Radboud Universiteit

# *Frustrations, memory, and complexity in physics and beyond*

Mikhail Katsnelson

# Main collaborators

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**Eugene Koonin and Yuri Wolf, National Institutes of Health**

# Epigraph with explanations

**All science is either physics of stamp collection (E. Rutherford)**


**In stamp collection we deal with history and complexity**

**But the same in biology, geology… To understand the origin of cats and mice we need to go billions years to the past**

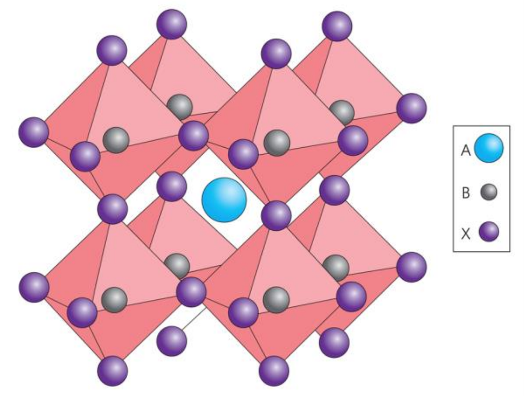
**Fundamental physical laws are local in time and space**

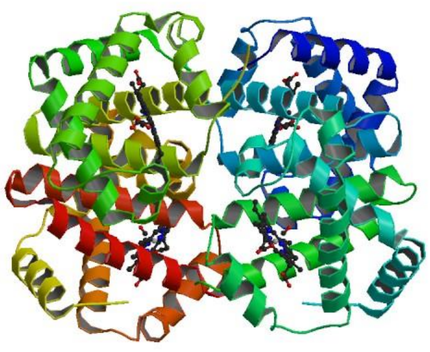
**What are the physical mechanisms of "stamp collection"?!**

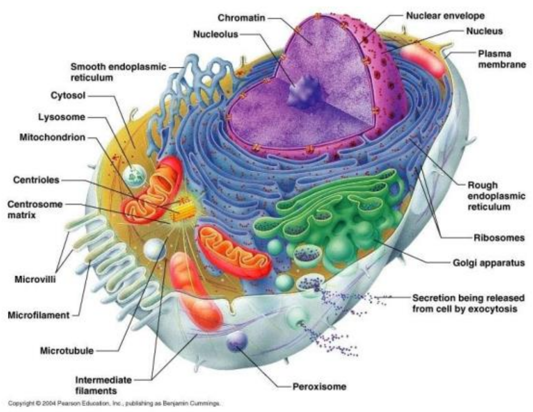
# Complexity

**Schrödinger: life substance is "aperiodic crystal" (modern formulation – Laughlin, Pines and others – glass)**

**Intuitive feeling: crystals are simple, biological structures are complex**

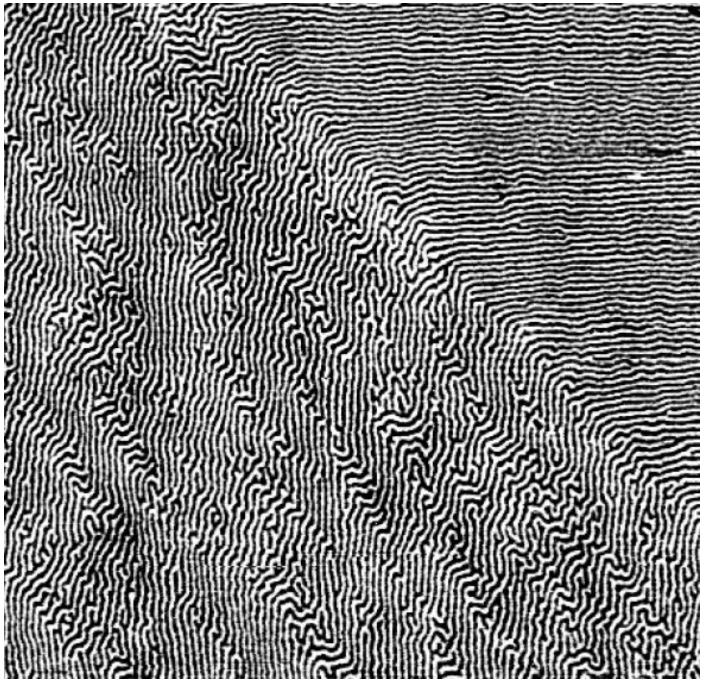





Origin and evolution of life: origin of complexity?

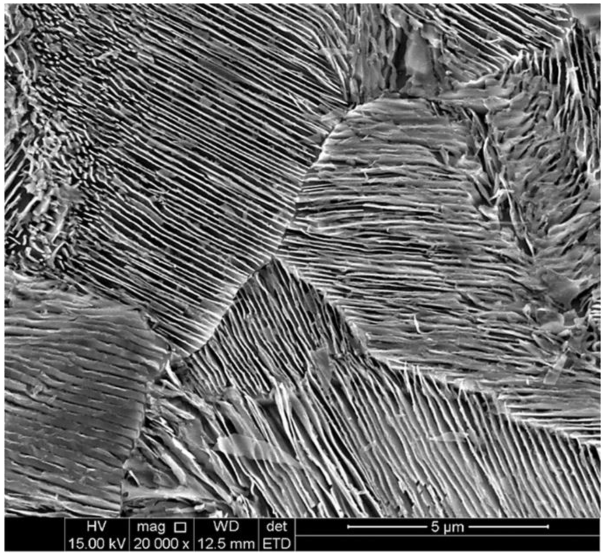
# Complexity ("patterns") in inorganic world



Stripe domains in ferromagnetic thin films

Stripes on a beach in tide zone

Microstructures in metals and alloys




Pearlitic structure in rail steel (Sci Rep 9, 7454 (2019))

Do we understand this? No, or, at least, not completely

# Outline

**Complexity vs criticality: holographic complexity**

**Pattern formation in physics: magnetic patterns as an example**

**Structural complexity from magnetic patterns to art objects**

**Self-induced glassiness and beyond: the role of frustration**

**Remarks on biological complexity and evolution**

# What is complexity?

- Something that we immediately recognize when we see it, but very hard to define quantitatively

- S. Lloyd, “Measures of complexity: a non-exhaustive list” – 40 different definitions

- Can be roughly divided into two categories:

- computational/descriptive complexities (“ultraviolet”)
- effective/physical complexities (“infrared” or inter-scale)

# Computational and descriptive complexities

- Prototype – the Kolmogorov complexity:

 the length of the shortest description (in a given language) of the object of interest

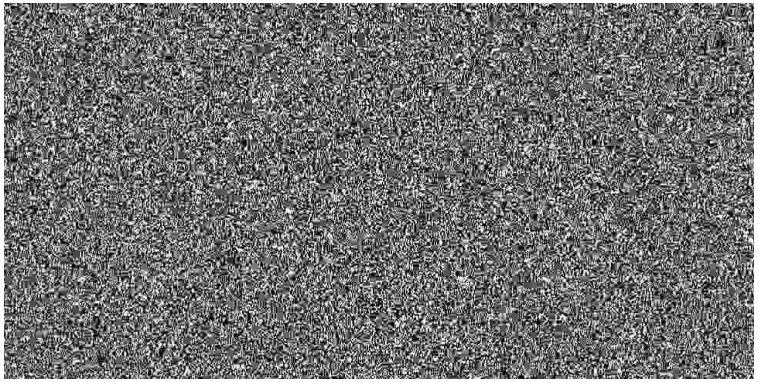
- Examples:

 - Number of gates (in a predetermined basis) needed to create a given state from a reference one

 - Length of an instruction required by file compressing program to restore image

# Descriptive complexity

- The more random – the more complex:



>

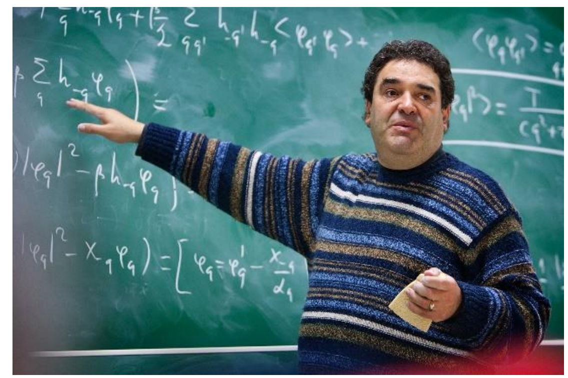
White noise
970 x 485 pixels, gray scale, 253 Kb

Vermeer "View of Delft"
750 x 624 pixels, colored, 234 Kb

# Descriptive complexity

- The more random – the more complex:

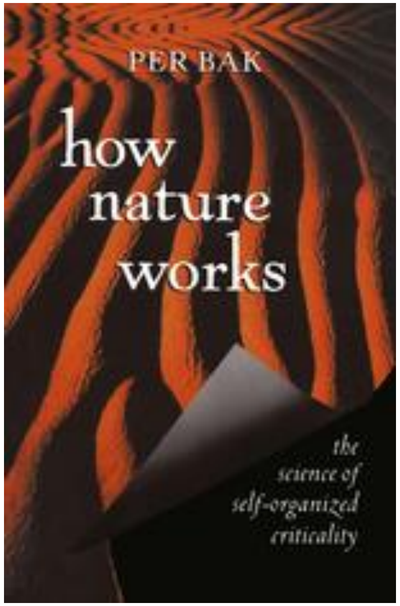
$\gg$



Paris japonica - 150 billion base pairs in DNA

Homo sapiens - 3.1 billion base pairs in DNA

# Attempts: Self-Organized Criticality

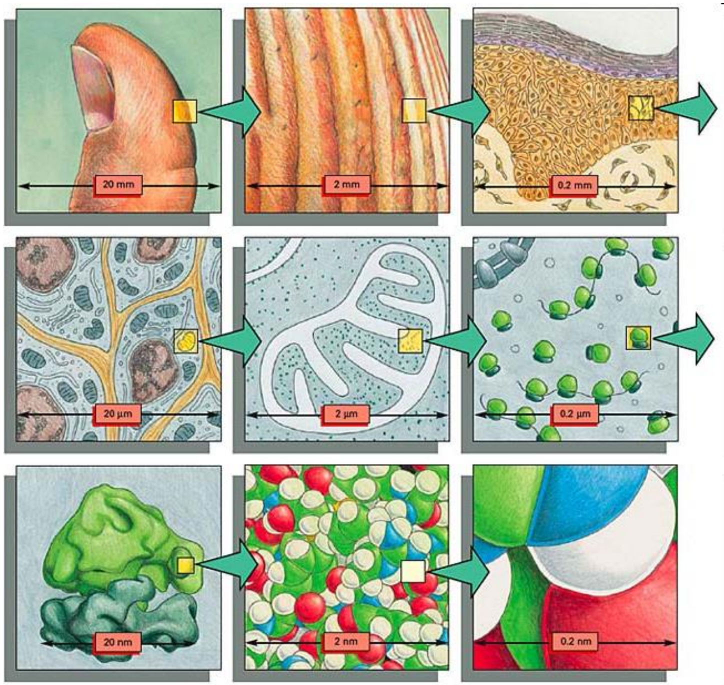



**Per Bak:** **Complexity *is* criticality**

**Some complicated (marginally stable) systems demonstrate self-similarity and "fractal" structure**

**This is intuitively more complex behavior than just white noise but can we call it "complexity"?**

**I am not sure – complexity is hierarchical**



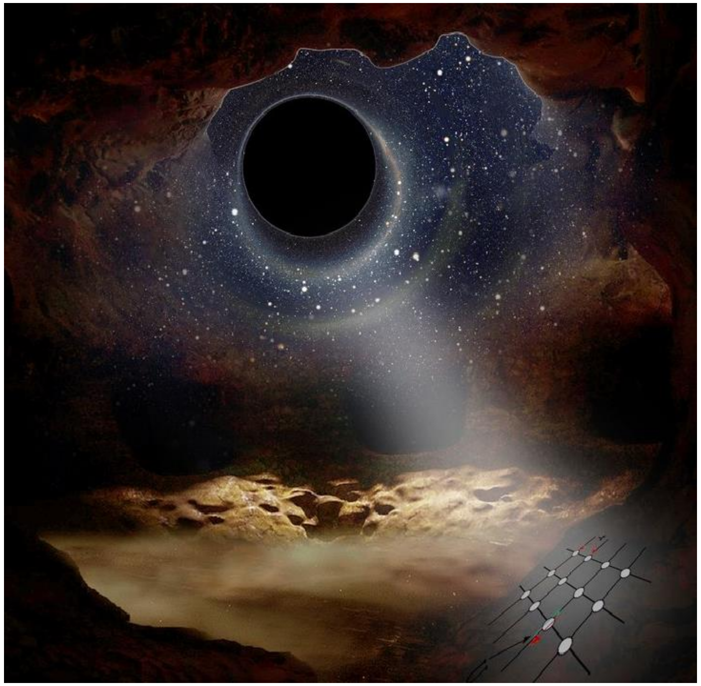
# Holographic principle and complexity

"Holographic principle" emerged as an attempt to resolve the information paradox in quantum gravity ('t Hooft 93, Susskind 94):

*A state of spacetime within a given subregion can be reconstructed from the state of its boundary*

The other way around:

*A d-dimensional quantum field theory can in principle be equivalent to a (d+1)-dimensional theory of gravity*



# Holographic complexity

**Additional coordinate: RG flow, motion along "scale" coordinate, from UV to IR**

**Two main definitions of holographic complexity**

**Complexity as volume (Susskind 2014, https://arxiv.org/abs/1402.5674)**

**Complexity as action (Brown et al, PRL 116, 191301 (2016))**

**Importantly: Both include integration over the "scale"**

# Holographic complexity II

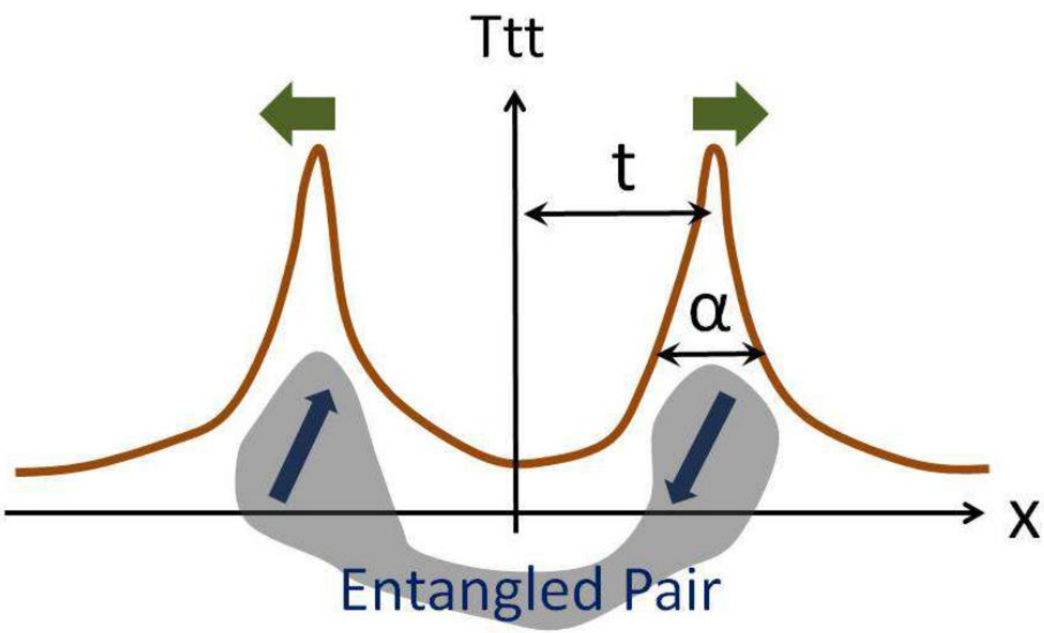
**Holographic local quench and effective complexity**

JHEP 08 (2018) 071

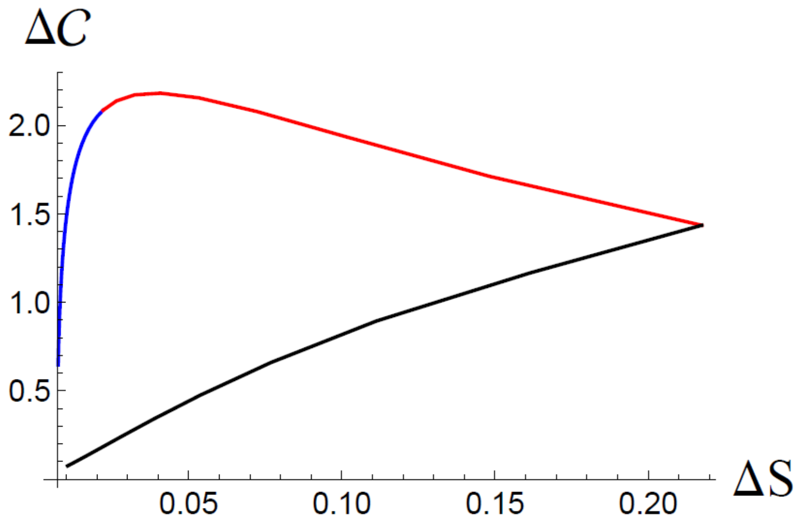
Dmitry Ageev, Irina Aref'eva, Andrey Bagrov and Mikhail I. Katsnelson

**Starting with 1+1 dimensional conformal field theory (that is, scale invariant!) and creating a local quench (putting *locally* energy into the system)**

**Pair of solitons is formed**



# Holographic complexity III




**Volume complexity is a nonmonotonous function of entanglement entropy**

**Action complexity reaches "Lloyd computational bound", that is, the fastest production of complexity (measured as a number elementary gates) consistent with Heisenberg uncertainty principle**

# Holographic complexity IV

Local quench → maximally fast growth of complexity??

**Criticality is not complexity but may be a prerequisite of quickly growing complexity!**

# Magnetic patterns

## Example: strip domains in thin ferromagnetic films

PHYSICAL REVIEW B **69**, 064411 (2004)

### Magnetization and domain structure of bcc $Fe_{81}Ni_{19}/Co$ (001) superlattices

R. Bručas, H. Hafermann, M. I. Katsnelson, I. L. Soroka, O. Eriksson, and B. Hjörvarsson

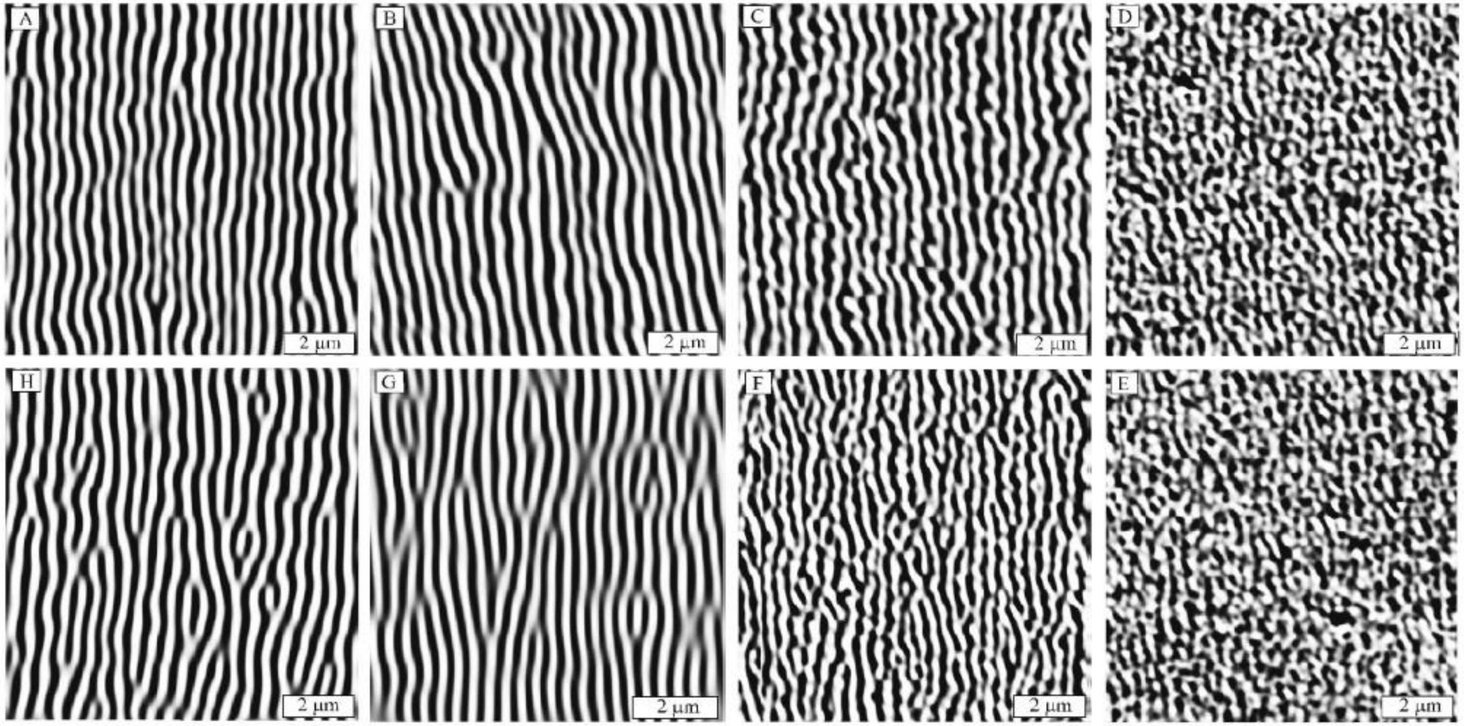
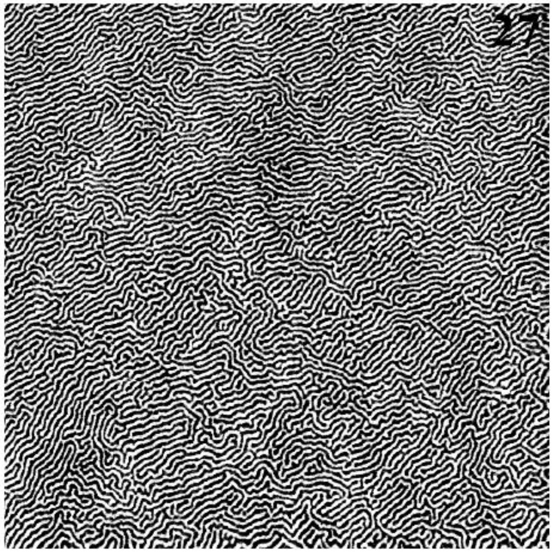
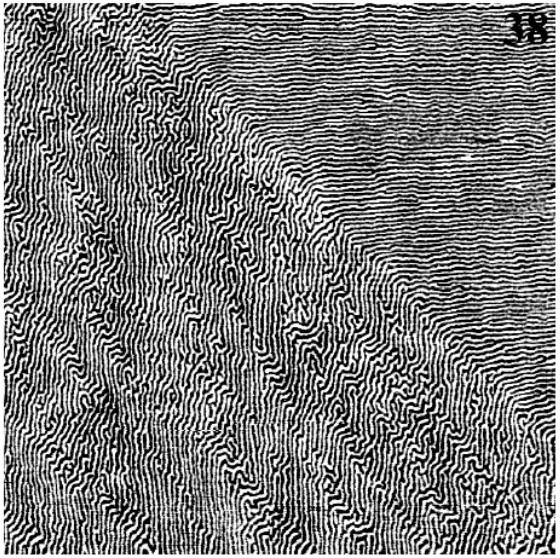
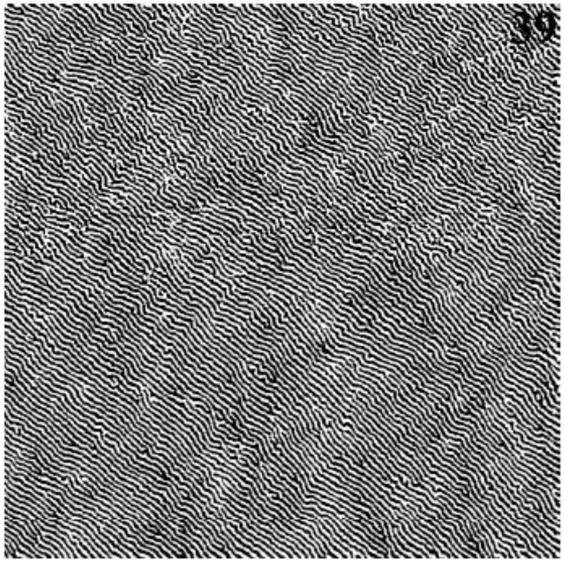


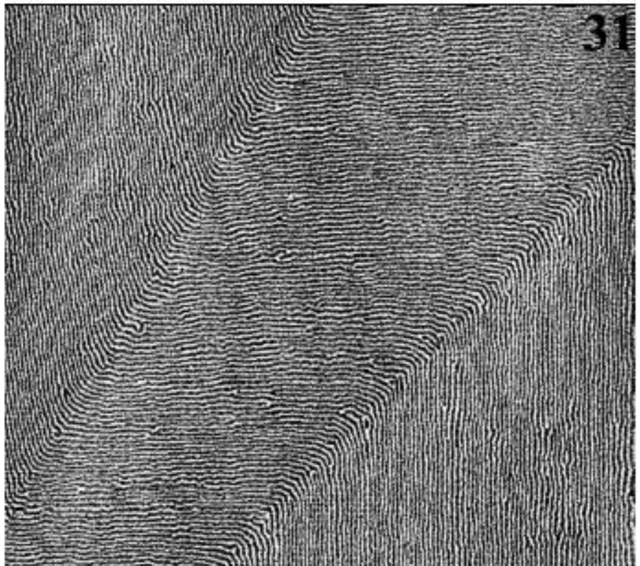

FIG. 2. The MFM images of the 420 nm thick $Fe_{81}Ni_{19}/Co$ superlattice at different externally applied in-plane magnetic fields: (a)—virgin (nonmagnetized) state; (b), (c), (d)—increasing field 8.3, 30, and 50 mT; (e), (f), (g)—decreasing field 50, 30, 8.3 mT; (h)—in remanent state.

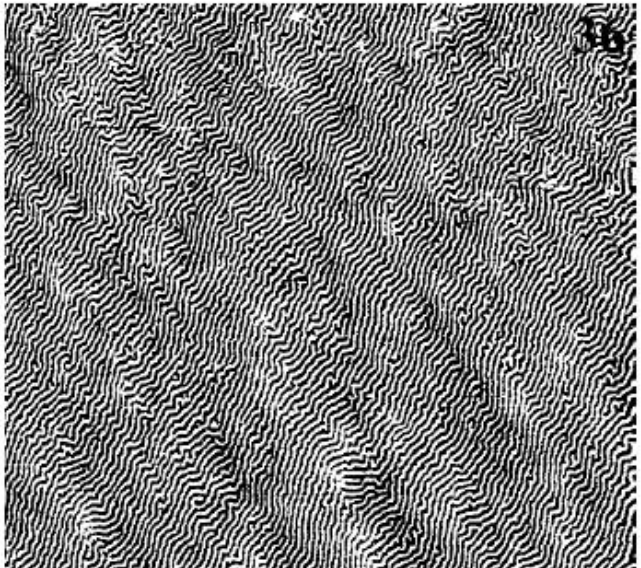
# Magnetic patterns II



# Magnetic patterns III

*Europhys. Lett.*, **73** (1), pp. 104–109 (2006)
DOI: 10.1209/epl/i2005-10367-8

**Topological defects, pattern evolution, and hysteresis in thin magnetic films**

P. A. Prudkovskii[1], A. N. Rubtsov[1] and M. I. Katsnelson[2]

$$H = \int \left( \frac{J_x}{2} \left( \frac{\partial \boldsymbol{m}}{\partial x} \right)^2 + \frac{J_y}{2} \left( \frac{\partial \boldsymbol{m}}{\partial y} \right)^2 - \frac{K}{2} m_z^2 - h m_y \right) \mathrm{d}^2 r +$$

$$+ \frac{Q^2}{2} \int \int m_z(\boldsymbol{r}) \left( \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} - \frac{1}{\sqrt{d^2+(\boldsymbol{r}-\boldsymbol{r}')^2}} \right) m_z(\boldsymbol{r}') \mathrm{d}^2 r \mathrm{d}^2 r'.$$

**Competition of exchange interactions (want homogeneous ferromagnetic state) and magnetic dipole-dipole interations (want total magnetization equal to zero)**

# Magnetic patterns IV

## Classical Monte Carlo simulations

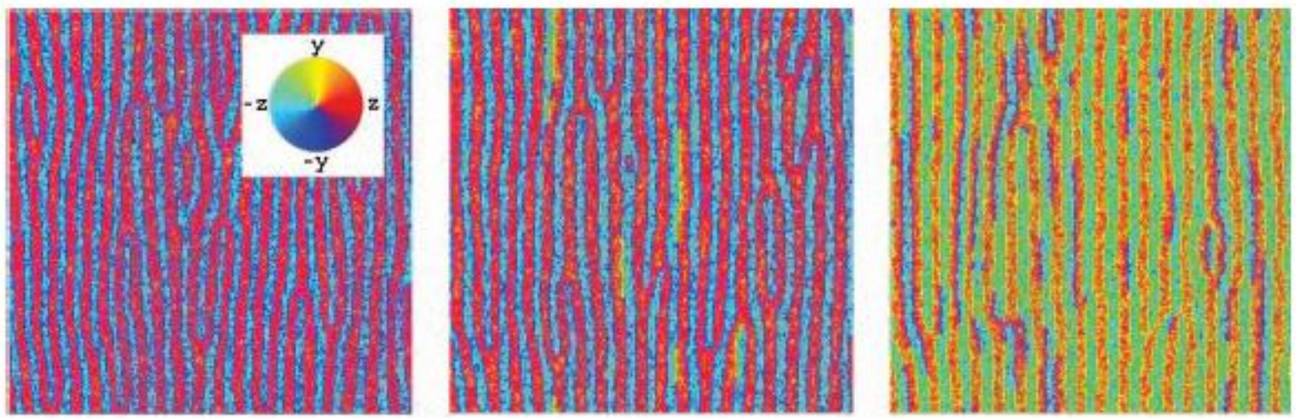



Fig. 2 – Snapshots of the stripe-domain system with the two-component order parameter at several points of the hysteresis loop for $\beta = 1$. The magnetic field is $h = 0$, $h = 0.3$, and $h = 0.6$, from left to right. The inset shows the color legend for the orientation of local magnetization.

**We know the Hamiltonian and it is not very complicated**

**How to describe patterns and how to explain patterns?**

# Structural complexity

## Multi-scale structural complexity of natural patterns

PNAS 117, 30241 (2020)

Andrey A. Bagrov[a,b,1,2], Ilia A. Iakovlev[b,1], Askar A. Iliasov[c], Mikhail I. Katsnelson[c,b], and Vladimir V. Mazurenko[b]

**The idea (from holographic complexity and common sense):**
**Complexity is dissimilarity at various scales**

**Let $f(x)$ be a multidimensional pattern**

$f_\Lambda(x)$ **its coarse-grained version (Kadanoff decimation, convolution with Gaussian window functions,…)**

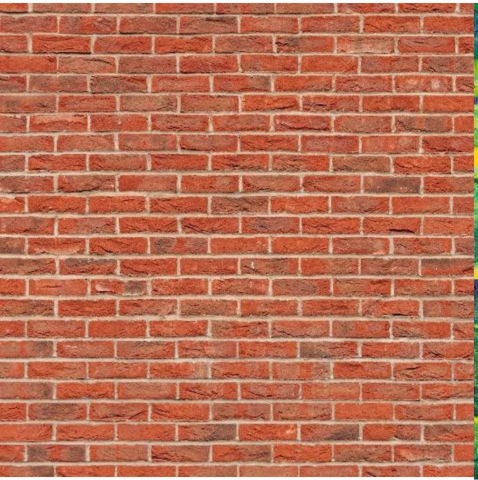
**Complexity is related to distances between** $f_\Lambda(x)$ and $f_{\Lambda+d\Lambda}(x)$

$$\langle f(x)|g(x)\rangle = \int_D dx\, f(x) g(x)$$

$$\Delta_\Lambda = |\langle f_\Lambda(x)|f_{\Lambda+d\Lambda}(x)\rangle - \frac{1}{2}\left(\langle f_\Lambda(x)|f_\Lambda(x)\rangle + \langle f_{\Lambda+d\Lambda}(x)|f_{\Lambda+d\Lambda}(x)\rangle\right)| = \frac{1}{2}|\langle f_{\Lambda+d\Lambda}(x) - f_\Lambda(x)|f_{\Lambda+d\Lambda}(x) - f_\Lambda(x)\rangle|,$$

$$\mathcal{C} = \sum_\Lambda \frac{1}{d\Lambda}\Delta_\Lambda \to \int |\langle \frac{\partial f}{d\Lambda}|\frac{\partial f}{d\Lambda}\rangle| d\Lambda, \text{ as } d\Lambda \to 0$$

# Art objects (and walls)



$C = 0.1076$

$C = 0.2010$

$C = 0.2147$

$C = 0.2765$

$C = 0.4557$

$C = 0.4581$

$C = 0.4975$

$C = 0.5552$

# Solution of an ink drop in water

**Entropy should grow, but complexity is not! And indeed…**

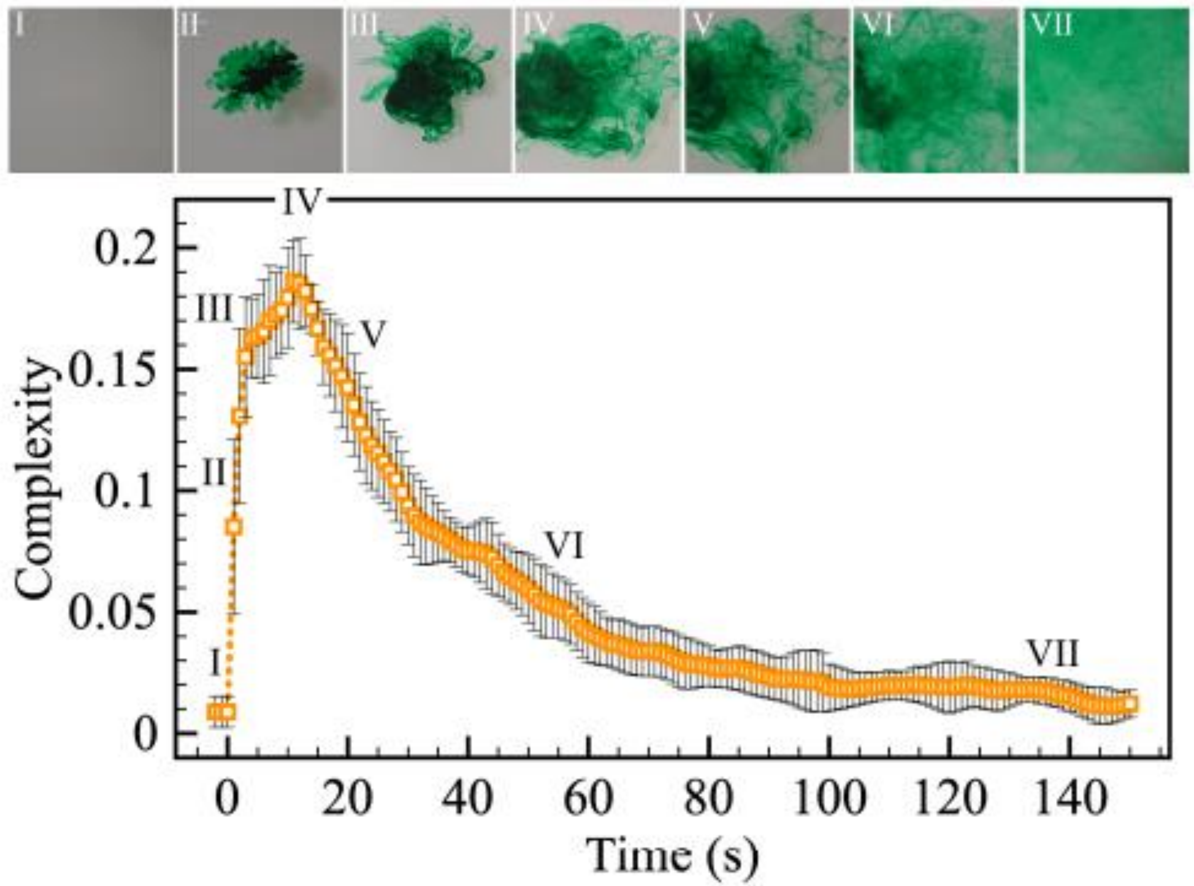



FIG. 7. The evolution of the complexity during the process of dissolving a food dye drop of 0.3 ml in water at 31°C.

# Structural complexity: 2D Ising model

**Can be used as a numerical tool to find $T_C$ from finite-size simulations**

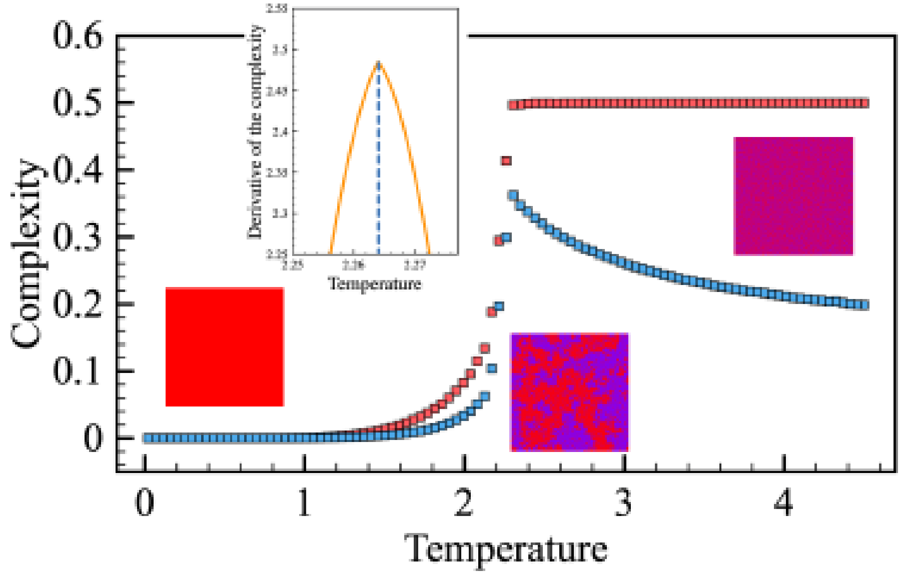
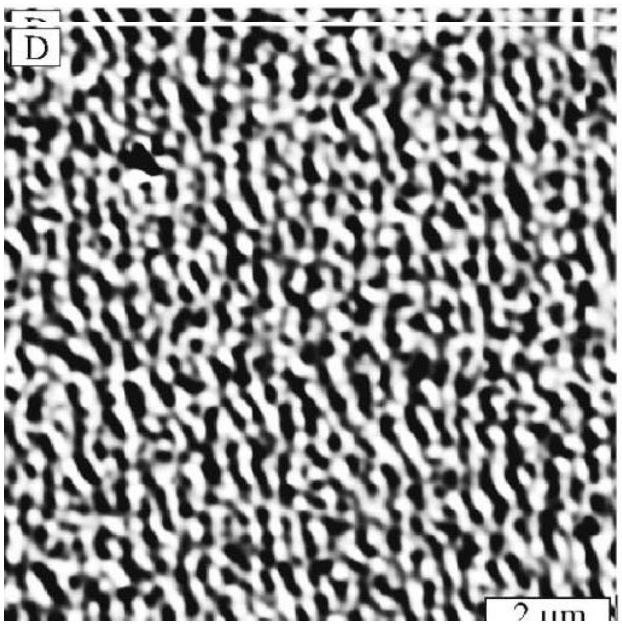



FIG. 2. Temperature dependence of the complexity obtained from the two-dimensional Ising model simulations. Red and blue squares correspond to the complexities calculated with $k \geq 0$ and $k \geq 1$, respectively. The size of error bars is smaller than the symbol size. Inset shows the first derivative of the complexity used for accurate detection of the critical temperature. Here we used $N = 8$, $\Lambda = 2$.

# Competing interactions and self-induced spin glasses

## Special class of patterns: “chaotic” patterns

PHYSICAL REVIEW B **69**, 064411 (2004)




**Hypothesis: a system wants to be modulated but cannot decide in which direction**

$$E_m = \int \int d\mathbf{r} d\mathbf{r}' m(\mathbf{r}) m(\mathbf{r}') \left[ \frac{1}{|\mathbf{r}-\mathbf{r}'|} - \frac{1}{\sqrt{(\mathbf{r}-\mathbf{r}')^2 + D^2}} \right]$$

$$= 2\pi \sum_{\mathbf{q}} m_{\mathbf{q}} m_{-\mathbf{q}} \frac{1-e^{-qD}}{q}, \qquad (13)$$

where $m_{\mathbf{q}}$ is a two-dimensional Fourier component of the magnetization density. At the same time, the exchange energy can be written as

$$E_{exch} = \frac{1}{2} \alpha \sum_{\mathbf{q}} q^2 m_{\mathbf{q}} m_{-\mathbf{q}}, \qquad (14)$$

so there is a finite value of the wave vector $q = q^*$ found from the condition

$$\frac{d}{dq} \left( 2\pi \frac{1-e^{-qD}}{q} + \frac{1}{2} \alpha q^2 \right) = 0 \qquad (15)$$

# Self-induced spin glasses II

PHYSICAL REVIEW B 93, 054410 (2016)

**Stripe glasses in ferromagnetic thin films**

Alessandro Principi* and Mikhail I. Katsnelson

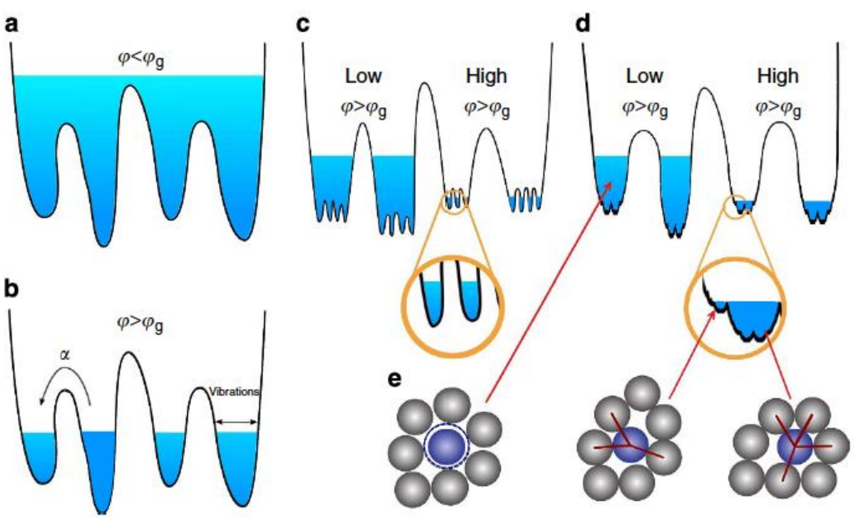
PRL 117, 137201 (2016) PHYSICAL REVIEW LETTERS week ending 23 SEPTEMBER 2016

**Self-Induced Glassiness and Pattern Formation in Spin Systems Subject to Long-Range Interactions**

Alessandro Principi* and Mikhail I. Katsnelson

**Development of idea of stripe glass, J. Schmalian and P. G. Wolynes, PRL 2000**

**Glass: a system with an energy landscape characterizing by infinitely many local minima, with a broad distribution of barriers, relaxation at "any" time scale and aging (at thermal cycling you never go back to *exactly* the same state)**




**Picture from P. Charbonneau et al,**

DOI: 10.1038/ncomms4725

Intermediate state between equilibrium and non-equilibrium, opportunity for history and memory ("stamp collection")

# Self-induced spin glasses III

**One of the ways to describe: R. Monasson, PRL 75, 2847 (1995)**

$$\mathcal{H}_\psi[m,\lambda] = \mathcal{H}[m,\lambda] + g\int dr[m(r) - \psi(r)]^2$$

**The second term describes attraction of our physical field $m(r)$ to some external field $\psi(r)$**

**If the system an be glued, with infinitely small interaction *g*, to macroscopically large number of configurations it should be considered as a glass**

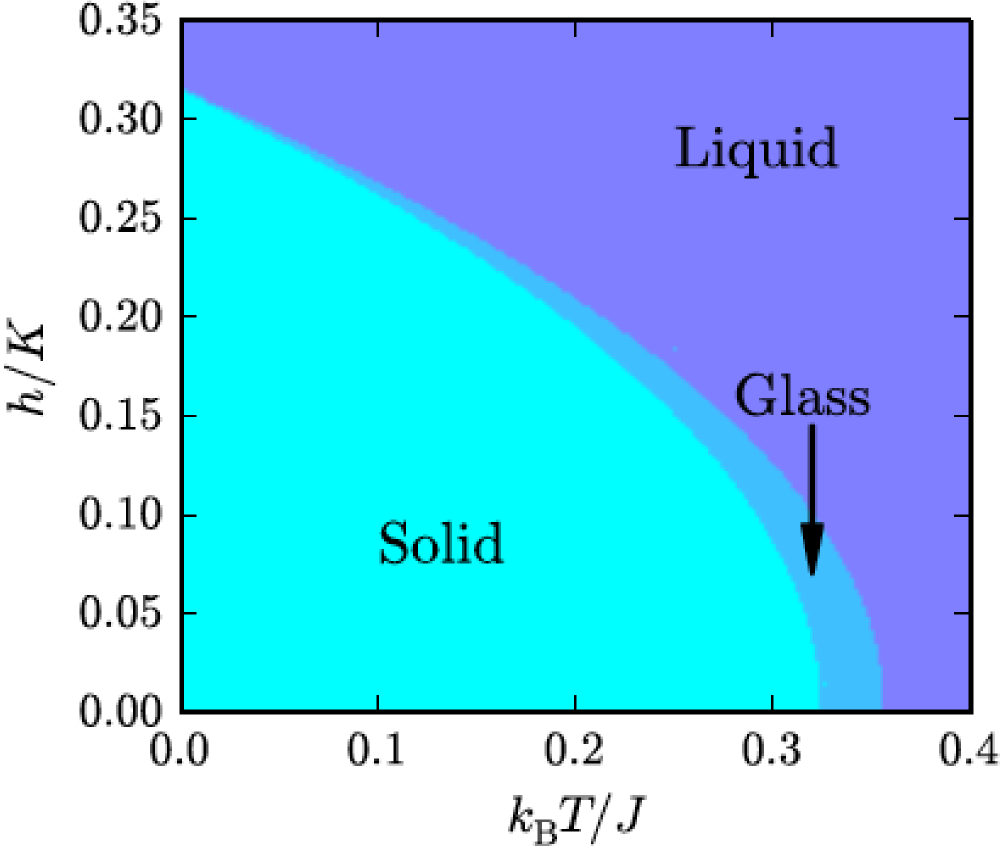
**Then we calculate** $F_g = \frac{\int \mathcal{D}\psi\, Z[\psi] F[\psi]}{\int \mathcal{D}\psi\, Z[\psi]}$ **and see whether the limits**

$F_{\mathrm{eq}} = \lim_{N\to\infty} \lim_{g\to 0} F_g$ **and** $F = \lim_{g\to 0} \lim_{N\to\infty} F_g$ **are different**

**If yes, this is self-induced glass**

**No disorder is needed (contrary to traditional view on spin glasses)**

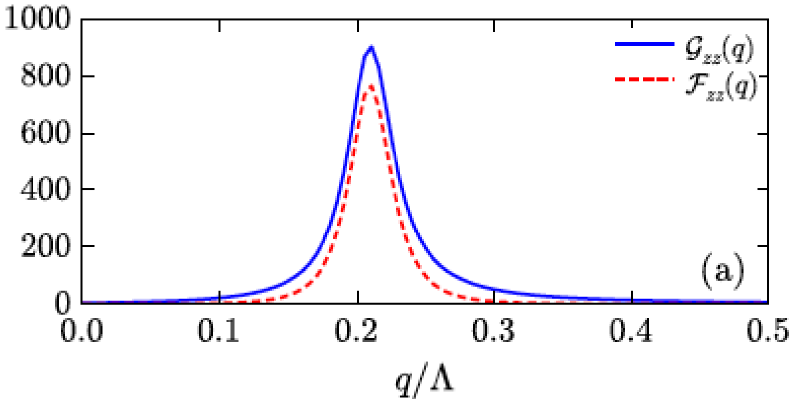
# Self-induced spin glasses IV




Phase diagram

**Maximum at**

$$q_0 \simeq [Q/(2J)]^{1/3} \neq 0$$




**q-dependence of normal and anomalous ("glassy", non-ergodic spin-spin correlators**

# Experimental observation of self-induced spin glass state: elemental Nd

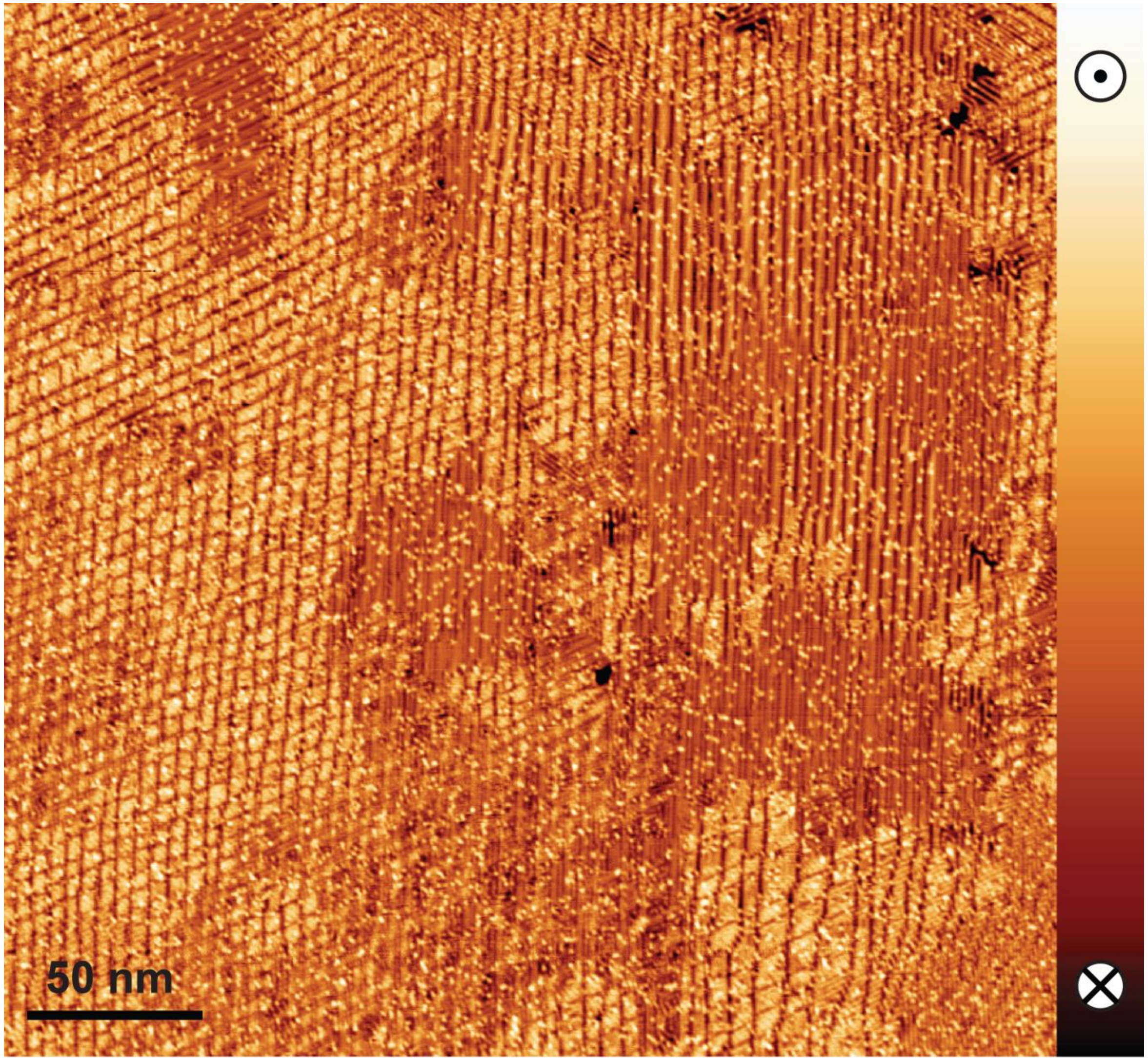
## Self-induced spin glass state in elemental and crystalline neodymium

*Science* **368**, 966 (2020)

Umut Kamber, Anders Bergman, Andreas Eich, Diana Iuşan, Manuel Steinbrecher, Nadine Hauptmann, Lars Nordström, Mikhail I. Katsnelson, Daniel Wegner*, Olle Eriksson, Alexander A. Khajetoorians*

**Spin-polarized STM experiment, Radboud University**


# Magnetic structure: no long-range



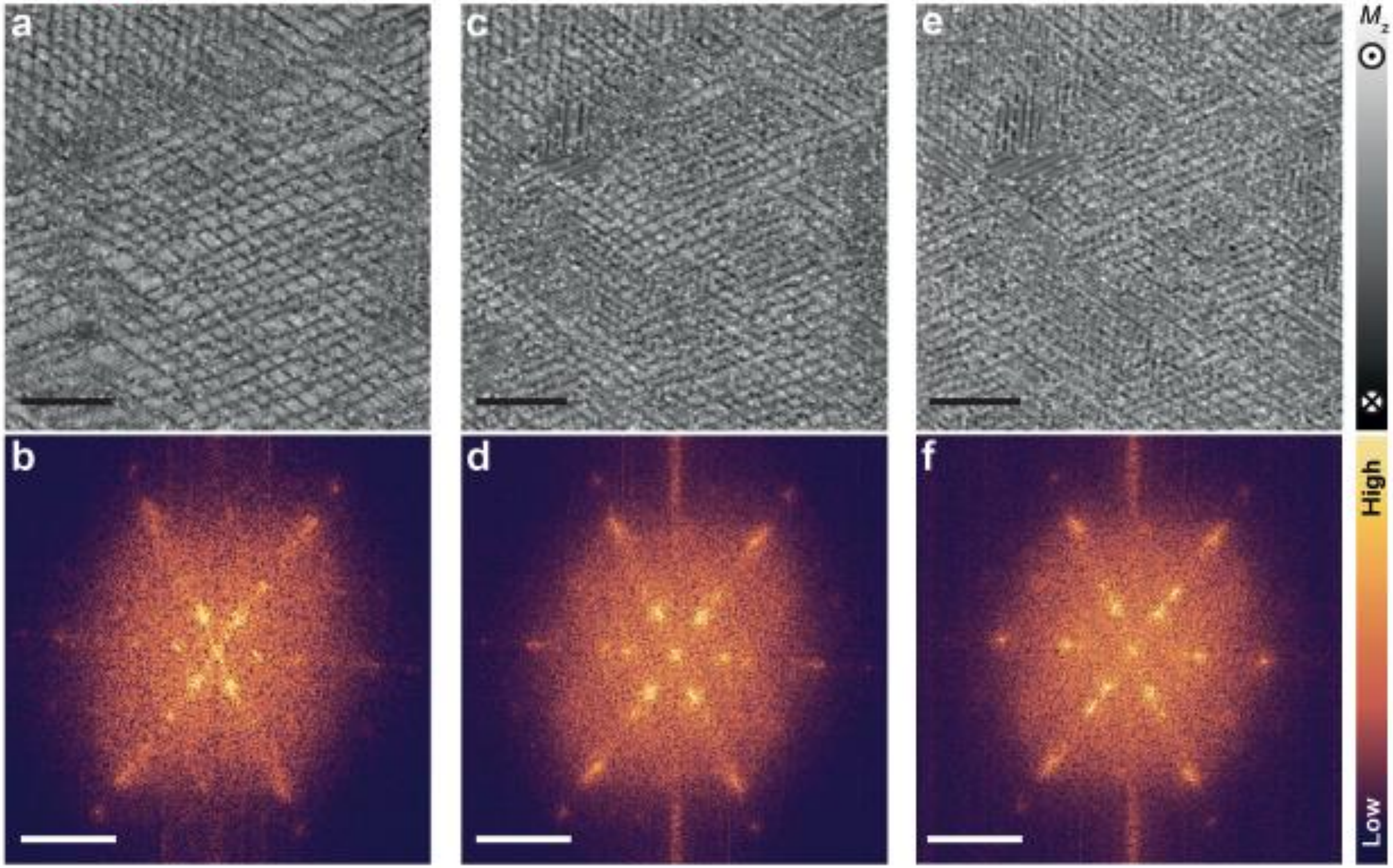

Cr bulk tip

*T: 1.3K*
*B: 0T*

✔ Short-range non-collinear order

✖ Long-range order

# Magnetic structure: local correlations

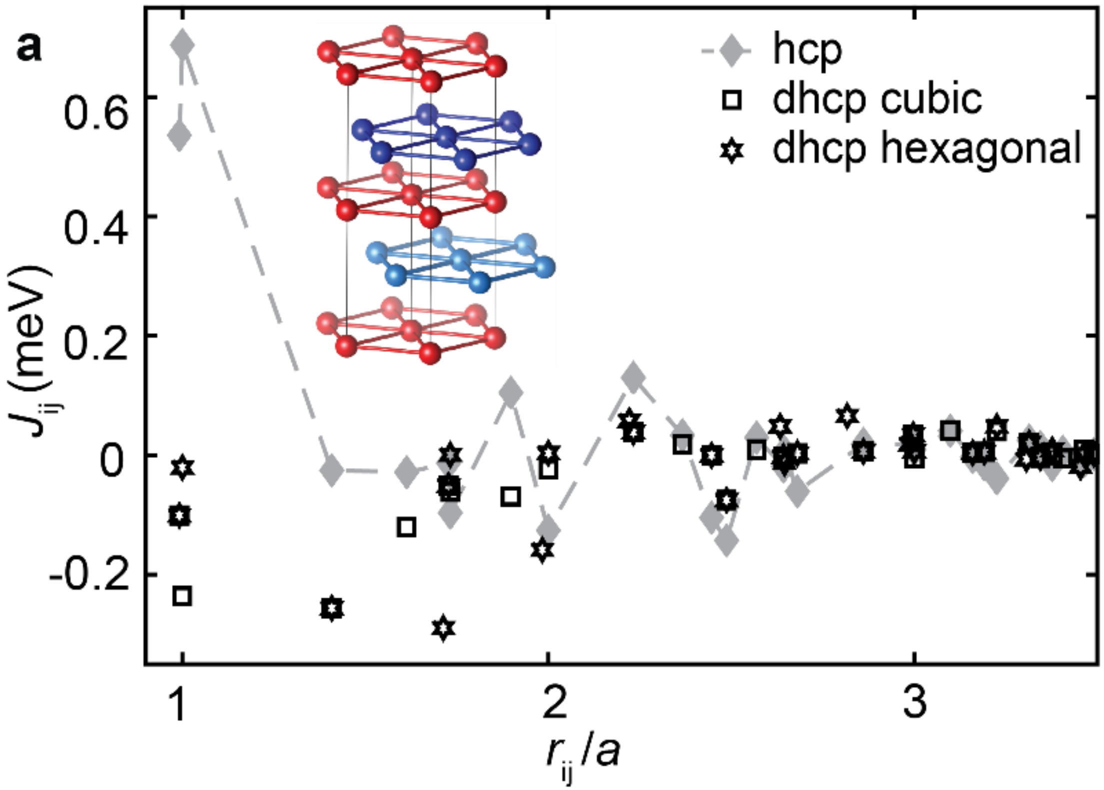



The most important observation: aging. At thermocycling (or cyling magnetic field) the magnetic state is not exactly reproduced

# *Ab initio*: magnetic interactions in bulk Nd

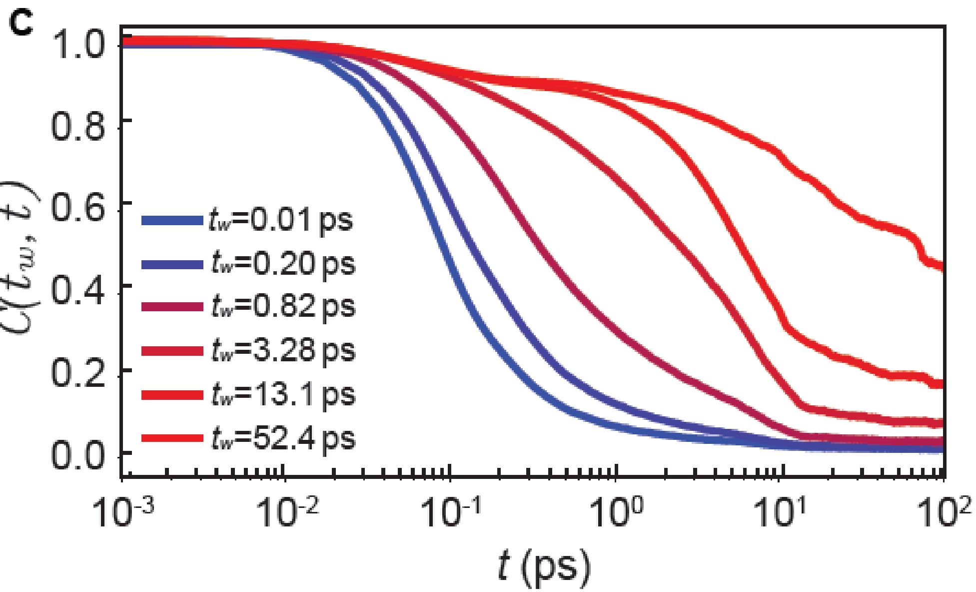
**Method: magnetic force theorem (Lichtenstein, Katsnelson, Antropov, Gubanov JMMM 1987)**

**Calculations: Uppsala team (Olle Eriksson group)**




- Dhcp structure drives competing AFM interactions
- Frustrated magnetism

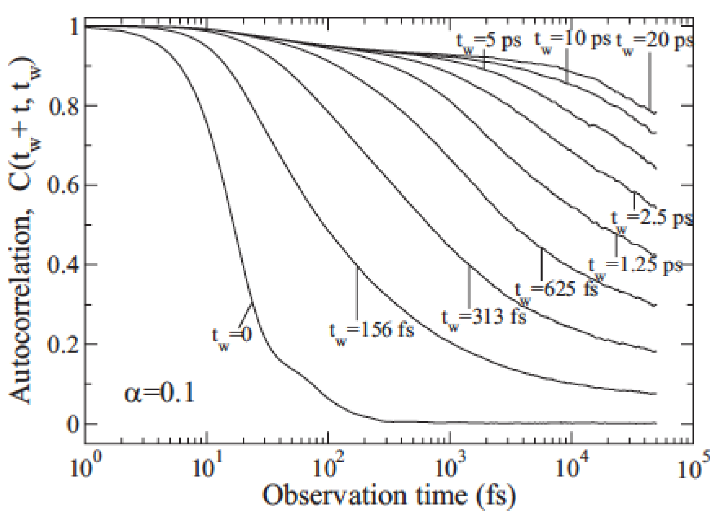
# Spin-glass state in Nd: spin dynamics




**Atomistic spin dynamics simulations**

**Typically spin-glass behavior**

Autocorrelation function $C(t_w, t) = \langle \boldsymbol{m}_i(t + t_w) \cdot \boldsymbol{m}_i(t_w) \rangle$ for dhcp Nd at $T$ = 1 K




**To compare: the same for prototype *disordered* spin-glass Cu-Mn**

**B. Skubic et al, PRB 79, 024411 (2009)**

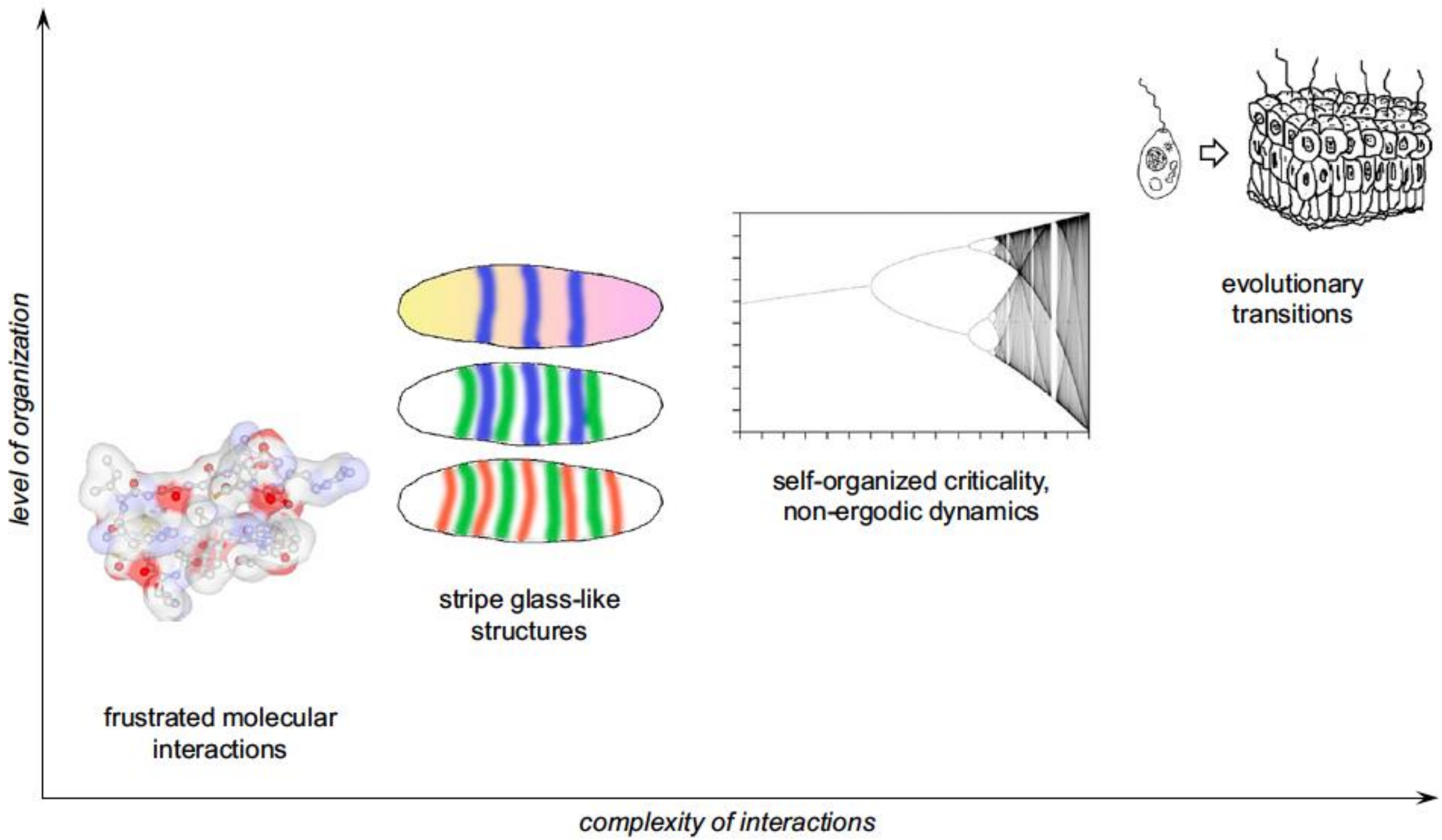
# Frustrations and biological complexity

## Physical foundations of biological complexity

Yuri I. Wolf[a], Mikhail I. Katsnelson[b], and Eugene V. Koonin[a,1]

E8678–E8687 | PNAS | vol. 115

**Competing interactions as universal mechanism of complexity?!**



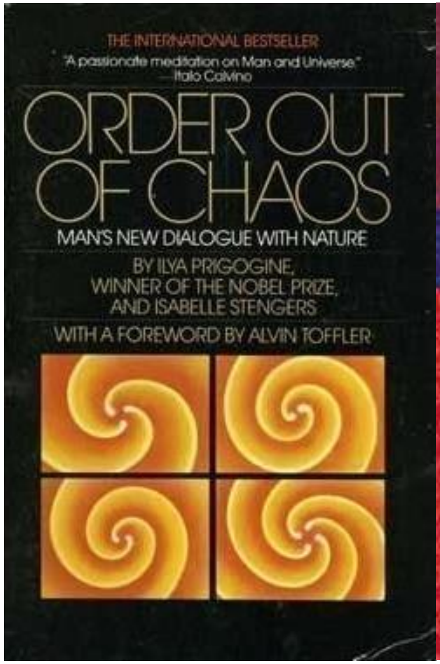
# Frustrations and biological complexity II

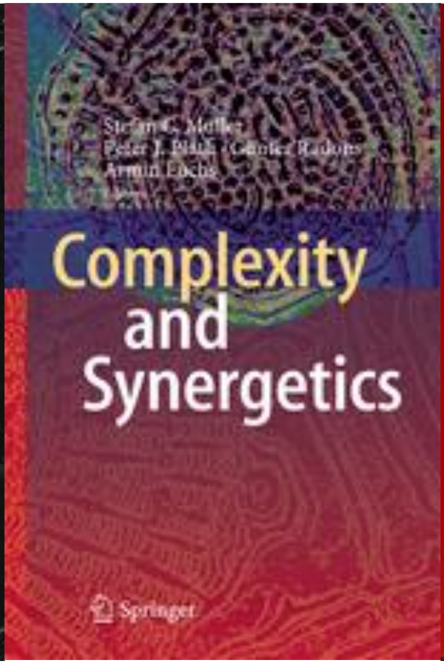
**Table 1. Competing interactions and frustrated states in biological evolution**

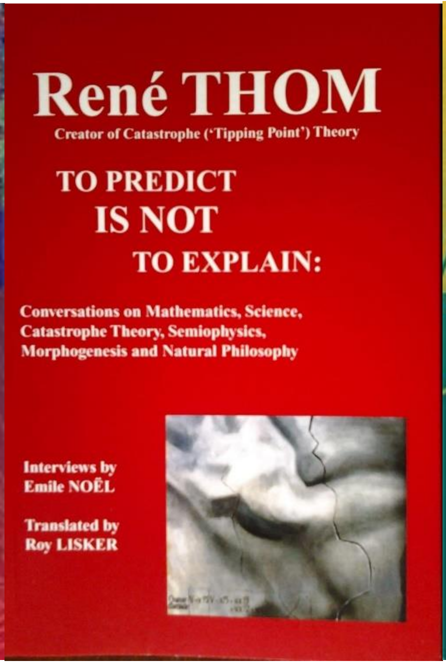
| System | Frustration-producing factors (competing interactions) | Emergent functional and evolutionary features |
|---|---|---|
| RNA | Short-range (within stem local hydrogen bonding, stacking) vs. long-range (long-distance hydrogen bonding, salt bridges) interactions between nucleotides | Complex 3D structures including ribozymes |
| Proteins | Short-range (Van der Waals) vs. long-range (hydrogen bonds, salt bridges) interactions between amino acid side chains | Stable conformations and semiregular patterns in protein structures; allostery enabled by transitions between energetically quasi-degenerate conformations |
| Macromolecular complexes | Within-subunit vs. between-subunit interactions | Elaborate complex organization, in particular nucleoproteins (ribosomes, chromatin) |
| **Cells** | **Membranes (confinement of chemicals) vs. channels/pores (transport of chemicals)** | **Compartments and cellular machinery dependent on electrochemical gradients** |
| **Autonomous (hosts) and semiautonomous (parasites) replicators** | **Replicator vs. parasite genomes** | **Self- vs. non-self-discrimination and defense; complex genomes of increasing size; primitive cells** |
| **Autonomous (hosts) and semiautonomous (parasites) reproducers/replicators** | **Host cells and viruses** | **Infection mechanisms, defense and counterdefense systems, evolutionary arms race; contribution to the origin of multicellular life forms** |
| Autonomous (hosts) and semiautonomous (parasites) reproducers/replicators | Host cells vs. transposons | Intragenomic DNA replication control; evolutionary innovation through recruitment of transposon sequences |
| Autonomous (hosts) and semiautonomous (parasites) reproducers/replicators | Host cells vs. plasmids | Beneficial cargo genes, plasmid addiction systems, efficient gene exchange and transfer mechanisms |
| **Emerging eukaryotic cells** | **Host (archaeal) cells vs. endosymbiont (α-proteobacteria, protomitochondria)** | **Eukaryotic cells with complex intracellular organization** |
| **Communities of unicellular organisms** | **Individual cells vs. cellular ensembles** | **Information exchange and quorum sensing mechanisms; replication control, programmed cell death, multicellularity** |
| Multicellular organisms | Soma vs. germline | Complex bodies, tissues and organ differentiation, sexual reproduction |
| Multicellular organisms | Dividing vs. quiescent cells | Aging, cancer, death |
| **Populations** | **Individual members vs. groups** | **Population-level cooperation; kin selection; eusocilaity** |
| Populations | Males vs. females (partners with unequal parental investment) | Sexual selection, sexual dimorphism |
| Ecosystems | Species in different niches | Interspecies competition, host–parasite and predator–prey relationships, mutualism, symbiosis |
| **Societies*** | — | — |

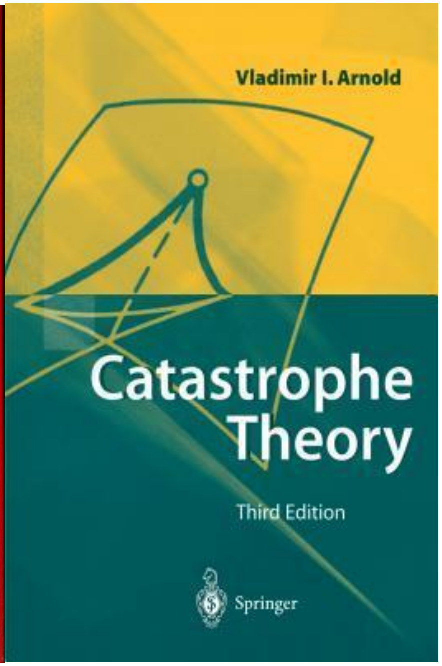
Those competing interactions and frustrated states that are deemed to directly contribute to MTE are shown in bold.
*We refrain from specifying the conflicts that drive the origin and evolution of human societies.

# To summarize: How it was in 1960th-1980th



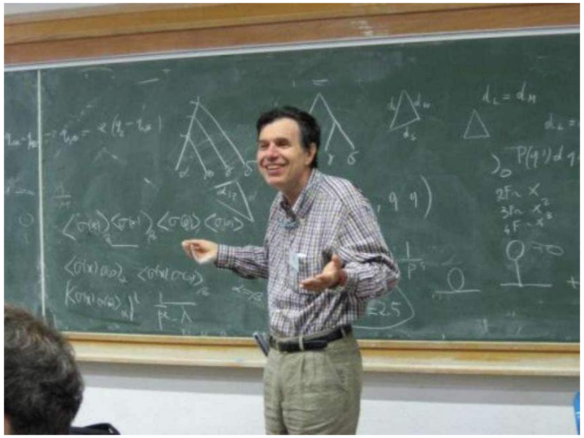

**People were very enthusiastic on applications of theory of dynamical systems: attractors, bifurcations, catastrophes – useful for sure but…**

**The distance from Benard convection cells to origin of life seems to be too far…**

# To summarize: Now

**Now we try statistical physics approached, our new key words are:**
**emergence, renormalization group flow, universality classes, spin glasses, broken replica symmetry, frustrations…**

**Giorgio Parisi, Nobel Prize in physics 2021**
"for the discovery of the interplay of disorder and fluctuations in physical systems from atomic to planetary scales."



**Will it help us?! Who knows…**

**THINK!!!**