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Θερινό Σχολείο Συνέδριο

Interdisciplinary Centre of Nonlinear Phenomena and Complex Systems (CeNoLi-ULB)

Department of Physics of Complex Systems and Statistical Mechanics

"Collective Dynamics Control in Physics and Biology:

Macroscopic Level: Aggregation & Self-Organization"

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> > omblex

Volos, July 12-21, 2017 @ University of Thessaly

<u>ODE 1 :</u> Non-standard Aggregation (the story of the genesis of a new paradigm)

Ode & Monte Carlo 1: Zeolites' Fractals

Ode & Monde Carlo 2: Ants Sharing Food

ODE 2: Seek a Shelter and Try to Settle Down

a history of a new paradigm **Non-standard Aggregation**:

Crystallization, Nucleation, Self-assembly And the role of intermediate crecursors



Josiah Willard Gibbs

stealing an idea from Gibbs to understand nucleation:

S



N*

 $[d \Delta G / d n(j)]=0 at n*(i)$

→ $\Delta G = n(j) \Delta G(j) - T\Delta S(n(j))$

Equilibrium Assumption



Fig. 1. Energetics of cubic cluster formation as a function of the cluster's size.





Capilary

Approximation $\rho_{cl} = \rho_{new}$. That is, the distinctive properties of the smallcondensed phase are size independent.

The surface tension, so-called surface free energy, is the same as for a planar interface of the new and the mother phase. That is equivalent to assume clusters with a sharp boundary. That is, $\alpha(R) = \alpha_{R \to \infty} + \mathcal{O}(R)$

Aggregation/coalescence aggregation segregation coalescence Ostwald ripening segregation disproportionation

Classical aggregation -- nucleation:

- Equilibrium, kinetics are "averaged out"
- Large critical nucleus, small isotropic molecules
- Single phases one for the liquid and one for the solid
- One reaction coordinate





ODE model I:

Bifurcations in multistep aggregation

"A new paradigm"

Kinetics and Thermodynamics of **Multistep Nucleation** and Self-Assembly in Nanoscale Materials Advances in Chemical Physics Volume 151 **Gregoire** Nicolis Dominique Maes WILEY

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

Kinetics of barrier crossing : formulation

 $ho,\ m$ order parameters

 $\lambda, \ \mu, \cdots$ control parameters

F Landau type free energy

L matrix of Onsager coefficients Transitions between states governed by

$$\frac{1}{t} \begin{pmatrix} \rho \\ m \end{pmatrix} = -\mathbf{L} \cdot \nabla F \left(\rho, \ m \right) + \begin{pmatrix} R_{\rho} \left(t \right) \\ R_{m} \left(t \right) \end{pmatrix}$$

where R_{ρ} , R_m are Gaussian white noises whose covariance matrix must satisfy fluctuation-dissipation type relationships

Kinetic potential and its bifurcation set

Requirements :

Switch as the control parameters are varied, from

 $F_1 \to S(2 - \text{well } U)$

to $F_1 \xrightarrow{\leftarrow} F_2 \to S \quad (3 - \text{well } U)$ "Parabolic umbilic" catastrophe scenario. Full unfolding by four control parameters

Simple Model Equations:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{\partial U}{\partial x} = -\lambda x - \mu x^2 + \gamma y^2 - x^3,$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = -\frac{\partial U}{\partial y} = -\lambda y + 2\gamma x y - y^3,$$

Steady states:

$$-\lambda x_S - \mu x_S^2 + \gamma y_S^2 - x_S^3 = 0,$$

$$-\lambda y_S + 2\gamma x_S y_S - y_S^3 = 0,$$



Fig. 4. Phase portraits of system (19) in the region of 3 stable steady states, $\lambda = -0.5$ (a) and in the region of 4 stable steady states, $\lambda = 0.5$ (b) with $\mu = 2$. The u's stand for the unstable states involved in the transitions. State F1 is in the far left of the diagrams and states S_+ , S_- in the far up right and down right parts.

In absence of external fields and other sources of asymmetry

$$U(x,y) = \frac{\lambda}{2} \left(x^2 + y^2\right) + \frac{\mu}{3}x^3 - \gamma xy^2 + \frac{1}{4} \left(x^4 + y^4\right)$$





where the k's are related to mean first passage times statistics associated to the Fokker-Planck equation

for
$$\lambda < 0$$

$$k \approx \frac{1}{2\pi} \left(\frac{\sigma_u^+}{|\sigma_u^-|} \right)^{1/2} (\sigma_{s_1} \sigma_{s_2})^{1/2}$$
$$\exp\left(\frac{U(unst) - U(st)}{\epsilon} \right)$$

for
$$\lambda > 0$$

$$\frac{1}{2} | -(k_1 + k_2 + k'_1) + \sqrt{(k_1 - k_2)^2 + k'_1^2 + 2k'_1 (k_1 + k_2)} |$$

$$(k_1 \rightarrow k_2 \text{ for } k'_1 < < k_1)$$

 $au^{-1} \ (F_1 o S)$: lowest eigenvalue

Optimization near the F₁ - F₂ coexistence Non -trivial cross-over at $\lambda = 0$



Fig. 6. Mean transition times between states F1 and S versus λ in the vicinity of $\lambda = 0$, obtained numerically from the Langevin equations (24) after an averaging over 5000 realizations. Dashed lines stand for linear fits in the regions $\lambda < 0$ and $\lambda > 0$. Parameter values $\mu = 2$, $\gamma = 1.6$ and $q^2 = 0.6$.

Biophysical Journal Volume 93 July 2007 1-12

Two-Step Mechanism of Homogeneous Nucleation of Sickle Cell Hemoglobin Polymers

Oleg Galkin,* Weichun Pan,* Luis Filobelo,* Rhoda Elison Hirsch,^{‡§} Ronald L. Nagel,[‡] and Peter G. Vekilov*



1) Barriers Around~ 100kT

2) Weak & Short ranged interactions compared to simple fluids.



Configuration coordinate

Proc Natl Acad Sci U S A. Aug 19; 100(17): 9826–9830. 2003

"Ordering of water molecules between phospholipid bilayers visualized by coherent anti-Stokes Raman scattering microscopy"



Monte Carlo Lattice Simulation I: Zeolite Aggregation (spatiotemporal model)

Including intermediate steps:



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

164701-2 Lutsko et al.

J. Chem. Phys. 132, 164701 (2010)



FIG. 1. A schematic demonstration of multistep versus standard synthetic pathways in a two-order parameter space accounting for the presence of partially structured intermediates.







Mean Field model (Lutsko, Basios et al 2010)

$$\frac{dN(t)}{dt} = -2k_{N-N(X)}N^2(t)X(t)$$
$$\frac{dX(t)}{dt} = k_{N-N(X)}N^2(t)X(t) - k_{X-S}X(t)S(t)$$
$$\frac{dS(t)}{dt} = k_{X-X}X^2(t) + k_{X-S}X(t)S(t)$$

$$k_{X-S} = K_{xs}S^{\alpha}$$







Reaction Steps N "monomers", X "intermediates", S "crystallite"

$$N_{i} + N_{j} + X_{kl} \stackrel{p_{N-N(X)}}{\to} \qquad X_{ij} + X_{kl} \qquad (1a)$$
$$X_{ij} + X_{kl} \stackrel{p_{X-X}}{\to} \qquad S_{ijkl} \qquad (1b)$$
$$X_{ij} + S_{m_{1}m_{2}, \cdots m_{l}} \stackrel{p_{X-S}}{\to} \qquad S_{ijm_{1}m_{2}, \cdots m_{l}} \qquad (1c)$$



Diffusion Steps (S does not diffuse,V is the empty site)

$$N_i + V_j \stackrel{p_{diff^{-N}}}{\to} V_i + N_j \tag{2}$$

$$V_i + X_{kl} \stackrel{p_{diff}-X}{\to} X_{ik} + V_l \tag{3}$$

Cooperativity in forming the solid:

$$p_{X-S}(S) = c_{X-S}S^{\alpha}$$





Mean Field model compatible with MC & previous work (Lutsko, Basios et al 2010)

$$\frac{dN(t)}{dt} = -2k_{N-N(X)}N^2(t)X(t)$$
$$\frac{dX(t)}{dt} = k_{N-N(X)}N^2(t)X(t) - k_{X-S}X(t)S(t)$$
$$\frac{dS(t)}{dt} = k_{X-X}X^2(t) + k_{X-S}X(t)S(t)$$

$$k_{X-S} = K_{xs}S^{\alpha}$$



Properties of the aggregates (II) Different initial conditions (a) homogeneous (b) seeding)





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

2004-2015





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Monte Carlo Lattice Simulation II: Food Aggregation in Ant Colonies (spatiotemporal model)

Same Pathways in Selforganization in biology!



Trophallaxis (food exchange):

Work partition and specialization by individuals, some gather food
(Foreagers 15%-20%) some keep it saving for "rainy days"(Domestics).
Ant Colony's Social Stomach fills up

Hierachical Systems in Social Biological Systems



credits:

Physical and Biological Determinants of Collective Behavioural Dynamics in Complex Systems Bochynek T, Robson SKA (2014) PLoS ONE 9(4): e95112. doi:10.1371/journal.pone.0095112

Experimental Set Up

Methods

Experimental nests (10 cmx10 cm x 0.2 cm) contained 200 workers of *F. fusca* no brood, no queen) (Fig. 1). The colonies were deprived of food for 1, 4 and 7 days prior to each experiment. Four nests were tested at a time. At the beginning of the experiment, we placed 1ml of radiolabeled sucrose 0.5M. For 3 hours, we monitored the spreading of the food inside the nest with a scintigraph.





Experimental setup













Radioactivity (counts/30s)

Buffin A et al. FASEB J 2012;26:2725-2733

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The FASEB Journal



Figure 4. Distribution of the radioactive pixels at the end of the 3 h of experiment.



Trophallaxis (food exchange):

Ant Colony's Social Stomach fills up by the combined action of: Foreagers (A) and Domestics (B)

THEORETICAL MODELLING

Two levels: (i) food exchange kinetics: $S+A \rightarrow A^*$ $A^*+B \rightarrow A+B^*$

(ii) ants diffussion



4.1.2 The reaction steps

In particular we start with the minimum number of food exchange steps, labeling the forward and backward steps as k_* and k^r_* respectively. (BOOKEEPING ISSUE ... ANY IDEA FOR A MORE "SHARP, SLIM AND CLEAN" LABELING CON-CERNING THE REACTION STEPS AND CONSTANS IS MUCH MUCH WELCOMED!)

 Filling up of the foragers: When they meet sugar sources, we assume that all foragers fill up at once. The sugar source is inexhaustible so it remains constant throughout the reaction.

$$S + A_n \xrightarrow{k_n} A_N + S$$

for n = 0, 1, 2, 3...N - 1.

2. Feeding the domestics: Encounters of foragers with domestics result in trophallaxis. The foragers give out part of their load in discrete quantal changing their "species" from n to n - 1 and the domestics stock it up changing from m to m + 1:

$$A_n + B_m \underset{\substack{k_{N-1+n+m}^r \\ k_{N-1+n+m}^r}}{\overset{k_{N-1+n+m}}{\rightleftharpoons}} A_{n-1} + B_{m+1}$$

for n = 0, 1, 2, 3...N and m = 0, 1, 2, 3...M - 1.

 Stocking up in the "collective stomach": Domestics engage in trophallaxis within the nest. The discrete quantal change of their "species" from m to m±1 is simply:

$$B_{m'} + B_m \stackrel{k_{N-1+n+m+m'}}{\underset{k_{N-1+n+m+m'}}{\rightleftharpoons}} B_{m'\pm 1} + B_{m\mp 1}$$



Level II: Social Stomach, density of food



WITHOUT DIFFUSION







Max Capacity: N =2



Max Capacity: N =3





Fractal Dimention & **Aggregation Index**



Figure 5. Aggregation index (AI) according to the radioactive surface (in pixels).



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ODE model II: (back to bifurcations)

Collective decision-making resulting from social behavior BV. & J.L. Deneubourg ULB

Emergence of specialized individuals (loaded-unloaded)

Two ants model



Kinetics of exchange : only depends on Q1 & Q2 (their loads) Two symetrical equations with the same parameters values for both ants



Emergence of specialized individuals (loaded-unloaded) Two ants model



Aggregation in a patchy environment



Probability of joining a shelter



$$P_i = \mu \left(1 - \frac{x_i}{S} \right)$$

 μ : maximal probability of joining x_i : number of sheltered individuals S: carrying capacity of shelter *i*

Probability of leaving (retention) a shelter



n et al, 2005; Amé et al, 2006; Halloy, et al, 2007; Garnier et al, 2008; Laurent et al, 201

Model

System of differential equations describes the time evolution of the population in each shelter x_i

$$\frac{dx_i}{dt} = P(x_i)x_e + Q(x_i)x_i$$
Input Output

i=1,...,*p*

(number of patches)

Total population:
$$N = x_e + \sum_{i=1}^{p} x_i$$

 \boldsymbol{x}_{e} (outside shelters) is homogeneously distributed outside the patches

Collective choice and crowding Bifurcation diagram (2 identical shelters; stationary states)



Amé et al, PNAS, 2006; Broly et al, 2012

Collective choice and crowding Experimental bifurcation diagram



Shelter supply influences the collective response

• Identical shelters

 $p {<} p_c$: Minimization of the number of equally occupied sites



 $p \ge p_c$: Dispersion, all shelters are equally occupied $x_1 = \dots$ = x_p Sempo et al, 2013, PloS One, JAE, 2013

Similar responses in different social situations



Queens of ants *Lasius niger*



Social spider Anelosimus eximius (Krafft)



Trail and traffic regulation (*Lasius niger*)

Jeanson et al, 2004; Dussutour et al, 2004; Tourneur, 2012; Devigne et al, 2011; Broly et al, 2014; Aron et al, in prep

Segregation: by-product of the aggregation & crowding

Exp: Individual discriminates between its own strain and a "foreign" strain Collective level: aggregation- segregation (no agonistic behaviour)



 β = (inter strain / intra strain) attraction

 $\beta=0$ high preference for their strain $\beta=1$ no preference $\beta>1$ preference for the other strain

 $Q_0 \approx \frac{1}{(O + \beta R)^2}; Q_R \approx \frac{1}{(R + \beta O)^2}$

(Rivault & Cloarec, 1999, Amé et al, 2004; Leoncini & Rivault, Ethology, 2005 Mailleux et al 2008; Astudillo et al, in prep)



Maintaining the cohesion when individuals present opposite preference



Theoretical results : Model Equations

Two equal groups with opposite preferences

$$\begin{aligned} \frac{dx_i}{dt} &= \frac{1}{m-1} \sum_{\substack{j=1, j \neq i}}^m \left[-\frac{\theta_i x_i}{k^n + (x_i + \beta_{xy} y_i)^n} + \frac{\theta_j x_j}{k^n + (x_i + \beta_{xy} y_i)^n} \right] \\ \frac{dy_i}{dt} &= \frac{1}{m-1} \sum_{\substack{j=1, j \neq i}}^m \left[-\frac{\theta_j y_i}{k^n + (\beta_{yx} x_i + y_i)^n} + \frac{\theta_i y_j}{k^n + (\beta_{yx} x_i + y_i)^n} \right] \\ &\quad i, j = 1, m, i \neq i \end{aligned}$$

$$\begin{split} &Nx = Ny = 2N, \\ &i=2, n = 2, \\ &\theta 1 > \theta 2, (X \text{ group likes shelter } 2 \& Y \text{ group likes shelter } 1) \\ &\beta xy = \beta yx = 1 \\ &Steady \text{ States from a 5}^{th} \text{ -degree equation} \\ &k \sim 2N \end{split}$$

Theoretical results : Phase diagram

Two equal groups with opposite preferences



Fig. 2. Bifurcation diagrams of the steady state solutions $x_1 + y_1$ of model 1 as a function of $R(\theta_1/\theta_2)$ for 4 values of k (k = 0.1, 0.3, 0.5, 0.8) (a) and state diagram as a function of R and k (b).

Stam. Nicolis et al Scientific Reports | 6:32703 | DOI: 10.1038/srep32703



two equal patches and its relationship with the model defined by eq. (4) (a). Positive feedback network conspecific and heterospecific interactions : symmetrical (b) and asymmetrical (c) case.

$$\frac{dx_1}{dt} = -\frac{x_1\left(1 - \frac{1}{s}(x_2 + y_2)\right)}{k^2 + (\beta_x y_1 + x_1)^2} + \frac{x_2\left(1 - \frac{1}{s}(x_1 + y_1)\right)}{k^2 + (\beta_x y_2 + x_2)^2}
\frac{dx_2}{dt} = \frac{x_1\left(1 - \frac{1}{s}(x_2 + y_2)\right)}{k^2 + (\beta_x y_1 + x_1)^2} - \frac{x_2\left(1 - \frac{1}{s}(x_1 + y_1)\right)}{k^2 + (\beta_x y_2 + x_2)^2}
\frac{dy_1}{dt} = -\frac{y_1\left(1 - \frac{1}{s}(x_2 + y_2)\right)}{k^2 + (\beta_y x_1 + y_1)^2} + \frac{y_2\left(1 - \frac{1}{s}(x_1 + y_1)\right)}{k^2 + (\beta_y x_2 + y_2)^2}
\frac{dy_2}{dt} = \frac{y_1\left(1 - \frac{1}{s}(x_2 + y_2)\right)}{k^2 + (\beta_y x_1 + y_1)^2} - \frac{y_2\left(1 - \frac{1}{s}(x_1 + y_1)\right)}{k^2 + (\beta_y x_2 + y_2)^2}$$
(4)

where $x_i = X_i/N$, $y_i = Y_i/N$, s = S/N, k = K/N and $t = \theta T/N^2$. We notice that $dx_1/dt + dx_2/dt = 0$ and $dy_1/dt + dy_2/dt = 0$ reflecting that throughout the process the numbers of individuals are conserved $(x_1 + x_2 = 1, y_1 + y_2 = 1)$. Notice that when $\ell \le 1$, although the rates still decrease with the populations already on the patches, the only solution is the homogeneous one, $x_i = y_i = 0.5$ (i = 1, 2), where the two populations are well-mixed among the two patches (see Supplemental Material A).

Figure 1a shows a tunical experimental setup corresponding to our theoretical formulation - two patches of a









Hybrid Animal – Robot Societies: Control via "info-allaxis"

Mixed groups of cockroaches and socially integrated robots

The robot is designed

- to mimic insect behavior patterns (sensors for wall detection, robots, cockroaches)
- Artificial agents and organisms interact ("robot is a conspecific") its influence on insects
- is the same as the influence of insects on insects



Collective decision making in mixed groups Robots mimick the behaviour of the animals

12 cockroaches & 4 robots, 2 identical shelters







Clear choice in 25 out 30 tests

Robots are with insects both like dark nests

(G. Sempo et al, 2006; J. Halloy et al, Science, 2007).

Collective decision making in mixed groups of robots and cockroaches (two different shelters) (II)

Insects prefer dark & Robots prefer light

 $\begin{array}{ll} \text{Robots and insects can present opposite preference for} \\ \text{shelters} & \theta_{\text{rlight}} < \theta_{\text{rdark}} \text{ and } \theta_{\text{light}} > \theta_{\text{dark}} \end{array}$



next step: TIME-Varying Networks & Aggregation



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Thanks to collaborating teams



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SCHOOL OF SCIENCE AND TECHNOLOGY

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thèmes de recherche

wato-organisationl self-organisation, emergent behaviour, non-linear dynamical systems in biology, dissipative structure, biological complex systems, collective intelligence in artificial systems.



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 Θ) and asymmetrical (c) case.

"Coordinated aggregation in complex systems", V. Basios, S.C. Nicolis, JL Deneubourg, Eur. Phys. J. ST 225 (6-7), 1143-7, 2016



Figure 5.5. Schematic of phase space slice through intersecting manifolds of stochastic system.

"Strong perturbations in nonlinear systems", V. Basios Eur. Phys. J. ST 6 (225), 1219-29, 2016