26ο Θερινό Σχολείο – Συνέδριο
«Δυναμικά Συστήματα και Πολυπλοκότητα» 14-20/7/2019

Πολυπλοκότητα και δυναμική της πληροφορίας: Ένα από τα κληροδοτήματα του Γρηγόρη Νίκολη

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ULB UNIVERSITÉ LIBRE DE BRUXELLES

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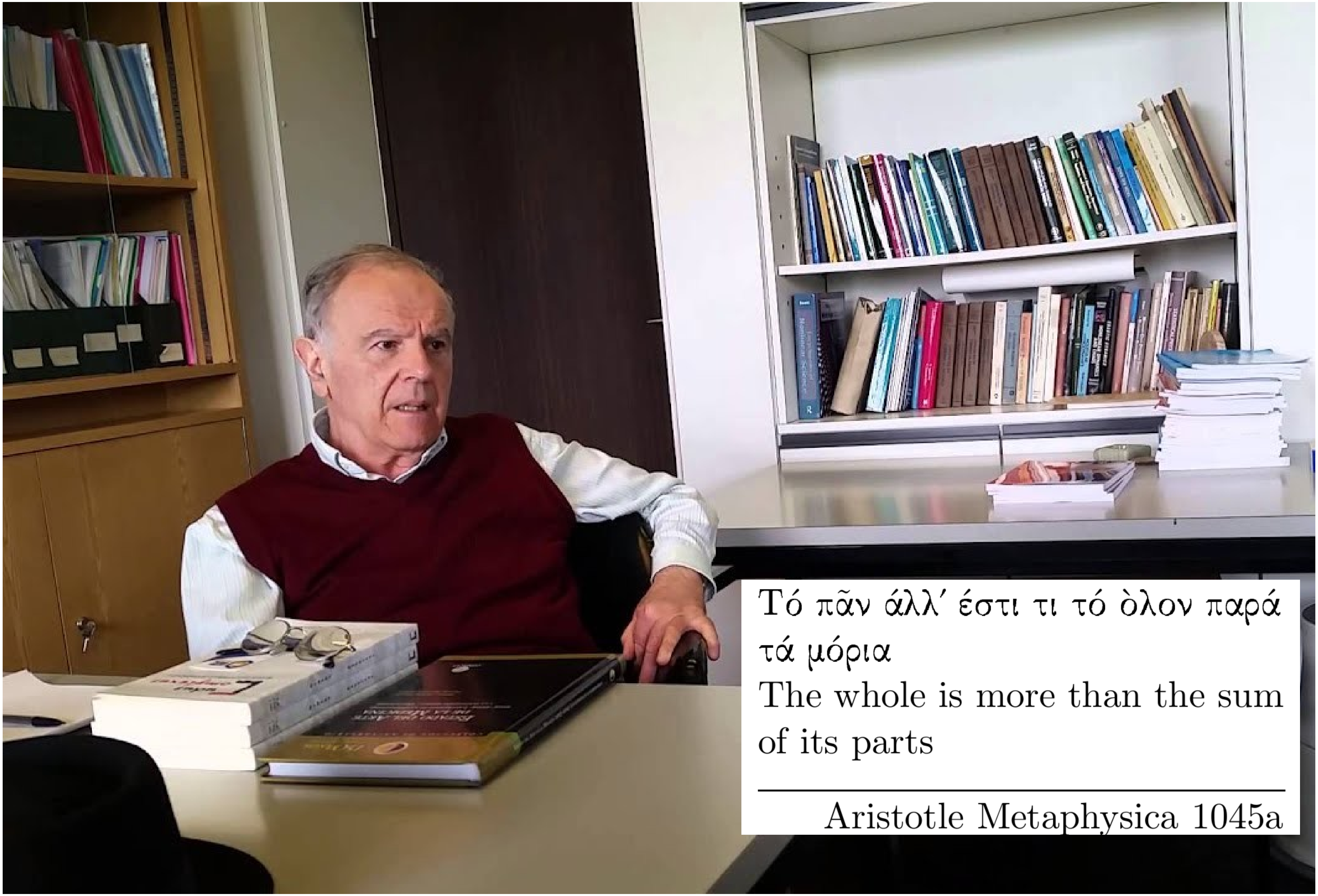
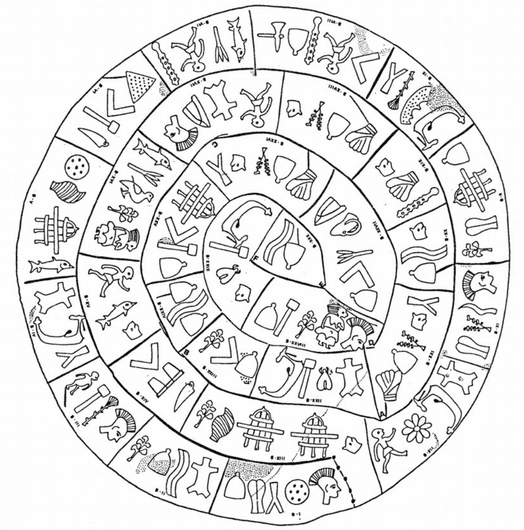
&
Département de Physique des Systèmes Complexes et Mécanique Statistique,
University of Brussels (ULB), Brussels.



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

Outline of the talk:



Prolegomena

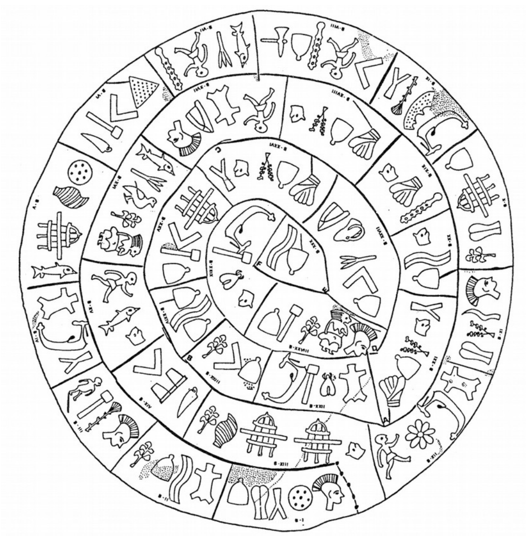
Part 1. Out of equilibrium:

Active Matter & New Materials

Part 2. Dynamics of Information:

Decision making in Collective Motion

Prolegomena



Part 1. Out of equilibrium:

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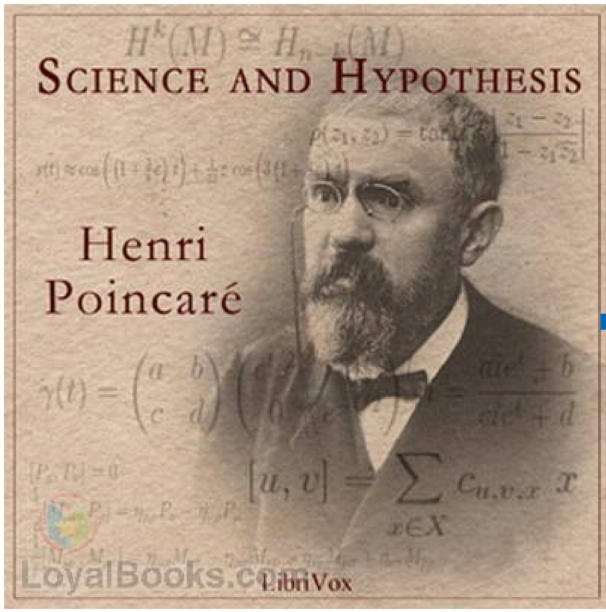
Gregoire's Nicolis Academic 'Family' Tree



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)
Second Law of Thermodynamics,
Dissipative structures,
Order out of Chaos,
Time's arrow

Gregoire Nicolis’ Encomium & Heritage:

Open Systems &
the 2nd Law of Thermodynamics

Dissipative Structures

Bifurcations & Chaos

Self-Organization & Pattern Formation

Constructive Role of Fluctuations & Chaos
(+ Stochastic Resonance)

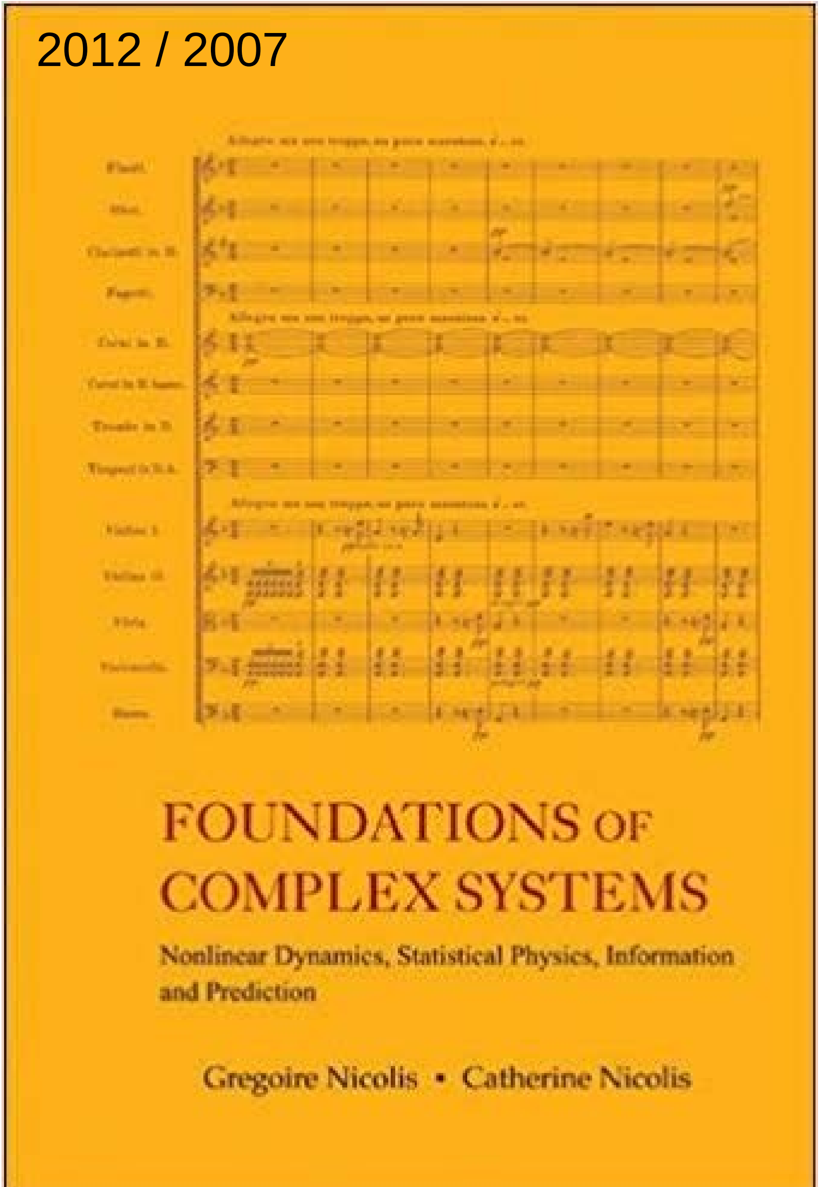
Self-reference & Nonlinear Feedback

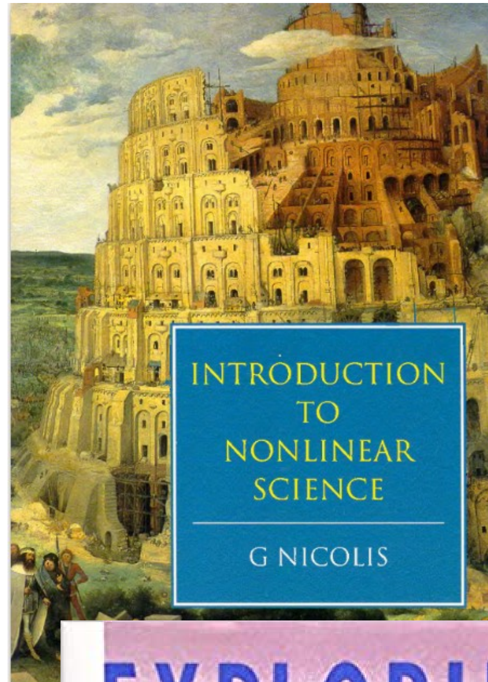
Information Dynamics
(+ Entropy & Symbolic Dynamics + Prediction)

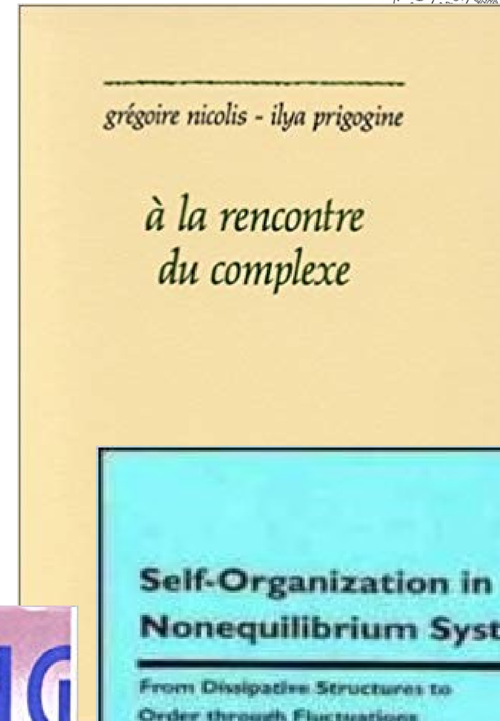
Emergence & Irreversibility

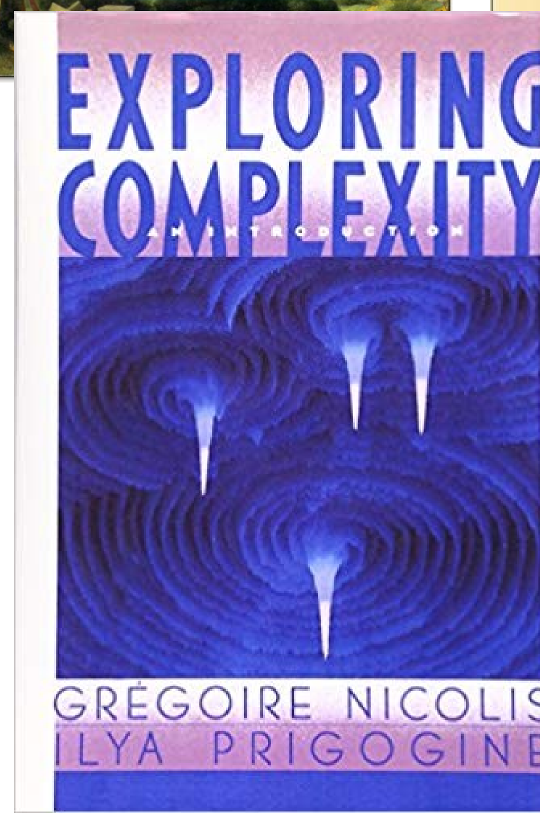
Complexity Science bookshelf

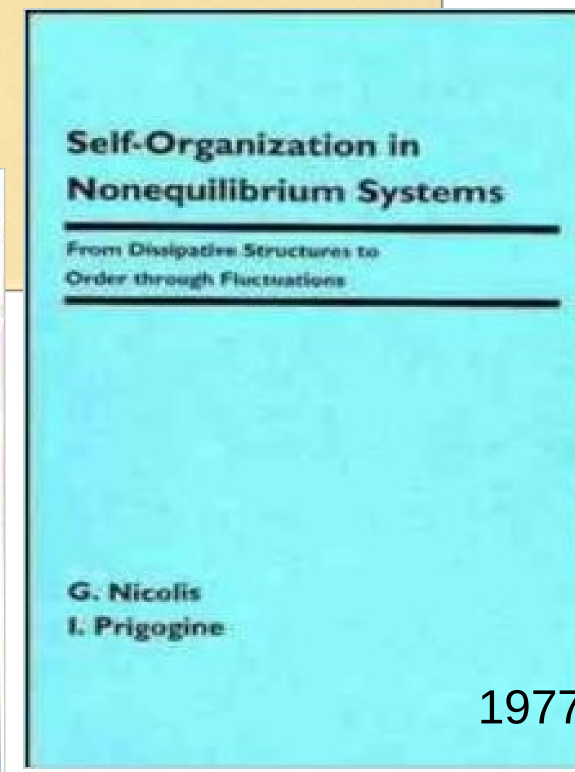
2012 / 2007











1977

Com<u>plex</u> =
many parts + nonlinear relations

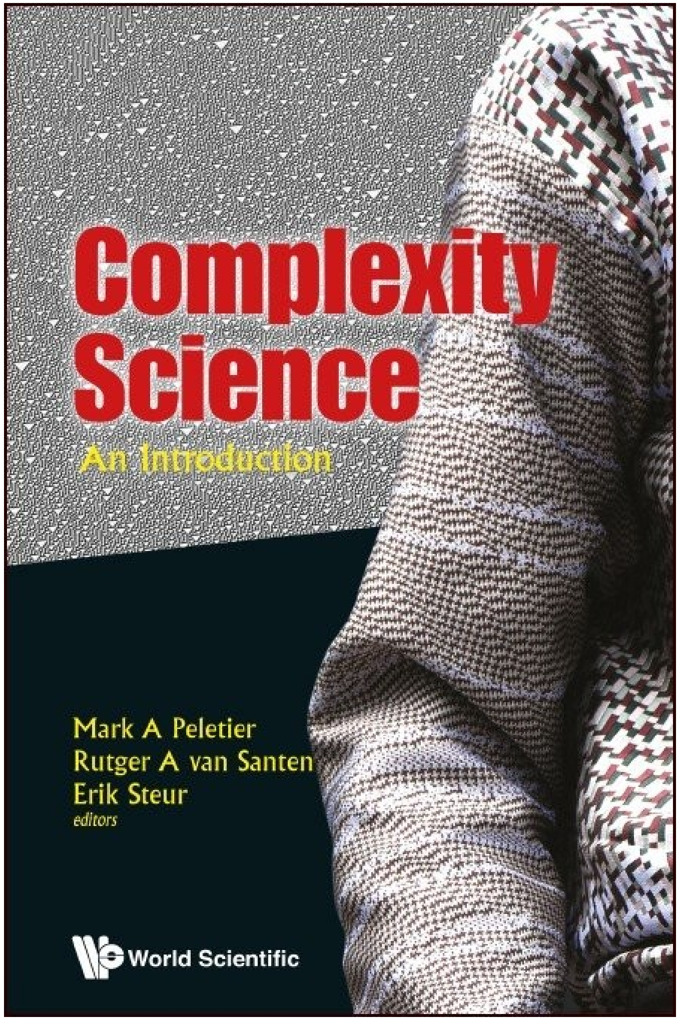
Chapter 1:
“The many facets of complexity”
by Grégoire Nicolis (2019)

Phenomenology of Complexity

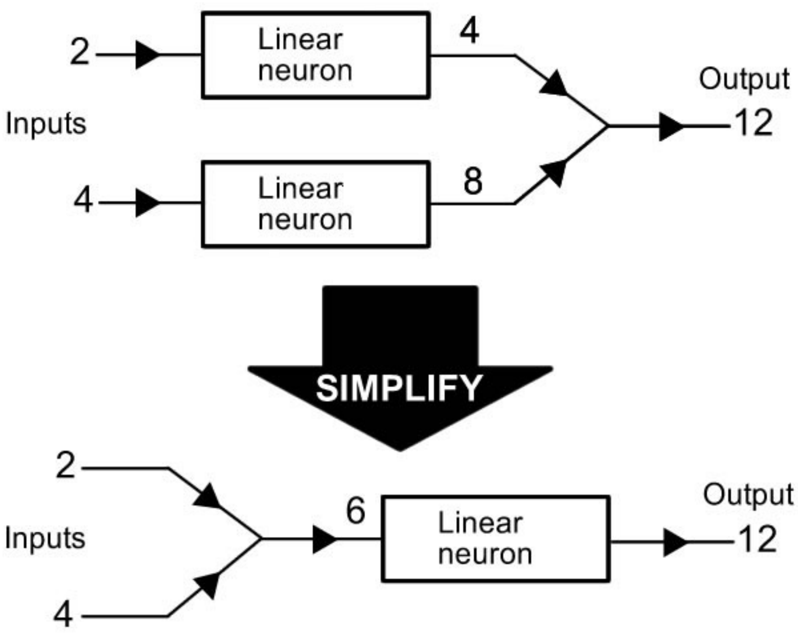
Formulation
- *a) Deterministic view*
- *b) Probabilistic approach*

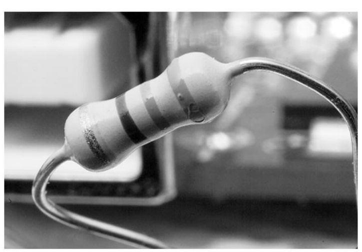
Emergence

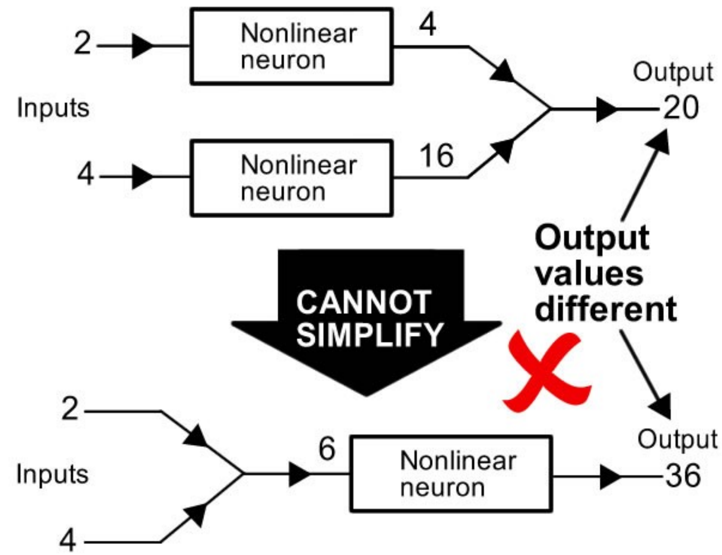
Complexity and Information

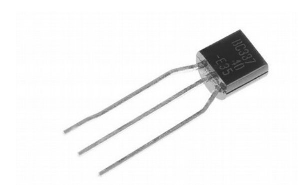


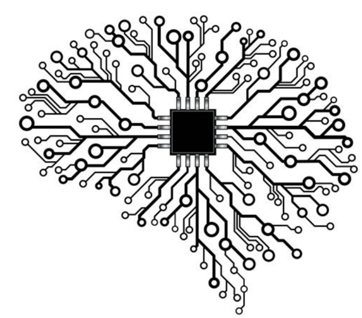
The Importance of Being Nonlinear: Information flow





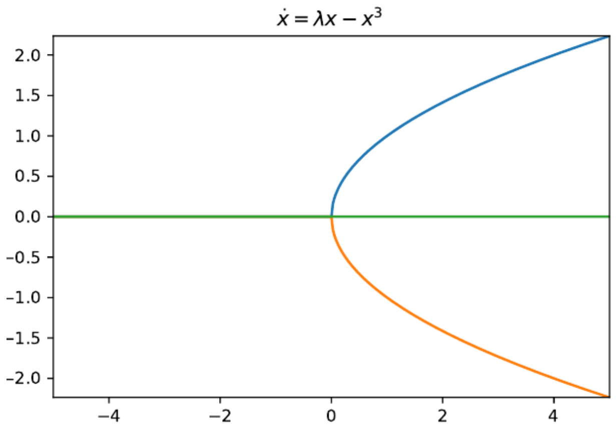


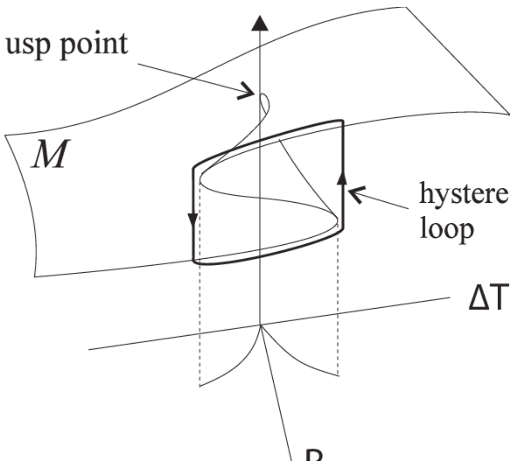




Only Nonlinear Elements can process information, i.e … compute !!!

The Importance of Being Nonlinear: Bifurcations & Multistability





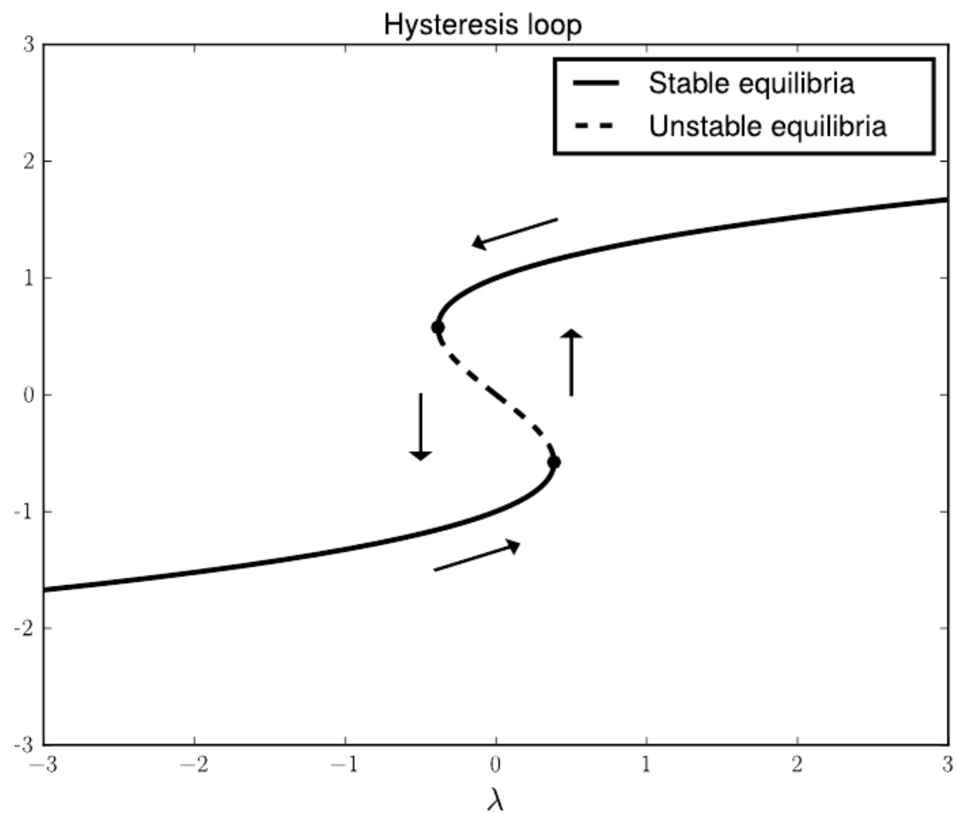


Figure 6.5: Bifurcation diagram for the ODE $x' = \lambda + x - x^3$.

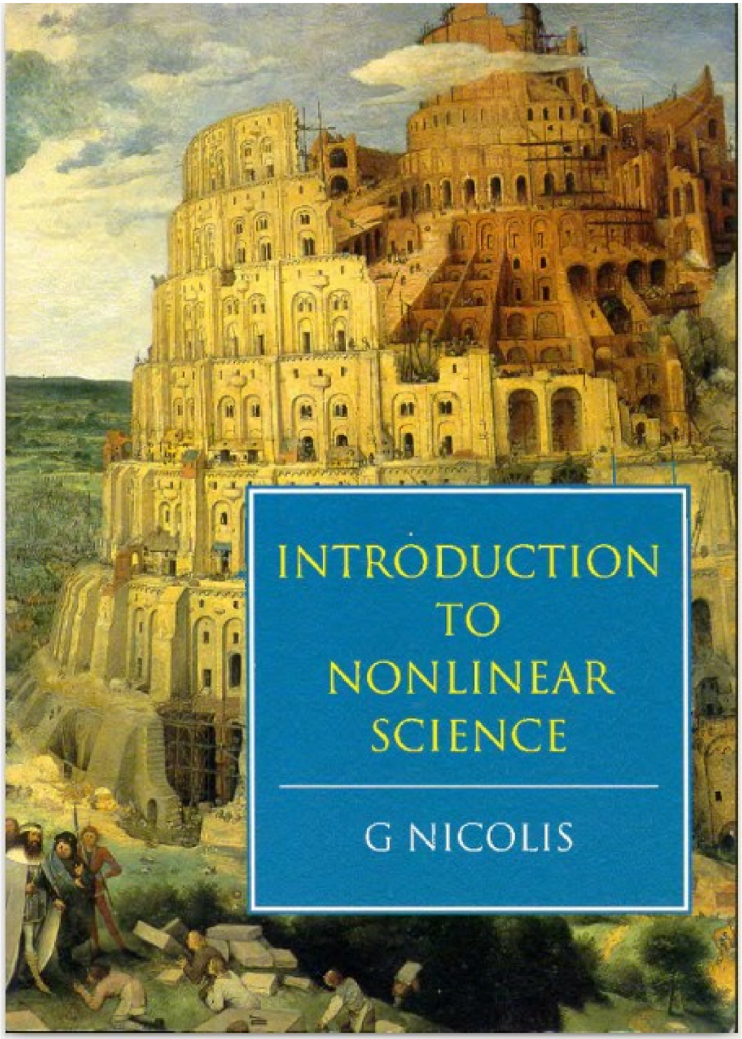
Only Nonlinear Elements can have dynamic memory !!! (Hysteresis)

“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.

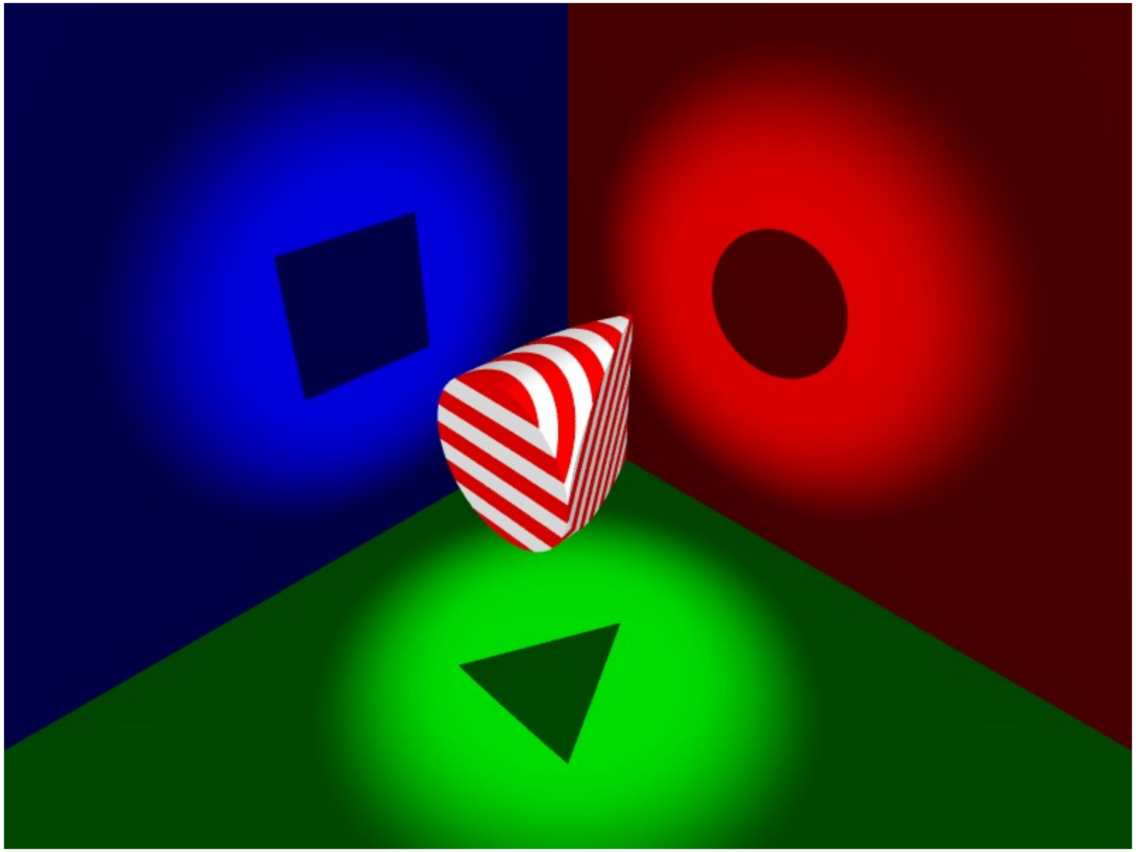
It uses an **extremely large variety of methods from very diverse disciplines**, but through the process of continual **switching between different views of the same reality** these methods are cross-fertilized and blended into a unique combination that gives them a marked added value.

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)



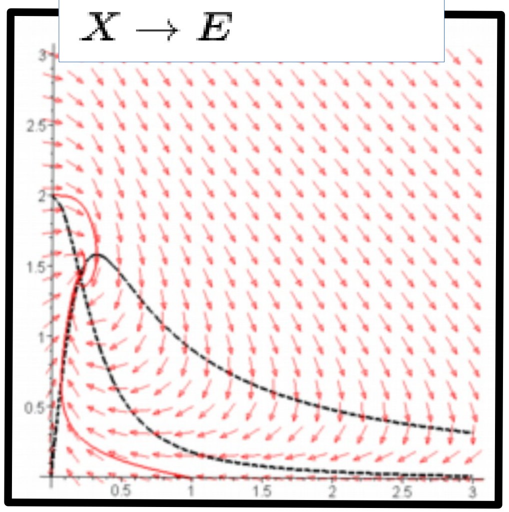
"…appropriate level of description …"

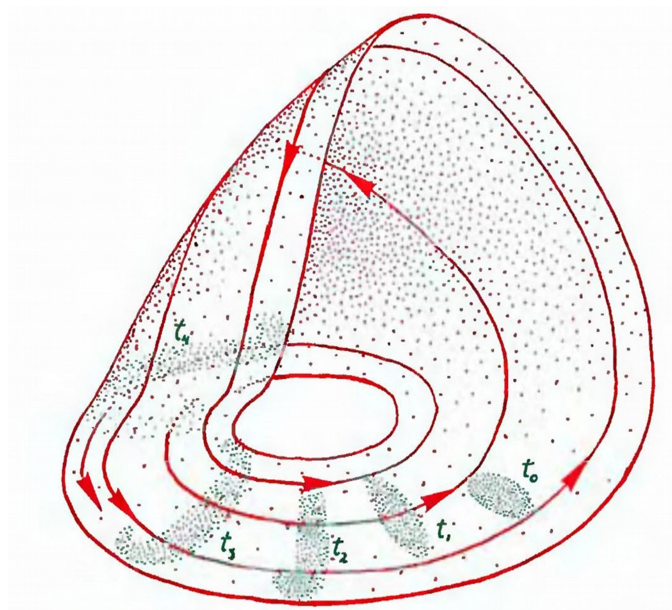


"…topological, geometric, metric …"

The Brusselator: nonlinear Feedback, Bifurcations, Chaos

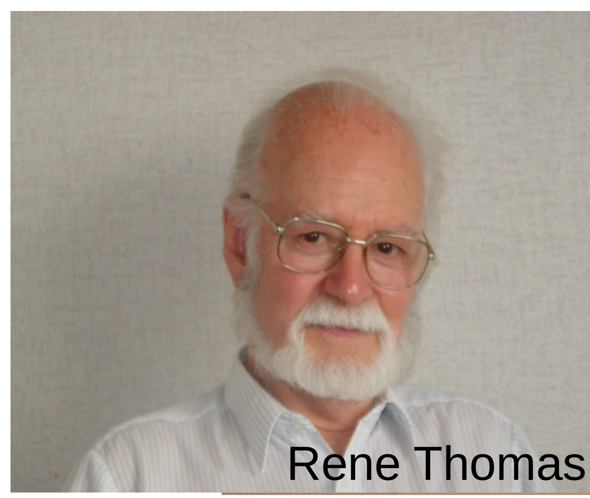
$$A \rightarrow X$$
$$2X + Y \rightarrow 3X$$
$$B + X \rightarrow Y + D$$
$$X \rightarrow E$$





Leonid Shilnikov

Joel Lebowitz, Mitchell Feigenbaum

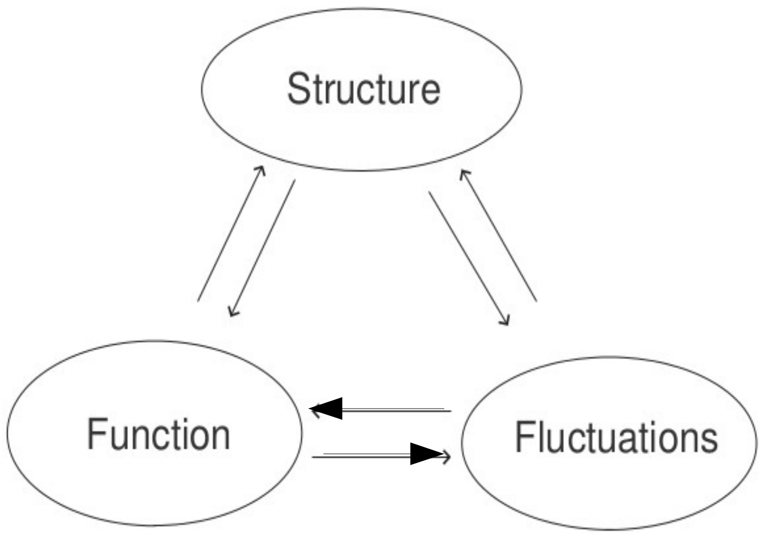


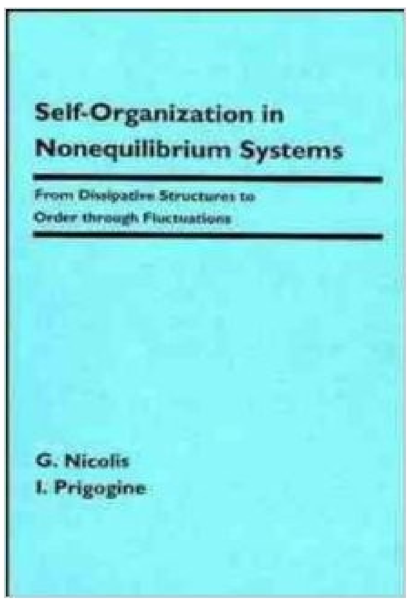
Rene Thomas

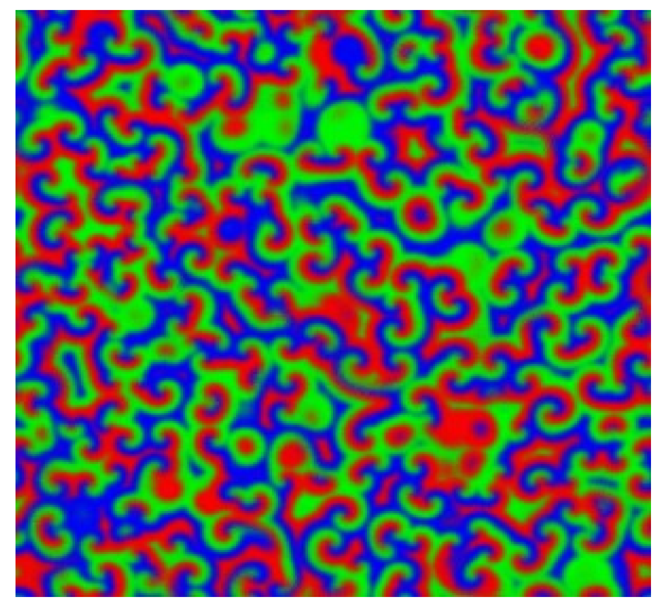
Otto Roessler

"...The fluctuations involved <u>are not</u> fluctuations in concentrations or other macroscopic parameters <u>but</u> fluctuations in the mechanisms leading to modifications of the [kinetic] equations..."

G. Nicolis and I. Prigogine

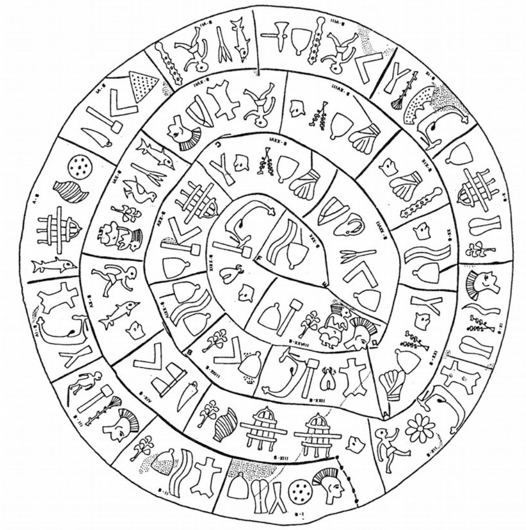






in: **"Self-Organization in Nonequilibrium Systems: From Dissipative Structures to Order through Fluctuations"**
discussing auto-catalytic reactions and Manfred Eigen's "hypercycles"

Outline of the talk:



Prolegomena

Part 1. Out of equilibrium:

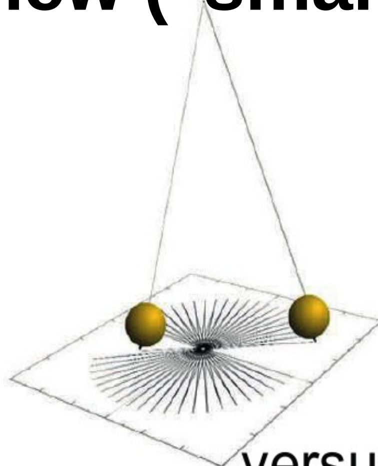
Active Matter & New Materials

Part 2. Dynamics of Information:

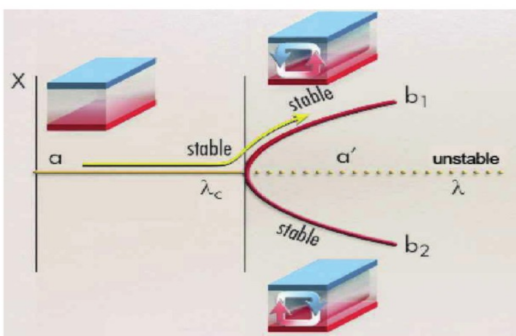
Decision making in Collective Motion

PART 1: ACTIVE MATTER

self-organization, dynamics, emergence, new ("smart")materials



versus



ition to Rayleigh–Bénard patterns arising beyond the instability of t

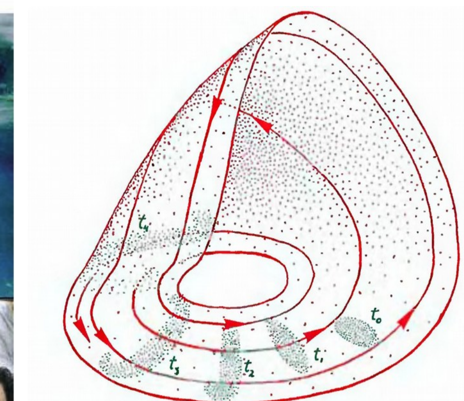


Fig. 1. Upper part: Simple pendulum. Lower part: Three manifestations of Complexity in everyday experience. Clockwise Bird flocking, the earth-atmosphere system, trading in the stock market.

Statistical Mechanics and Thermodynamics Presiding to the Self-organization of Matter

with thanks to Pierre Gaspard
(ULB)

Non (-) equilibrium or Nonequilibrium?

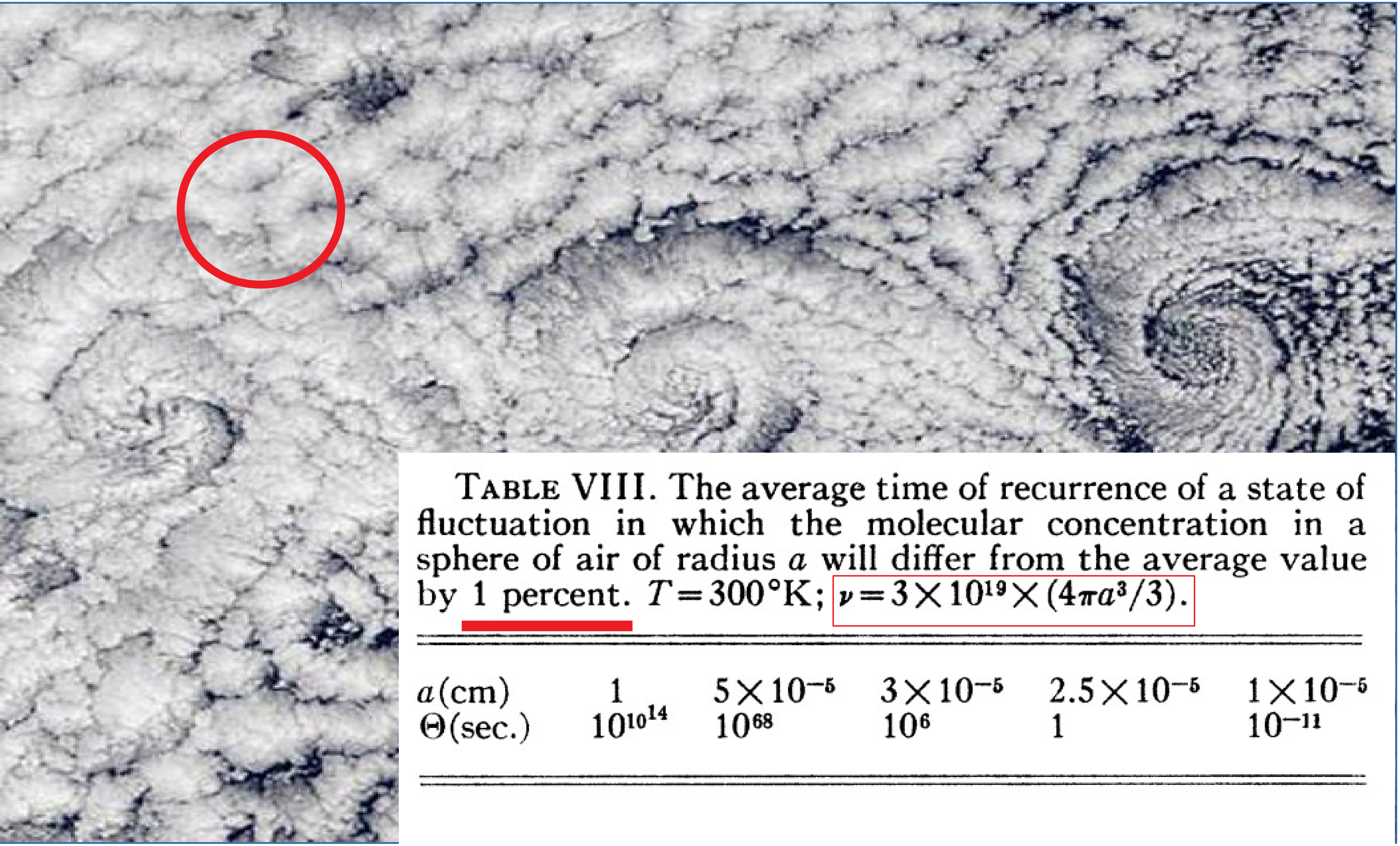


TABLE VIII. The average time of recurrence of a state of fluctuation in which the molecular concentration in a sphere of air of radius a will differ from the average value by 1 percent. $T=300°K$; $\nu=3\times10^{19}\times(4\pi a^3/3)$.

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

EQUILIBRIUM VERSUS NONEQUILIBRIUM

ΔG = free energy supply by reactive event

2nd law of thermodynamics
entropy production rate

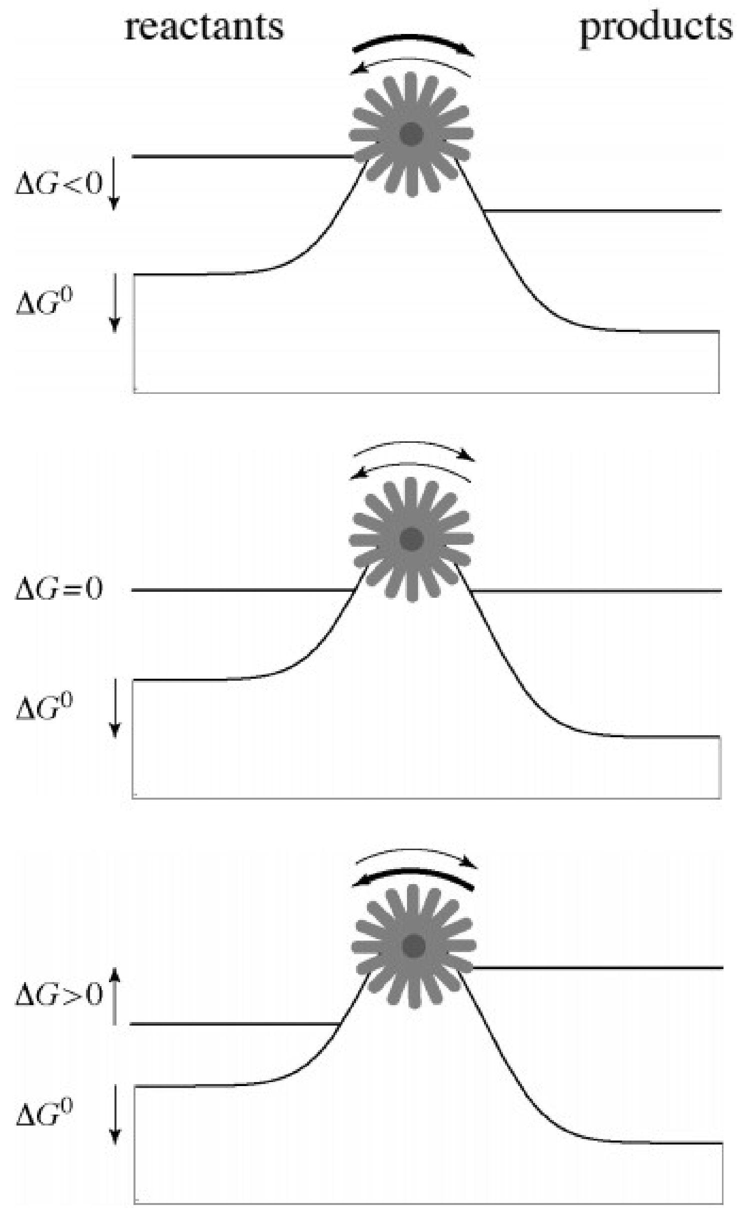
$$\frac{d_i S}{dt} = -\frac{\Delta G}{T} \times \text{rate} \geq 0$$

Th. De Donder
I. Prigogine
P. Glansdorff
G. Nicolis

out of equilibrium:
$\Delta G < 0$
rate > 0

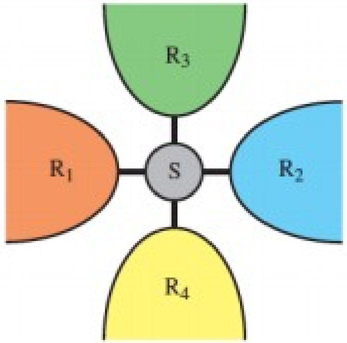
equilibrium:
$\Delta G = 0$
rate $= 0$

out of equilibrium:
$\Delta G > 0$
rate < 0



PRINCIPLES OF DYNAMICAL ORDERING AT THE NANOSCALE

FLUCTUATION THEOREM FOR CURRENTS



fluctuating currents: $\mathbf{J} = \Delta\mathbf{N}/t,\ \Delta\mathbf{r}/t$

ex:
- electric currents in open quantum systems
- rates of chemical reactions
- velocity of a molecular motor

De Donder affinities or thermodynamic forces: (non-fluctuating) $\mathbf{A} = \frac{\Delta \mathbf{G}}{kT}$ (free energy sources)

Stationary probability distribution $P_{\mathbf{A}}(\mathbf{J})$:

- No directionality at equilibrium $\mathbf{A} = 0$
- Directionality out of equilibrium $\mathbf{A} \neq 0$

$$\frac{P_{\mathbf{A}}(\mathbf{J})}{P_{\mathbf{A}}(-\mathbf{J})} \underset{t\to\infty}{\approx} \exp(\mathbf{A}\cdot\mathbf{J}\,t)$$

consequence of microreversibility

The thermodynamic entropy production is always non-negative:

$$\frac{1}{k_{\mathrm{B}}}\frac{d_{\mathrm{i}}S}{dt} = \mathbf{A}\cdot\langle\mathbf{J}\rangle_{\mathbf{A}} \geq 0$$

COUPLING BETWEEN THE CURRENTS

D. Andrieux & P. Gaspard, J. Chem. Phys. **121** (2004) 6167; J. Stat. Phys. **127** (2007) 107

THEOREM OF NONEQUILIBRIUM DYNAMICAL ORDERING

Out of equilibrium, the typical histories are more probable than the corresponding time-reversed histories: **dynamical order.**

$$\frac{\text{Prob(typical history)}}{\text{Prob(time - reversed history)}} \approx \exp\left(\frac{\Delta_{\mathrm{i}}S}{k_{\mathrm{B}}}\right)$$

P. Gaspard, J. Stat. Phys. **117** (2004) 599; C. R. Phys. **8** (2007) 598

BIOMOLECULAR MOTORS & PROCESSORS

Rotary motor: F_1-ATPase + filament/bead

K. Kinosita and coworkers (2001,2004)
Itoh et al., Nature **427** (2004) 465

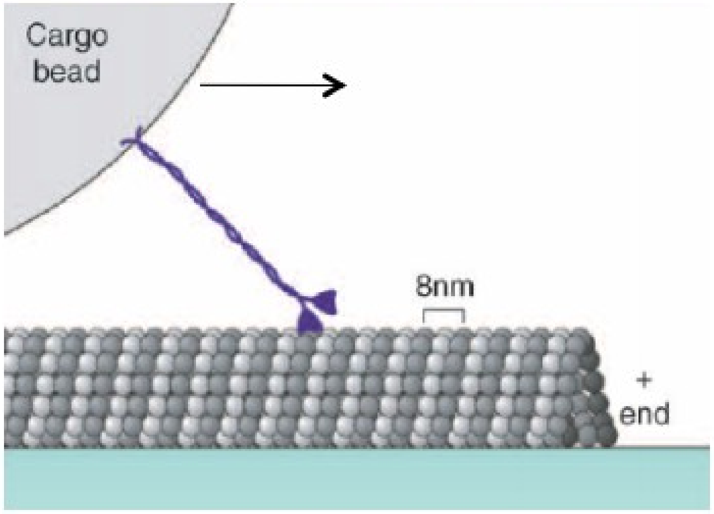
ATP hydrolysis drives the rotation.

A mechanical force is also applied.

$T = 300$ K
power = 10^{-18} Watt

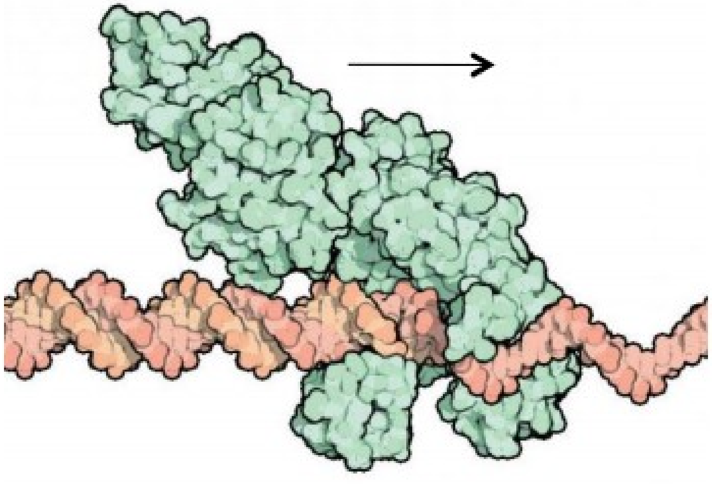
ATP hydrolysis/synthesis
is coupled to
mechanical motion/force.

Linear motor: kinesin-microtubule

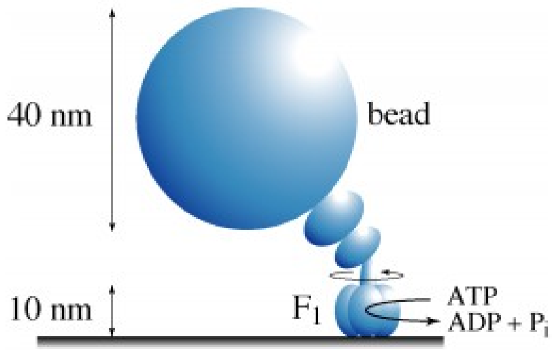


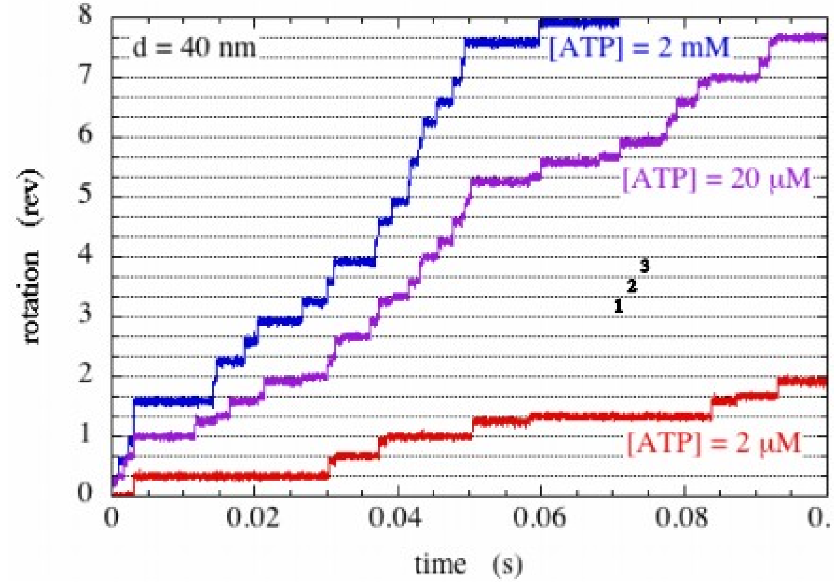
Wikipedia

Information processor: DNA polymerase

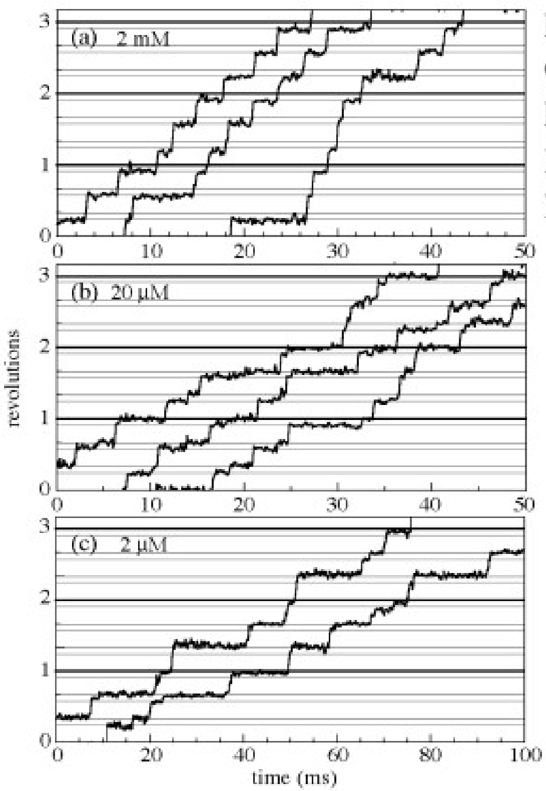


NONEQUILIBRIUM DIRECTIONALITY IN THE F_1-ATPase MOTOR





Simulations of random trajectories:
P. Gaspard & E. Gerritsma,
J. Theor. Biol. **247** (2007) 672



Random trajectories
observed in experiments:
R. Yasuda, H. Noji, M. Yoshida,
K. Kinosita Jr. & H. Itoh,
Nature **410** (2001) 898

at equilibrium:
…212132131223132…
(random)

detailed balance between
forward and backward rotations,
zero currents

out of equilibrium:
…123123123123123…
(more regular)

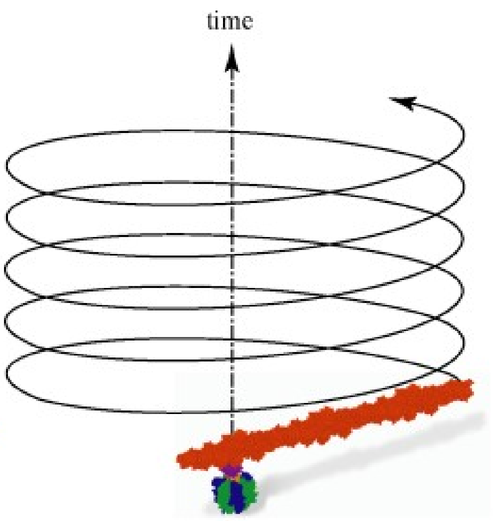
directionality of motion:
non-zero currents,
dynamical order

OUT-OF-EQUILIBRIUM MOLECULAR MACHINES

Nanosystems sustaining fluxes of matter or energy, dissipating energy supply

Examples:
- rotary or linear molecular motors
- ribosome: translation from mRNA to proteins
- RNA or DNA polymerase: transcription or replication

Equilibrium:	***Nonequilibrium:***
• no flux $\langle J_\gamma \rangle = 0$	• flux $\langle J_\gamma \rangle \neq 0$
• no entropy production $\frac{d_i S}{dt} = 0$	• entropy production $\frac{d_i S}{dt} > 0$
• no energy supply needed	• energy supply required
• in contact with one reservoir	• in contact with several reservoirs
• structure in 3D space	• dynamics in 4D space-time
• no directionality	• directionality, **dynamical order**, **function**

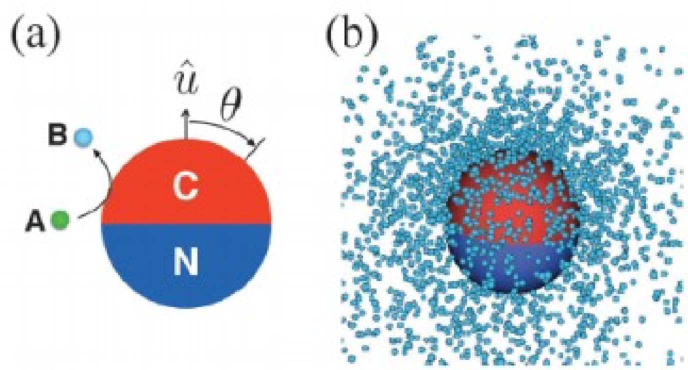


P. Gaspard, in A. S. Mikhailov & G. Ertl, Editors, *Engineering of Chemical Complexity* (World Scientific, 2013) pp. 51-77

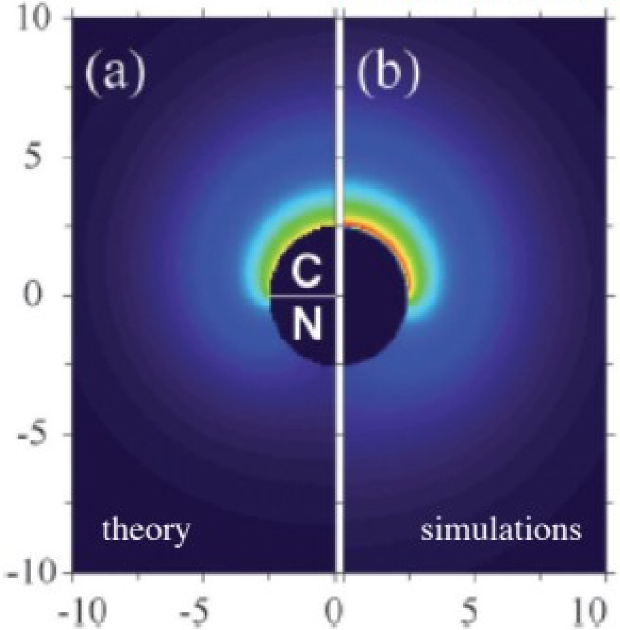
SELF-PHORETIC (self-steering) MOTORS

PROPULSION BY SELF-DIFFUSIOPHORESIS

The fluid flow is modified by the interaction of reactant A and product B with the active particle.



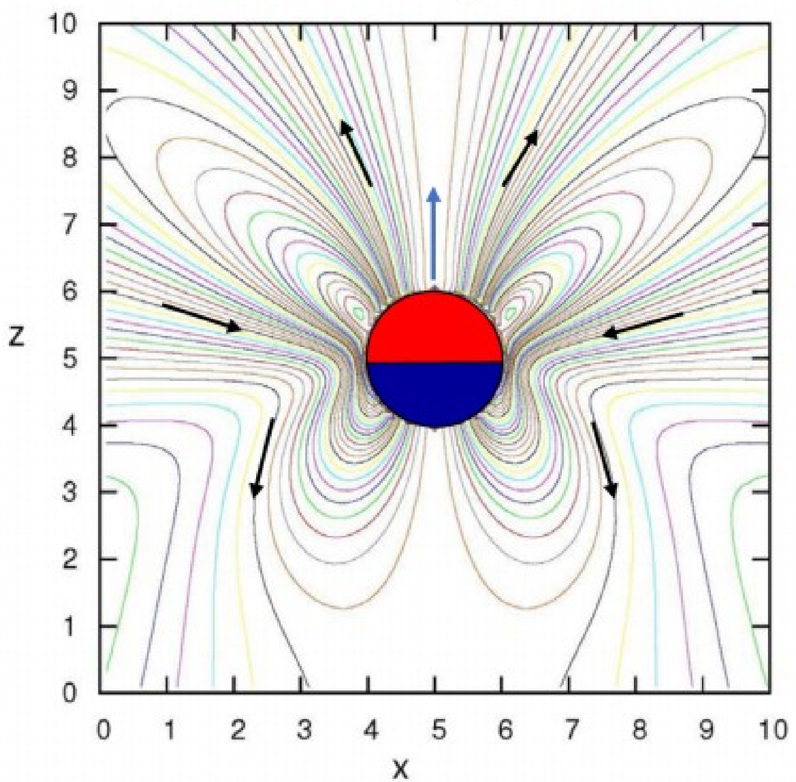
Janus particle with catalytic (C) and non-catalytic (N) hemispheres



concentration field of product B

M.-J. Huang, J. Schofield & R. Kapral, Soft Matter **12** (2016) 5581

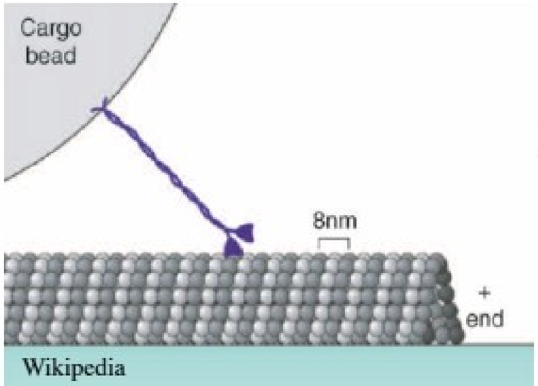
fluid velocity field



S. Y. Reigh, M.-J. Huang, J. Schofield & R. Kapral, Phil. Trans. R. Soc. A **374** (2016) 20160140

MECHANOCHEMICAL COUPLING FOR ENERGY TRANSDUCTION

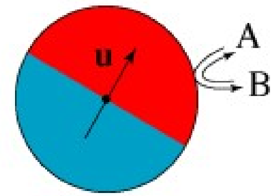
MOLECULAR MOTORS

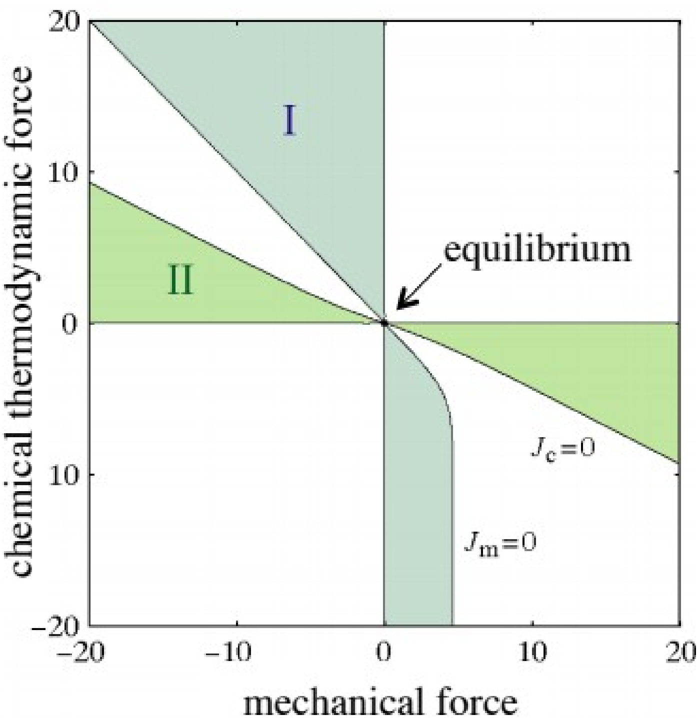


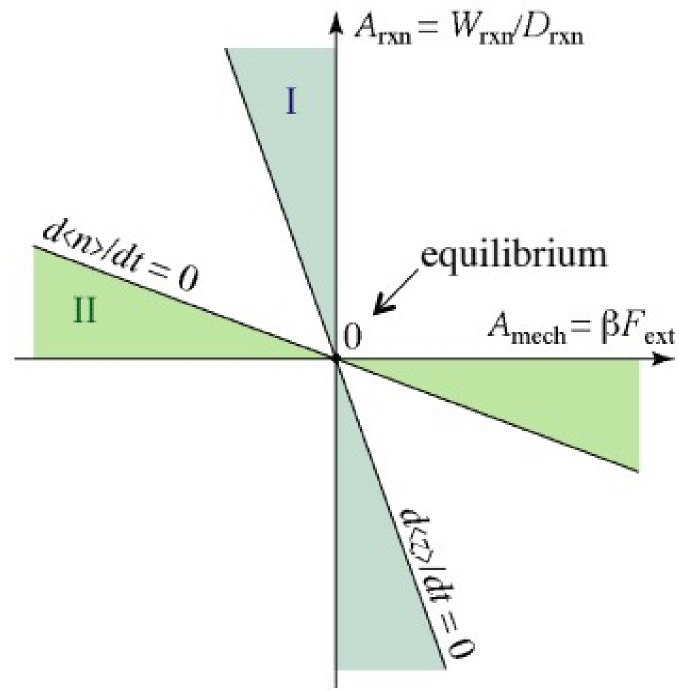
ACTIVE PARTICLES

I: mechanical work

II: fuel synthesis





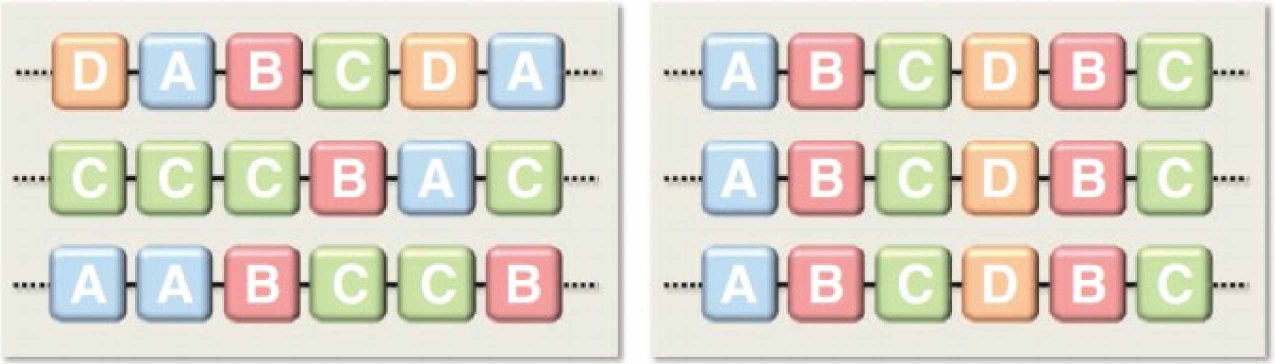


P. Gaspard & R. Kapral, Adv. Phys. X **4** (2019) 1602480

MOLECULAR INFORMATION PROCESSING

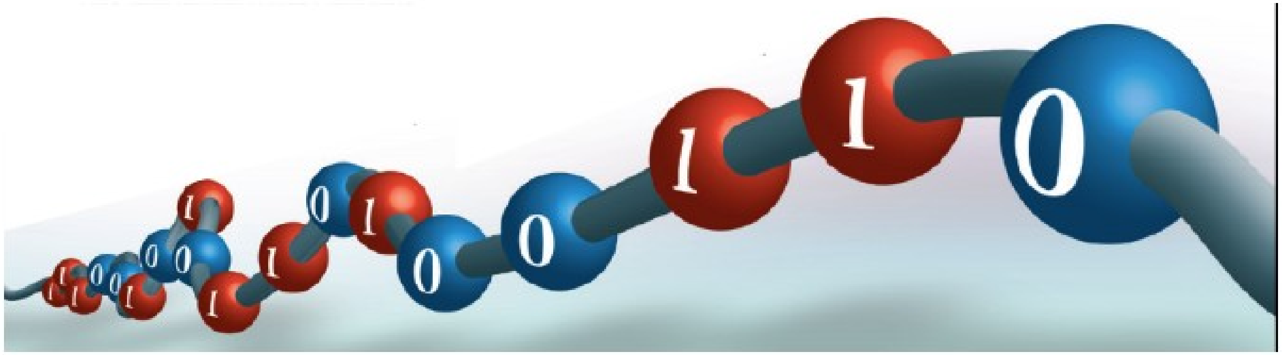
INFORMATION STORAGE IN COPOLYMERS

Jean-François Lutz, Makoto Ouchi, David R. Liu, and Mitsuo Sawamoto, *Sequence-Controlled Polymers*, Science **341** (2013) 628



Precise molecular encoding of synthetic polymer chains. In most synthetic copolymers, monomer units (represented here as colored square boxes A, B, C, and D) are distributed randomly along the polymer chains (**left**). In sequence-controlled polymers, they are arranged in a specific order in all of the chains (**right**). Monomer sequence regularity strongly influences the molecular, supramolecular, and macroscopic properties of polymer materials.

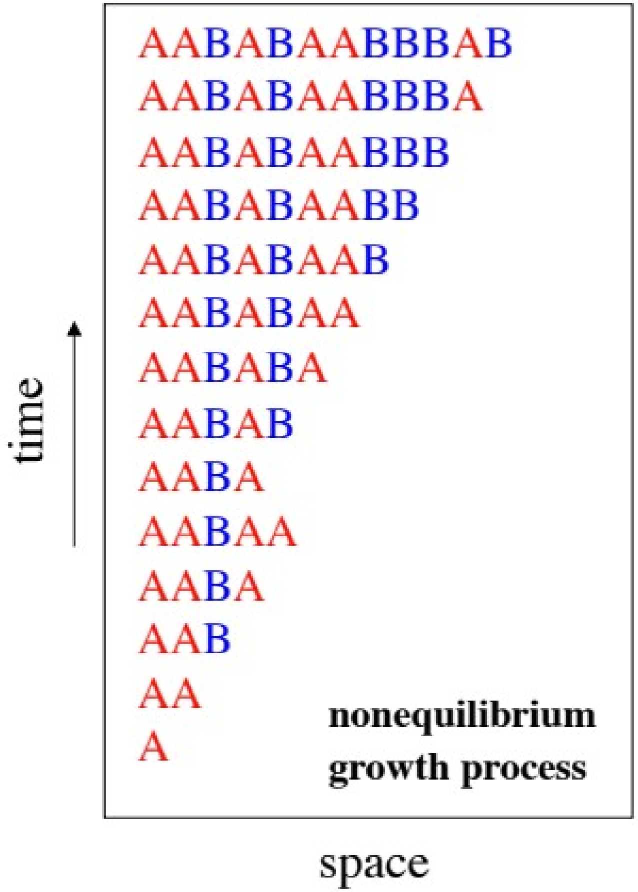
Howard Colquhoun and Jean-François Lutz, *Information-containing macromolecules*, Nature Chemistry **6** (2014) 455

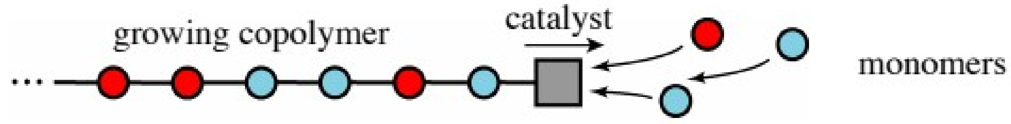


COPOLYMERIZATION PROCESSES

statistical copolymer = spatial support of information

= aperiodic crystal by E. Schrödinger, *What is Life?* (1944)

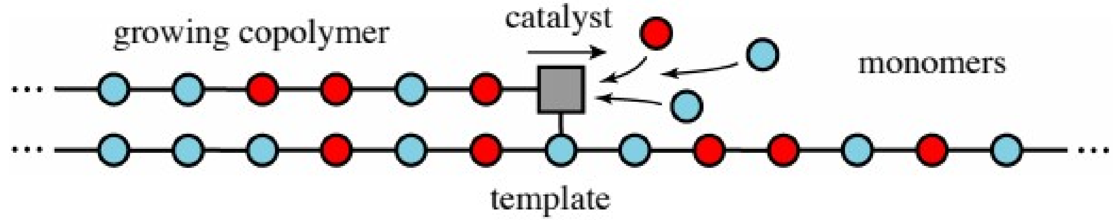




free copolymerization:

statistical copolymers

ex: ethylene/1-octene copolymer



template-directed copolymerization:

ex: DNA replication

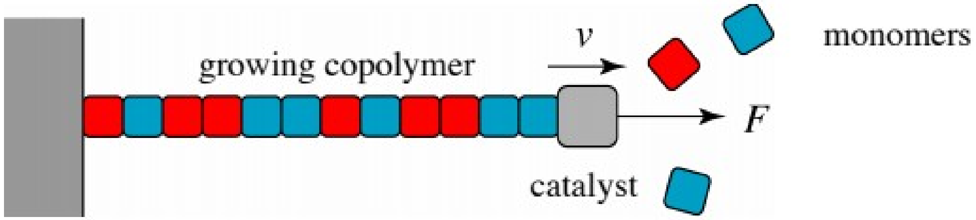
DNA-mRNA transcription

mRNA-protein translation

D. Andrieux & P. Gaspard, *Nonequilibrium generation of information in copolymerization processes*
Proc. Natl. Acad. Sci. U.S.A. **105** (2008) 9516

THERMODYNAMICS OF COPOLYMERIZATION

free copolymerization



growth velocity: v

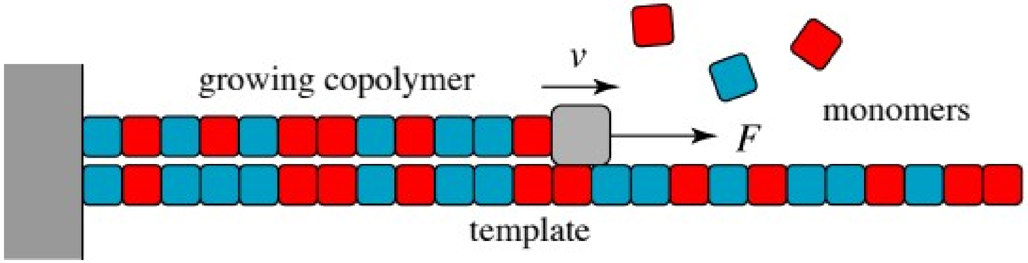
free-energy driving force: $\varepsilon = -\frac{g}{k_B T}$

sequence disorder: D

entropy production rate:

$$\frac{1}{k_B}\frac{d_i S}{dt} = v\left[\varepsilon + D(\text{sequence})\right] \geq 0$$

template-directed copolymerization



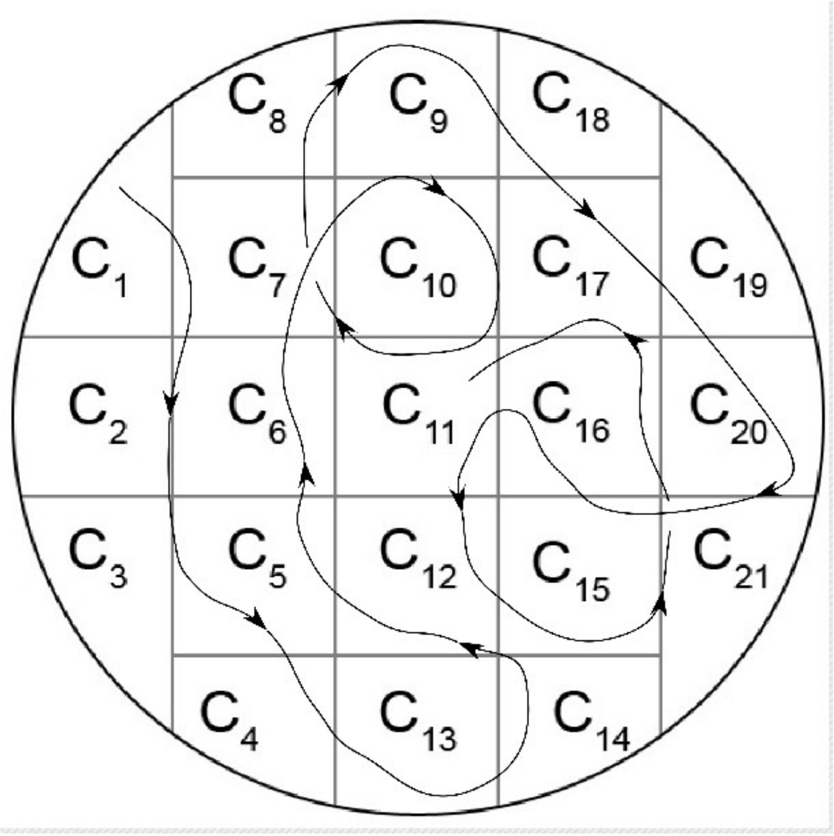
mutual information between the copy and the template: I

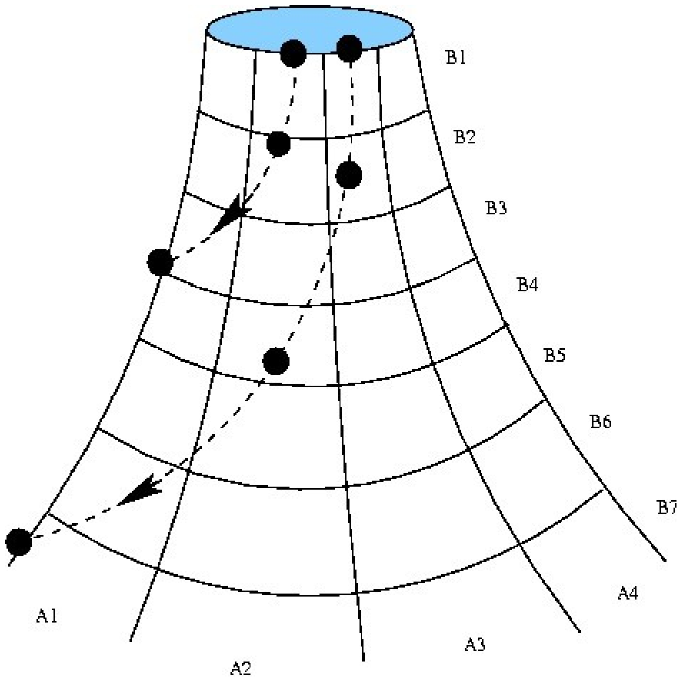
entropy production rate:

$$\frac{1}{k_B}\frac{d_i S}{dt} = v\left[\varepsilon + D(\text{copy}) - I(\text{copy,template})\right] \geq 0$$

D. Andrieux & P. Gaspard, *Nonequilibrium generation of information in copolymerization processes*
Proc. Natl. Acad. Sci. U.S.A. **105** (2008) 9516

“Coarse Graining”
“Symbolic Dynamics”





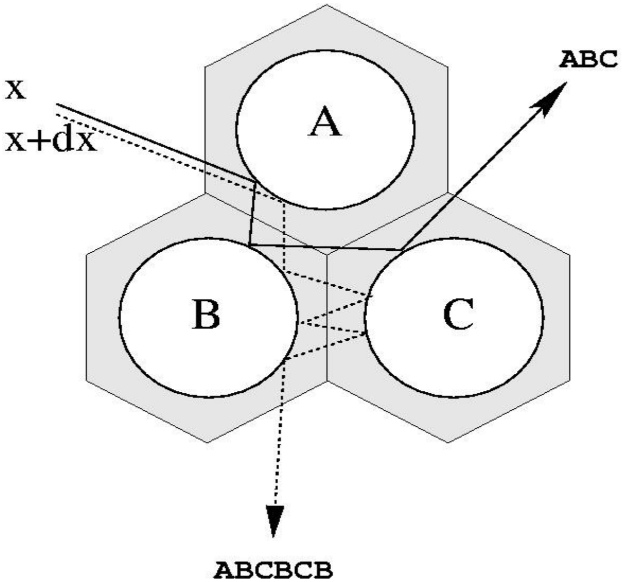
Poincaré (1890s) & Maxwell:
Nonlinear dynamical systems can exhibit sensitive dependence on initial conditions

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

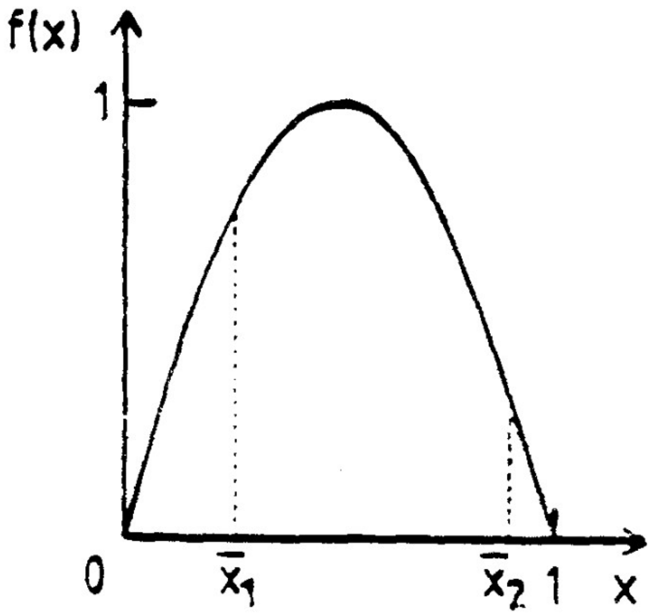
Sinai: a physical billiard can be ergodic.



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)

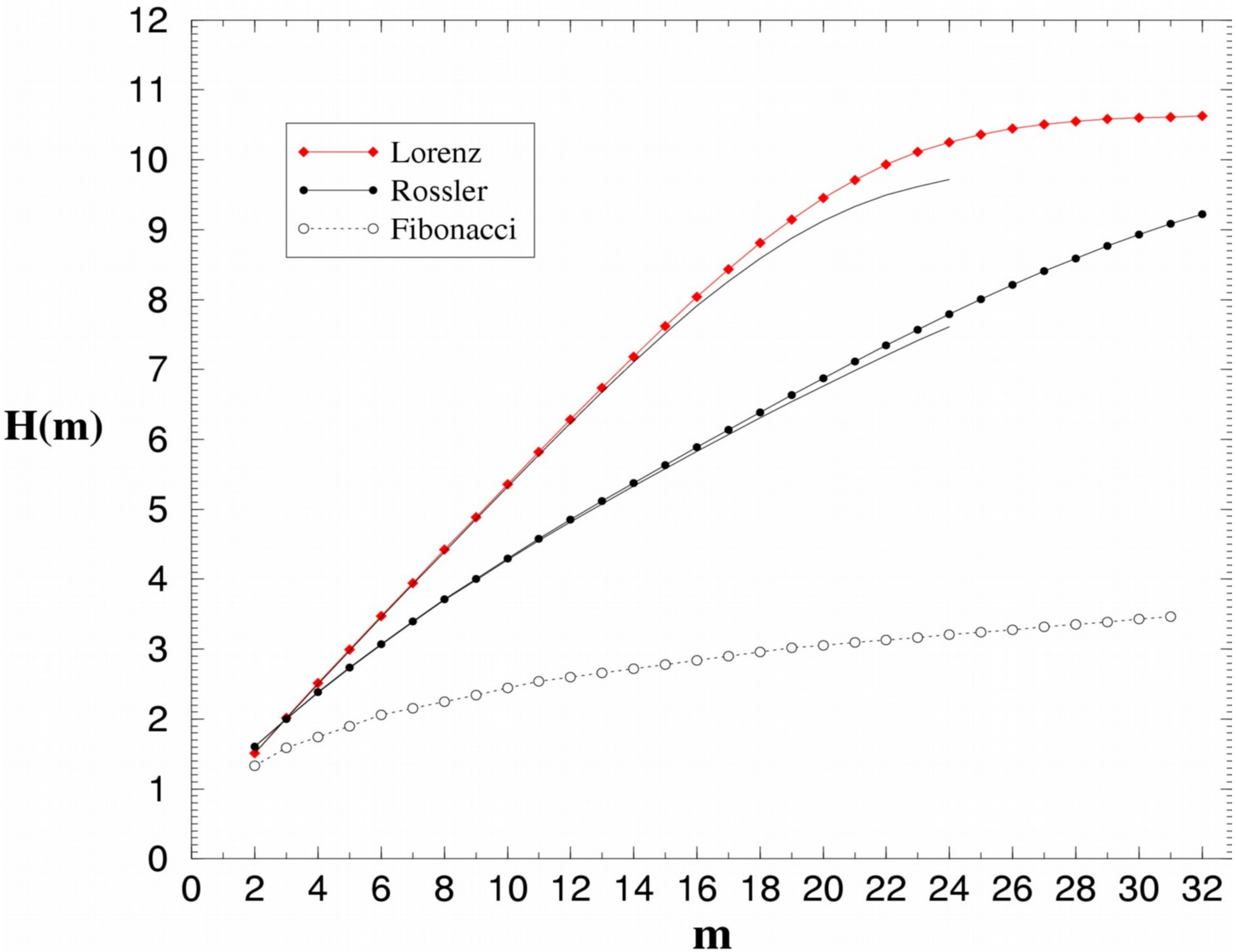
Shannon-McMillan Theorem :
The probability of a word of length m to appear
is "penalized" according to Entropy scaling w.r.t. its length

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

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.

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



$$H = hm$$

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

$$H = \log(m)$$

- 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

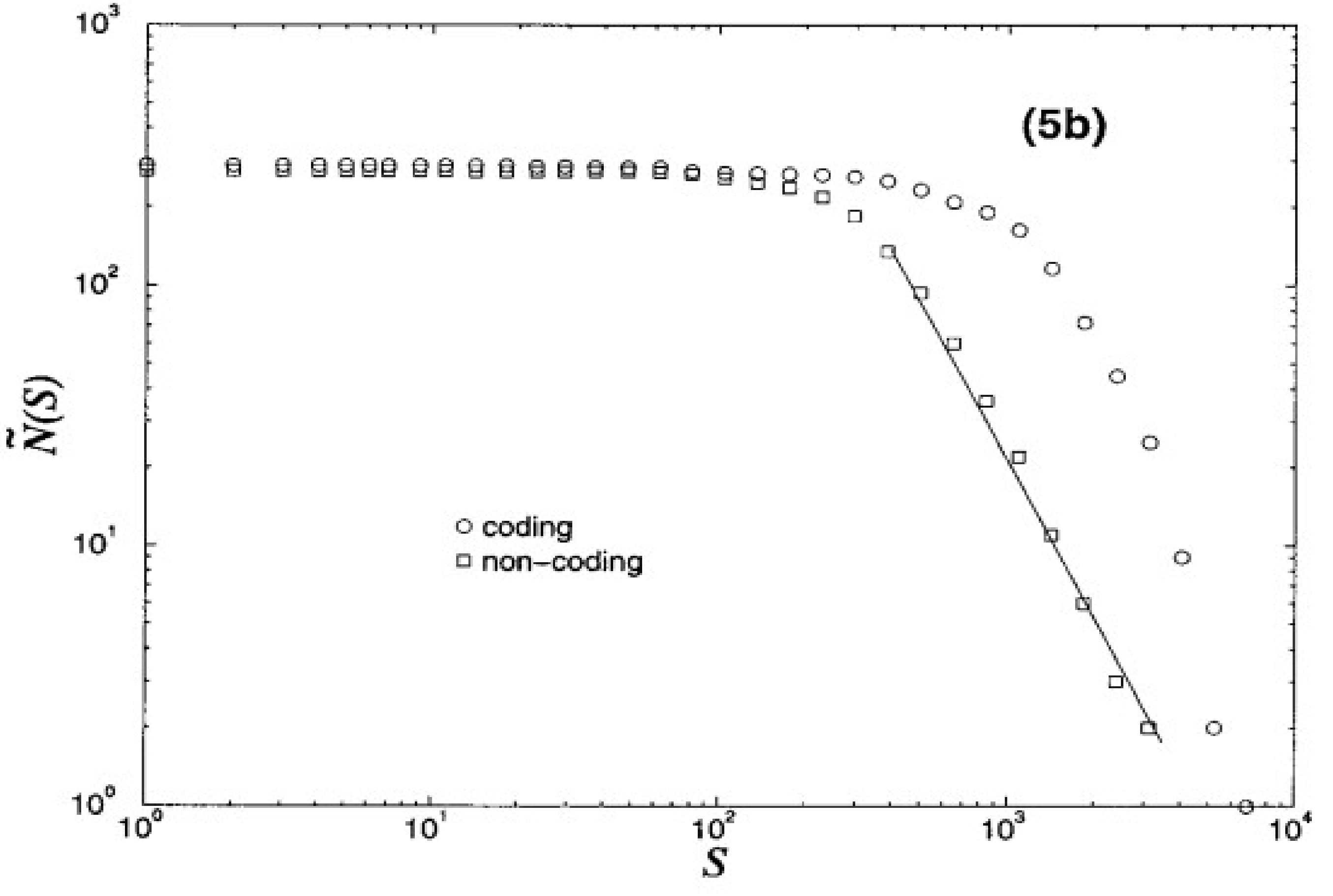
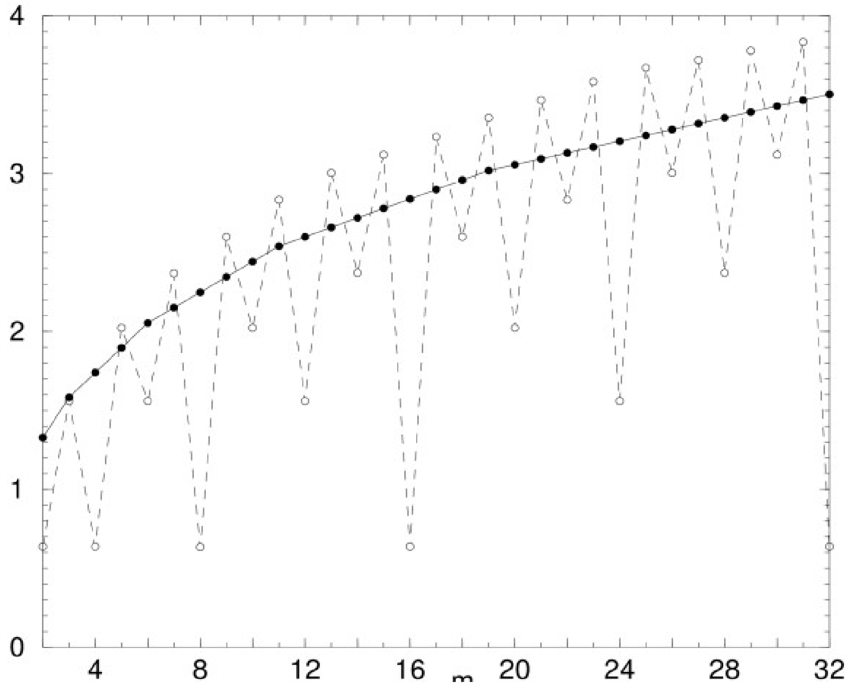


Fig. 5. The number of coding and non-coding regions of size $\geqslant S$, $\tilde{N}(S)$, for three fungal DNA sequences. The straight lines have the following slopes: (5a) $-\mu = -0.8$, (5b) $-\mu = -1.8$ and (5c) $-\mu = -1.3$.



META-SELECTION RULES:

Syntax, Context & Semantics

“We are no where”

“We are now here”

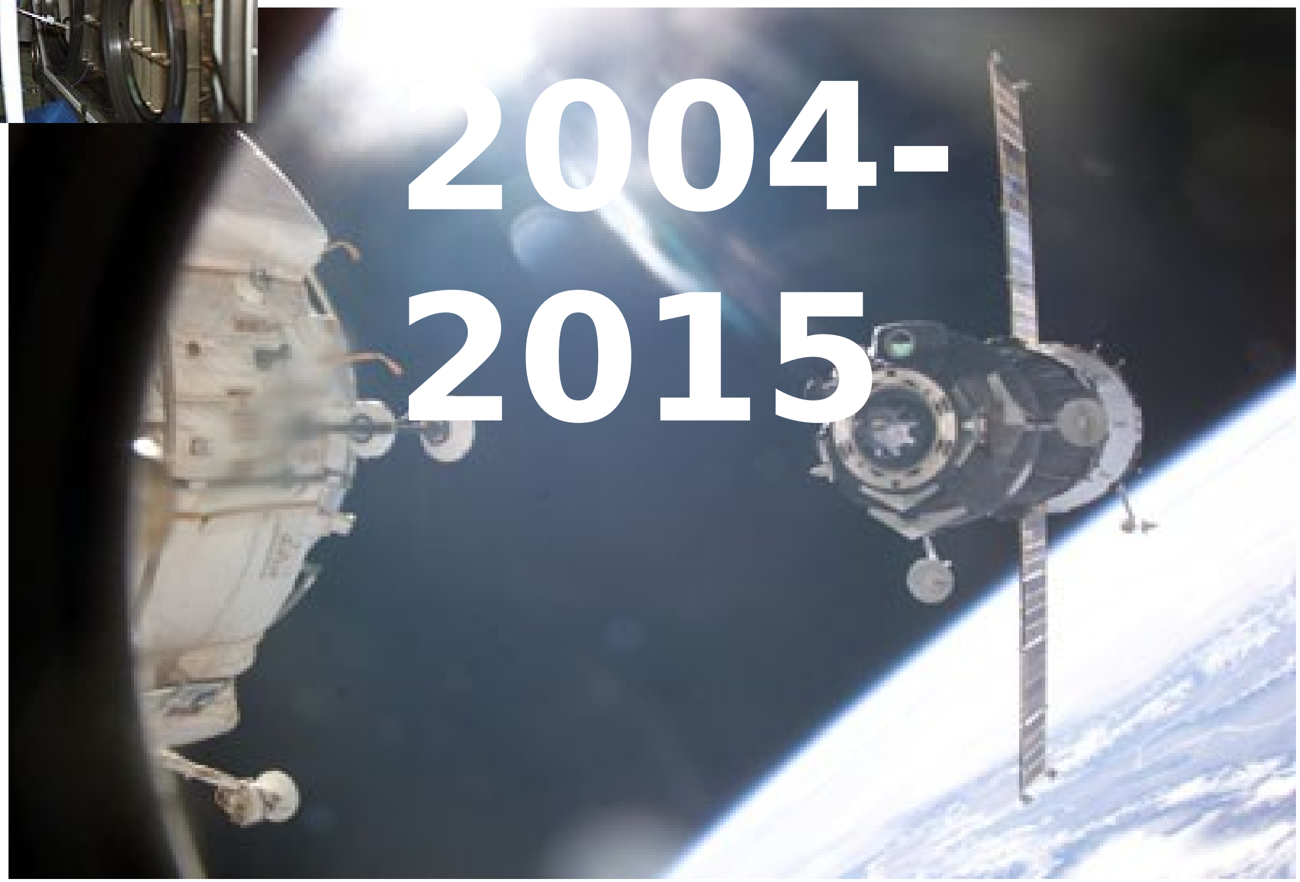
AUTOMATICITY & context:
K. Karamanos and G. Nicolis,
"Symbolic dynamics and entropy analysis of Feigenbaum limit sets",
Chaos, Solitons & Fractals 10(7), 1135-1150 (1999).

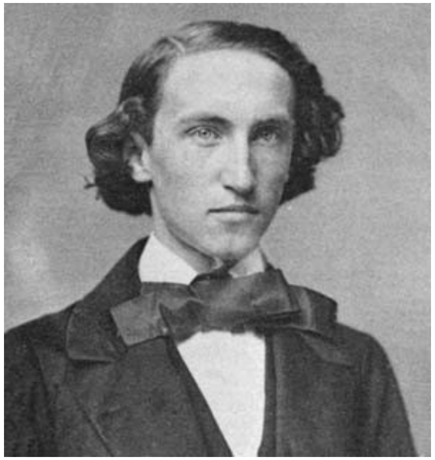
META-SELECTION RULES, context & the 'Nicolis-Ebeling Conjecture':

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)

A new paradigm of nucleation and self-assembly

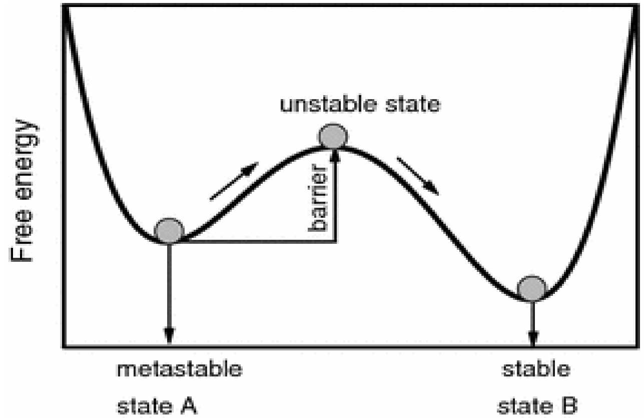
Complex Matter Science initiative at ESA
&
the SOYUZ missions in ISS





Josiah Willard Gibbs (1839 - 1903)

stealing an idea from Gibbs to understand nucleation:



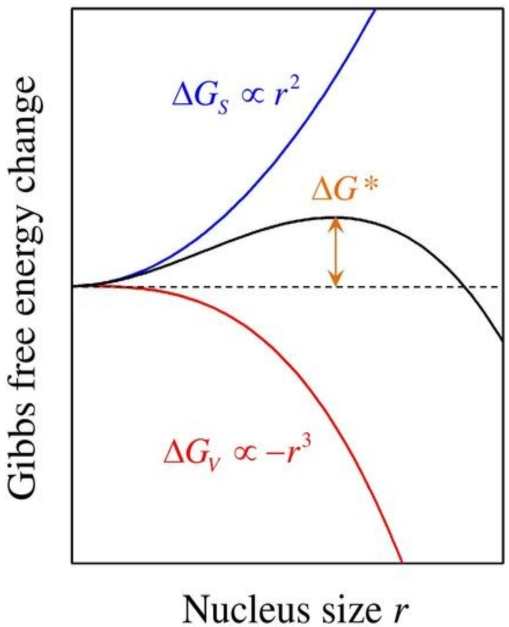
$$\Delta G = r(i)\, \Delta G(i) - T\Delta S(r(i))$$

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

Equilibrium Assumption

$$N \rightleftharpoons N^* \longrightarrow S$$

a)



- Gibbs free energy change of nucleation

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

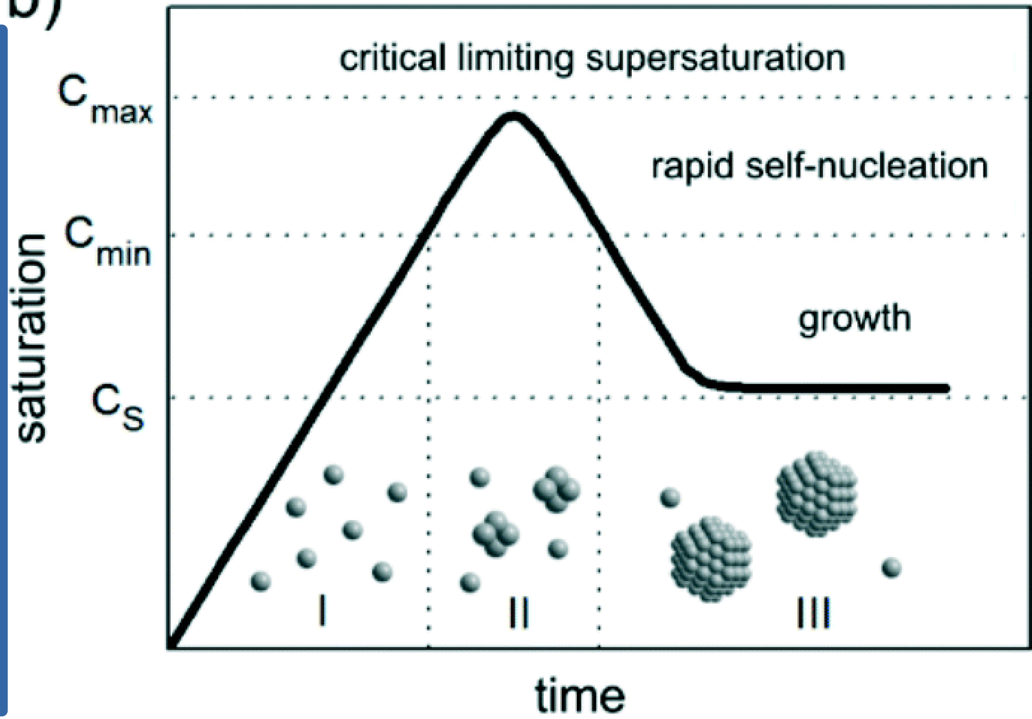
- Critical nucleus size

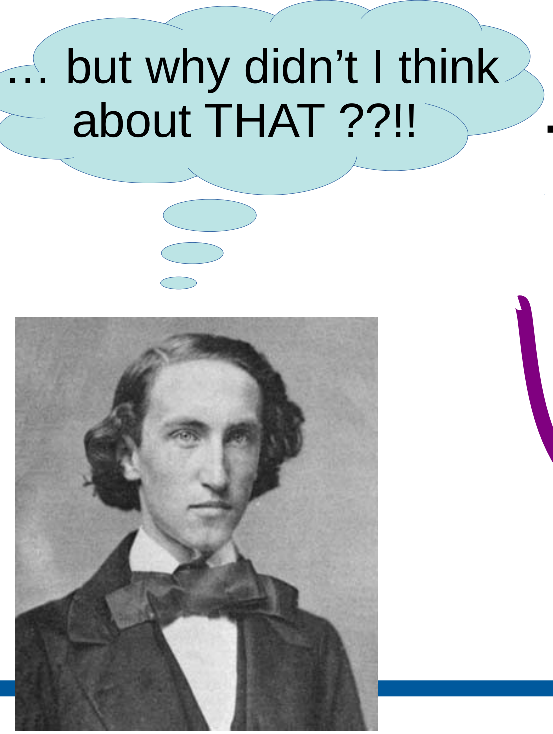
$$r^* = \frac{2\gamma T_m}{\Delta H_m \Delta T}$$

- Energy barrier towards nucleation

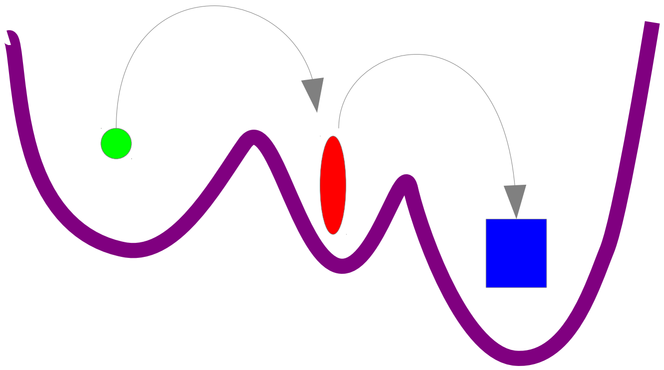
$$\Delta G^* = \frac{16\pi}{3} \cdot \frac{\gamma^3 T_m^2}{\Delta H_m^2 \Delta T^2}$$

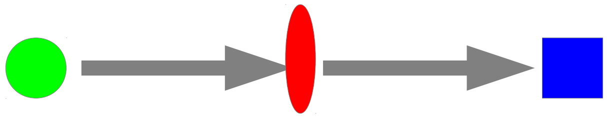
b)



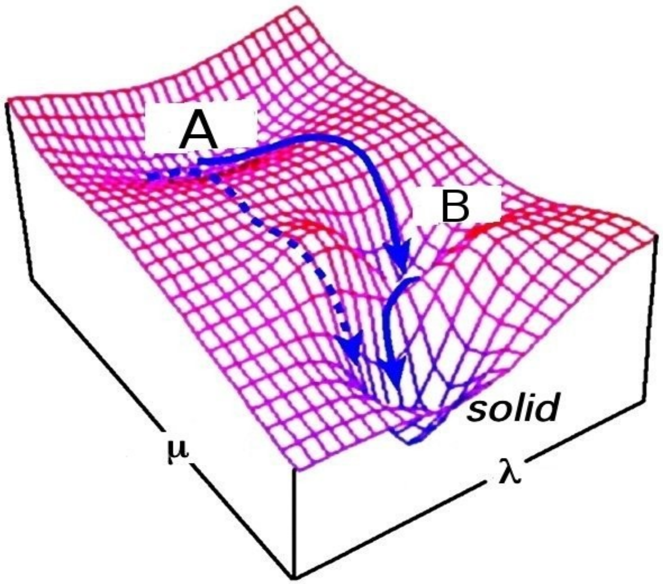


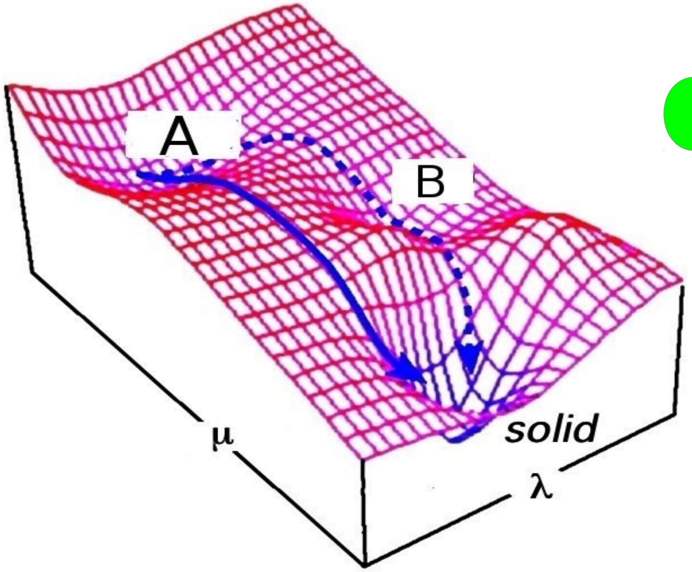
TWO-steps, ONE order-parameter

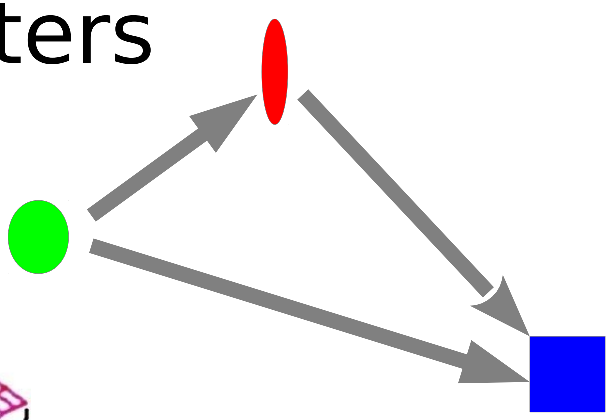




TWO-steps, TWO order-parameters



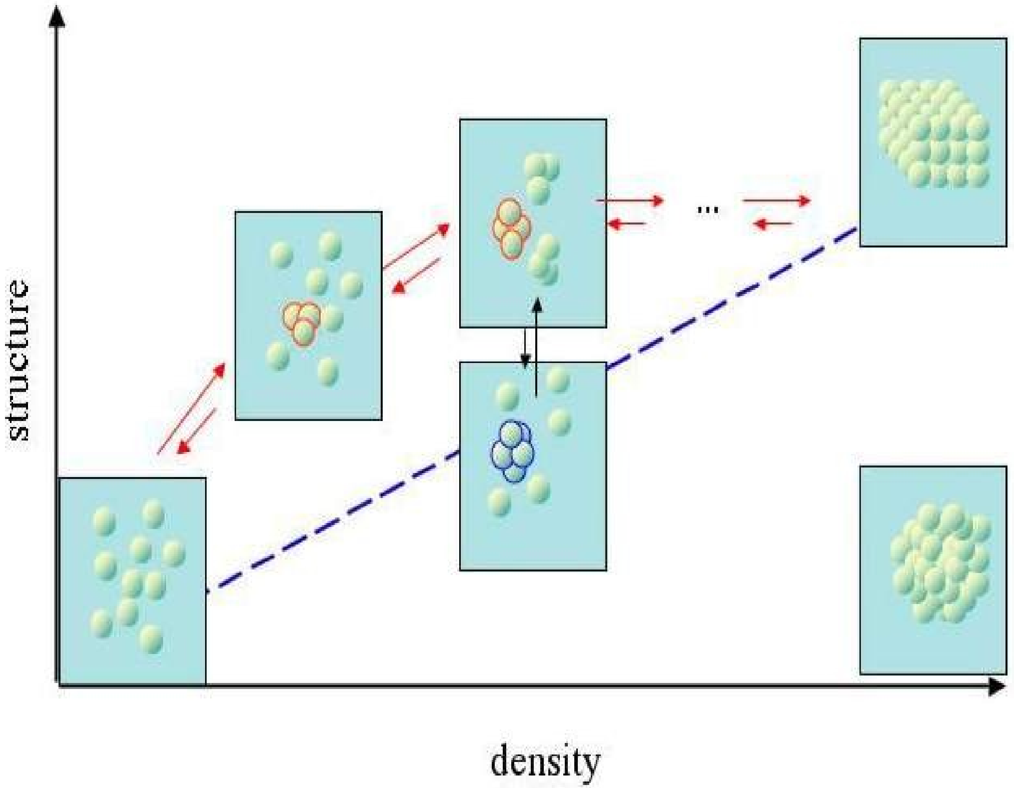




Non standard nucleation mechanisms with combined structural and density fluctuations

- 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

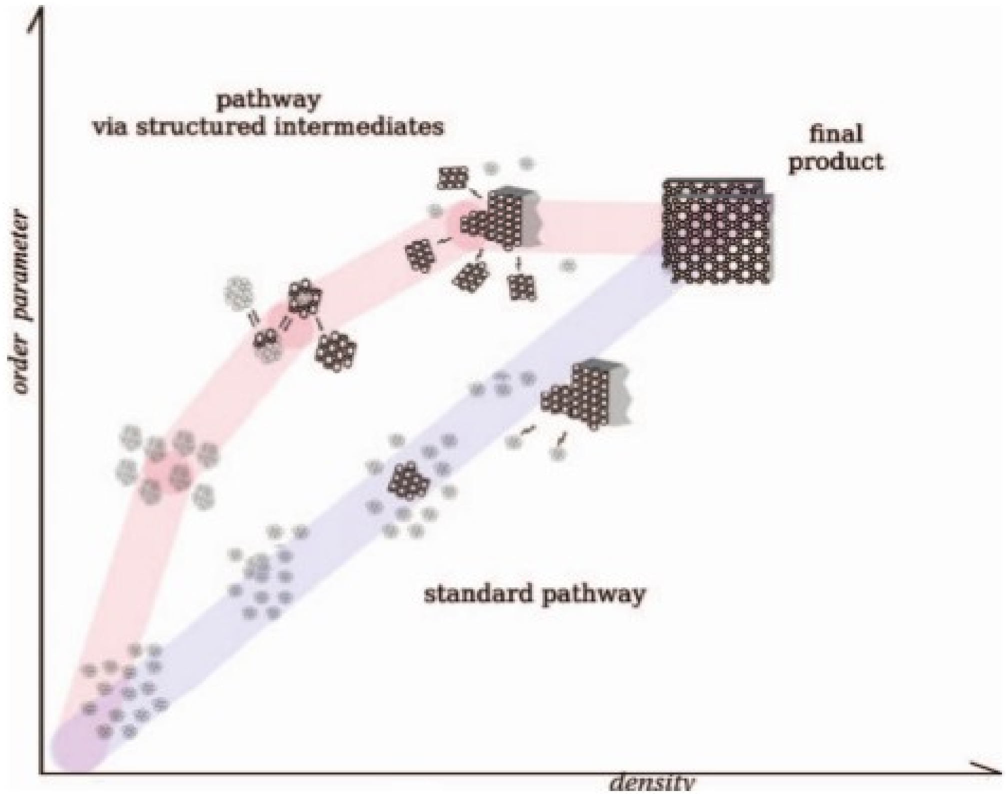
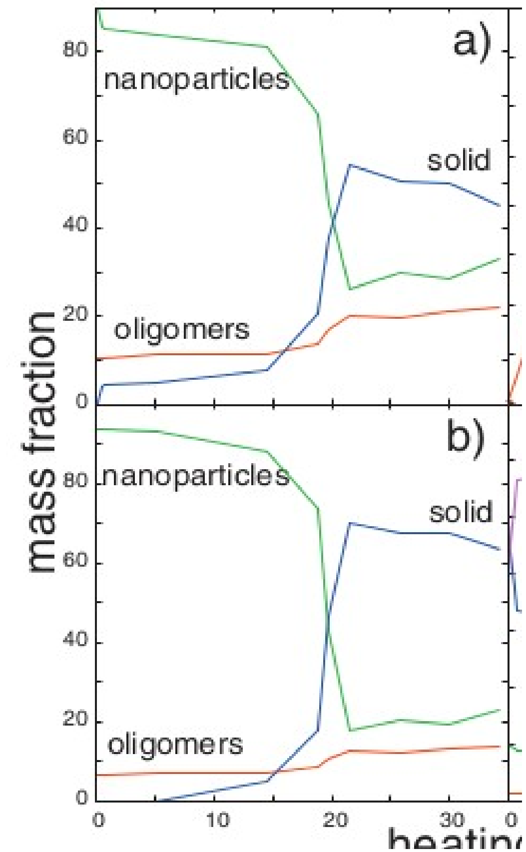


FIG. 1. A schematic demonstration of multistep versus standard synthetic



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

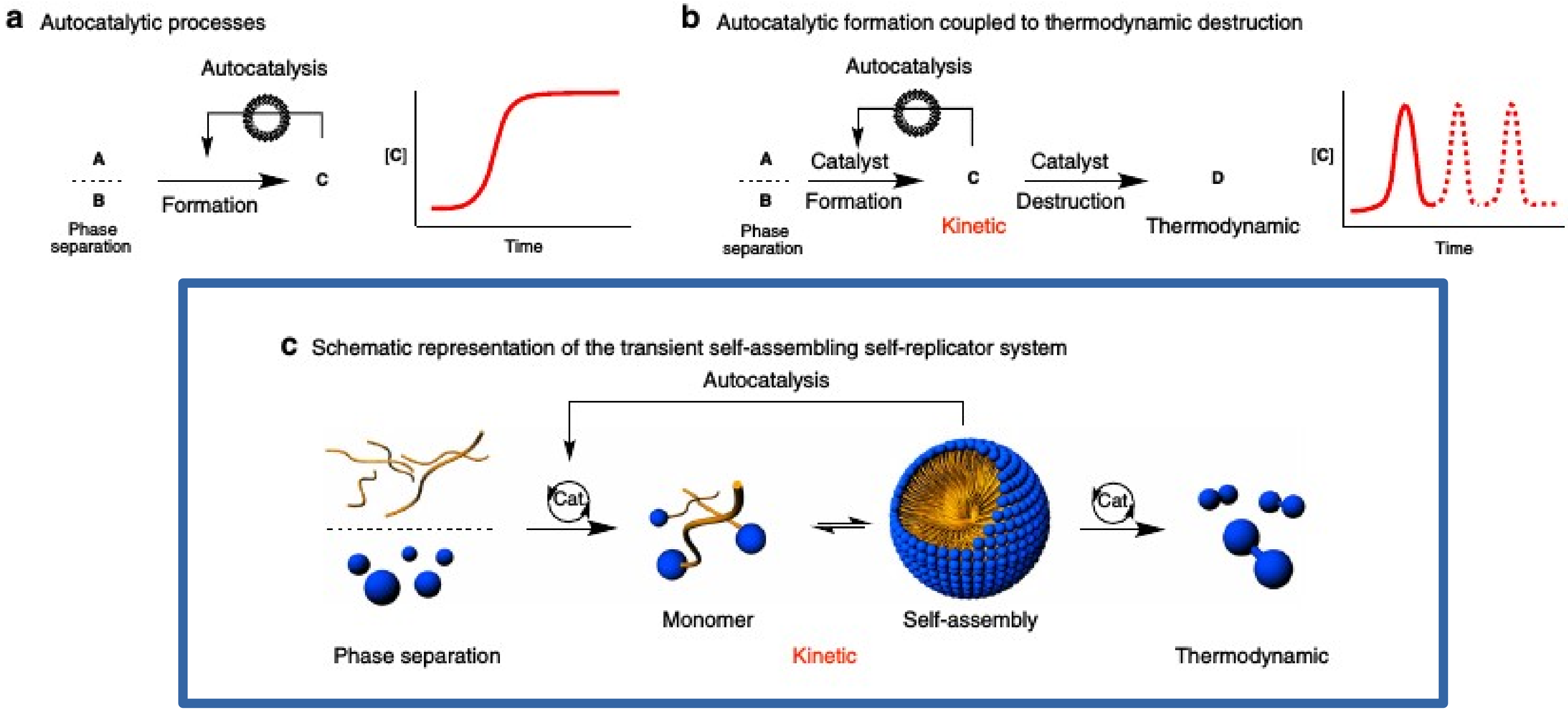
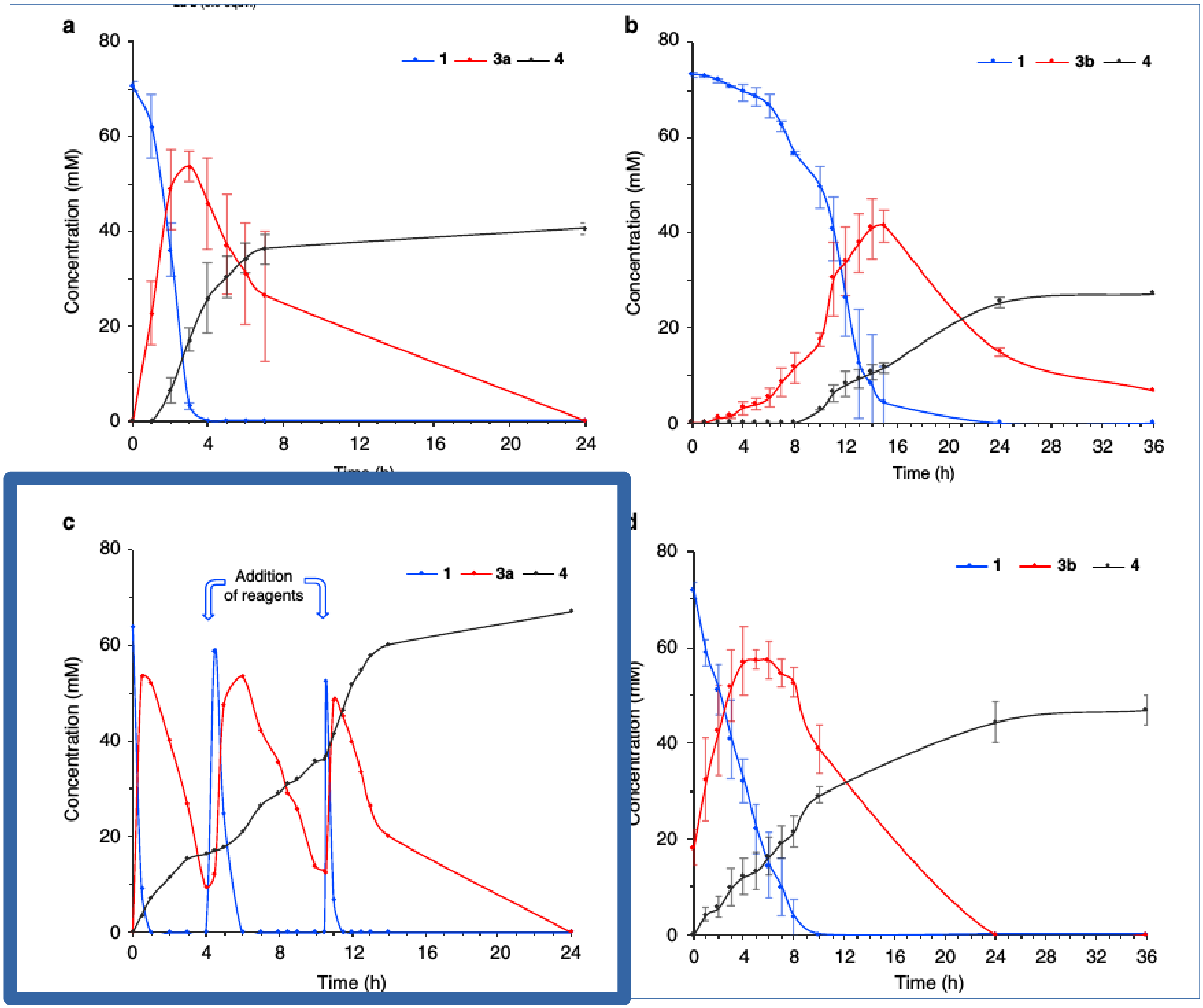


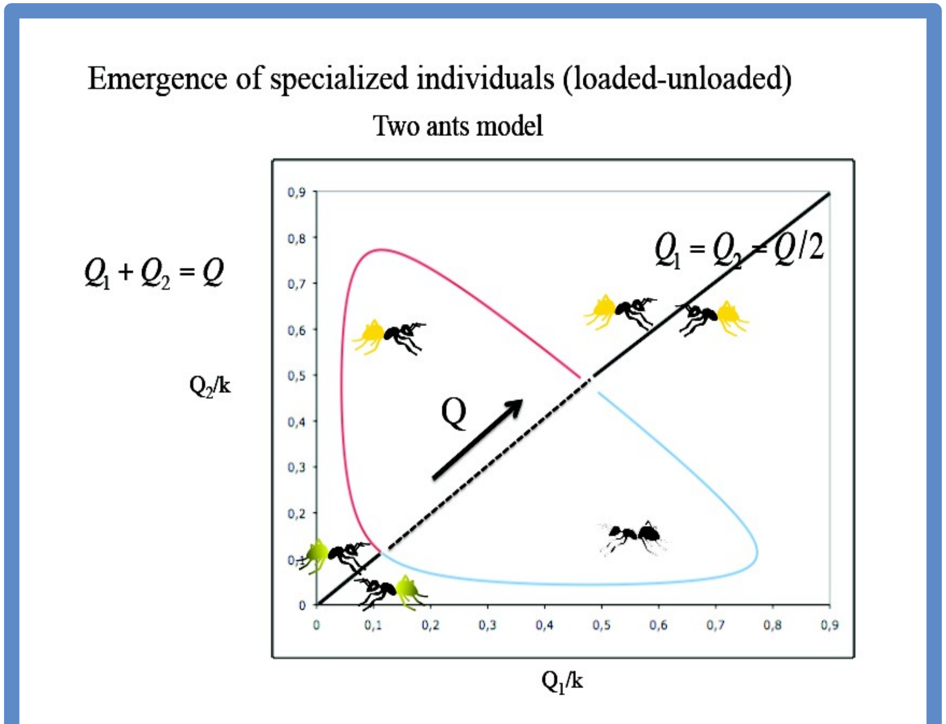
Fig. 1 Examples of autocatalysis. **a** An autocatalytic system based on phase separation. **b** An autocatalytic system based on phase separation, coupled to thermodynamic destruction, that in a closed set-up experiment will evolve towards thermodynamic equilibrium. **c** Schematic representation of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

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

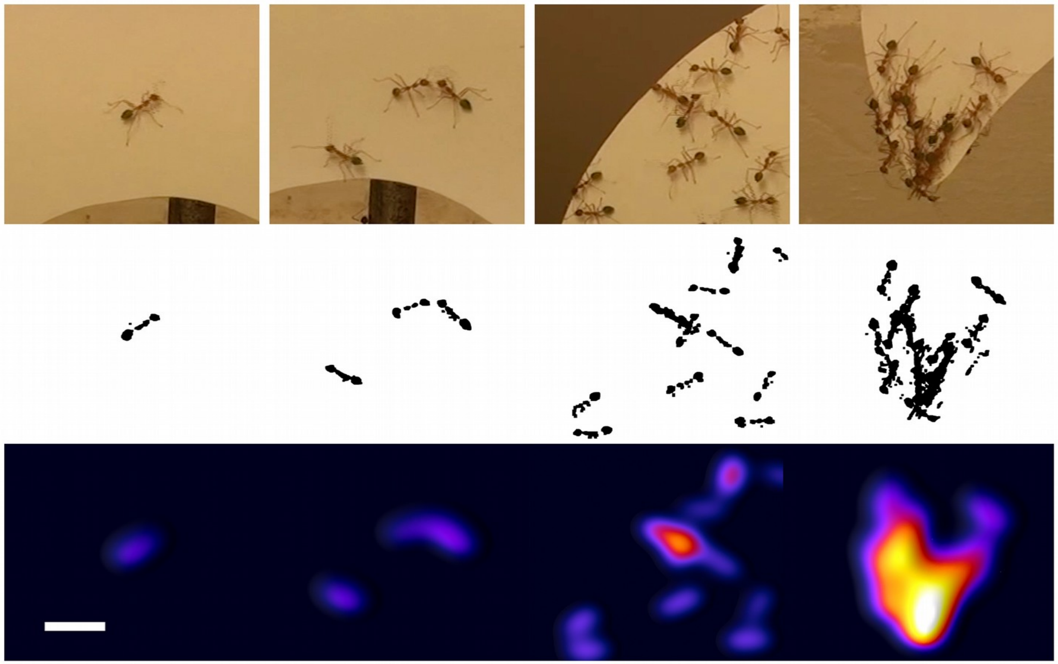


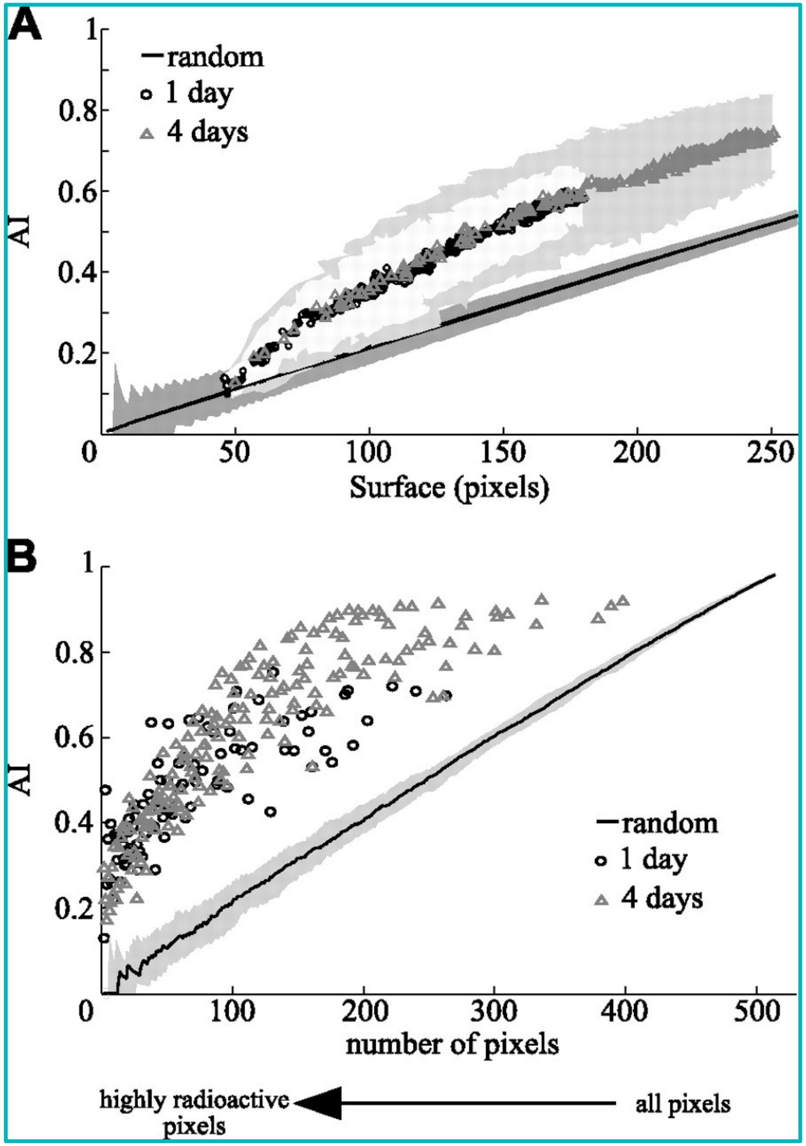
Diversion: “many-step aggregation in social animals”

Trophallaxis Colony's Social Stomach filling up



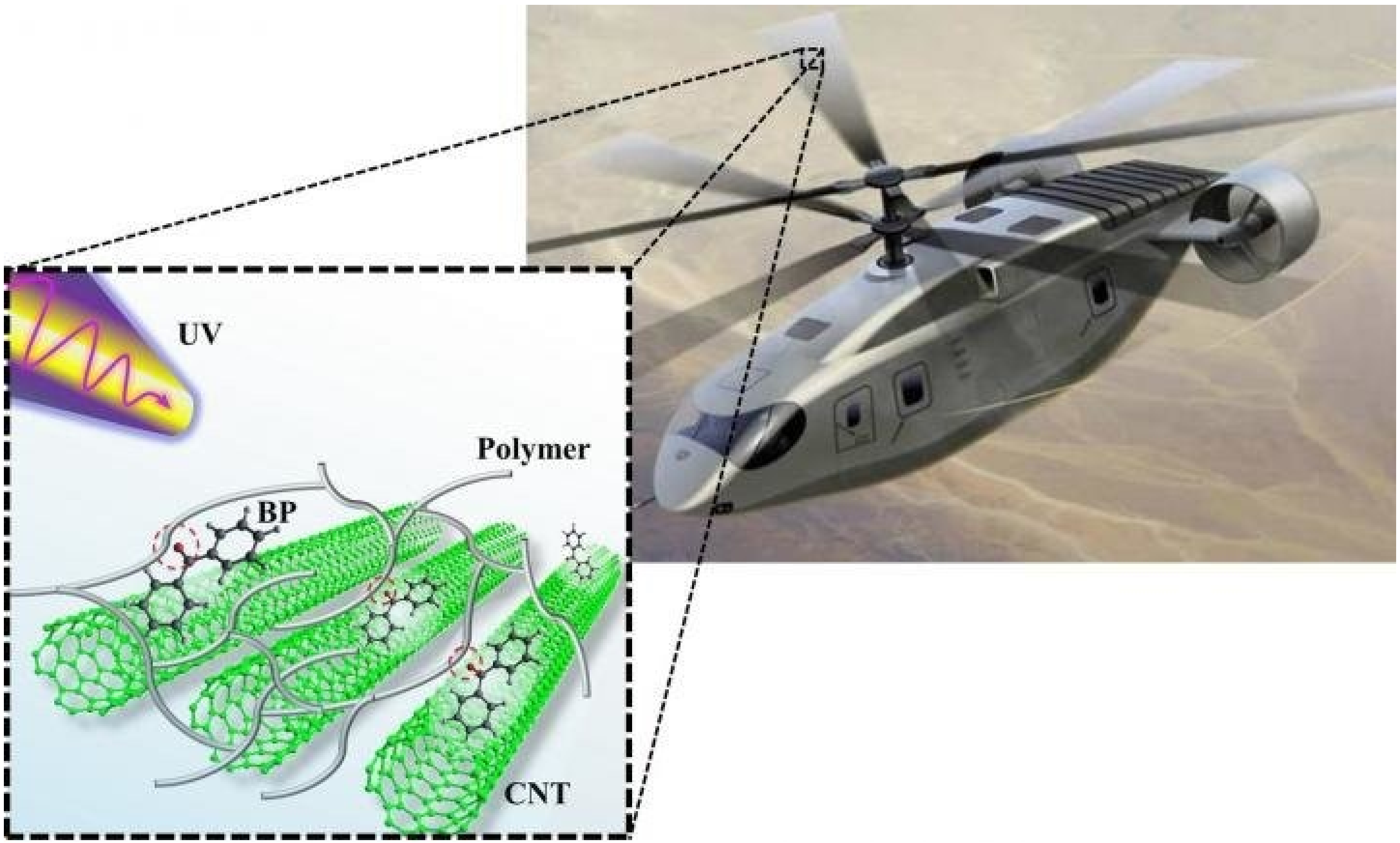
Hierachical Self-assembly and Phoresis in Biological Communities
(what if … molecules were ants ??? ;-)





End of Diversion:
“many-step aggregation in social animals”

Matter is Active:
self-organized, adaptive, ‘smart’, information-processing, materials



Materials Science meets Biology* to capture CO_2

CO_2(g) Dissolution and Disassociation.

$$CO_2(g) \leftrightarrow CO_2(aq) \quad (1)$$

$$CO_2(aq) + H_2O(l) \leftrightarrow H_2CO_3 \quad (2)$$

$$H_2CO_3 \leftrightarrow HCO_3^- + H^+ \quad (3)$$

$$HCO_3^- \leftrightarrow CO_3^{2-} + H^+ \quad (4)$$

Ureolysis.

$$CO(NH_2)_2 + H_2O \rightarrow NH_2COOH + NH_3 \quad (5)$$

$$NH_2COOH + H_2O \rightarrow NH_3 + H_2CO_3 \quad (6)$$

$$H_2CO_3 \leftrightarrow HCO_3^- + H^+ \quad (7)$$

$$2NH_3 + 2H_2O \leftrightarrow 2NH_4^+ + 2OH^- \quad (8)$$

$$HCO_3^- + H^+ + 2OH^- \leftrightarrow CO_3^{2-} + 2H_2O \quad (9)$$

Overall Ureolysis and $CaCO_3$ Precipitation.

$$NH_2CONH_2 + 2H_2O \Leftrightarrow 2NH_4^+ + CO_3^{2-} \quad (10)$$

$$Ca^{2+} + CO_3^{2-} \Leftrightarrow CaCO_3(s) \quad (11)$$

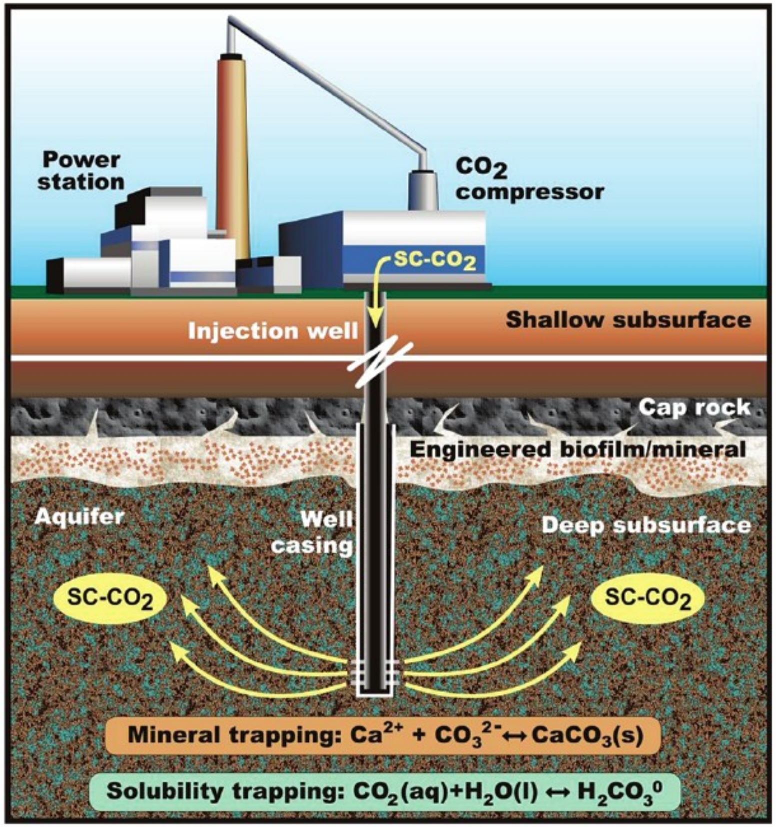


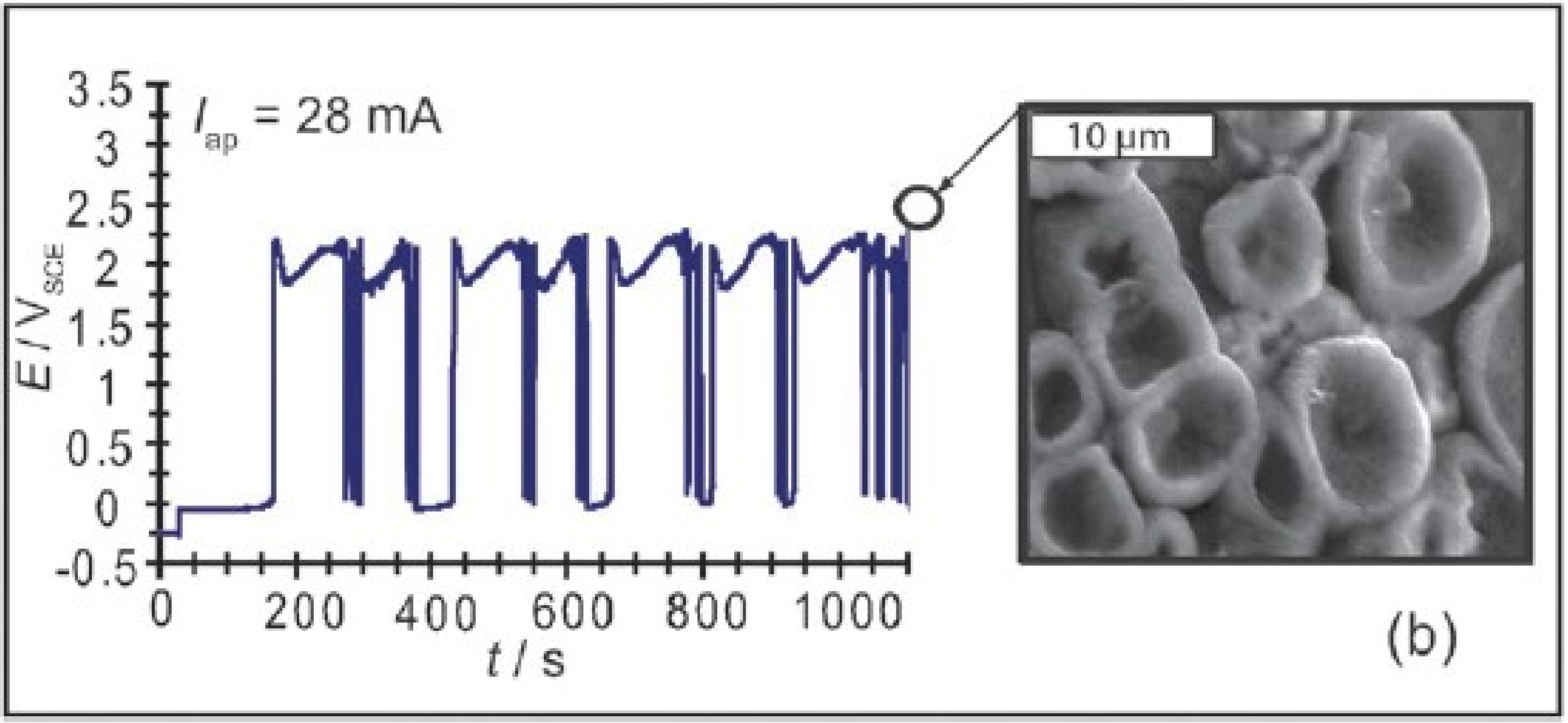
FIGURE 1. Schematic representation of microbially enhanced carbon capture and storage.

(*) Ref. kindly provided by **Dr. Delora Gaskins (ULB)**

“Microbially Enhanced Carbon Capture and Storage by Mineral-Trapping and Solubility-Trapping”
A.C. Mitchell et al, *Environ. Sci. Technol. 2010, 44, 5270–5276*

Oscillations as a sculptor*

Fe| 0.75 M H_2SO_4 + 20 mM Cl^- galvanostatic oscillations



(*) Ref. kindly provided by **Ms. Dimitra Spanoudaki (ULB)**
Sazou et al., PCCP, 8841(11), 2009

www.foresight.cnr.it/working-groups/wg-materials

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Pierre Gaspard, Vasileios Basios (ULB)
Theory & Research

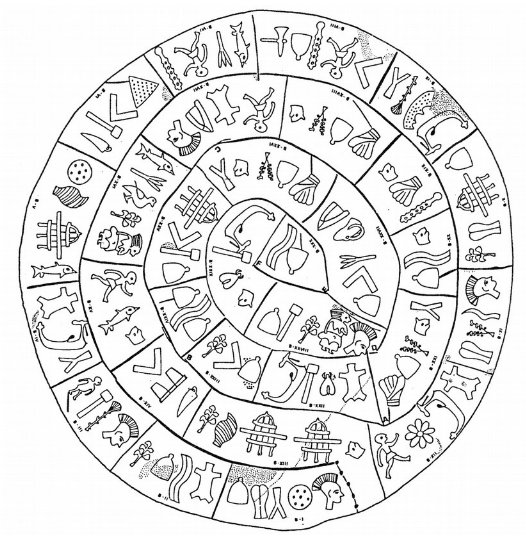
WG Materials

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

Pier-Francesco Moretti (CNR)
Support & Experimental Infrastructure



Outline of the talk:

Prolegomena

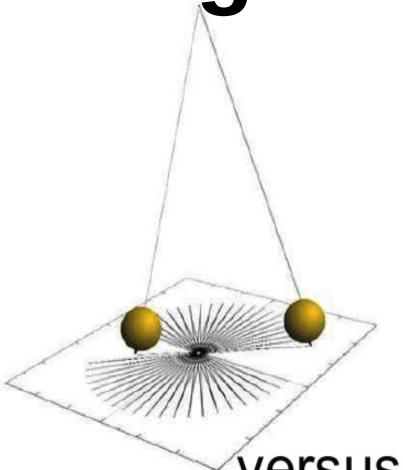
Part 1. Out of equilibrium:

Active Matter & New Materials

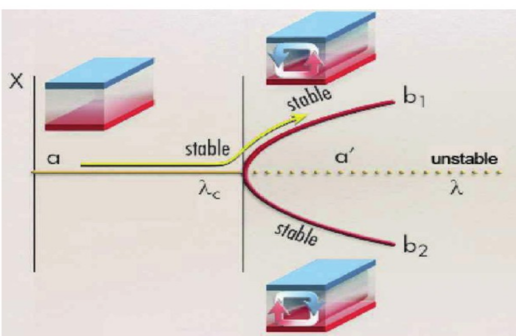
Part 2. Dynamics of Information:

Decision making and Collective Motion

PART 2: Dynamics of Information Decision making and Collective Motion



versus



ition to Rayleigh–Bénard patterns arising beyond the instability of t

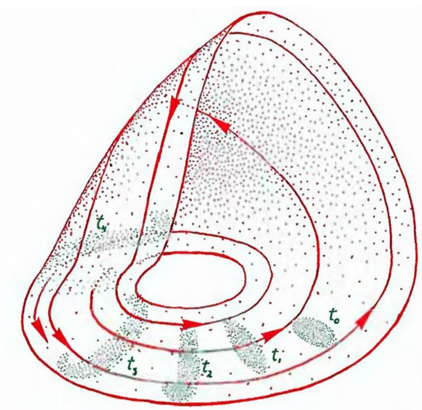
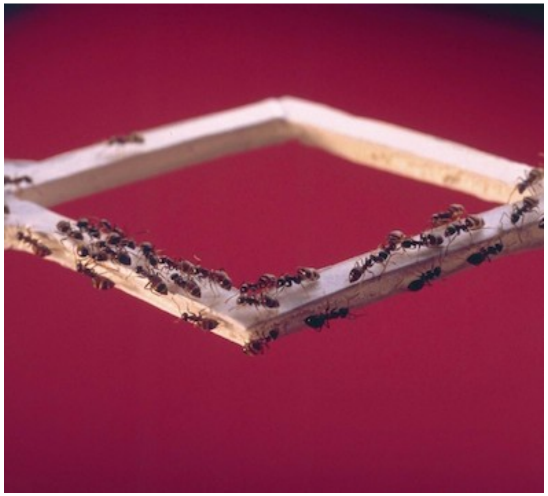
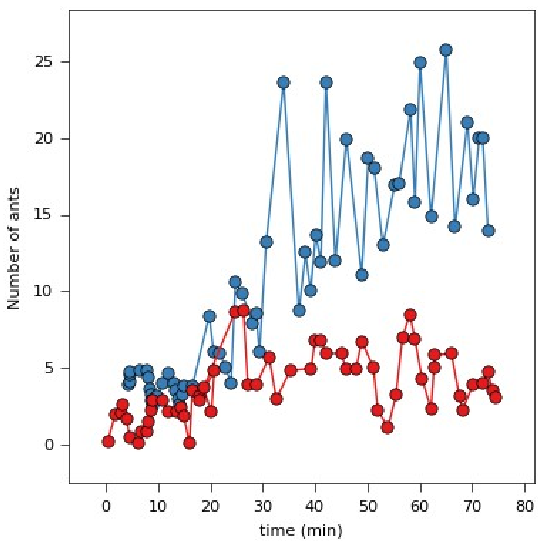
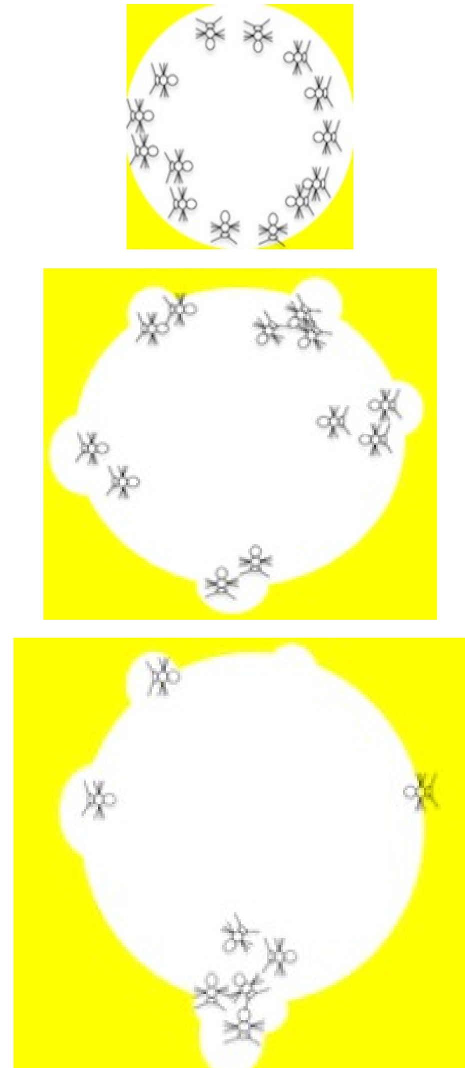


Fig. 1. Upper part: Simple pendulum. Lower part: Three manifestations of Complexity in everyday experience. Clockwise Bird flocking, the earth-atmosphere system, trading in the stock market.

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



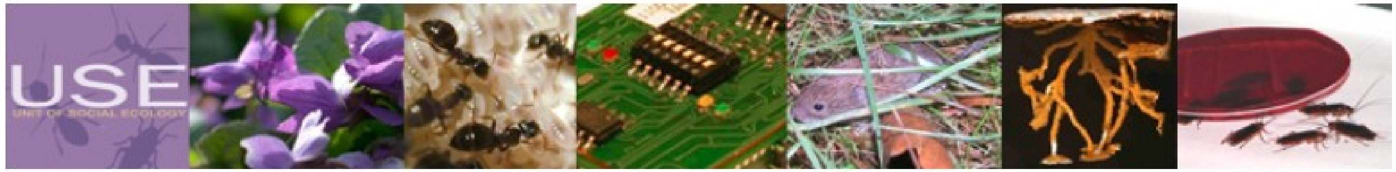




Pitchfork Bifurcation

Spatio-temporal Pattern Formation

Coordinated Aggregation: History & Hysteresis



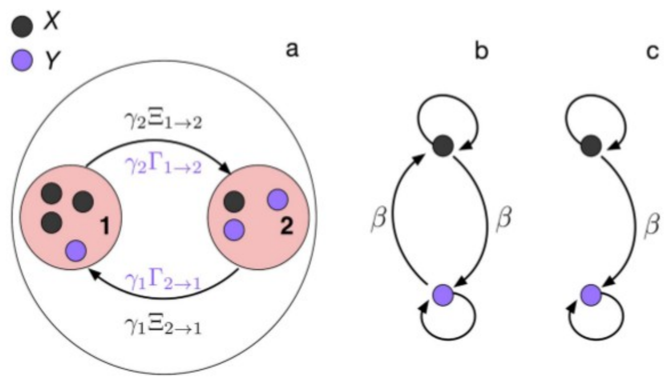


Figure 1. Experimental setup for the study of aggregation/segregation dynamics in an environment containing two equal patches and its relationship with the model defined by eq. (4) (**a**). Positive feedback networks of conspecific and heterospecific interactions : symmetrical (**b**) and asymmetrical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

"Coordinated aggregation in complex systems: an interdisciplinary approach"
Eur. Phys. J. ST 225, 1143-7 (2016)
V. Basios, S.C. Nicolis, J.L. Deneubourg

Real Soldier-Crab decision making monitoring & data

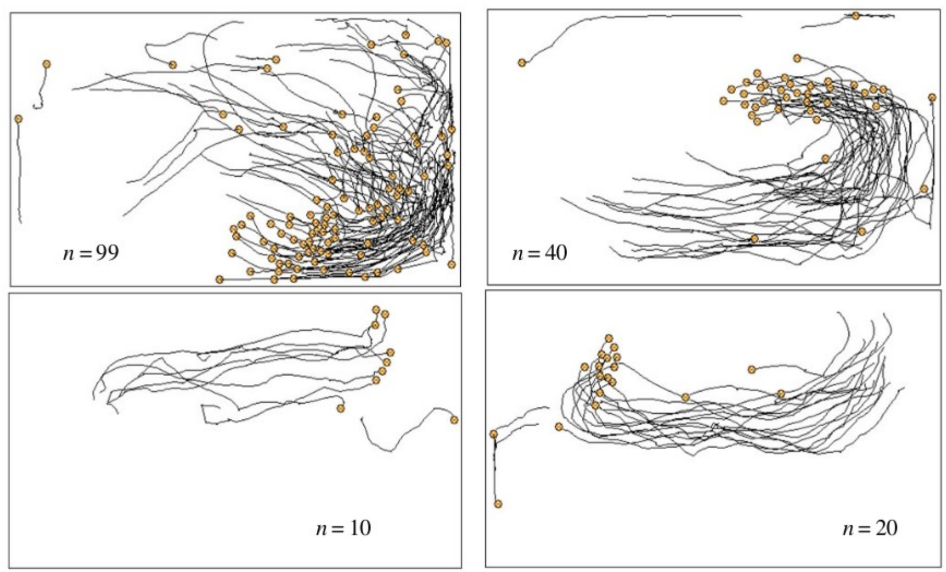
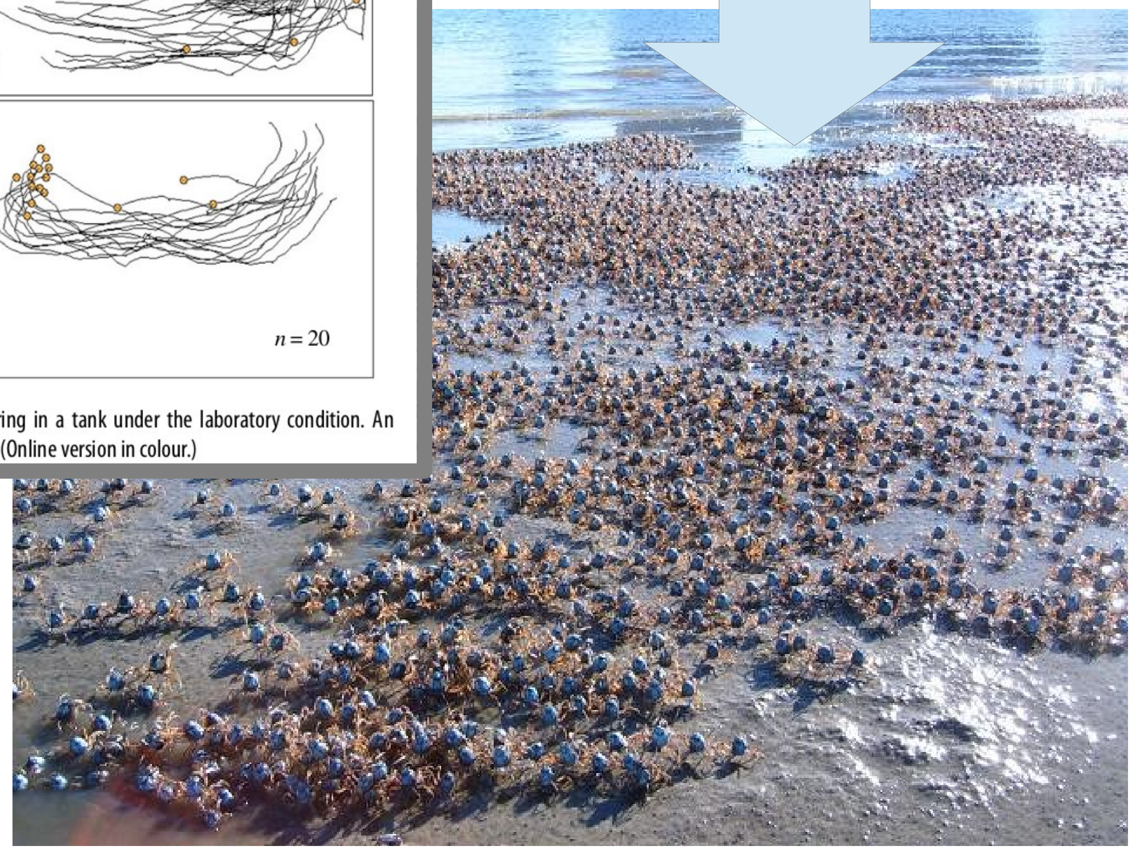
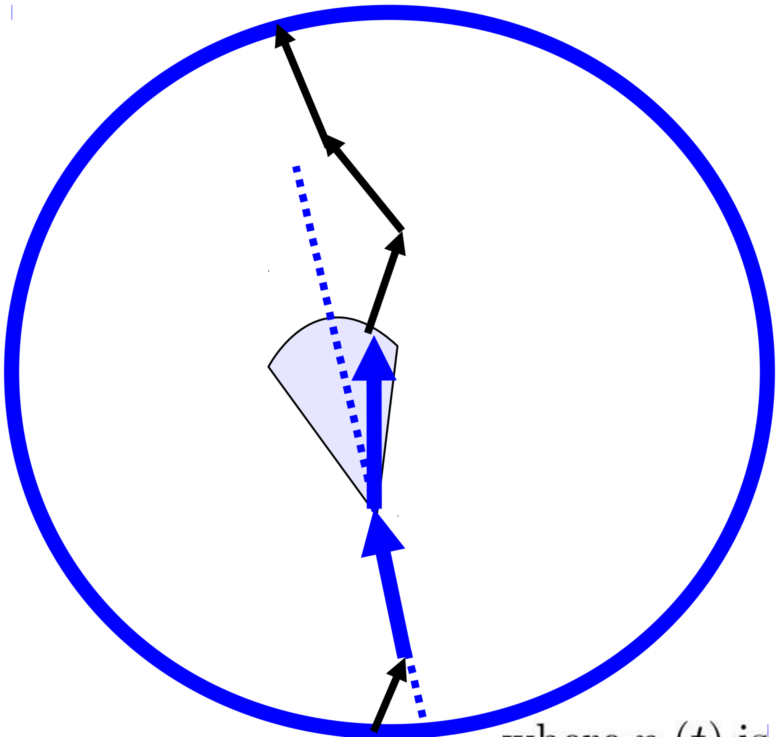


Figure 3. Snapshots of the real soldier crabs, *Mictyris guinotae*, wandering in a tank under the laboratory condition. An individual is represented by a circle accompanied by its previous trajectory. (Online version in colour.)



The standard Viscek Model of Flocking Behaviour:



$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \vec{v}_i(t)\Delta t, \quad i = 1, \ldots, N, \quad \vec{r}_i, \vec{v}_i \in \mathbb{R}^2$$

$$\vec{v}_i(t+\Delta t) = \begin{pmatrix} \cos\vartheta_i(t) & -\sin\vartheta_i(t) \\ \sin\vartheta_i(t) & \cos\vartheta_i(t) \end{pmatrix} \cdot \vec{v}_i(t), \quad i = 1, \ldots, N,$$

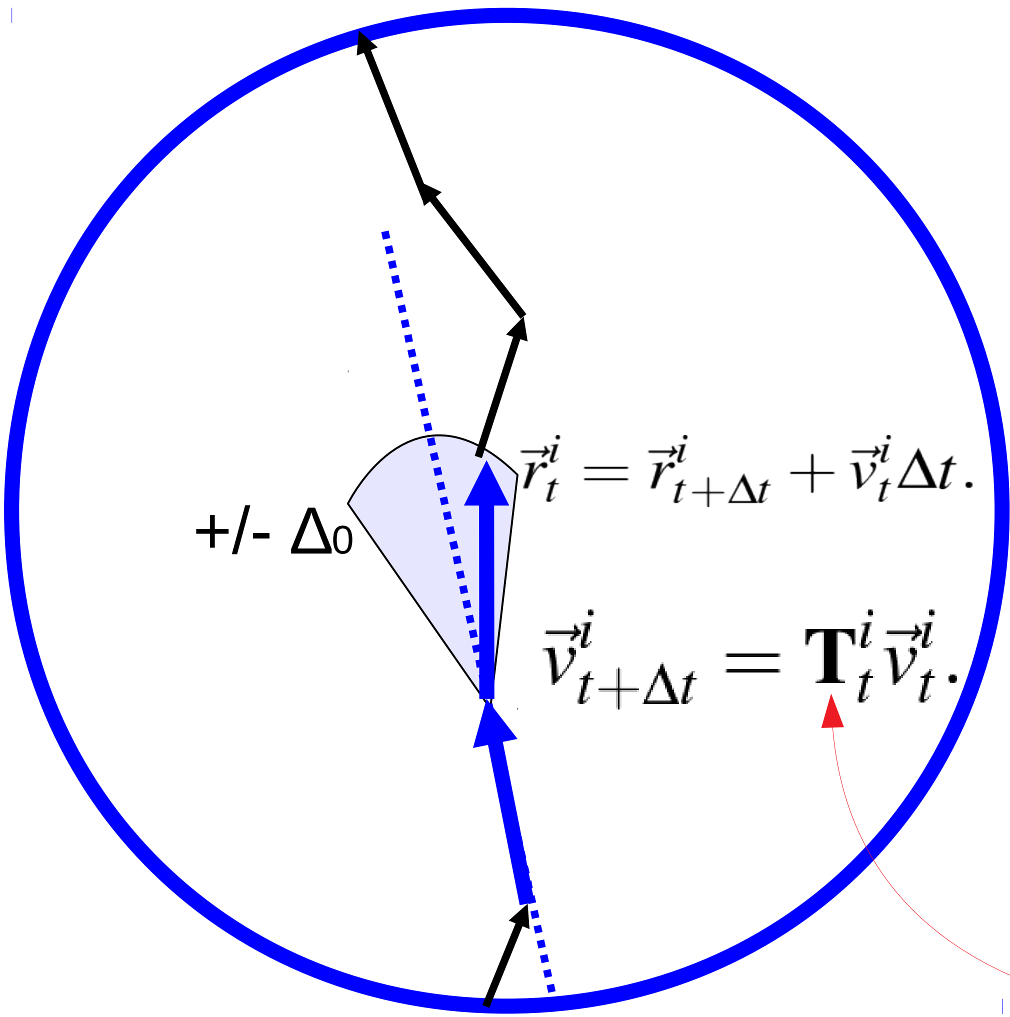
$$\vartheta_i(t+\Delta t) = \langle\vartheta_i(t)\rangle_r + \eta_i(t) \quad i = 1, \ldots, N \tag{3}$$

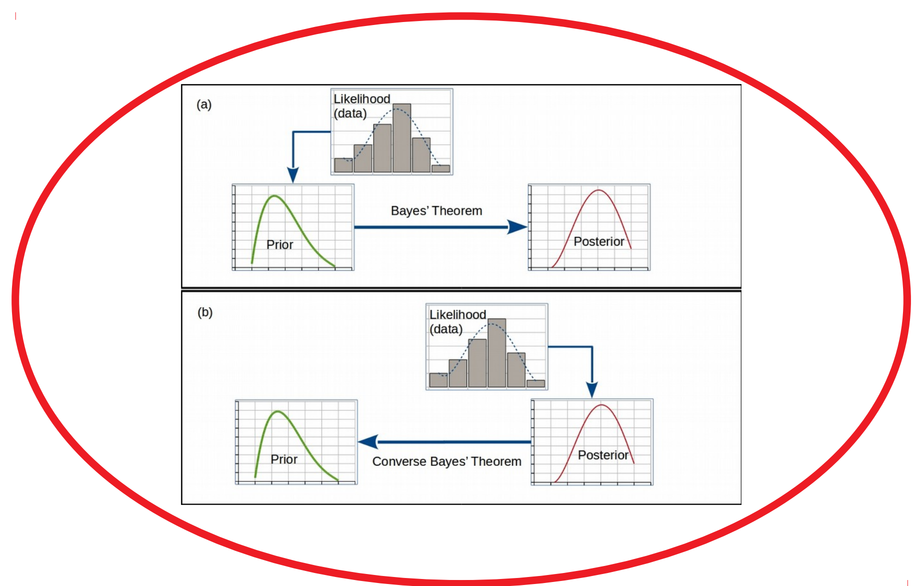
where $\eta_i(t)$ is a "noise" term taken randomly (at each time step again) from the uniform distribution $[-\eta/2, \eta/2]$, and $< \vartheta_i(t) >_r$ is the average angle of all particles inside a disk of radius r with the particle i at its center.

"Emergence of coherent motion in aggregates of motile coupled maps"
A. Garsia Cantu-Ros, C. Antonopoulos, V. Basios, *Chaos, Solitons & Fractals 44 (2011) 574.*

1) Provided an <u>inner steering</u> mechanism for the Vicsek Model

2) Provided the "particles" with an <u>inner</u> Decision making process based on Bayesian-Inverse-Bayesian Inference



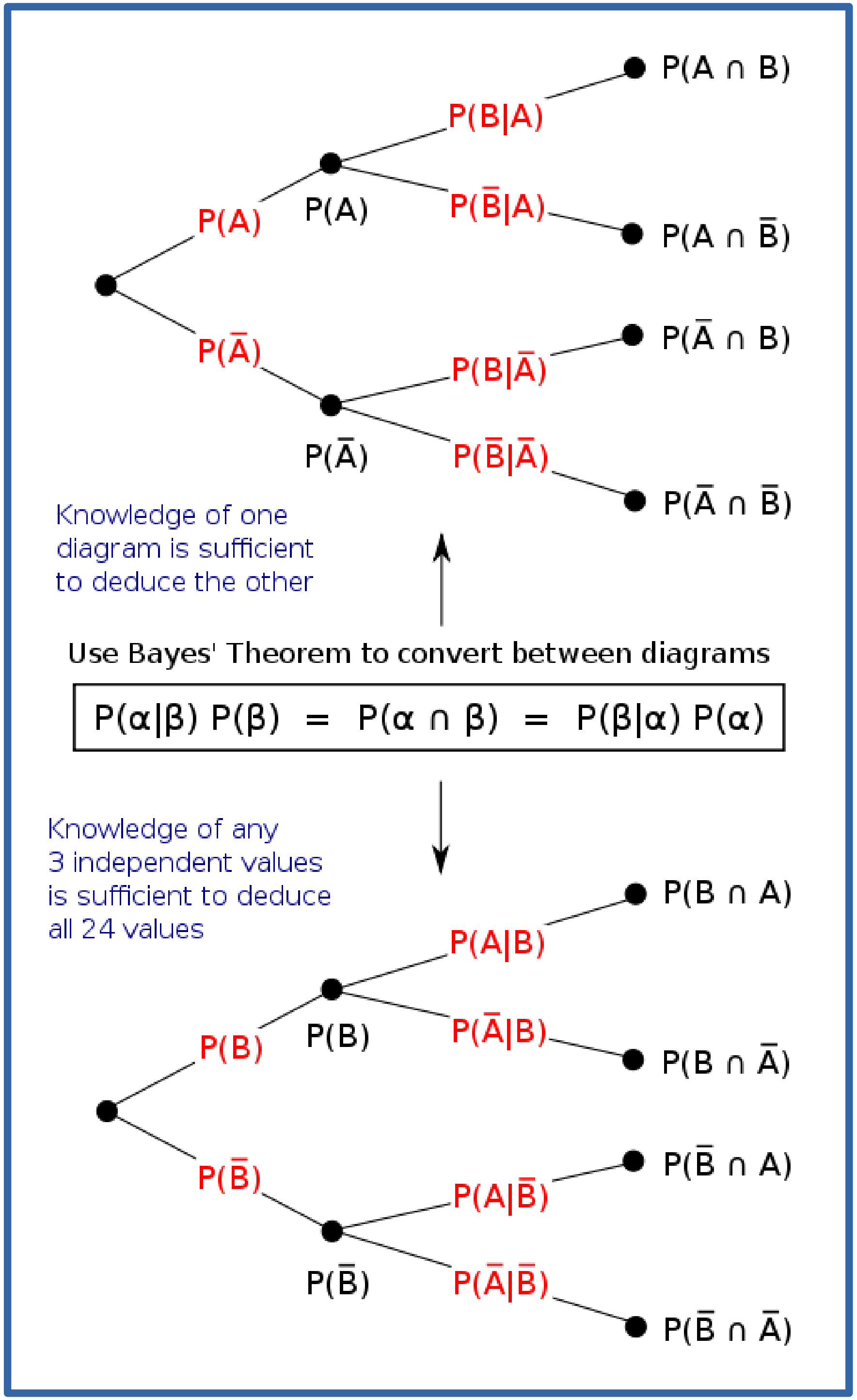


Bayes Inference: Rescaling Chance due to Bayes Theorem

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

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.



Rule of Three !!!

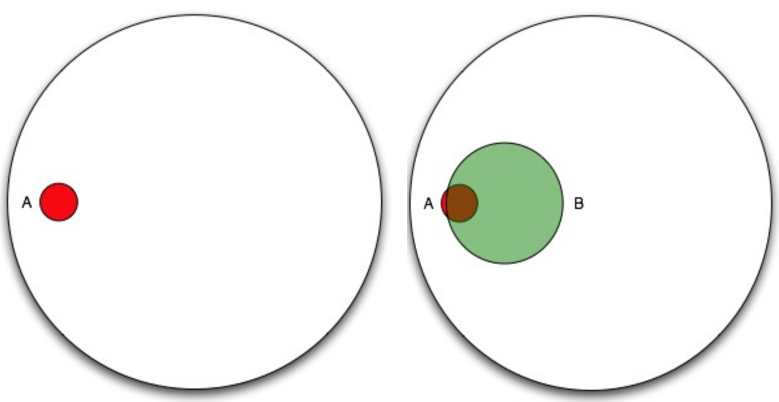
Reduction to Unity !!

Renormalization !

An Example of Bayesian Inference: Medical Test for disease A by test B (1/3)

$P_{(A)} = .005$	the probability that the disease will be present in any particular person
$P_{(\sim A)} = 1 — .005 = .995$	the probability that the disease will not be present in any particular person
$P_{(B\|A)} = .99$	the probability that the test will yield a positive result [B] **if** the disease is present [A]
$P_{(\sim B\|A)} = 1 — .99 = .01$	the probability that the test will yield a negative result [~B] **if** the disease is present [A]
$P_{(B\|\sim A)} = .05$	the probability that the test will yield a positive result [B] **if** the disease is not present [~A]
$P_{(\sim B\|\sim A)} = 1 — .05 = .95$	the probability that the test will yield a negative result [~B] **if** the disease is not present [~A]

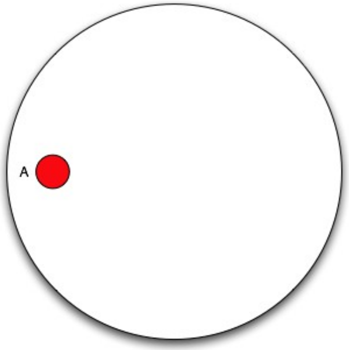
$$P(A \mid B) = \frac{P(B \mid A) P(A)}{P(B)}$$

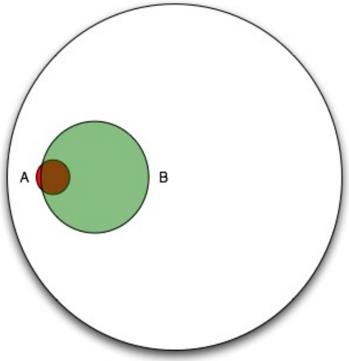


Example: Medical Test for disease A by test B (2/3)

$P_{(A)} = .005$	the probability that the disease will be present in any particular person
$P_{(\sim A)} = 1 - .005 = .995$	the probability that the disease will not be present in any particular person
$P_{(B\|A)} = .99$	the probability that the test will yield a positive result [B] **if** the disease is present [A]
$P_{(\sim B\|A)} = 1 - .99 = .01$	the probability that the test will yield a negative result [~B] **if** the disease is present [A]
$P_{(B\|\sim A)} = .05$	the probability that the test will yield a positive result [B] **if** the disease is not present [~A]
$P_{(\sim B\|\sim A)} = 1 - .05 = .95$	the probability that the test will yield a negative result [~B] **if** the disease is not present [~A]

$P_{(B)} = [P_{(B\|A)} \times P_{(A)}] + [P_{(B\|\sim A)} \times P_{(\sim A)}] = [.99 \times .005] + [.05 \times .995] = .0547$	the probability of a positive test result [B], irrespective of whether the disease is present [A] or not present [~A]
$P_{(\sim B)} = [P_{(\sim B\|A)} \times P_{(A)}] + [P_{(\sim B\|\sim A)} \times P_{(\sim A)}] = [.01 \times .005] + [.95 \times .995] = .9453$	the probability of a negative test result [~B], irrespective of whether the disease is present [A] or not present [~A]

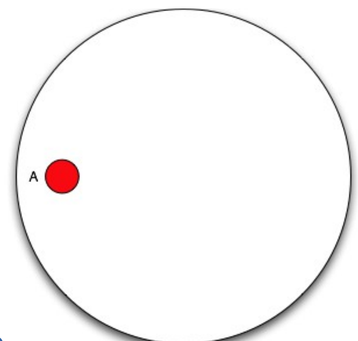




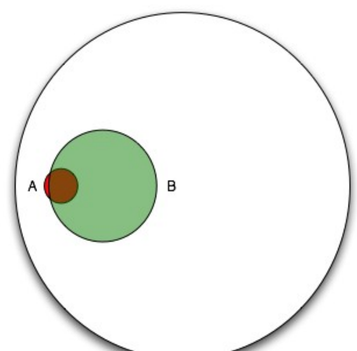
Example: Medical Test for disease A by test B (3/3)

$P_{(A)} = .005$	the probability that the disease will be present in any particular person
$P_{(\sim A)} = 1 - .005 = .995$	the probability that the disease will not be present in any particular person
$P_{(B\|A)} = .99$	the probability that the test will yield a positive result [B] **if** the disease is present [A]
$P_{(\sim B\|A)} = 1 - .99 = .01$	the probability that the test will yield a negative result [~B] **if** the disease is present [A]
$P_{(B\|\sim A)} = .05$	the probability that the test will yield a positive result [B] **if** the disease is not present [~A]
$P_{(\sim B\|\sim A)} = 1 - .05 = .95$	the probability that the test will yield a negative result [~B] **if** the disease is not present [~A]

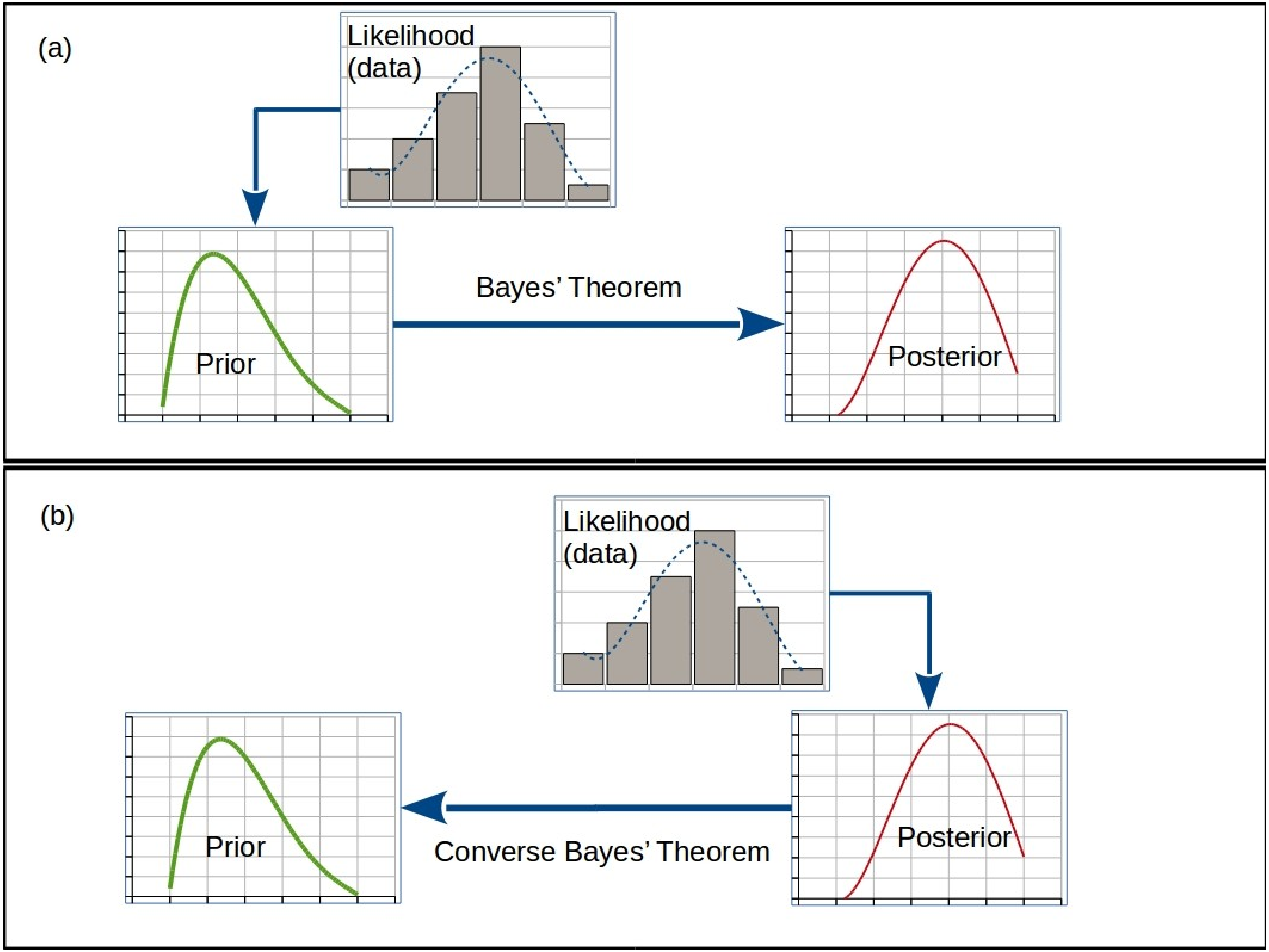
$P_{(B)} = [P_{(B\|A)} \times P_{(A)}] + [P_{(B\|\sim A)} \times P_{(\sim A)}]$ $= [.99 \times .005] + [.05 \times .995] = .0547$	the probability of a positive test result [B], irrespective of whether the disease is present [A] or not present [~A]
$P_{(\sim B)} = [P_{(\sim B\|A)} \times P_{(A)}] + [P_{(\sim B\|\sim A)} \times P_{(\sim A)}]$ $= [.01 \times .005] + [.95 \times .995] = .9453$	the probability of a negative test result [~B], irrespective of whether the disease is present [A] or not present [~A]



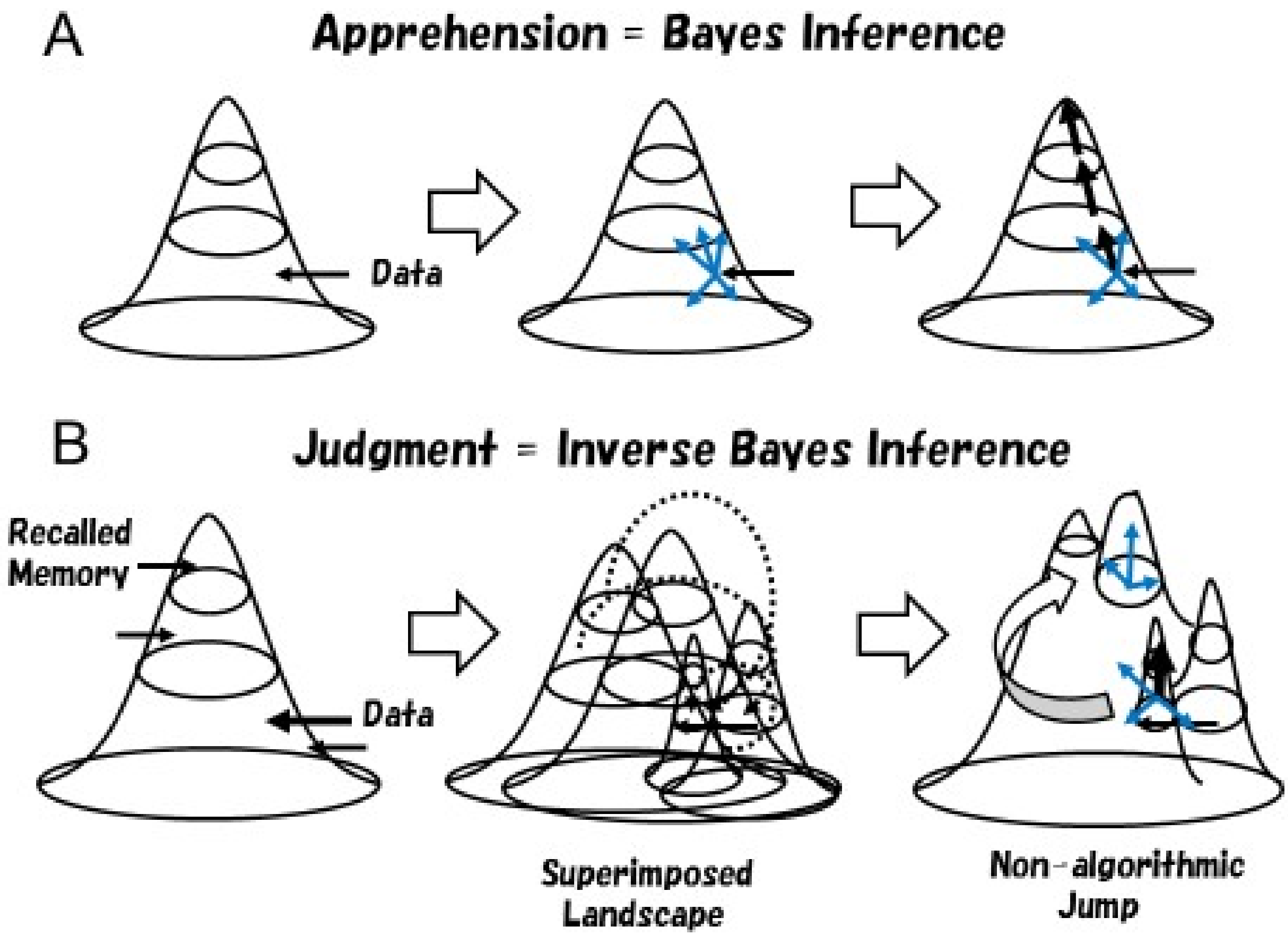
$P_{(A\|B)} = [P_{(B\|A)} \times P_{(A)}] / P_{(B)}$ $= [.99 \times .005] / .0547 = .0905$	the probability that the disease is present [A] **if** the test result is positive [B] (i.e., the probability that a positive test result will be a true positive)
$P_{(\sim A\|B)} = [P_{(B\|\sim A)} \times P_{(\sim A)}] / P_{(B)}$ $= [.05 \times .995] / .0547 = .9095$	the probability that the disease is not present [~A] **if** the test result is positive [B] (i.e., the probability that a positive test result will be a false positive)
$P_{(\sim A\|\sim B)} = [P_{(\sim B\|\sim A)} \times P_{(\sim A)}] / P_{(\sim B)}$ $= [.95 \times .995] / .9453 = .99995$	the probability that the disease is absent [~A] **if** the test result is negative [~B] (i.e., the probability that a negative test result will be a true negative)
$P_{(A\|\sim B)} = [P_{(\sim B\|A)} \times P_{(A)}] / P_{(\sim B)}$ $= [.01 \times .005] / .9453 = .00005$	the probability that the disease is present [A] **if** the test result is negative [~B] (i.e., the probability that a negative test result will be a false negative)



Bayesian Inverse Bayesian non-linear feedback decision process



Tito-Fortunato Arrechi (2013),
Yukio-Pegio Gunji & Vasileios Basios (2014)

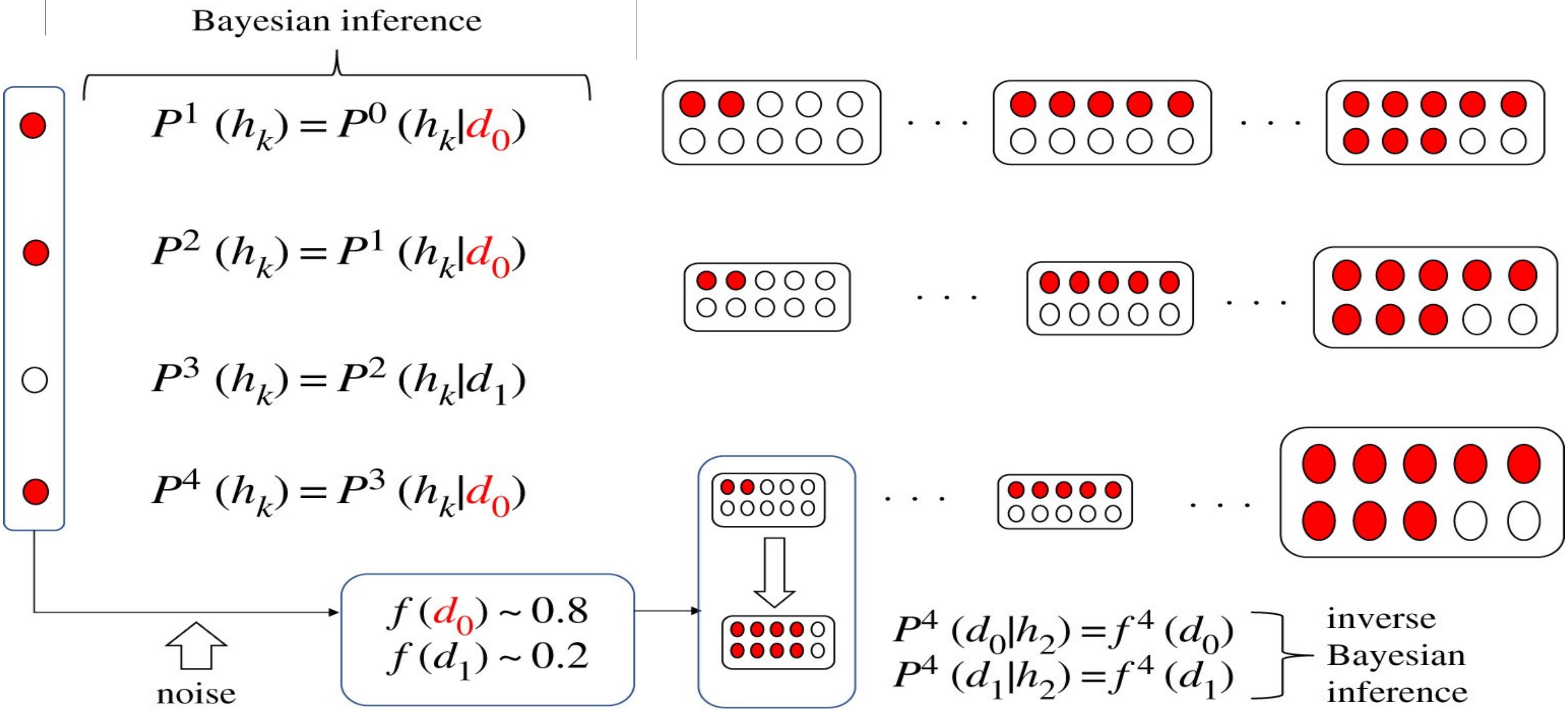


data (d_0, d_1...)

BIB

hypotheses

(h_0 = 20:80, h_1=50:50, h_3=80:20)



Modified "Vicsek Model" with:

Bayesian & Inverse Bayesian Inference Process (BIB) as internal steering

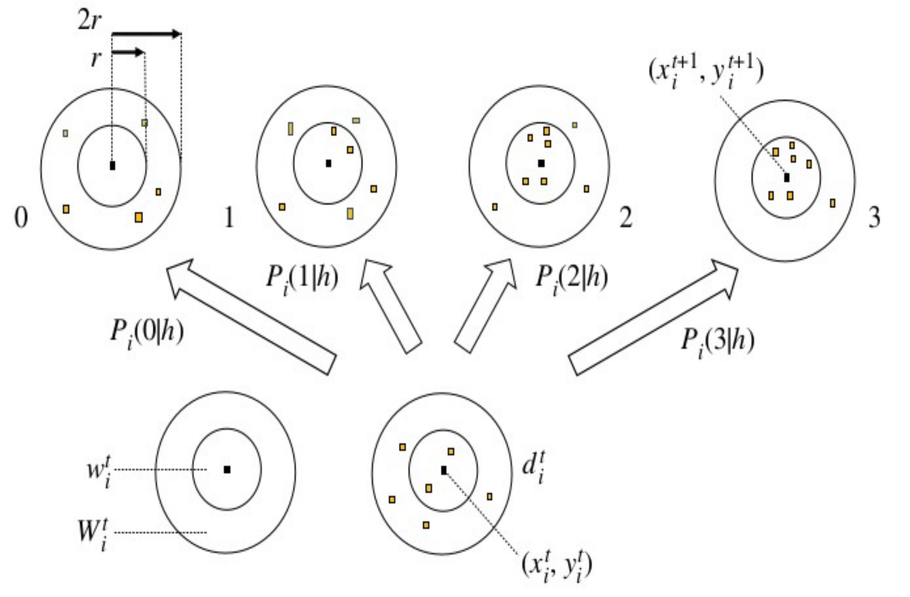


Figure 5. Schematic diagram of data and hypothesis adopted by a time series of real soldier crabs. (Online version in colour.)

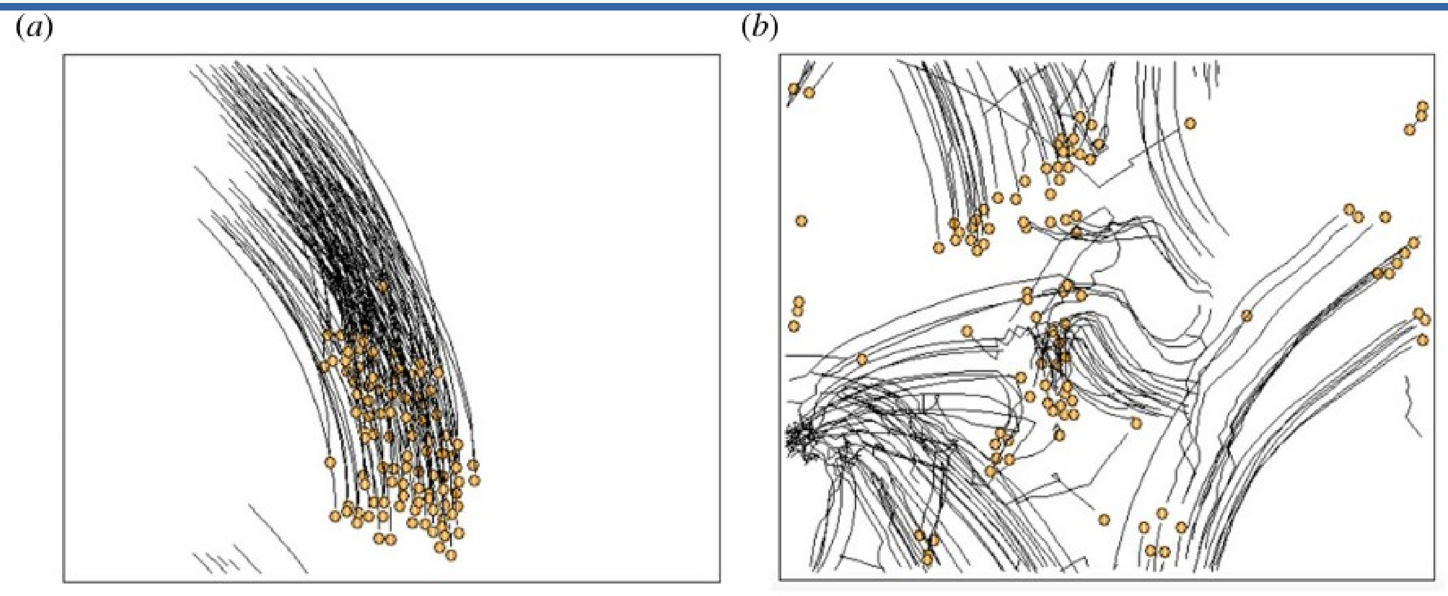


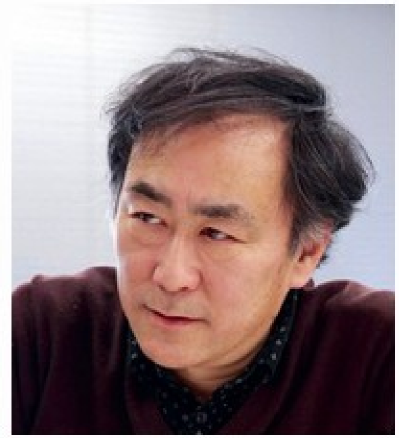
Figure 10. Snapshots of the swarm model based on BIB inference. Swarming phase (*a*) and dispersing phase (*b*). (Online version

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

November 2018

Inverse Bayesian inference in swarming behaviour of soldier crabs

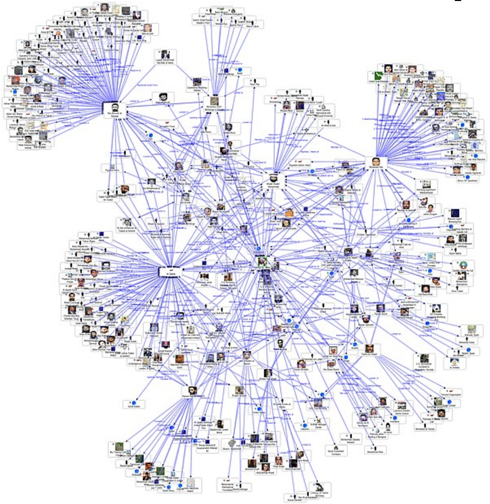
Yukio-Pegio Gunji[1], Hisashi Murakami[2], Takenori Tomaru[3] and Vasileios Basios[4]



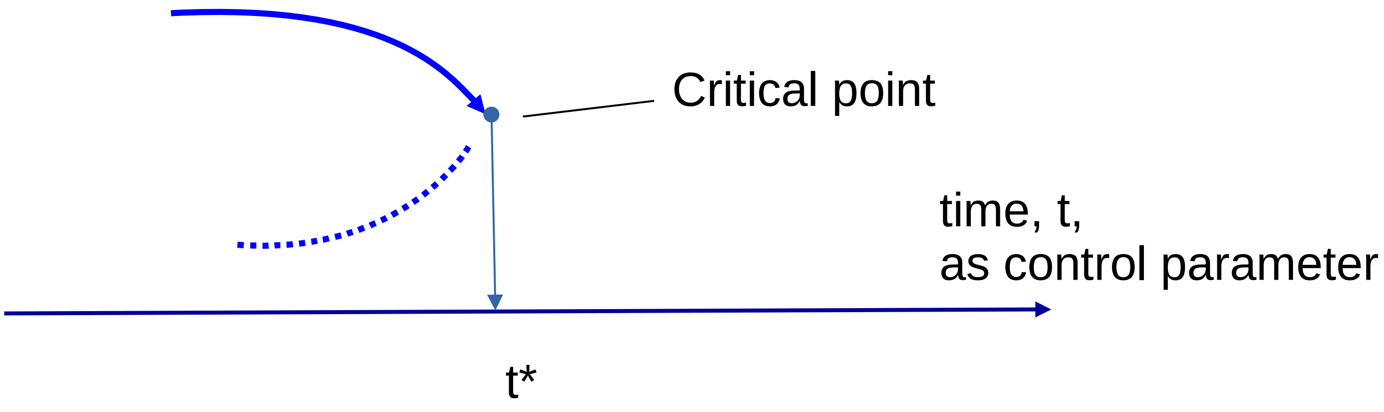
WASEDA University

Complexity Science in Sociology & Economics

Networks (social, transactions, epidemic …), Optimization.



Prediction of potentially disastrous state transitions.

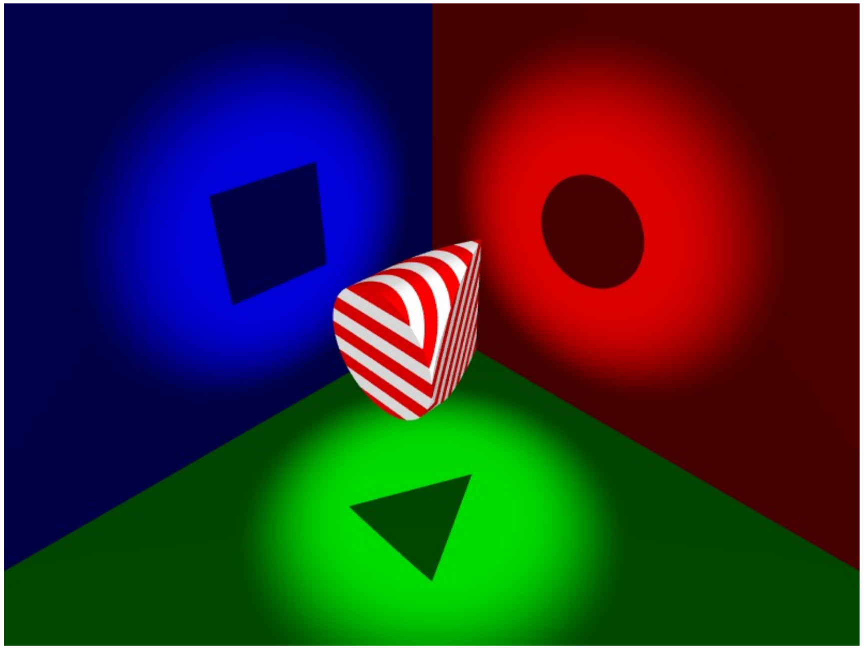


“Nonlinear science introduces a new way of thinking based on a subtle interplay between qualitative and quantitative techniques, between topological, geometric and metric considerations, between deterministic and statistical aspects.

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