

Radboud Universiteit



***Multiscale structural complexity of
natural and unnatural patterns***

Mikhail Katsnelson

Main collaborators

Andrey Bagrov, Askar Iliasov, Anna Kravchenko, Ilya Schurov
Radboud University, Nijmegen

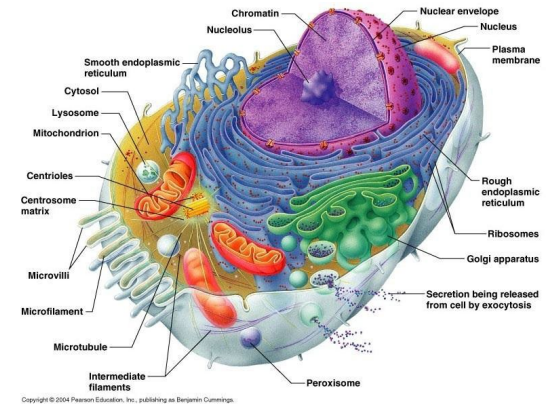
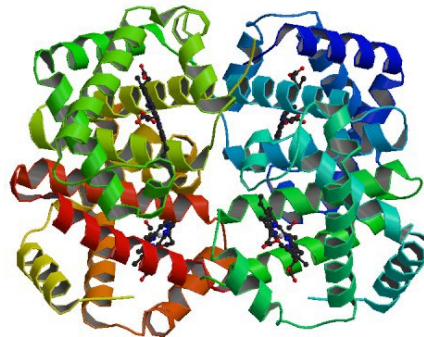
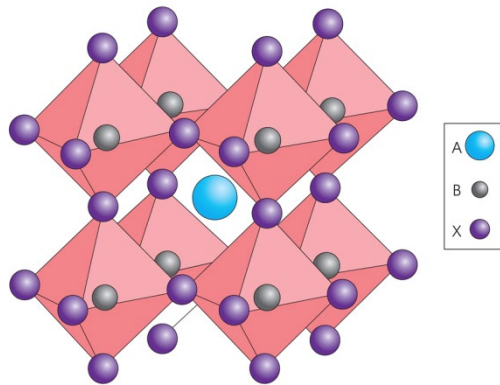
Vladimir Mazurenko, Ilya Iakovlev, Oleg Sotnikov
Ural Federal University, Ekaterinburg

Veronica Dudarev
University of British Columbia, Vancouver

Complexity

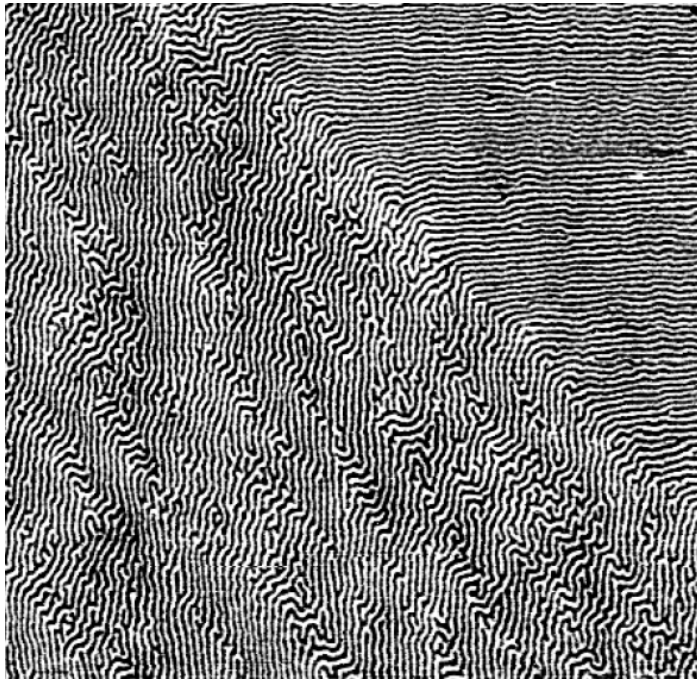
Schrödinger: life substance is “aperiodic crystal” (modern formulation – Laughlin, Pines and others – glass)

Intuitive feeling: crystals are simple, biological structures are complex



Origin and evolution of life: origin of complexity?

Complexity (“patterns”) in inorganic world

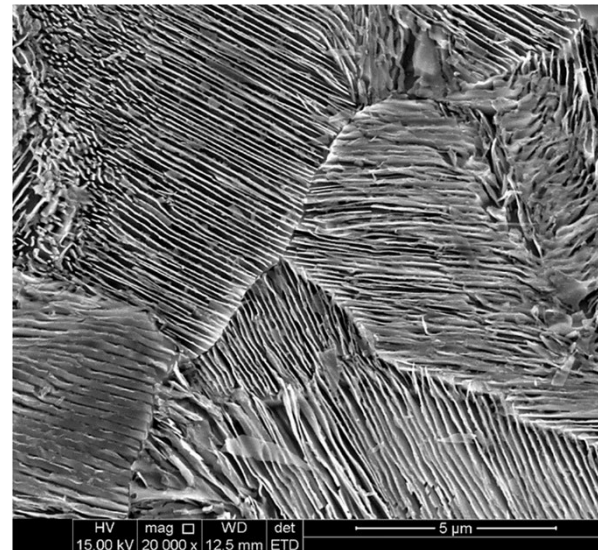


Stripe domains in ferromagnetic thin films

Microstructures in metals and alloys



Stripes on a beach in tide zone



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

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

What is complexity?

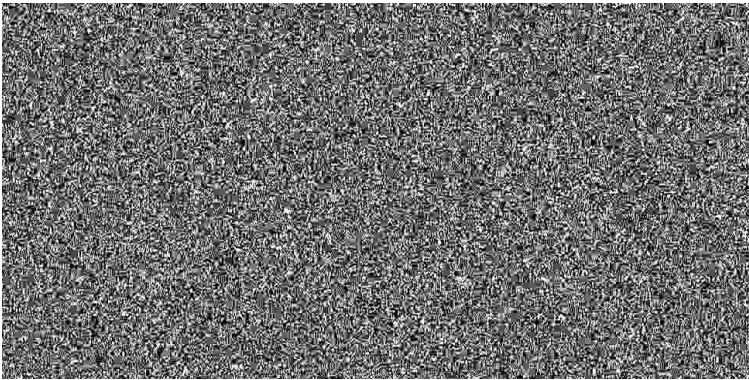
- Something that we immediately recognize when we see it, but very hard to define quantitatively
- S. Lloyd, “Measures of complexity: a non-exhaustive list” – 40 different definitions
- Can be roughly divided into two categories:
 - computational/descriptive complexities (“ultraviolet”)
 - effective/physical 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”

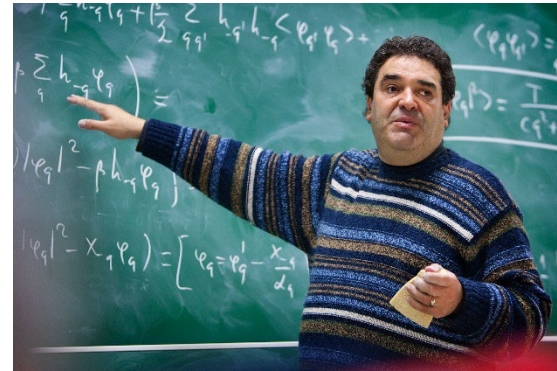
750 x 624 pixels, colored, 234 Kb

Descriptive complexity II

The longer instruction – the more complex?

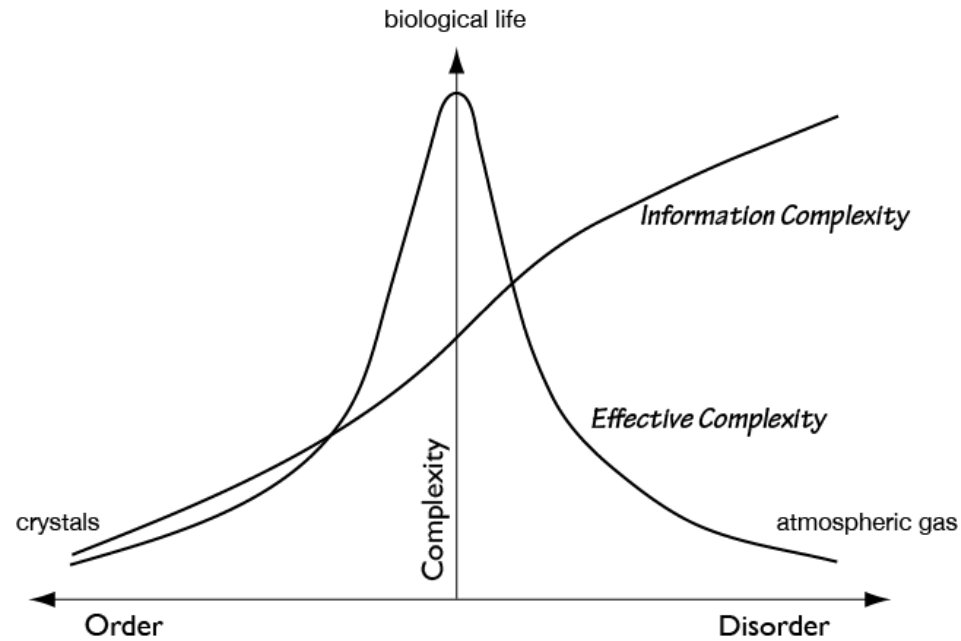


Paris japonica - 150
billion base pairs in
DNA



Homo sapiens - 3.1
billion base pairs in
DNA

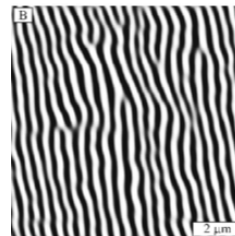
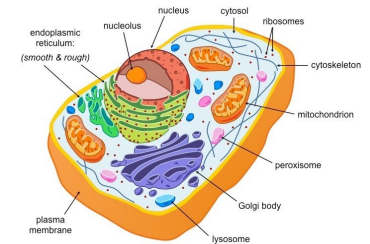
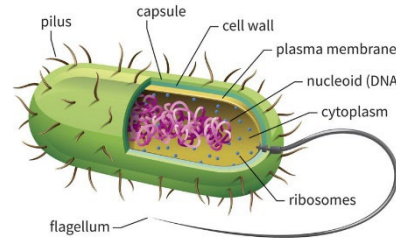
Effective complexity



Can we come up with a quantitative measure?..

Not a mere philosophical question...

- What happens at the major evolutionary transitions?
- Why are simple neural algorithms capable of solving complex many-body problems?
- Why do many natural patterns appear to be universal?

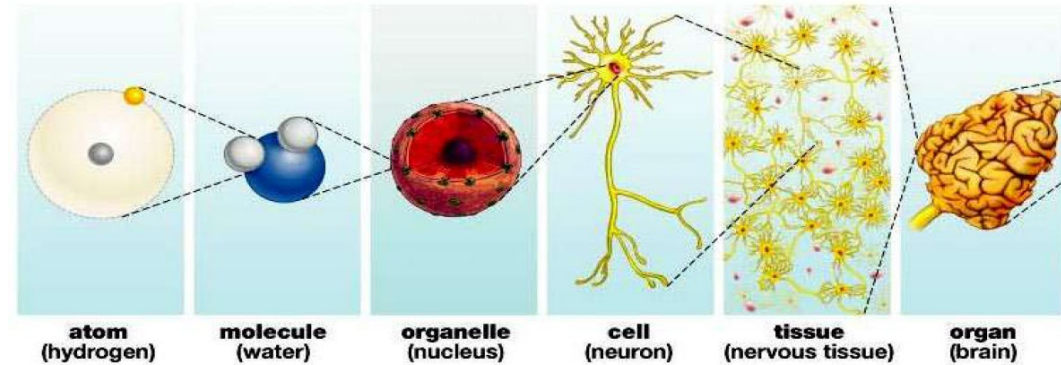
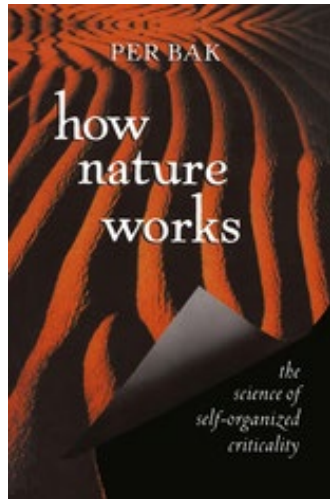


Attempts: Self-Organized Criticality?

Per Bak: Complexity *is* criticality

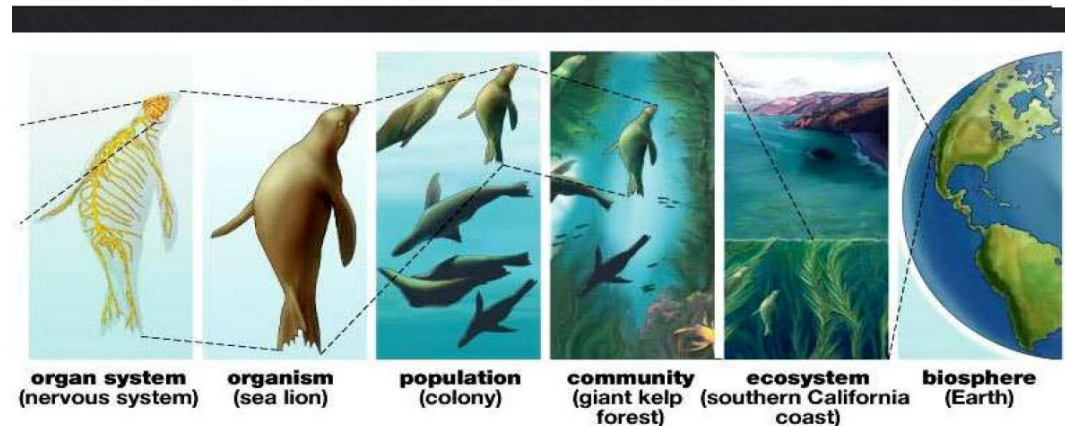
Some complicated (marginally stable) systems demonstrate self-similarity and “fractal” structure

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



But: complexity is hierarchical!

Our idea is dissimilarity at different scales



Multiscale 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

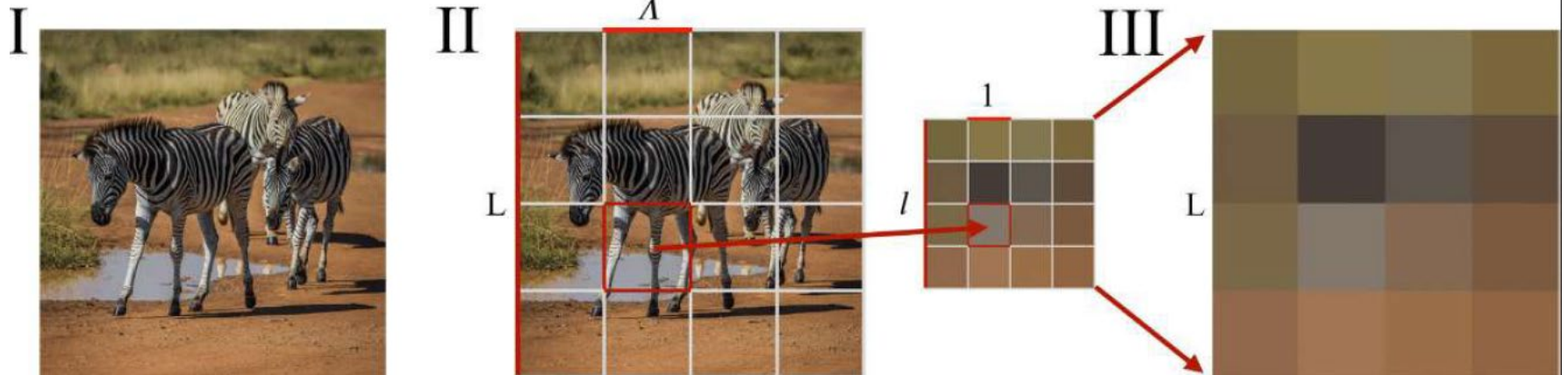
The idea (from holographic complexity and common sense):
Complexity is **dissimilarity** at various scales

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 $f_{\Lambda+d\Lambda}(x)$

Structural complexity II



$$\Delta_{\Lambda} = |\langle f_{\Lambda}(x) | f_{\Lambda+d\Lambda}(x) \rangle -$$

$$\frac{1}{2} (\langle f_{\Lambda}(x) | f_{\Lambda}(x) \rangle + \langle f_{\Lambda+d\Lambda}(x) | f_{\Lambda+d\Lambda}(x) \rangle) | =$$

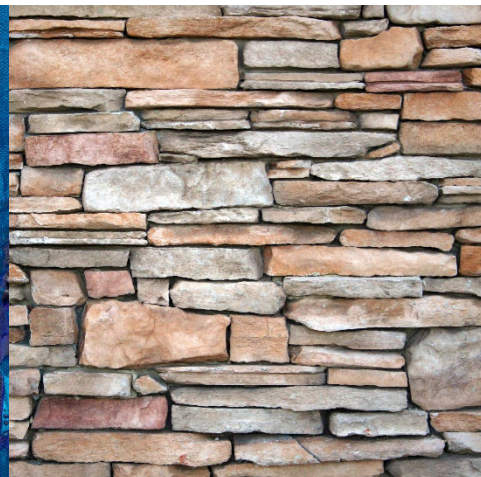
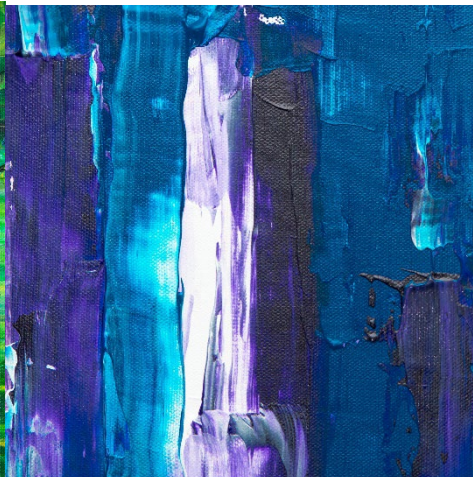
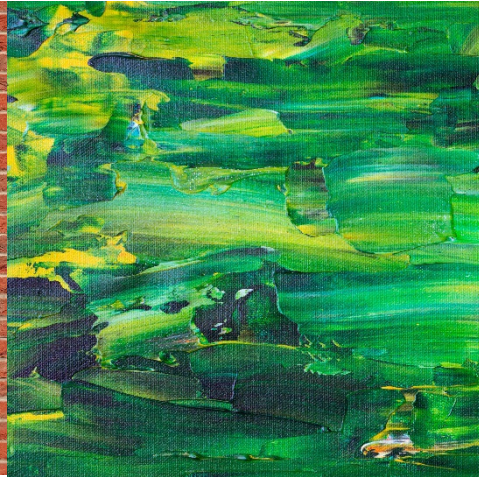
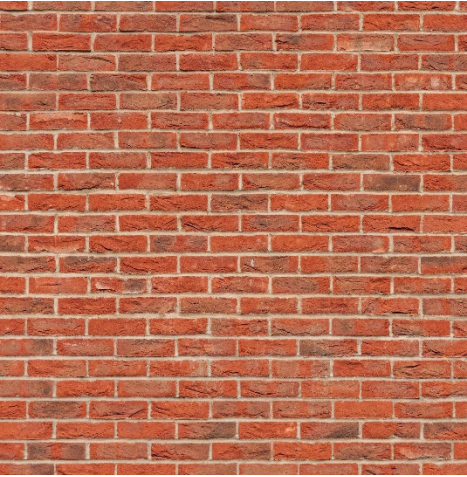
$$\frac{1}{2} |\langle f_{\Lambda+d\Lambda}(x) - f_{\Lambda}(x) | f_{\Lambda+d\Lambda}(x) - f_{\Lambda}(x) \rangle|,$$

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

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

Different ways of coarse-graining: average, “winner takes all” (Kadanoff decimation), cut-off in reciprocal space for Fourier image (Wilson RG...)

Art objects (and walls)

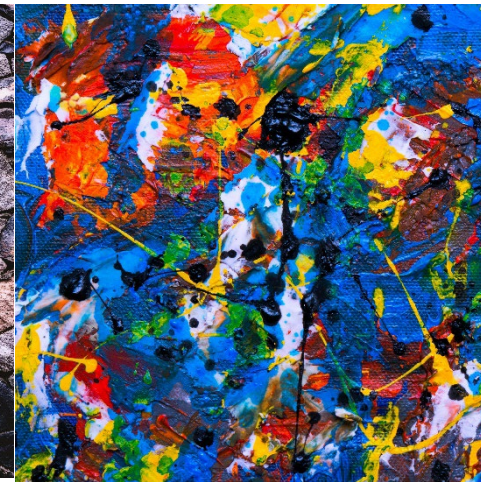


$C = 0.1076$

$C = 0.2010$

$C = 0.2147$

$C = 0.2765$



$C = 0.4557$

$C = 0.4581$

$C = 0.4975$

$C = 0.5552$

Other objects



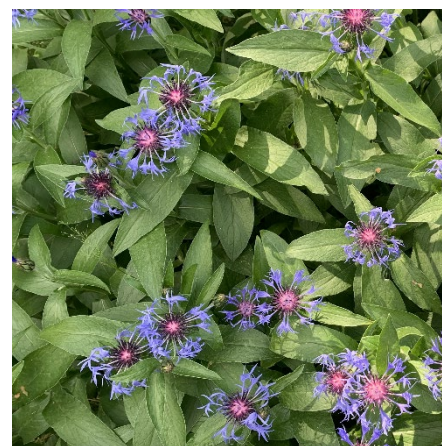
$C = 0.353$



$C = 0.152$



$C = 0.204$



$C = 0.260$



$C = 0.167$



$C = 0.316$



$C = 0.209$

*Photos by V. V.
Mazurenko*

Solution of an ink drop in water

Entropy should grow, but complexity is not! And indeed...

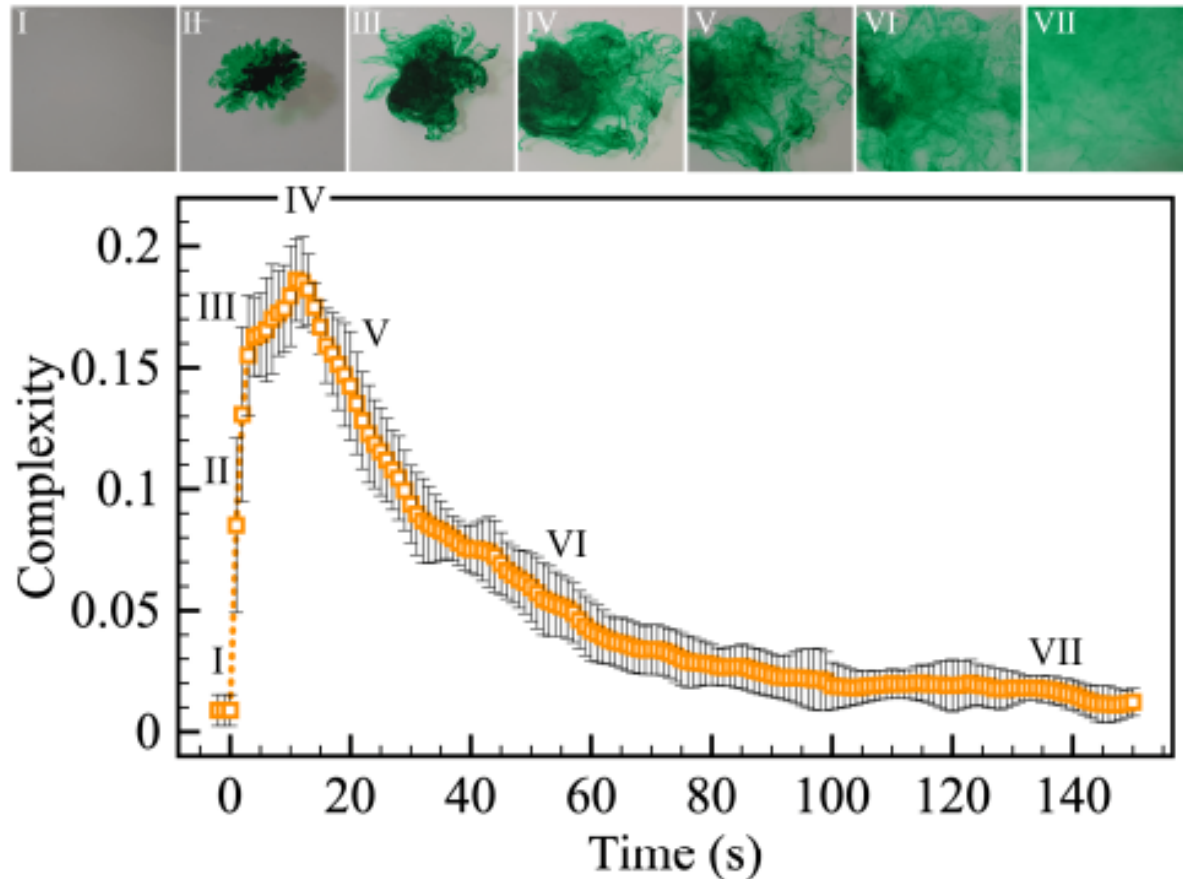
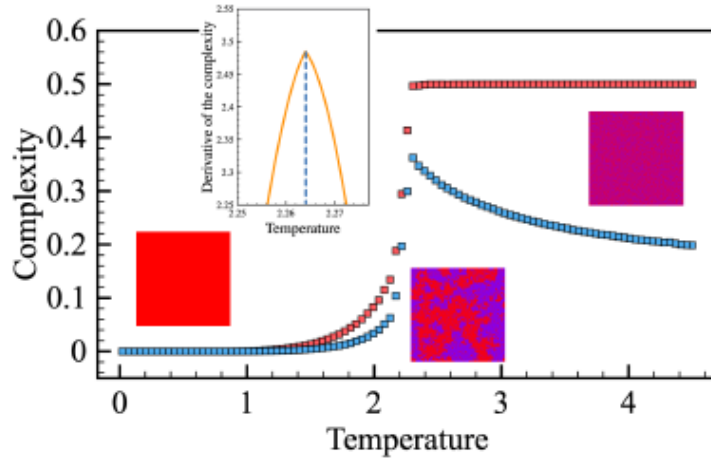


FIG. 7. The evolution of the complexity during the process of dissolving a food dye drop of 0.3 ml in water at 31°C.

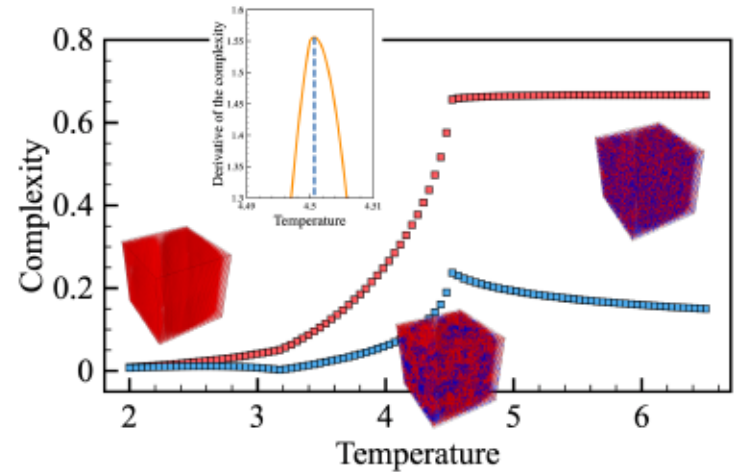
Structural complexity: Ising model

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

2D



3D



Different ways of coarse-graining give different pictures but T_C is always a cusp

Structural complexity: Magnetic patterns II

Simulations of magnetic systems $H = -J \sum_{nn'} \mathbf{S}_n \mathbf{S}_{n'} - \mathbf{D} \sum_{nn'} [\mathbf{S}_n \times \mathbf{S}_{n'}] - \sum_n B S_n^z$

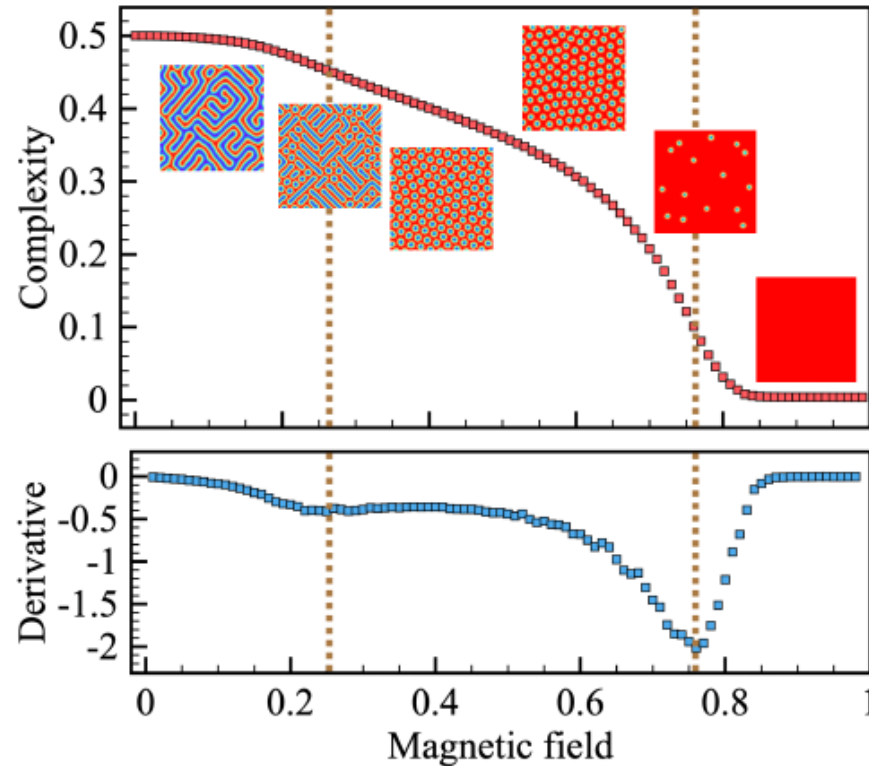


FIG. 4. (a) Magnetic field dependence of the complexity obtained from the simulations with spin Hamiltonian containing DM interaction with $J = 1$, $|\mathbf{D}| = 1$, $T = 0.02$. The error bars are smaller than the symbol size. (b) Complexity derivative we used for accurate detection of the phases boundaries.

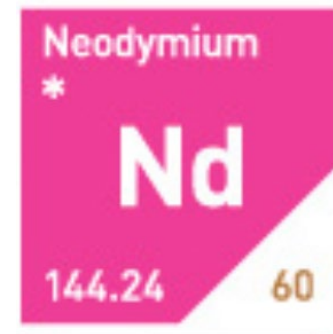
Experimental observation of self-induced spin glass state: elemental Nd

Self-induced spin glass state in elemental and crystalline neodymium

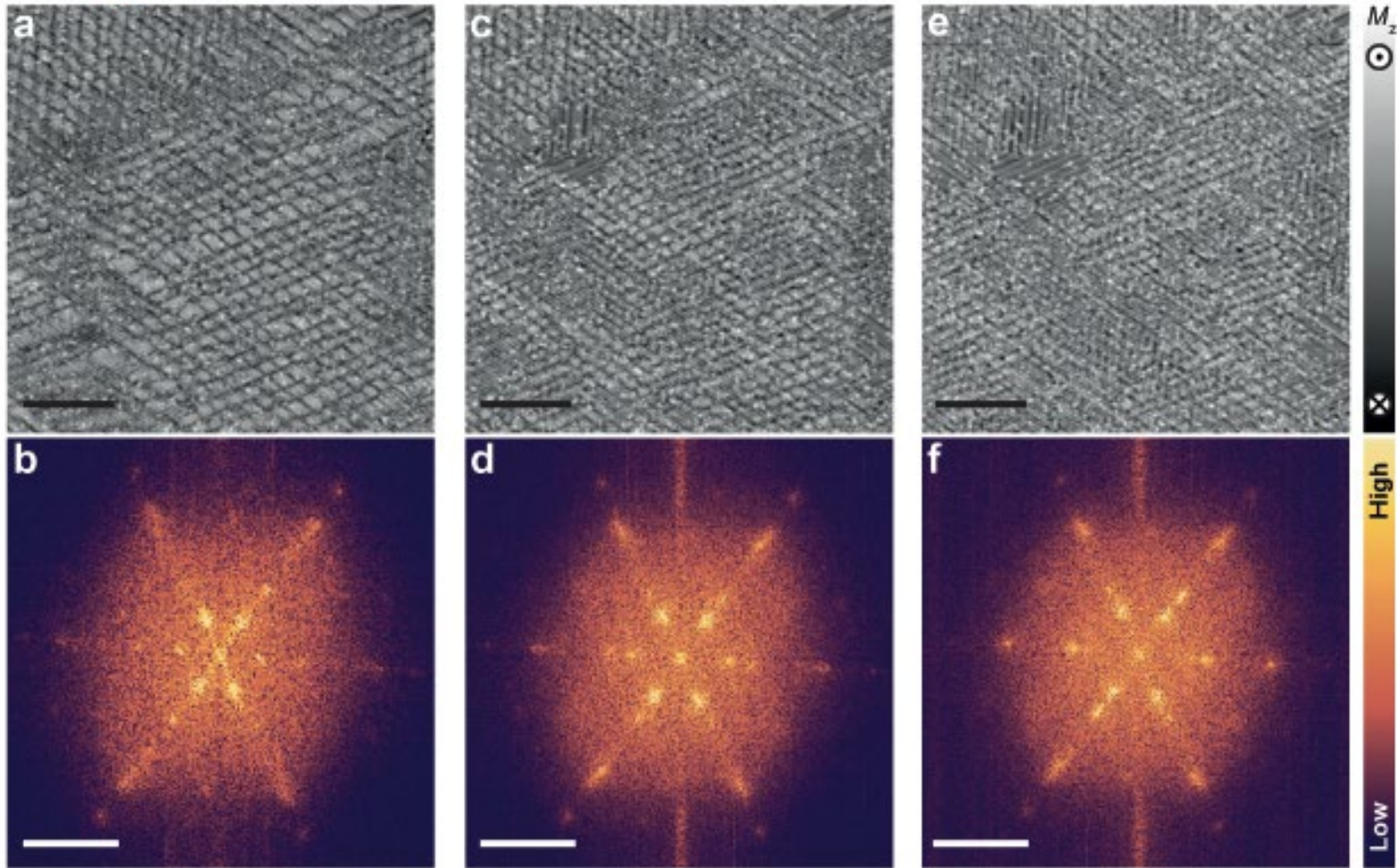
Science **368**, 966 (2020)

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: local correlations



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

Order from disorder

Thermally induced magnetic order from glassiness in elemental neodymium

NATURE PHYSICS | VOL 18 | AUGUST 2022 | 905-911

Benjamin Verlhac¹, Lorena Niggli¹, Anders Bergman², Umut Kamber¹, Andrey Bagrov^{1,2}, Diana Luşan², Lars Nordström², Mikhail I. Katsnelson¹, Daniel Wegner¹, Olle Eriksson^{2,3} and Alexander A. Khajetoorians¹✉

Glassy state at low T
and long-range order
at T increase

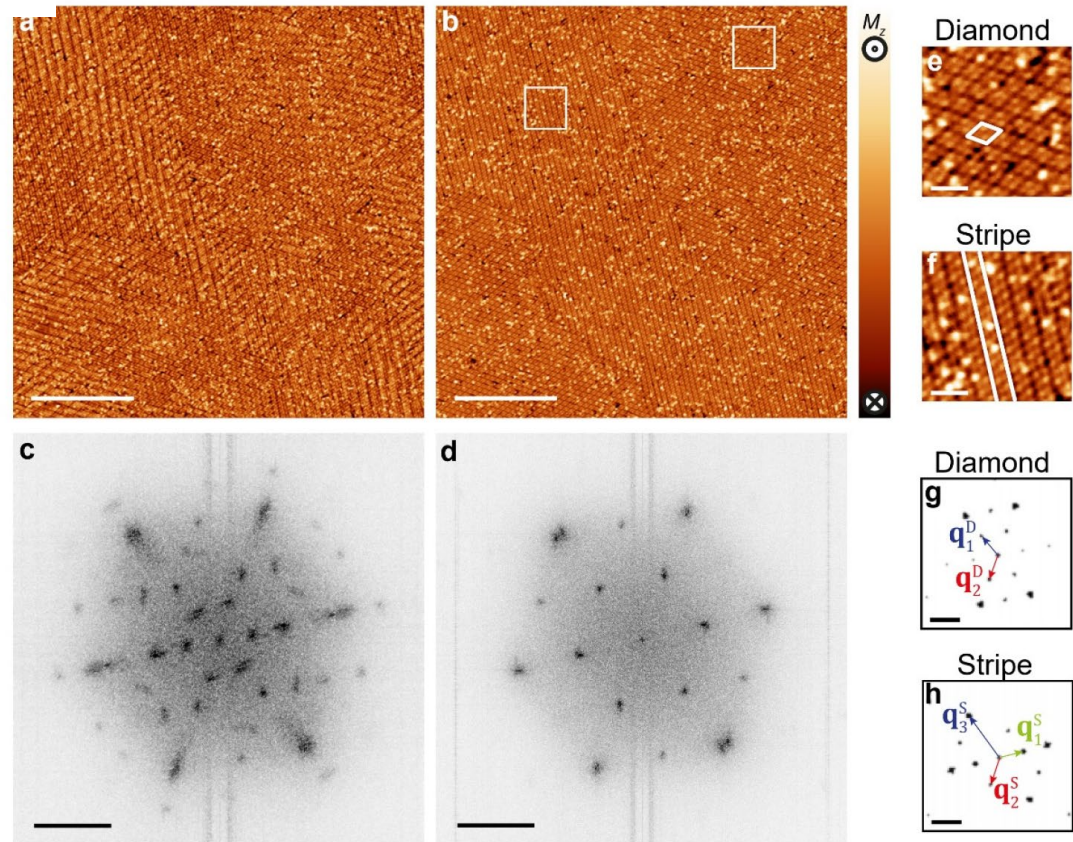
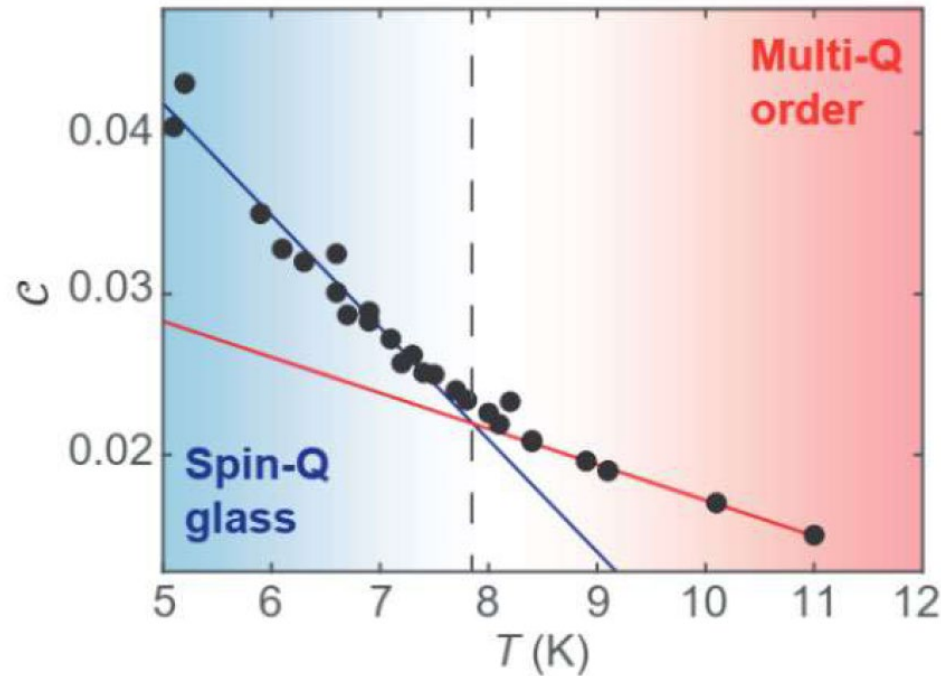
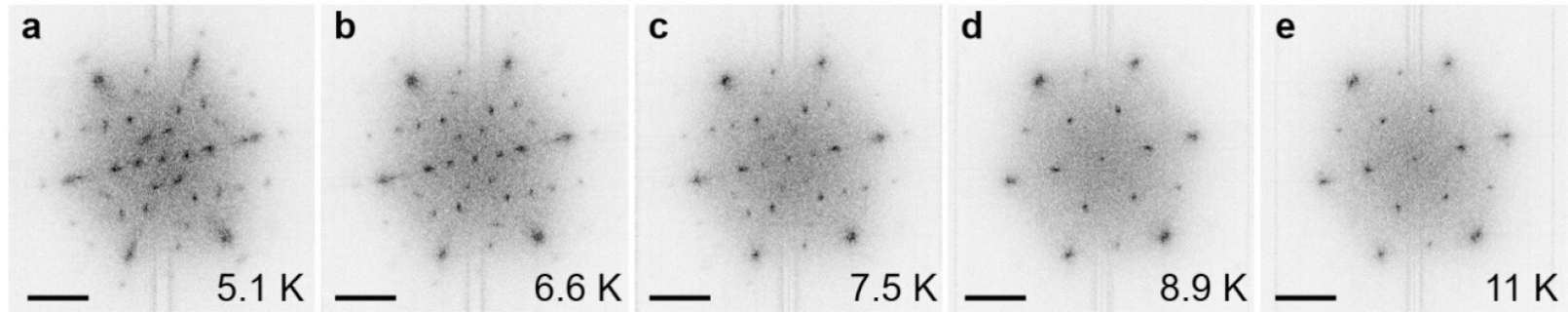


Figure 2: Emergence of long-range multi-Q order from the spin-Q glass state at elevated temperature. a,b. Magnetization images of the same region at $T = 5.1$ K and 11 K, respectively ($I_t = 100$ pA, a-b, scale bar: 50 nm). c,d. Corresponding Q-space images (scale bars: 3 nm⁻¹), illustrating the changes from strong local (i.e. lack of long-range) Q order toward multiple large-scale domains with well-defined long-range multi-Q order. e,f. Zoom-in images of the diamond-like (e) and stripe-like (f) patterns (scale bar: 5 nm). The locations of these images is shown by the white squares in b. g,h. Display of multi-Q state maps of the two apparent domains in the multi-Q ordered phase, where (g)

$T=5$ K (a,c): spin glass
 $T=11$ K(b,d): (noncollinear) AFM

Order from disorder II



Phase transition at approx. 8K (seen via our complexity measure)

Certification of quantum states

Certification of quantum states with hidden structure of their bitstrings

npj Quantum Information (2022)8:41

O. M. Sotnikov¹, I. A. Iakovlev¹, A. A. Iliasov², M. I. Katsnelson^{1,2}, A. A. Bagrov^{1,2,3} and V. V. Mazurenko¹✉

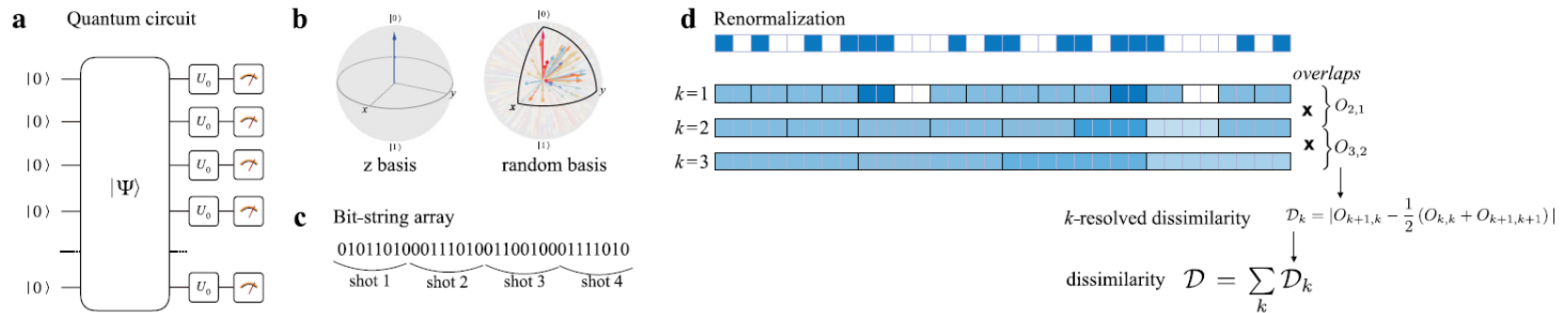


Fig. 1 Protocol for computing dissimilarity of a quantum state. **a** First, one prepares a state on a quantum device and chooses the measurement basis by applying rotational gates U_0 to individual qubits. **b** In this paper, we work with σ^z and random bases whose Bloch sphere representations are shown in the picture. We say that the set of measurements is performed in a random basis if, for each shot of measurement, a random vector belonging to the highlighted sector of the Bloch sphere is uniformly sampled and the corresponding parameters of gate U_0 are applied. **c** A number of measurements is performed and their outcomes — bitstrings of length N — are then stacked together in a one-dimensional binary array of length $N \times N_{\text{shots}}$ that serves as a classical representation of the quantum state. **d** The array is coarse-grained in several steps (indexed with k). Different schemes can be employed, but here we use plain averaging with fixed filter size Λ . In the picture, blue and white squares in the top line correspond to ‘0’ and ‘1’ bits in the array shown in (c), and black rectangles depict the blocks where averaging occurs at every step of coarse-graining. Overlap-based dissimilarities \mathcal{D}_k between subsequent arrays are computed and summed up to the overall dissimilarity \mathcal{D} . See Methods section for more details.

First make at least two complementary measurements, then analyze the measurement results (relation to Bohr’s complementarity principle)

Certification of quantum states II

Two-dimensional map can be used to characterize the type of quantum states

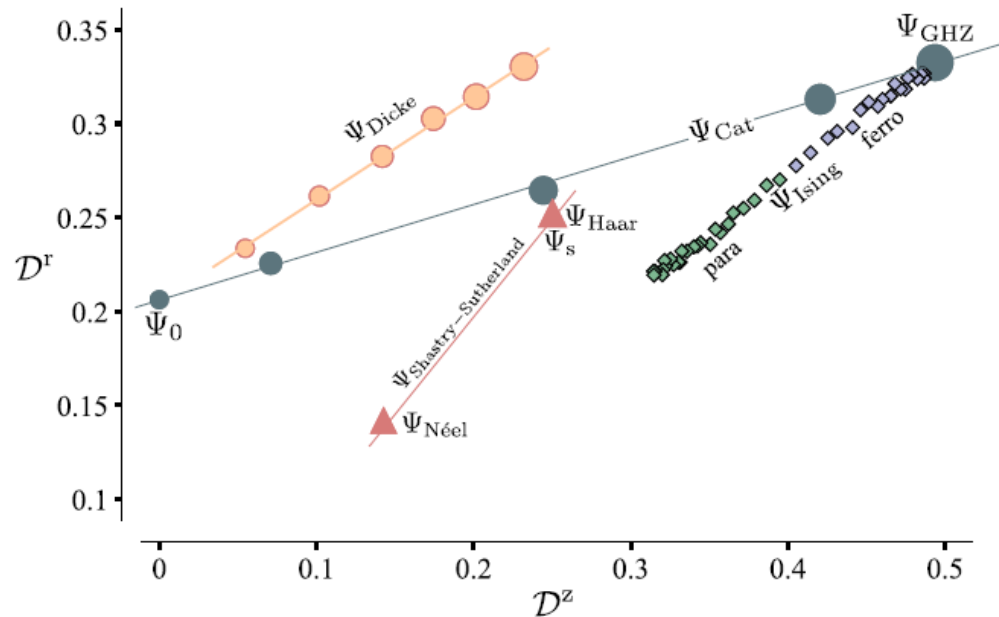


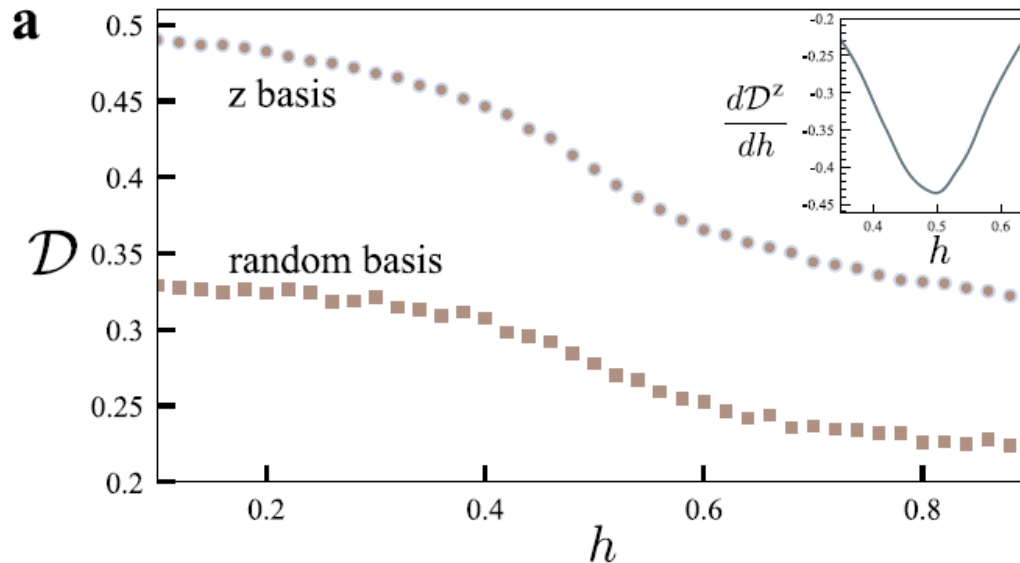
Fig. 10 Dissimilarity map. Low-dimensional representation of the 16-qubit quantum states studied in this work with respect to their dissimilarity calculated in σ^z and random bases. Ψ_0 , Ψ_s , Ψ_{Haar} denote the trivial $|0\rangle^{\otimes N}$, the singlet and the random quantum states, respectively.

Certification of quantum states III

One can characterize a type of quantum states and, again, find
(quantum) critical point

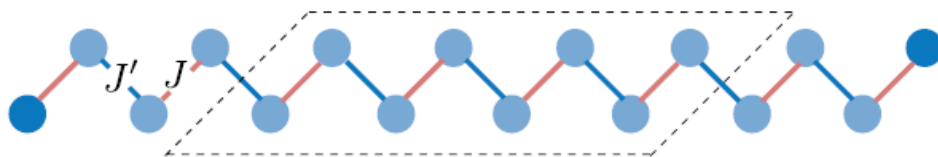
Ising in transverse field $H = J \sum_{ij} \hat{S}_i^z \hat{S}_j^z + h \sum_i \hat{S}_i^x$

1D chain; quantum critical point at $h_c = 0.5|J|$



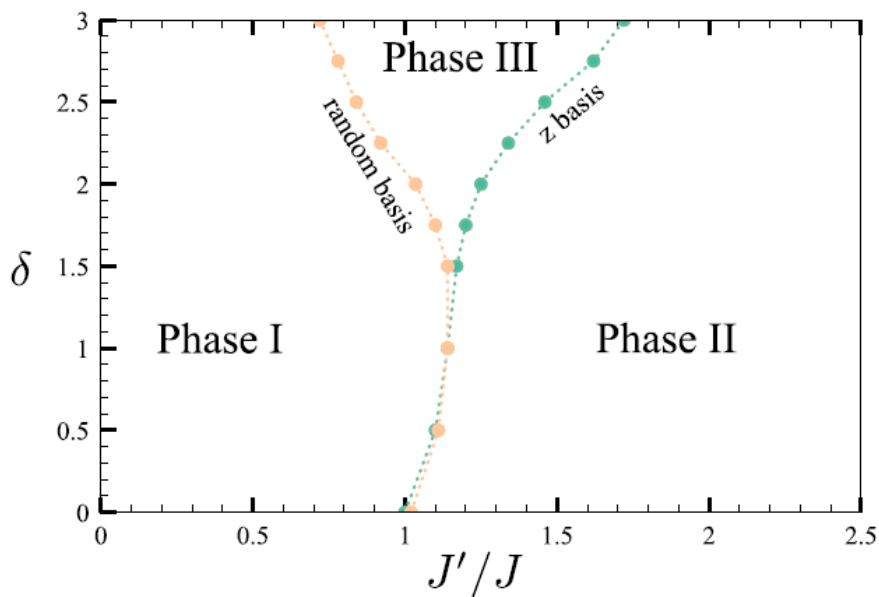
Certification of quantum states IV

The way to detect topological phases

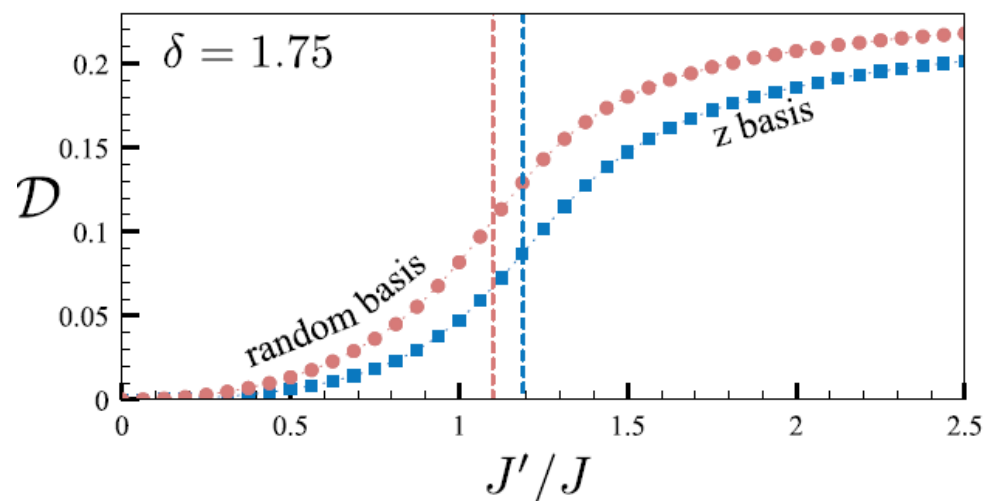


$$H_{\text{XXZ}} = J \sum_{ij \in \mathbf{O}} (\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \delta \hat{S}_i^z \hat{S}_j^z) + J' \sum_{ij \in \mathbf{E}} (\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \delta \hat{S}_i^z \hat{S}_j^z)$$

Three different phases: trivial (I), topological (II), antiferromagnetic (III)



Phase diagram constructed from dissimilarity (MSC), from maxima of its derivatives



Dissimilarities with different basis show different phase boundaries

Psychology of human visual perception

We wanted definition of complexity in agreement with our intuitive understanding of complexity – did we succeed?

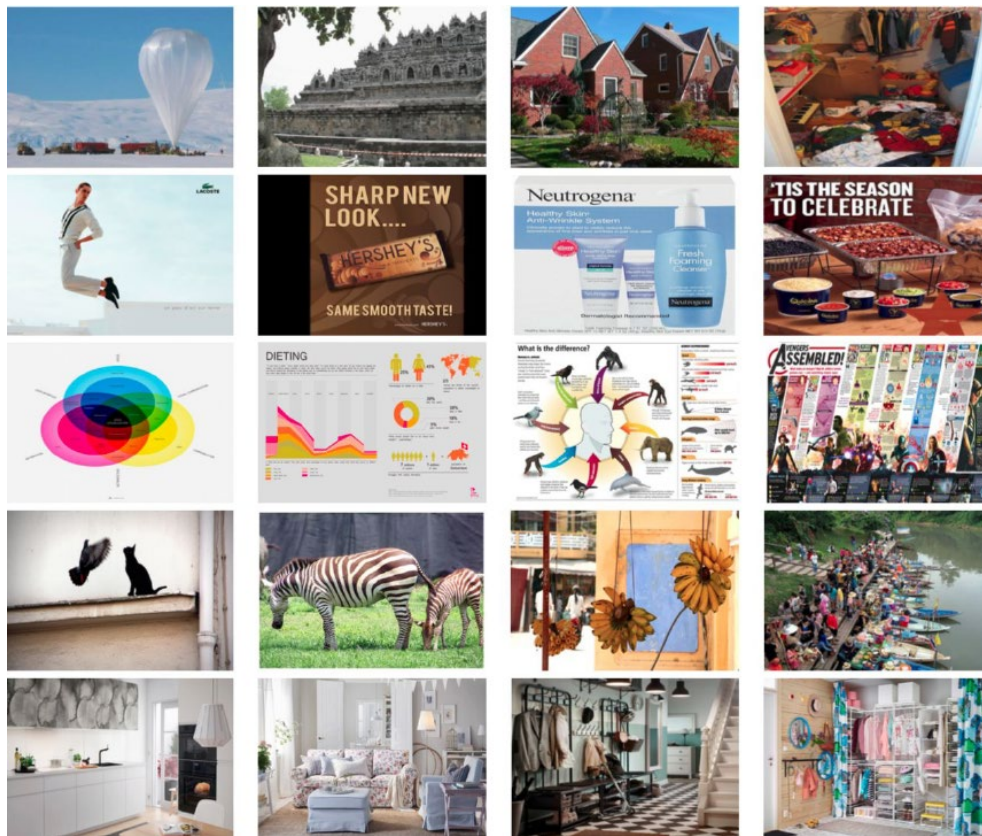
Multiscale structural dissimilarity in human perception of visual complexity

Anna Kravchenko, Andrey Bagrov, MIK, Veronica Dudarev (in preparation)

To analyze: **SAVOIAS: A Diverse, Multi-Category Visual Complexity Dataset**

[Elham Saraei](#), [Mona Jalal](#), [Margrit Betke](#); [arXiv:1810.01771](#)

- Multiple domains: Scenes, Advertisements, Infographics, Objects, Interior design, Art, and Suprematism
- Well-studied for other existing complexity measures
- Obtained by crowdsourcing more than 37,000 pairwise comparisons of images, rankings converted into 1-100 scale



Human visual perception II

Choosing coarse-graining method

There are many ways to do coarse graining

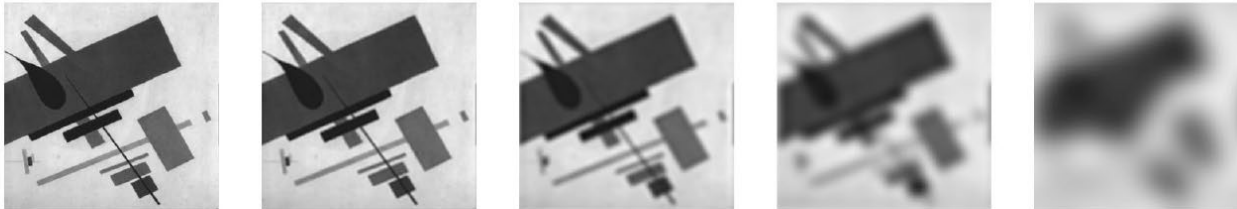
Evidence suggests processing on early layers of visual cortex can be approximated by Fourier Transform (Campbell and Robson 1968, Ochs 1979, Kulikowski and Bishop 1981, Olshausen 2003, Kesserwani 2002)

DFT:

$$F(k, l) = \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} f(i, j) e^{-i2\pi(\frac{ki}{N} + \frac{lj}{N})}$$

Inverse Fourier transform:

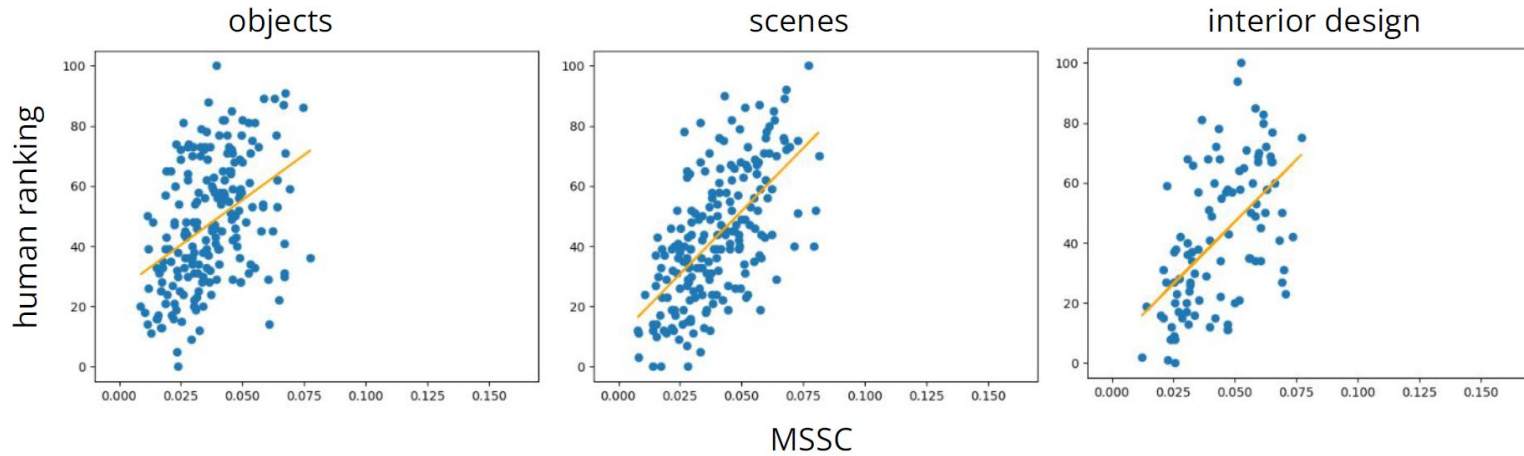
$$f(a, b) = \frac{1}{N^2} \sum_{k=0}^{N-1} \sum_{l=0}^{N-1} F(k, l) e^{i2\pi(\frac{ka}{N} + \frac{lb}{N})}$$



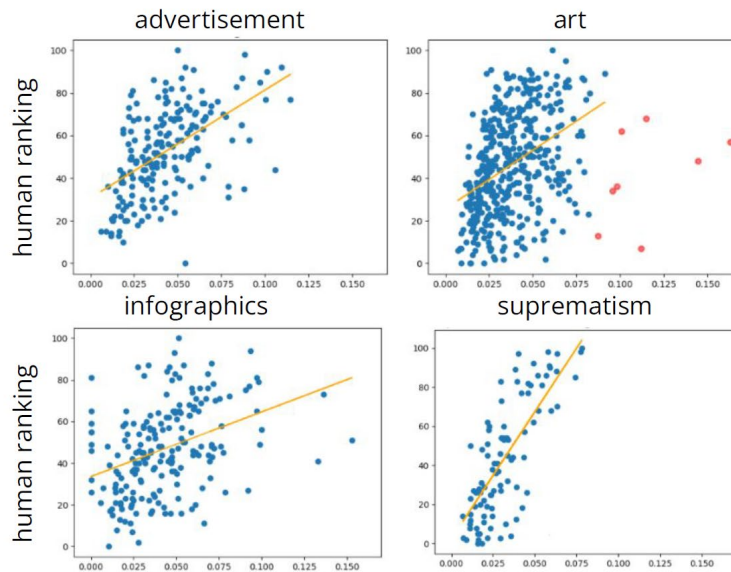
The best correlation is reached when making coarse-graining of Fourier images which can be interesting by itself

Human visual perception III

Natural scenes



Man-made images



- Worse correlation
 - Obvious outliers
- What does this imply?

Human visual perception IV

Comparison with existing measures

		edge density	compression ratio	number of regions	feature congestion	subband entropy	MSSC	max r
natural	scenes	0.16	0.3	0.57	0.42	0.16	0.62	0.57
	objects	0.28	0.16	0.29	0.3	0.1	0.46	0.3
Human-made	suprematism	0.18	0.6	0.84	0.48	0.39	0.76	0.84
	interior design	0.61	0.68	0.67	0.58	0.31	0.60	0.68
	advertisements	0.54	0.56	0.41	0.56	0.54	0.52	0.56
symbolic	art	0.48	0.51	0.65	0.22	0.33	0.42	0.65
	infographics	0.57	0.55	0.38	0.52	0.61	0.38	0.61

From (Saree et al. 2018)

Surpasses state-of-the-art on natural scenes, falls below state-of-the-art methods for images conveying information

What is missing in our definition? **Contextual** complexity (that is, cultural references)

Human visual perception V

Perceptual vs. conceptual complexity: art as a language

Outliers:

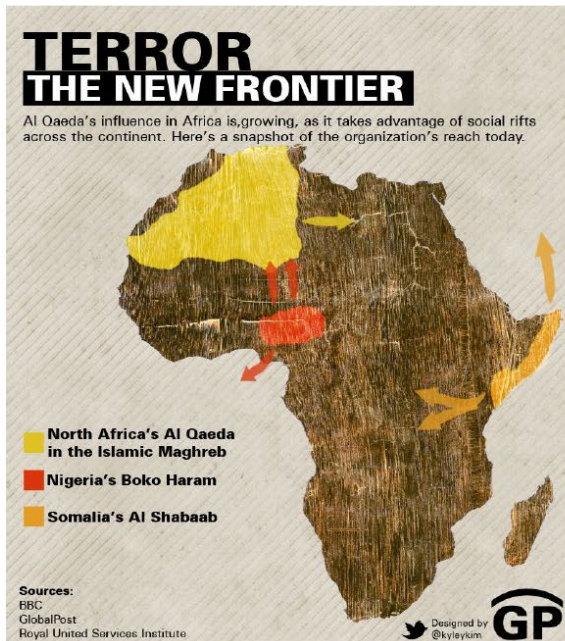


Visually straining but conceptually boring

Paintings identified as outliers, having been excluded from prediction by a threshold greater than two standard deviations, exhibited the same distinctive visual characteristic: broad lines featuring contrasting colors (9). This artistic style can be visually straining, however, it's relatively simplistic in terms of information conveyed through it.

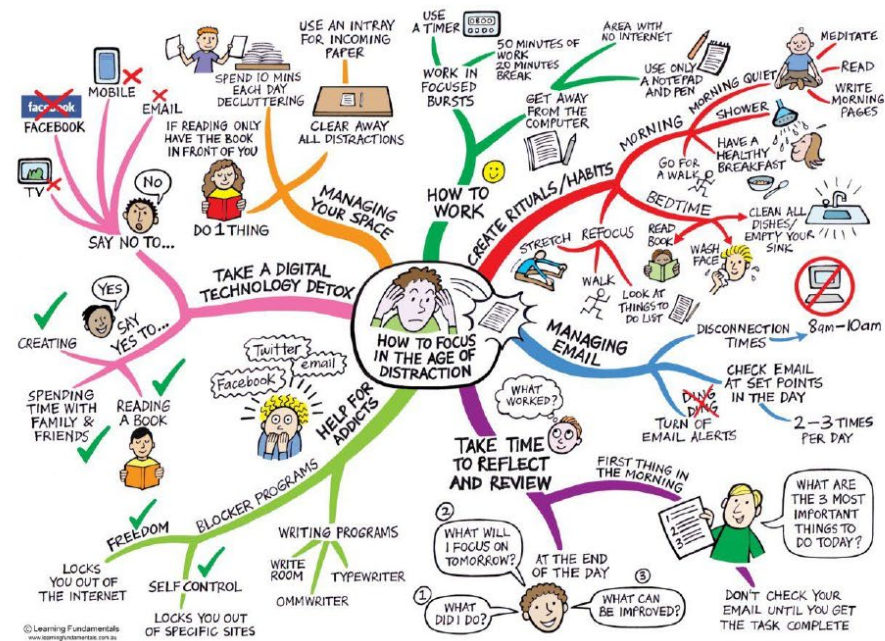
Human visual perception VI

Perceptual vs. conceptual complexity: infographics



30 in human ranking

same MSSC value



86 in human ranking

Letters as just images vs letters as symbols

Other applications –biology

bioRxiv preprint doi: <https://doi.org/10.1101/2024.04.26.591304>

Long range segmentation of prokaryotic genomes by gene age and functionality

Yuri I. Wolf¹, Ilya V. Schurov², Kira S. Makarova¹, Mikhail I. Katsnelson², Eugene V. Koonin¹

Multilevel structural complexity was used to analyze observed patterns in prokaryotic genomes vs predictions of various models

To summarize: computationally simple but useful concept

THANK YOU!