between topological, geometric and metric considerations, between deterministic and statistical aspects.

It uses an extremely large variety of methods from very diverse disciplines, but through the process of continual switching between different views of the same reality these methods are cross-fertilized and blended into a unique combination that gives them a marked added value.

Most important of all, nonlinear science helps to identify the appropriate level of description in which unification and universality can be expected.”

“Introduction to Nonlinear Science”
by Gregoire Nicolis
(Cambridge Univ. Press, 1995)

Gregoire Nicolis’ 60 years celebration, June 1999, ULB, Brussels

Gregoire Nicolis (1929-2018) interviewed in his study room at *ULB – CeNoLi* circa 2015