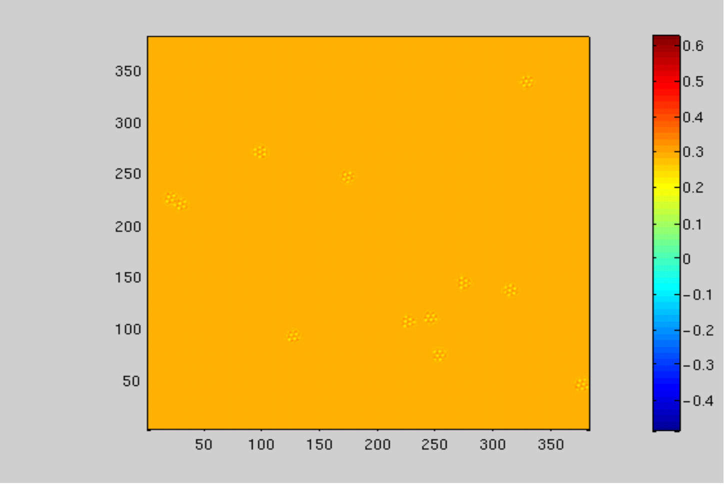
Emergence in physical and biological systems far from equilibrium



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NSF-EAR-0221743, NSF-EF-0526747, NSF-DMR-06-04435 & DOE-2005-05818

Outline

- Emergence and complexity
- Signatures of emergence in equilibrium
- Emergence far from equilibrium
  - Patterns
  - Turbulence
- Emergence and biological complexity
  - Microbes and phages
  - The genetic code
  - Universal biology
- Exploiting emergence to model nature
  - Modeling a complex geophysical landscape

Complex systems have ...

- Strong fluctuations
- Unpredictable and nonlinear dynamics
- Multiple scales of space and time
- Emergent structure

- Active components
- Nested feedback loops
- Multiple layers of system dynamics

Complexity – why now?

- Development of the sciences …
  - Pick the low hanging fruit first
  - Reductionist approach valid
- But ultimately must encounter problems where strong interactions lead to …
  - Emergent phenomena
- And then …
  - Complexity

4 August 1972, Volume 177, Number 4047 SCIENCE

More Is Different

Broken symmetry and the nature of the hierarchical structure of science.

P. W. Anderson

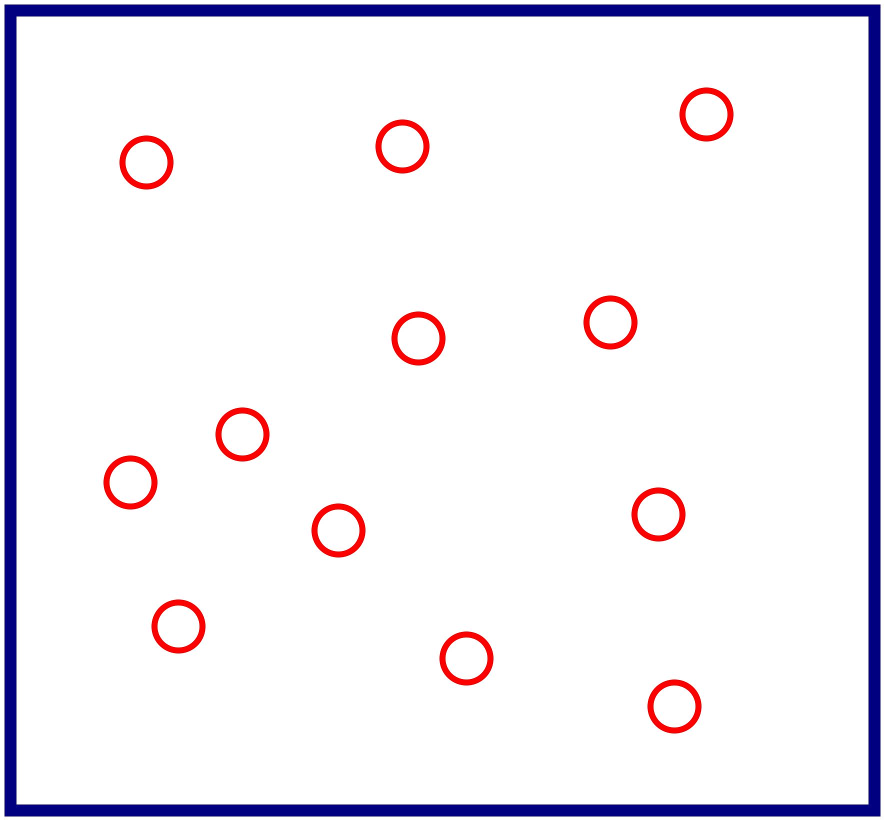
less relevance they seem to have to the very real problems of the rest of science, much less to those of society.

The constructionist hypothesis breaks down when confronted with the twin difficulties of scale and complexity. The behavior of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity entirely new properties appear, and the understanding of the new behaviors requires re-

Let’s do an experiment to see something critical about emergence!

Emergence of the solid state

- **Atoms in a box**
  - Fluid state
- **Low temperature**
  - Crystalline solid forms
- **Characteristics different from fluid state**
  - Periodic crystal lattice
  - Static shear rigidity



Emergence of the solid state

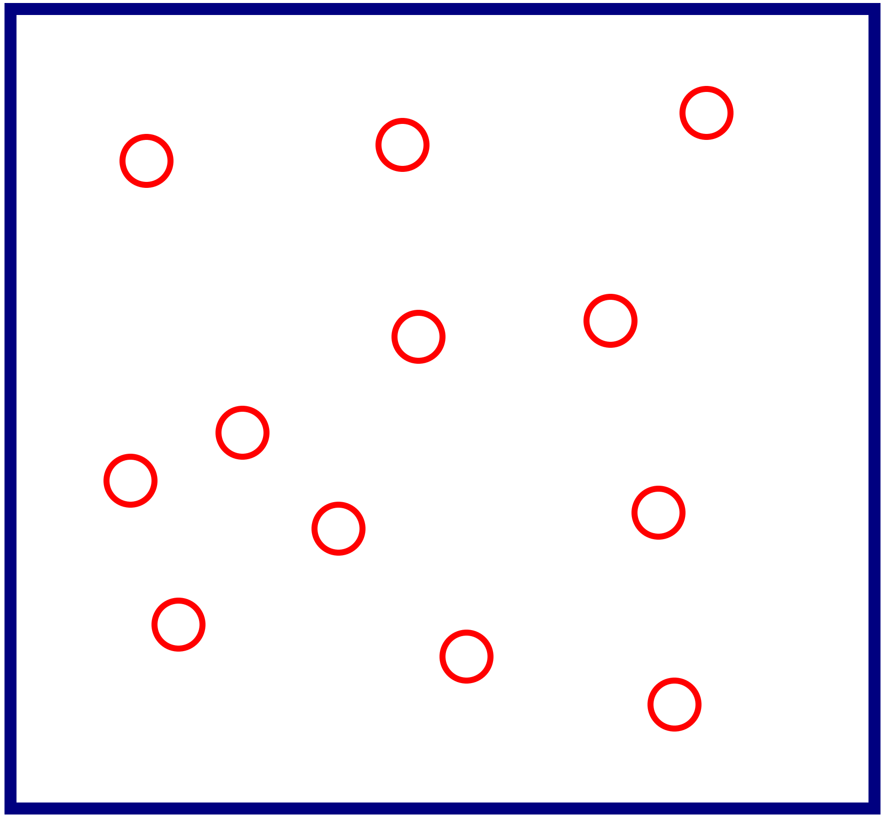
Q: ***Why is this interesting?***

A: ***Because the underlying physics of the crystal is <u>exactly</u> the same as the fluid!***

- **Total Energy =**

  Kinetic energy+ Potential energy

- **Lowering temperature <u>has not changed</u> the interactions between the atoms**



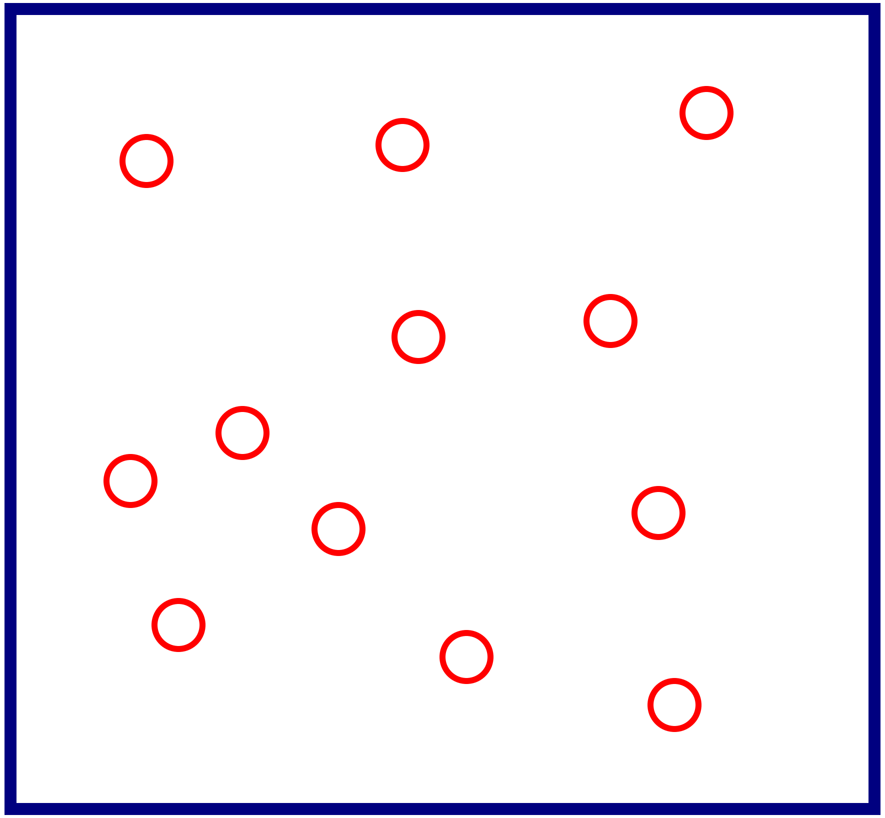
Emergence of the solid state

Conclusion:

Although the pairwise interactions between atoms did not change

the correlations between them changed when the temperature was lowered

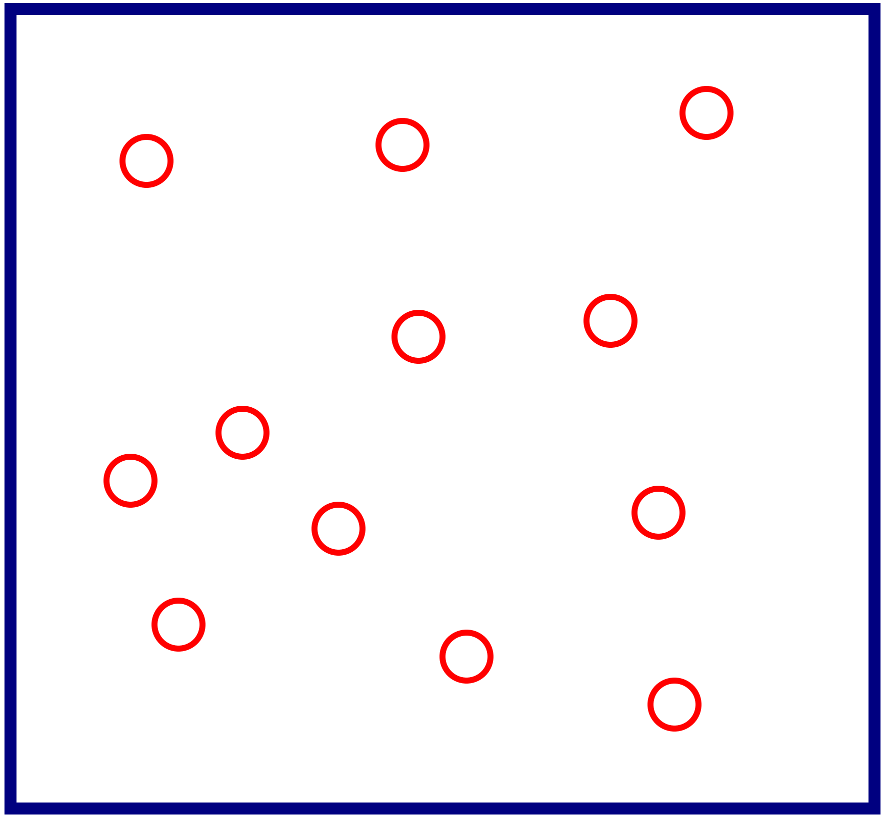
So the solid state emerged as if by magic out of the fluid state!



Emergence: the big deal

The solid state has its own new laws of physics!

- New long-range forces that are completely distinct from the original forces between the atoms
  - Elasticity!
    - Response of solid to external disturbances completely different from that of a fluid
    - The springs between atoms are emergent
- Origin of these new laws: the collective, statistical behaviour of the atoms

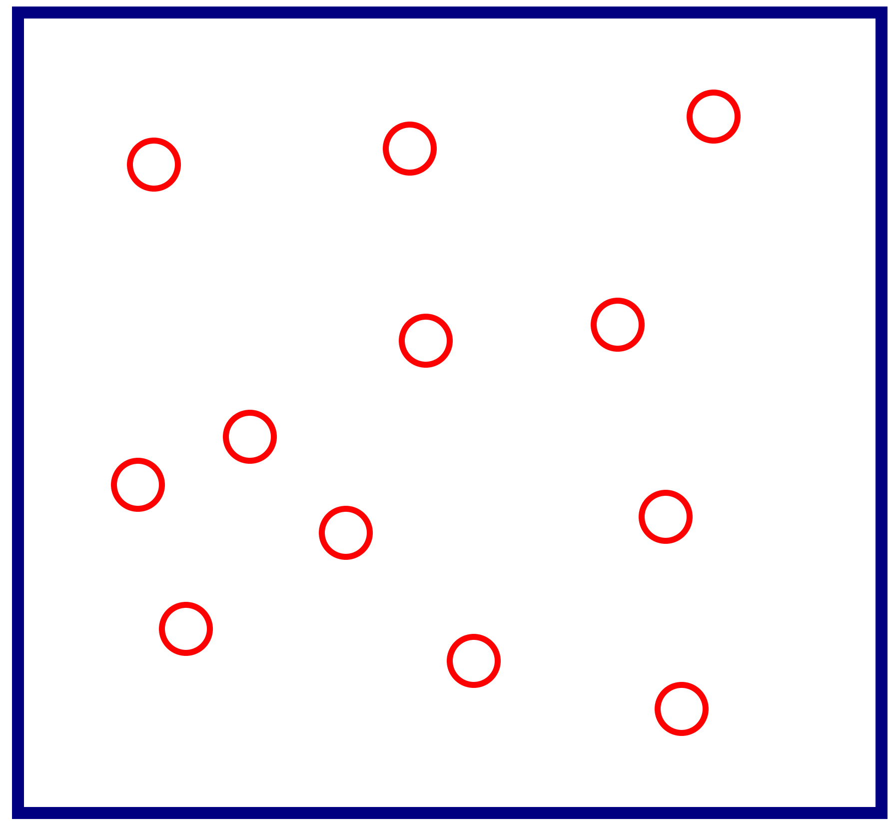


Emergence: new laws of physics?

The solid state has its own new "laws of physics"!

Really?

Well, yes! At the level of description of a solid, the actual interactions between the atoms cannot be detected --- only the continuum mechanics of the solid is observable!

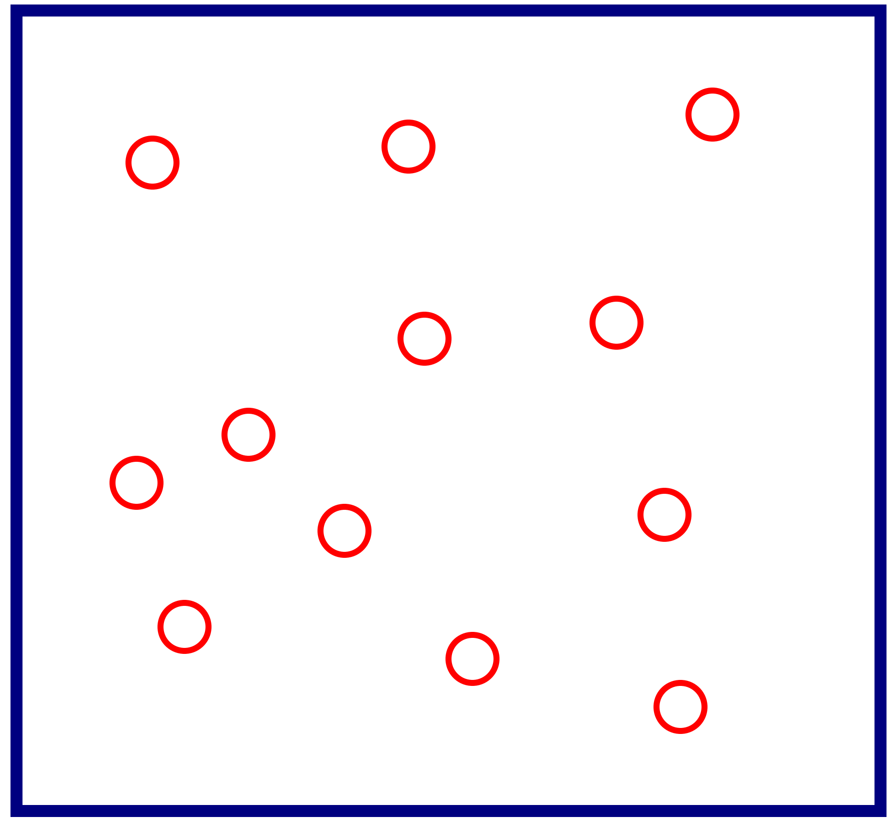


Emergence: new laws of physics?

This is why it took so long for the existence of atoms to be deduced!

Q: So where do atoms and their interactions matter?

A: The elastic forces are characterized by phenomenological parameters such as shear modulus that can only be computed from the atomic level of description.



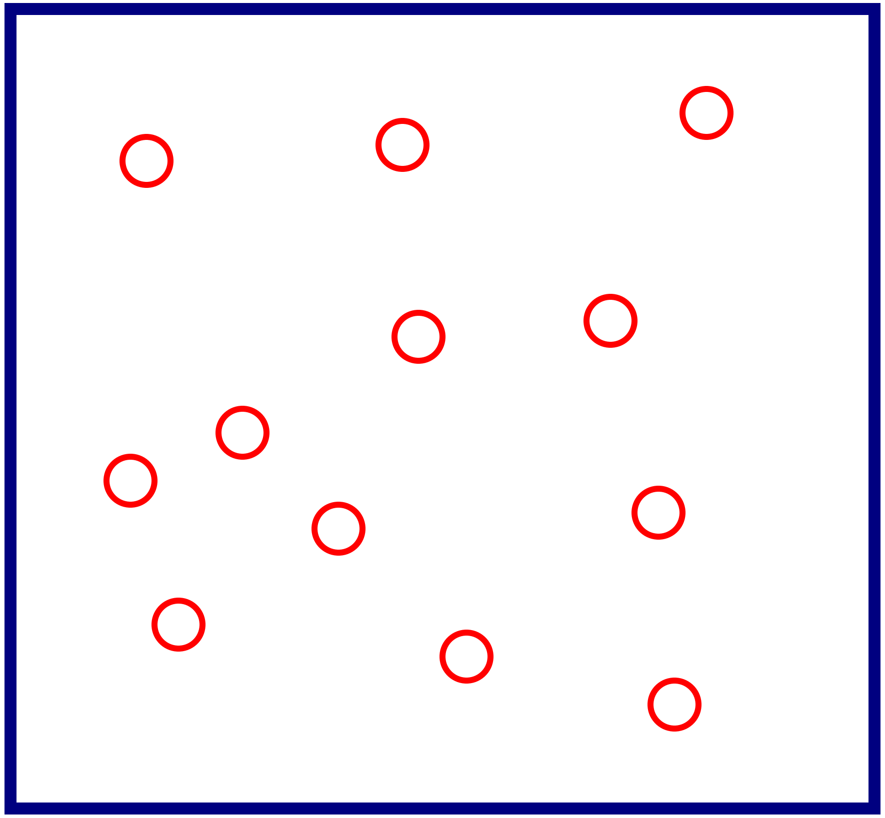
When we do atomic physics or chemistry, we do not need to take into account the mass of the top quark!

Emergence: new laws of physics?

Summary:

- **Emergent levels of description absorb the properties of lower levels of description into phenomenological parameters**
  - **Typically a small number!**
- **This makes "fundamental physics" hard, because one "goes against the flow" of emergence**
  - **Dooms reductionism!**
- **But collective properties of matter can be understood, and should be understood, without requiring knowledge "all the way down"**

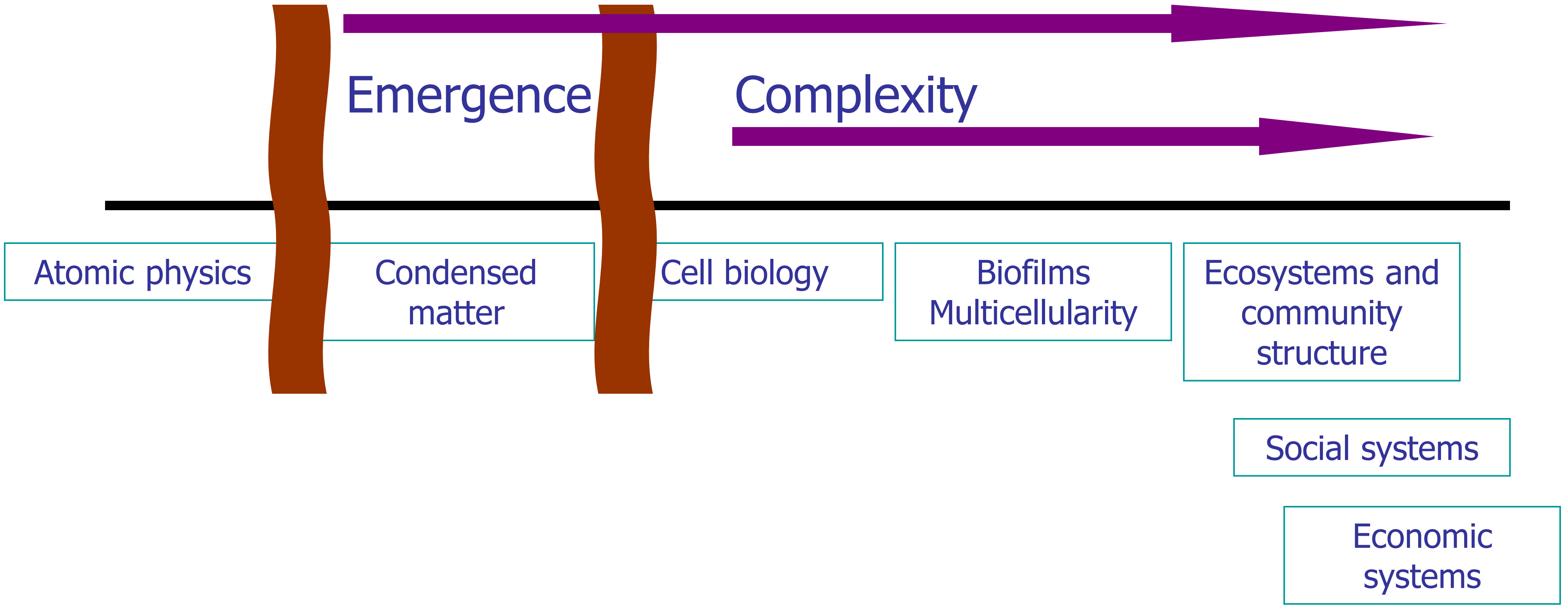
So we must be careful to only ask the right questions …



Characteristics of emergence

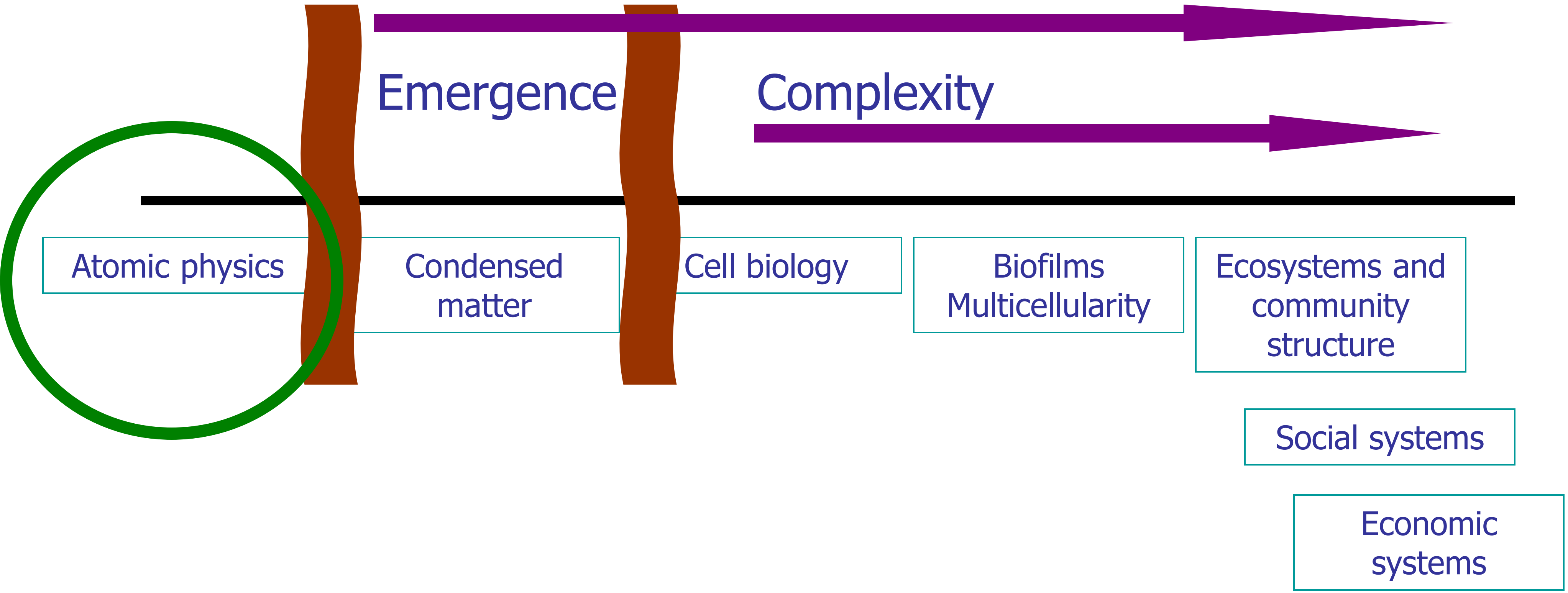
- **Emergence is associated with loss of uniqueness**
  - **Fluid state still possible at low temperature but much less likely than solid state**
  - **Phase transitions separate states**
    - **Collective, only well-defined for thermodynamically large systems**
- **New, collective properties arise in emergent states**
  - **Crystals, magnets, superconductors, quantum hall effects …**
  - **Turbulence? Gravity? Life?**
  - **Do emergent phenomena bring molecules to life?**

Emergence => complexity



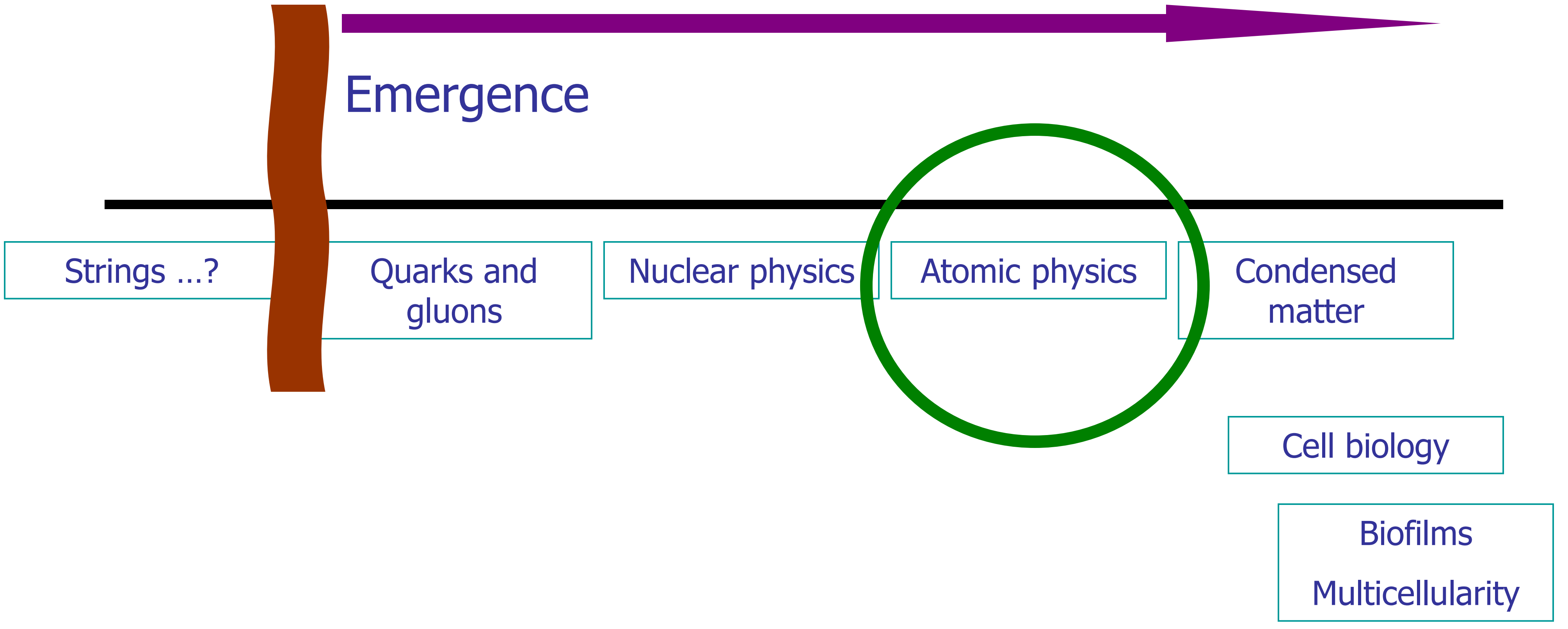
- **Emergence begins with strongly interacting condensed matter**

Emergence => complexity



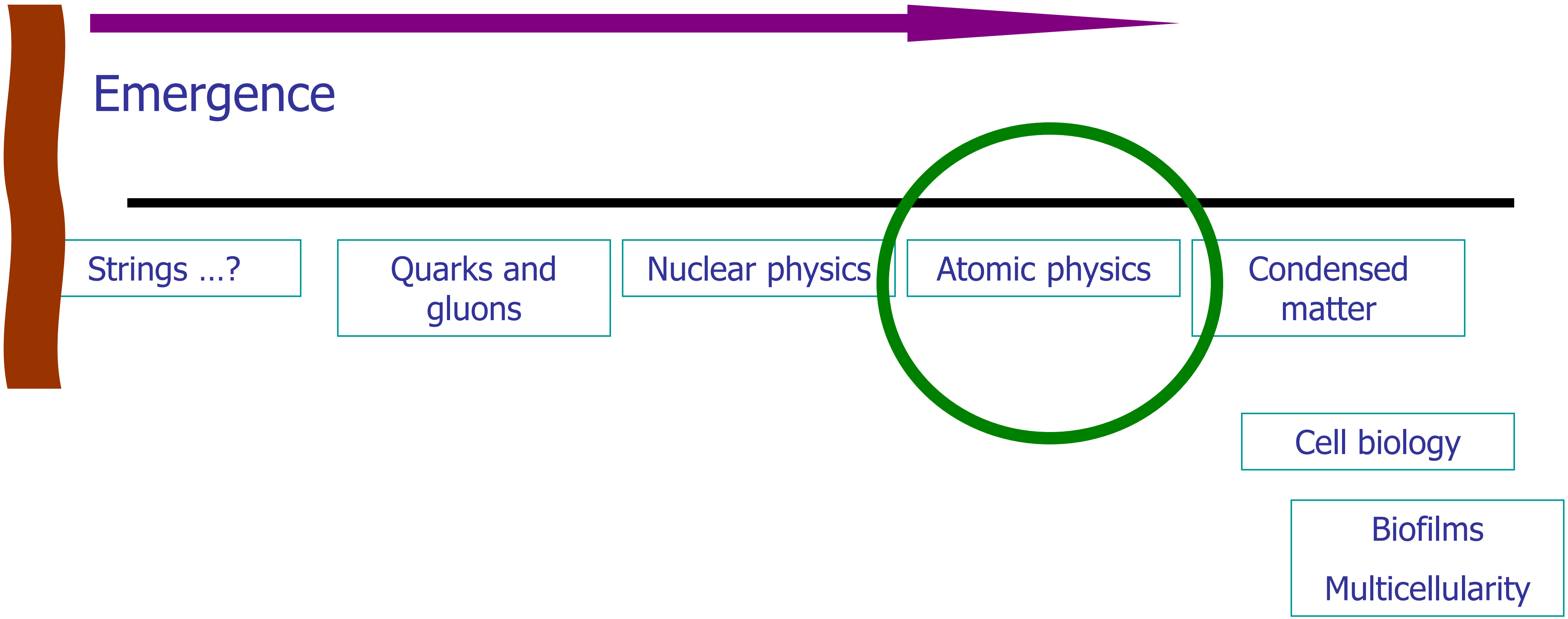
- **Emergence begins with strongly interacting condensed matter**
  … or does it?

Emergence => complexity



- **Emergence at every level of description!**

Emergence => complexity



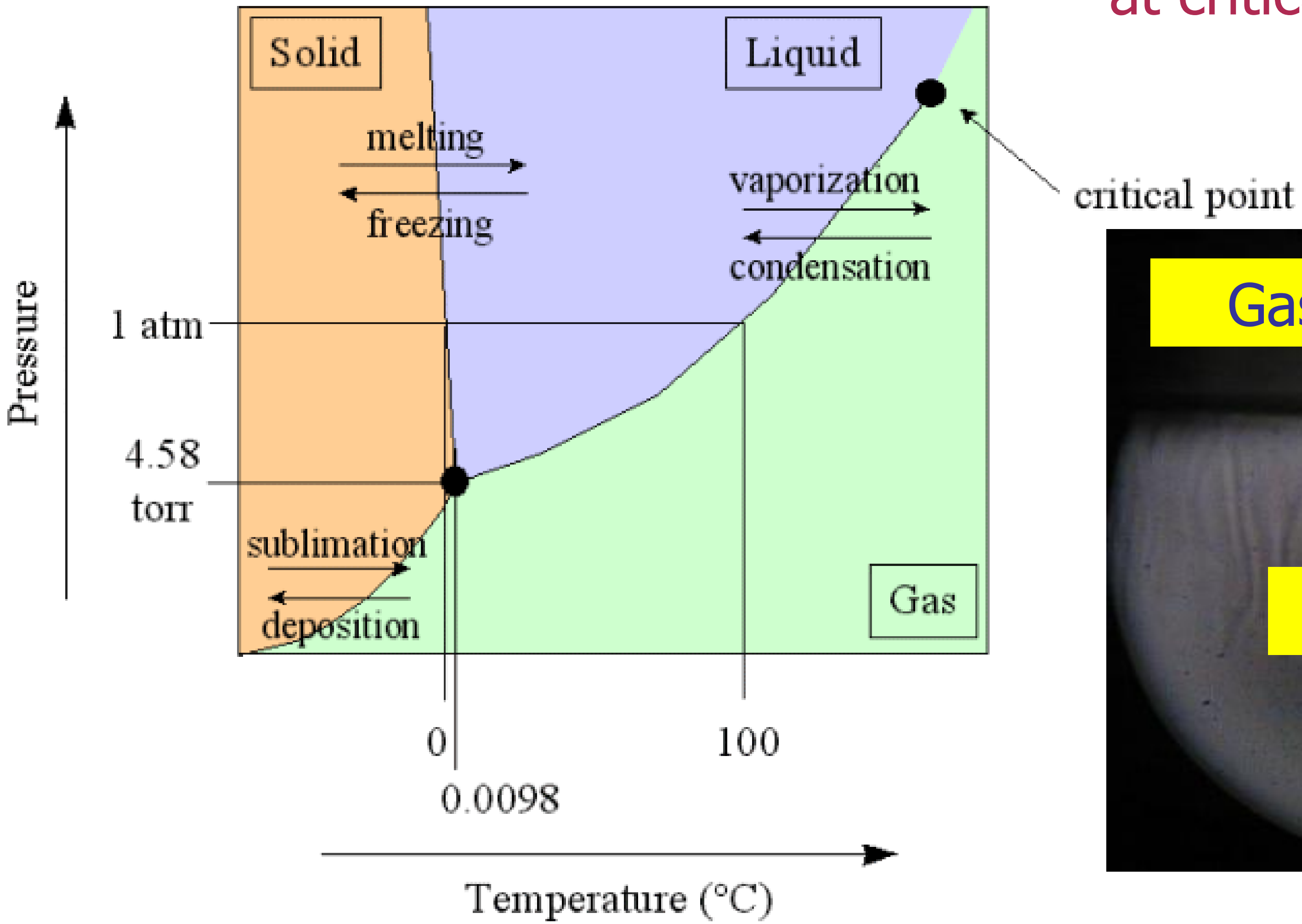
- **Are the most fundamental interactions emergent?**

Signatures of emergence

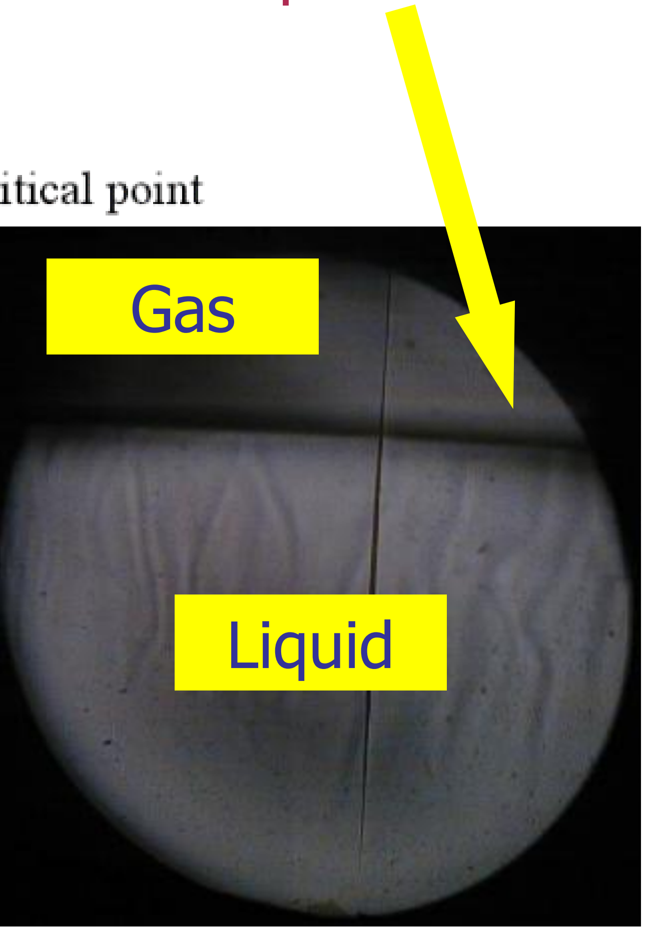
Scaling, phase transitions, fluctuations

Critical point in a fluid

http://www.exo.net/~pauld/workshops/cset/csetthermo.htm

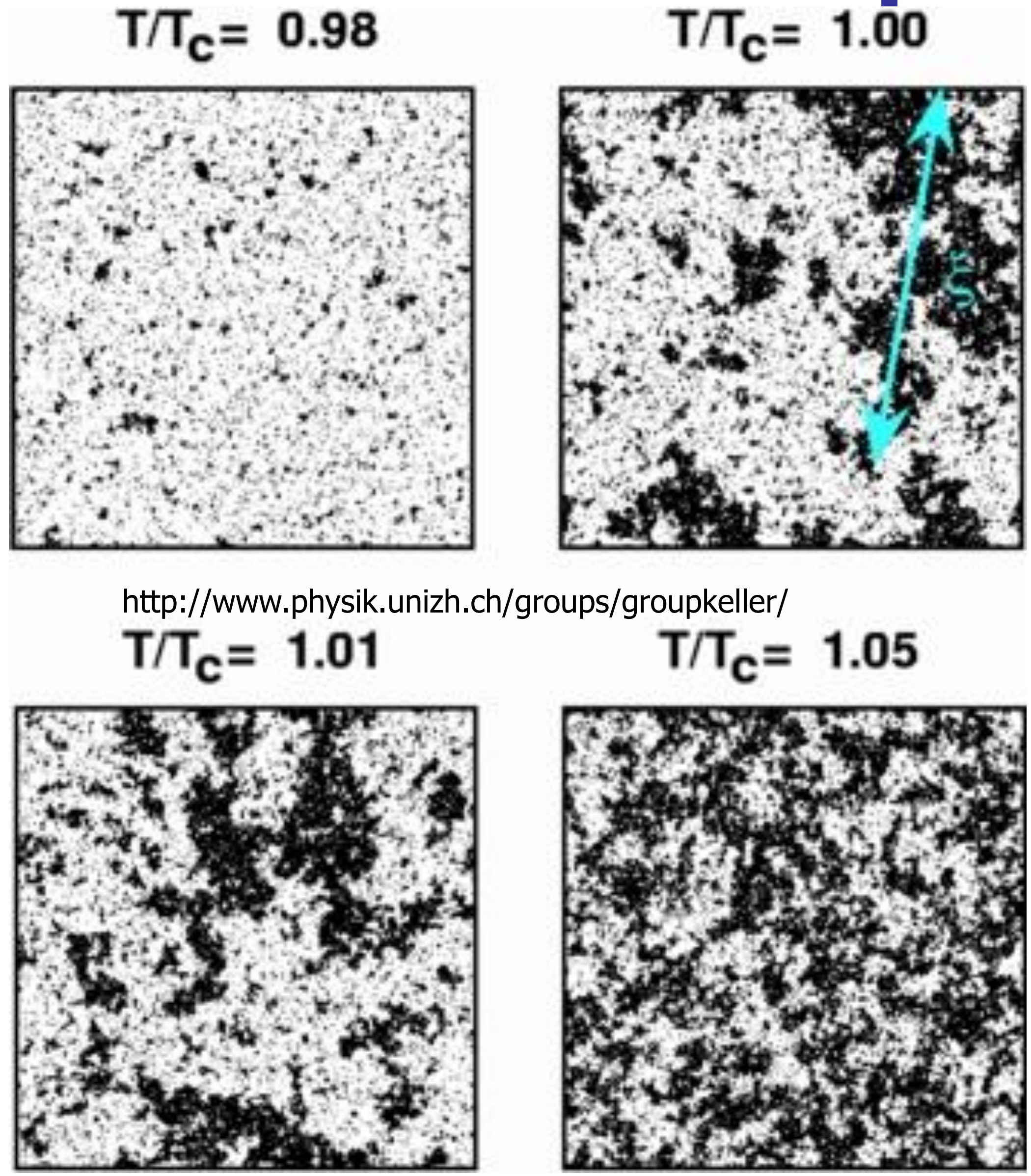


Meniscus vanishes at critical point



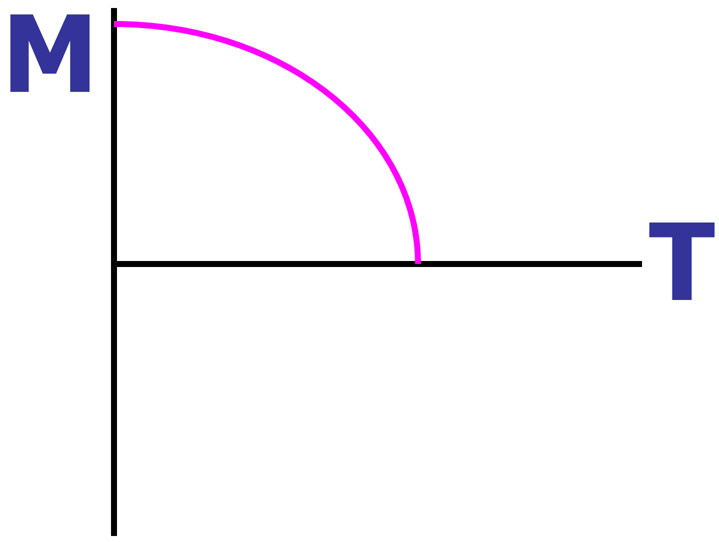
Large fluctuations near a critical point

- **Density in a fluid near its critical point**
  - **Black = high density**
  - **White = low density**
- **Note: size of domains grow as T → T_c**
- **Self-similarity and power law behaviour of correlations as T → T_c**

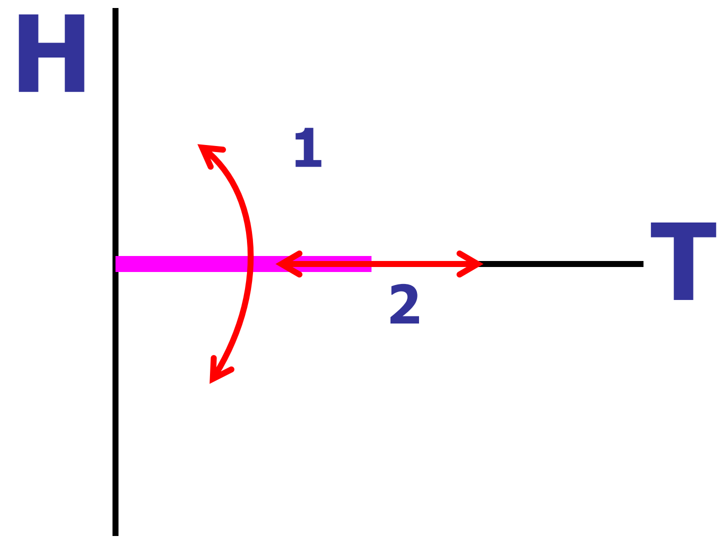


http://www.physik.unizh.ch/groups/groupkeller/

Critical phenomena in magnets



$M \sim M_0[|T-T_c|/T_c]^\beta$ for $H=0$ as $T \to T_c$



Critical isotherm: $M \sim H^{1/\delta}$ for $T=T_c$

- Widom (1963) pointed out that both these results followed from a *similarity formula*:

$$M(t,h) = |t|^\beta f_M(h/t^\Delta)$$

where $t \equiv (T-T_c)/T_c$ for some choice of exponent Δ and scaling function $f_M(x)$

Critical phenomena in magnets

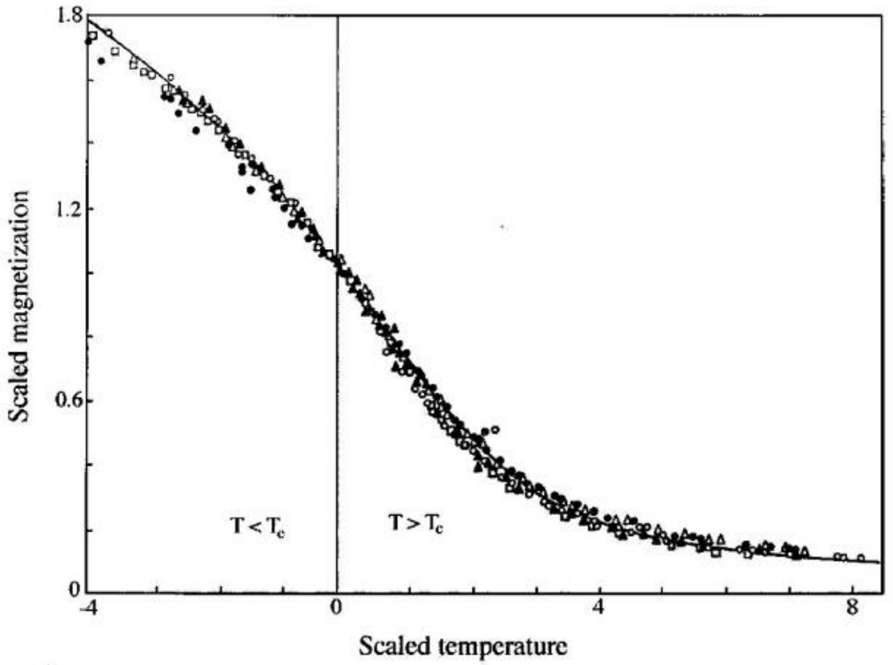


FIG. 1. Experimental *MHT* data on five different magnetic materials plotted in scaled form. The five materials are $CrBr_3$, EuO, Ni, YIG, and Pd_3Fe. None of these materials is an idealized ferromagnet: $CrBr_3$ has considerable lattice anisotropy, EuO has significant second-neighbor interactions. Ni is an itinerant-electron ferromagnet, YIG is a ferrimagnet, and Pd_3Fe is a ferromagnetic alloy. Nonetheless, the data for all materials collapse onto a single scaling function, which is that calculated for the $d=3$ Heisenberg model [after Milošević and Stanley (1976)].

- **M(H,T) ostensibly a function of two variables**
- **Plotted in appropriate scaling variables get ONE universal curve**
- **Scaling variables involve critical exponents**

Stanley (1999)

Turbulence as emergent

“The last great unsolved problem of classical physics” … but not yet complex

Leonardo Da Vinci

Nikuradse's pipe experiment (1933) to measure the friction factor f

$$f = \Delta P / l \rho U^2$$

Pipe diameter is 25-100 mm
Pipe length is ~ 70 diameters

Monodisperse sand grains
0.8mm glued to sides of pipe

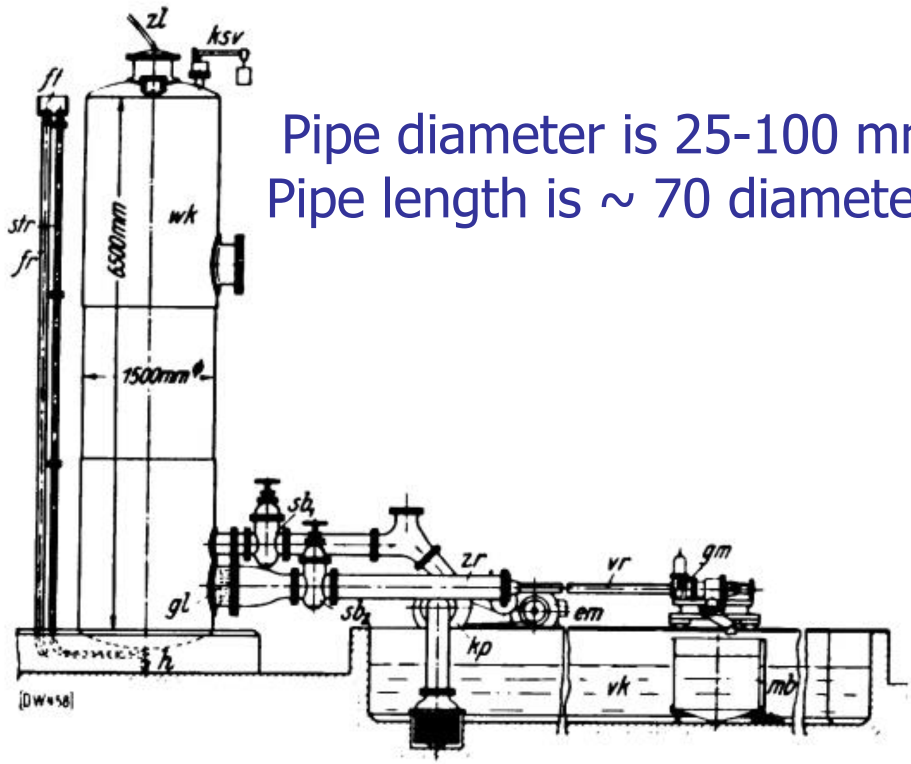


Figure 3.- Test apparatus.

em = electric motor
kp = centrifugal pump
vk = supply canal
wk = water tank
vr = test pipe
zl = supply line
str = vertical pipe
fr = overflow pipe
ft = trap
h = outlet valve
zr = feed line
mb = measuring tank
gm = velocity measuring device
ksv = safety valve on water tank
sb_1 = gate valve between wk and kp
sb_2 = gate valve between wk and zr
gl = baffles for equalizing flow

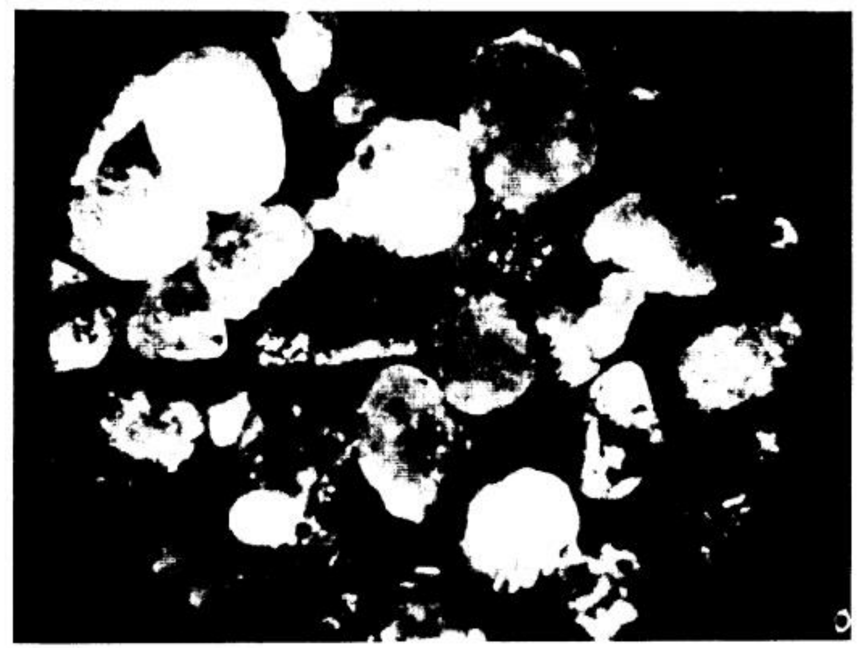


Figure 4.- Microphotograph of sand grains which produce uniform roughness. (Magnified about 20 times.)

Friction factor in turbulent rough pipes

Laminar

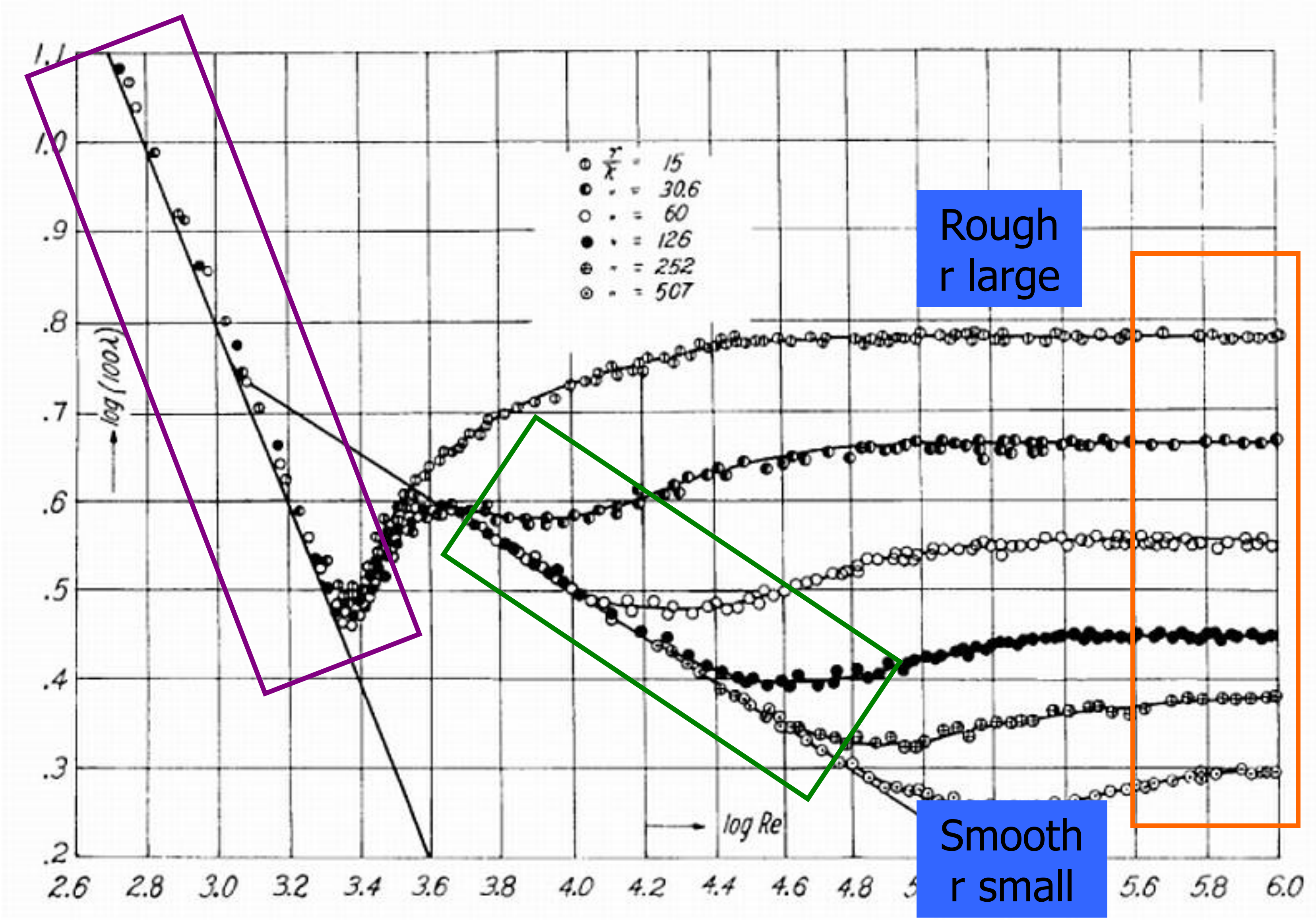
f ~ 12/Re

Blasius

f ~ Re$^{-1/4}$

Strickler

f ~ (r/D)$^{1/3}$



Emergent scaling in turbulence?

PRL **96,** 044503 (2006) PHYSICAL REVIEW LETTERS week ending 3 FEBRUARY 2006

Roughness-Induced Critical Phenomena in a Turbulent Flow

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Intermittency and rough-pipe turbulence

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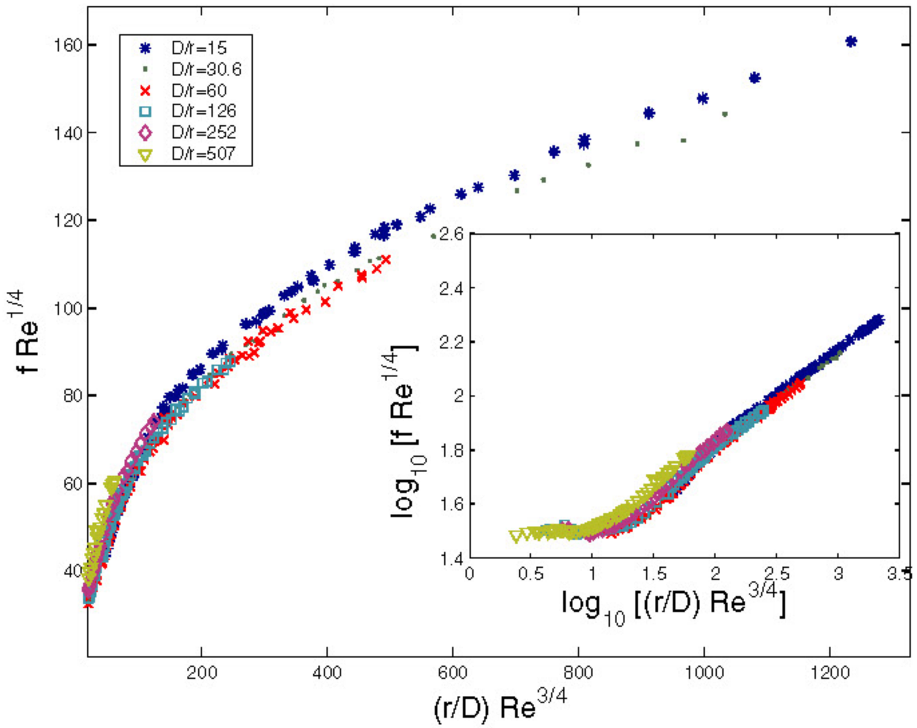
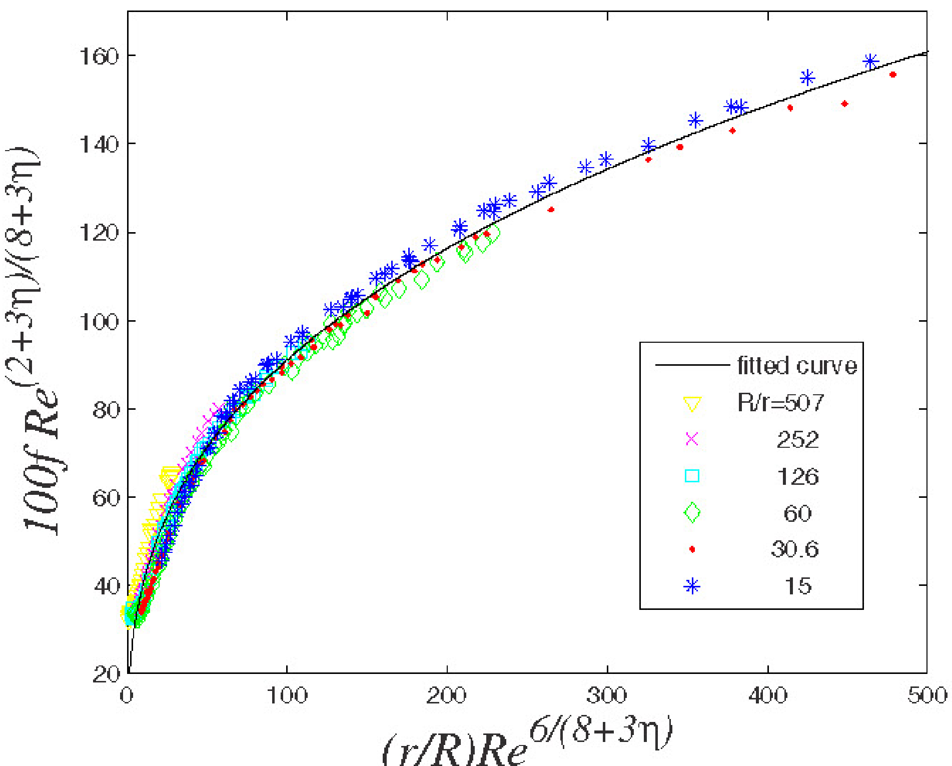
(Received 23 February 2008; published 15 May 2008)



Mean field (Kolmogorov 41) exponents



Intermittency corrections included

Emergent rigidity far from eqm.

Pattern formation outside of equilibrium

M. C. Cross

Department of Physics, California Institute of Technology 114-3ℓ

P. C. Hohenberg

AT&T Bell Laboratories, MH 1D-268, Murray Hill, New Jersey 07

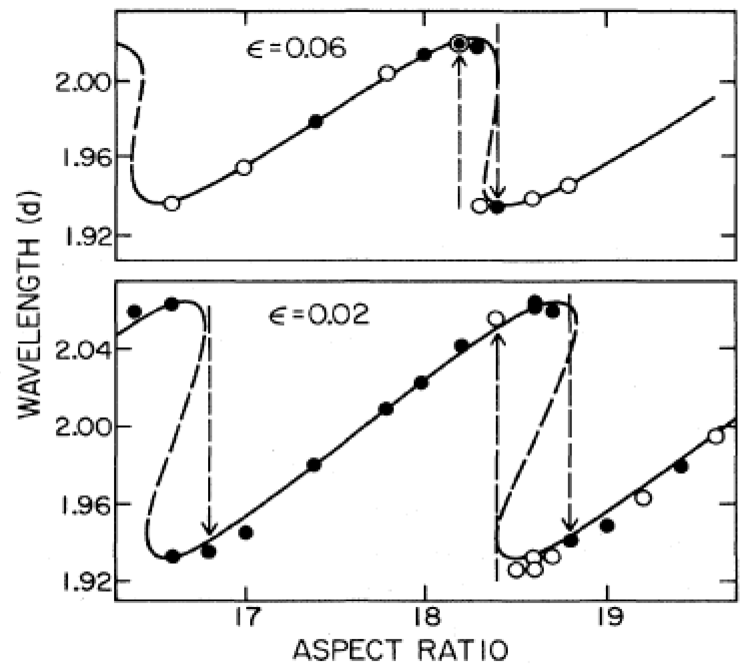


FIG. 63. Wavelength of rolls in the straight supercritical section of a Taylor-Couette system, selected by a control parameter ramp, plotted as a function of aspect ratio L, defined in terms of the length of the straight portion. The control parameter reaches subthreshold values due to an outer cylinder wall sloping at an angle $\alpha=0.03$ at one end of the cylinder. Solid circles were measured with increasing aspect ratio, open circles with decreasing L; dashed arrows correspond to the observed hysteresis. Solid and dashed lines are theoretical predictions of Cross (1984) based on Eq. (9.38) with the pinning strength h used as a fit parameter. The values of ε shown correspond to the control parameter in the straight portion. (From Ahlers *et al.*, 1986.)

• Generalized rigidity: action at a distance or long-range forces. This feature is well demonstrated by experiments on the Taylor-Couette system with ramped sidewalls over a portion of the length. Here the nature of the ramp may be used to control the steady-state "lattice spacing" (i.e. the roll width) arbitrarily far away (Sec. IX.B.2.d).

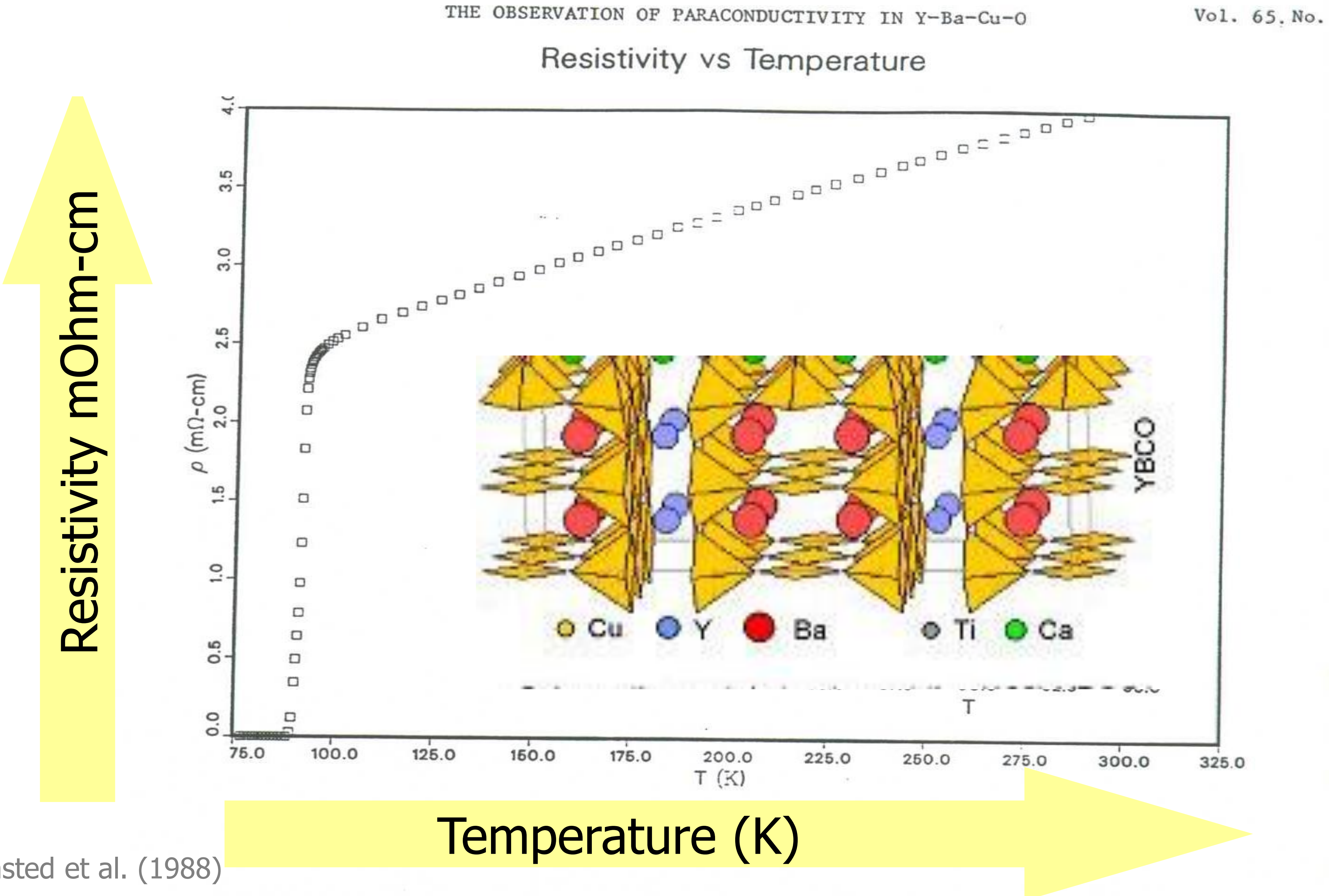
Emergence and biological complexity

Why do we care about emergence in biology?

- **Steven Jay Gould, New York Times, Feb 19, 2001**
  - **“Homo sapiens possesses between 30,000 and 40,000 genes... In other words, our bodies develop under the directing influence of only half again as many genes as the tiny roundworm ....”**
  - **“The collapse of the doctrine of one gene for one protein, and one direction of causal flow from basic codes to elaborate totality, marks the failure of reductionism for the complex system that we call biology.”**
  - **“First, the key to complexity is not more genes, but more combinations and interactions generated by fewer units of code — and many of these interactions (as emergent properties, to use the technical jargon) must be explained at the level of their appearance, for they cannot be predicted from the separate underlying parts alone.”**

So how can awareness of emergence help us understand life?

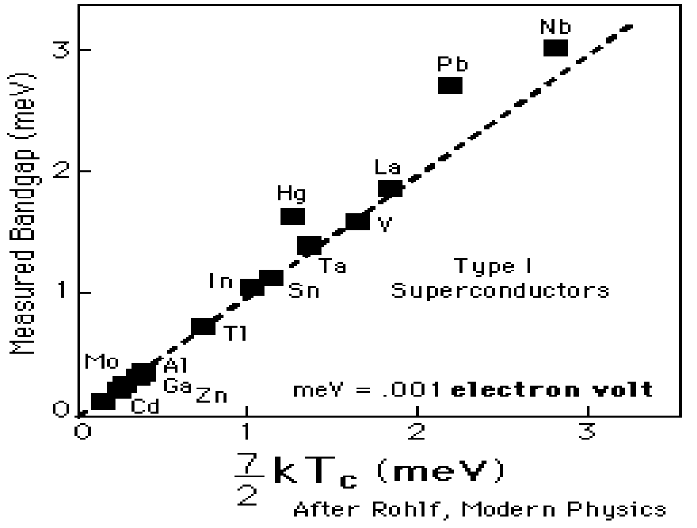
What brings molecules to life?

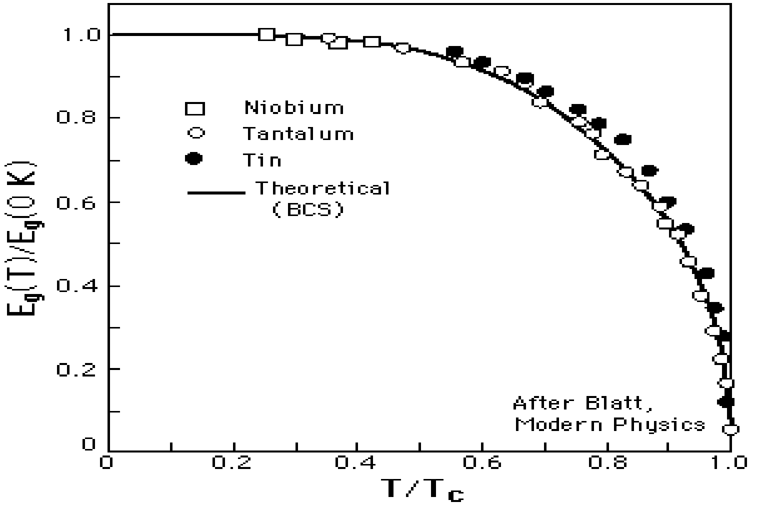


Olmsted et al. (1988)

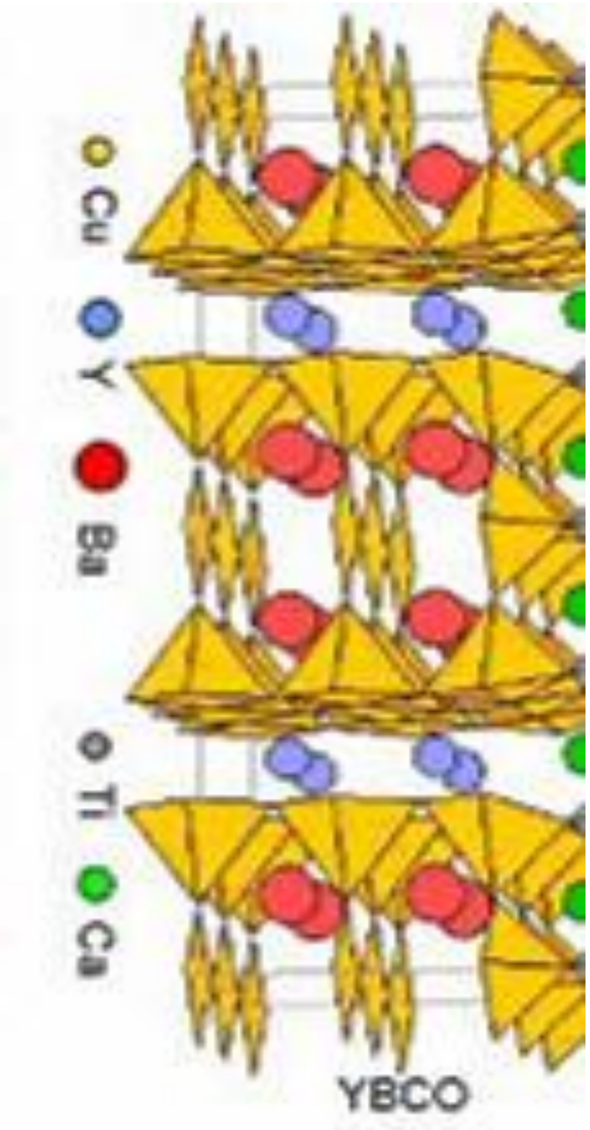
Superconductivity – it's not about the atoms

- **Example: Bardeen-Cooper-Schrieffer theory of superconductivity**
  - Most successful many-body theory
  - Spectacular agreement with experiment:
    - Universal ratios: $\Delta/k_B T_c = 3.53$
    - Universal functions: $\Delta(T)$
  - Predictions same for all materials to which the theory applies





Superconductivity – it's not about the atoms



- **BCS model leaves out much physics and all chemistry**
  - No atoms, no phonons, no electronic band structure
  - Just hopping electrons that can pair
  - Cooperativity is the essence!
- **But poor ability to predict T_c.**
  - Must ask what is the regime of validity of the theory

J. Eckstein

Superconductivity – it's not about the atoms

- **Moral of the story:**
  - Focus on the <u>process</u>, not the <u>realization</u>
    - Process = quantum dynamics of correlated electrons
    - Realization = Y-Ba-Cu-O atoms that you need to mix up in the lab to create something that manifests the process
  - Cannot explain superconductivity by just thinking about atoms: must understand their <u>cooperative</u> behavior.
- **Focus on what really matters!**

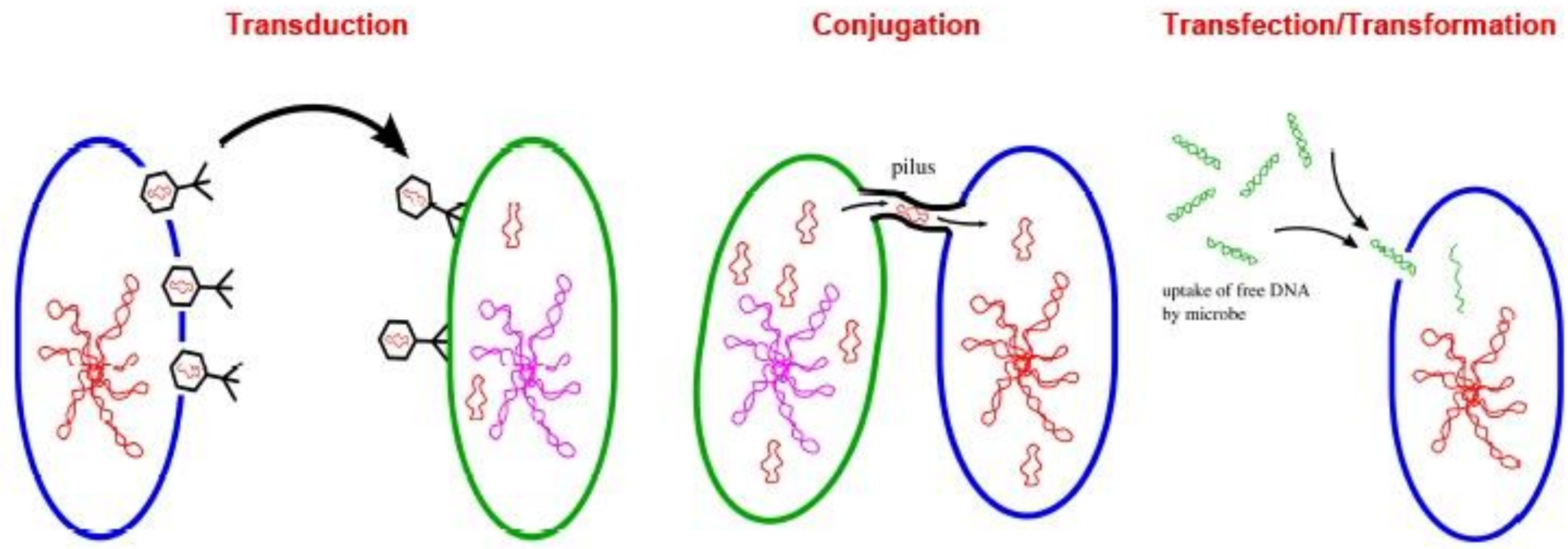
Life – it's not about the molecules

- **Moral of the story:**
  - Focus on the <u>process</u>, not the <u>realization</u>
    - Process = evolution
    - Realization = C, H, N, O, P, … atoms that you need to mix up in the lab to create something that manifests the process
  - Cannot explain life by just thinking about atoms: must understand their <u>cooperative</u> behavior.
- **Focus on what really matters!**

What matters for early life?

Cooperative effects

Horizontal gene transfer



Microbes can do this … but what happens when they all do it?

Spread of antibiotic resistance genes

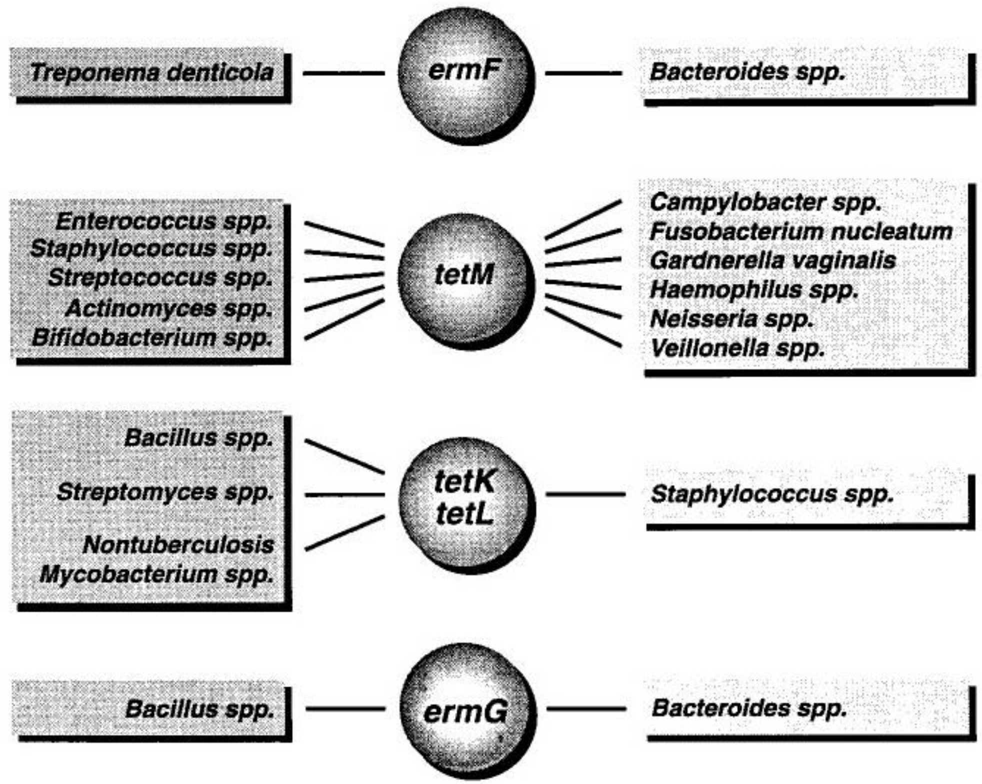


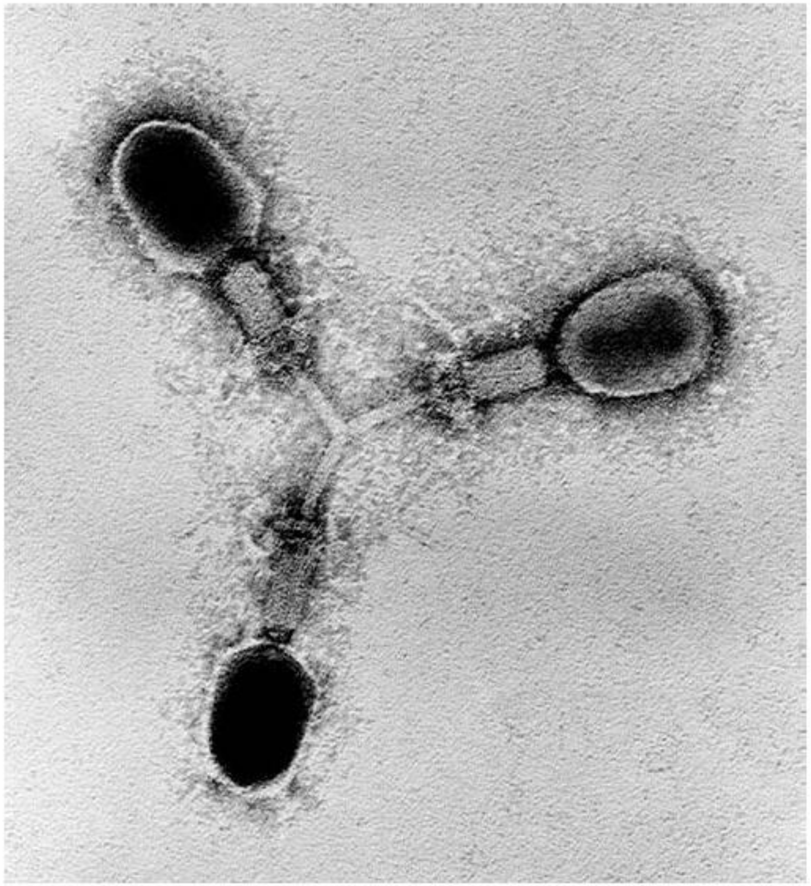
FIG. 1. Evidence that broad-host-range transfer of resistance genes occurs readily in nature (18–20). In each of the cases depicted here, virtually identical copies of the gene in the circle have been found in the species listed in the boxes connected to the circle. Such examples do not prove direct transfer between the species listed but indicate that there is some way for genes to move, whether directly or indirectly, between these genera.

Salyers & Amabile-Cuevas (1997)

- **Virtually identical copies of resistance genes found in distantly related bacteria**
  - **Genes are being expressed**
- **Genes cross species and phylum boundaries**
  - **Gram-positive/enteric**
  - **Bacteroides/enteric**
- **Genes cross physical locations**
  - **Bacteroides spp. (colon)/Bacillus spp. (soil)**

Gene transfer between host and virus

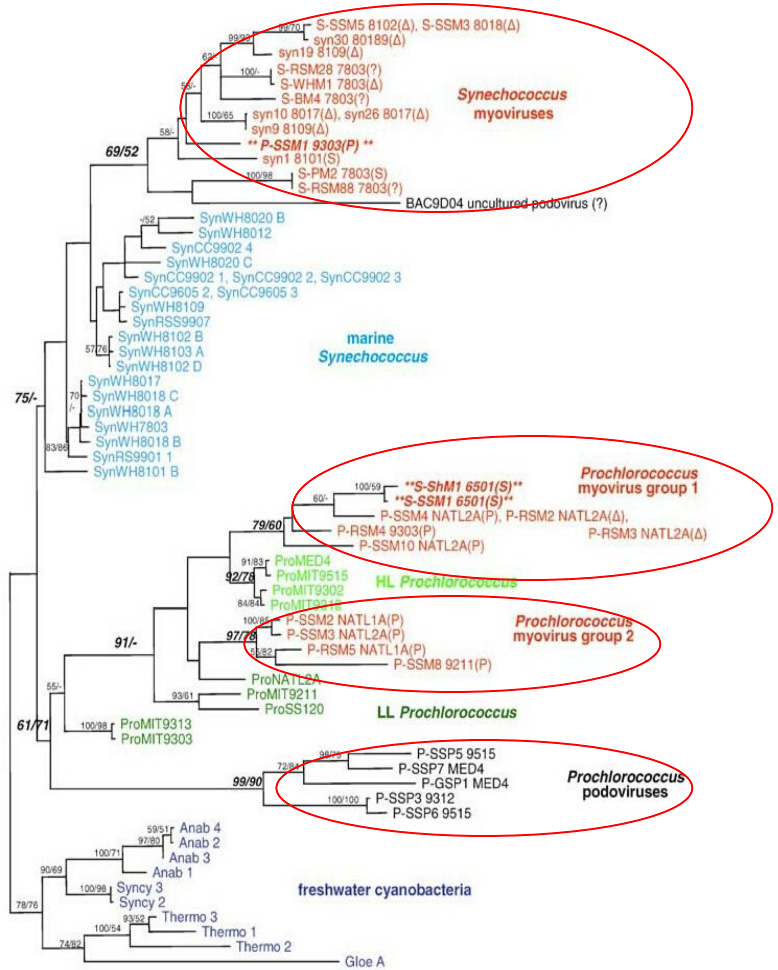
Sullivan et al. , PlosBiol (2006)



DOI: 10.1371/journal.pbio.0040264.g001

Cyanophages—viruses that infect photosynthetic marine bacteria—not only possess genes for photosynthesis but also exchange genetic material with their cyanobacterial hosts.

Hill, PlosBiol (2006)



PsbA gene acquired by phage

Phylogeny of psbA gene in cultured cyanobacteria and cyanophages

Is there a benefit to microbes of viruses?

"Therefore, mounting evidence indicates that host-like genes acquired by phages undergo a period of diversification in phage genomes and serve as a genetic reservoir for their hosts. Thus, a complex picture of overlapping phage and host gene pools emerges, where genetic exchange across these pools leads to evolutionary change for host and phage. Fully understanding the mechanisms of microbial and phage coevolution clearly requires an improvement in our ability to quantify horizontal gene transfer at the whole and partial gene level and in our ability to accurately estimate the relative fluxes into and out of these pools." (Sullivan et al. 2006)

Yes: microbe-phage interactions create a global reservoir of photosynthetic genes, benefiting both microbes and phages. **(E. Anderson (1966), N. Anderson (1970), S. Sonea (1988, 2001), M. Syvanen (1984) & many others, including L. Villareal, Weinbauer, Ochman, Lawrence, Groisman, Hatfull, Hendrix, Brussow …)**

Emergence of the canonical genetic code

<table>
<tr><th></th><th>U</th><th>C</th><th>A</th><th>G</th><th></th></tr>
<tr><td rowspan="4">U</td><td rowspan="2">Phe</td><td rowspan="4">Ser</td><td rowspan="2">Tyr</td><td rowspan="2">Cys</td><td>U</td></tr>
<tr><td>C</td></tr>
<tr><td rowspan="2">Leu</td><td rowspan="2">STOP</td><td>STOP</td><td>A</td></tr>
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<tr><td>Met</td><td>G</td></tr>
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<tr><td>C</td></tr>
<tr><td rowspan="2">Glu</td><td>A</td></tr>
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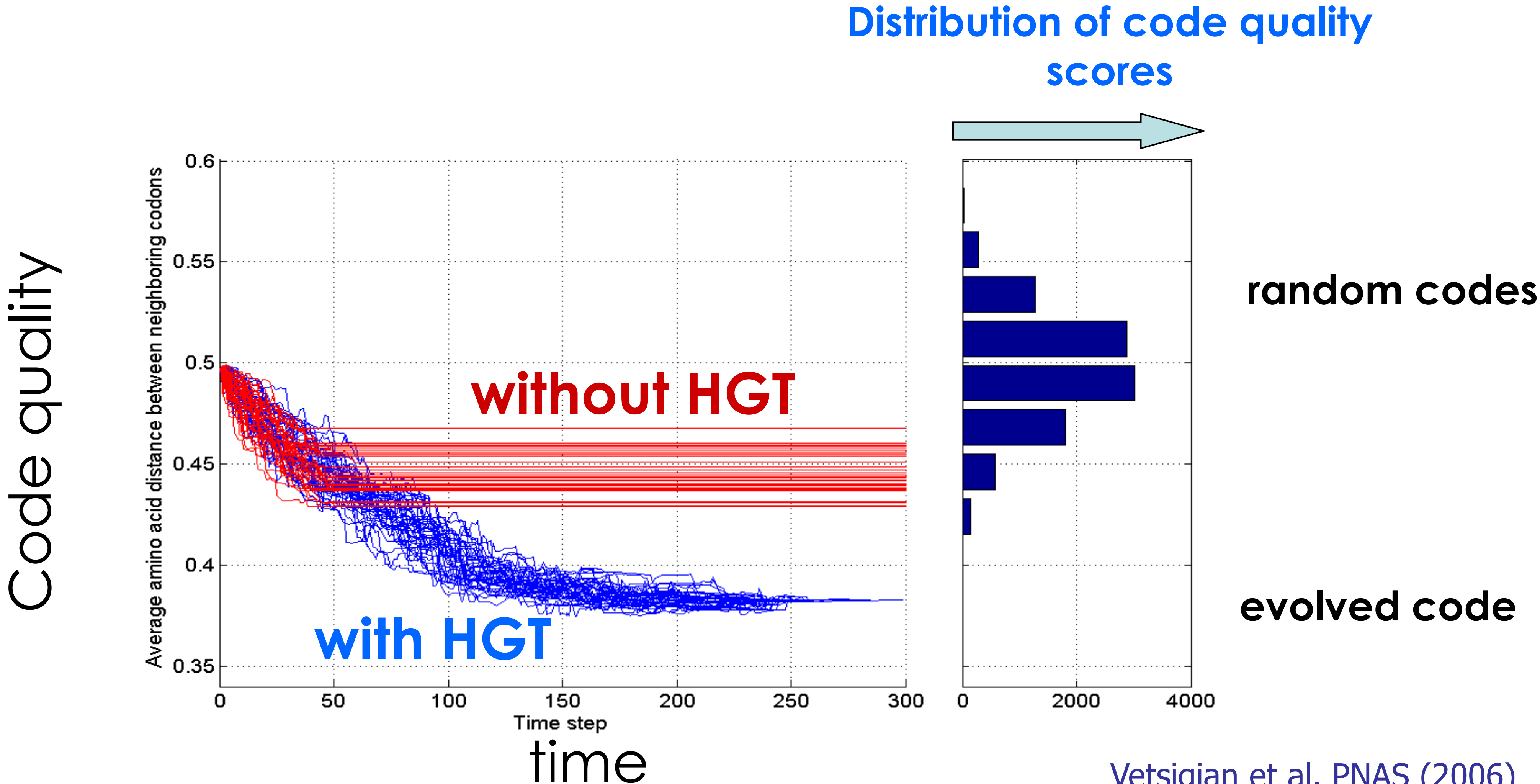
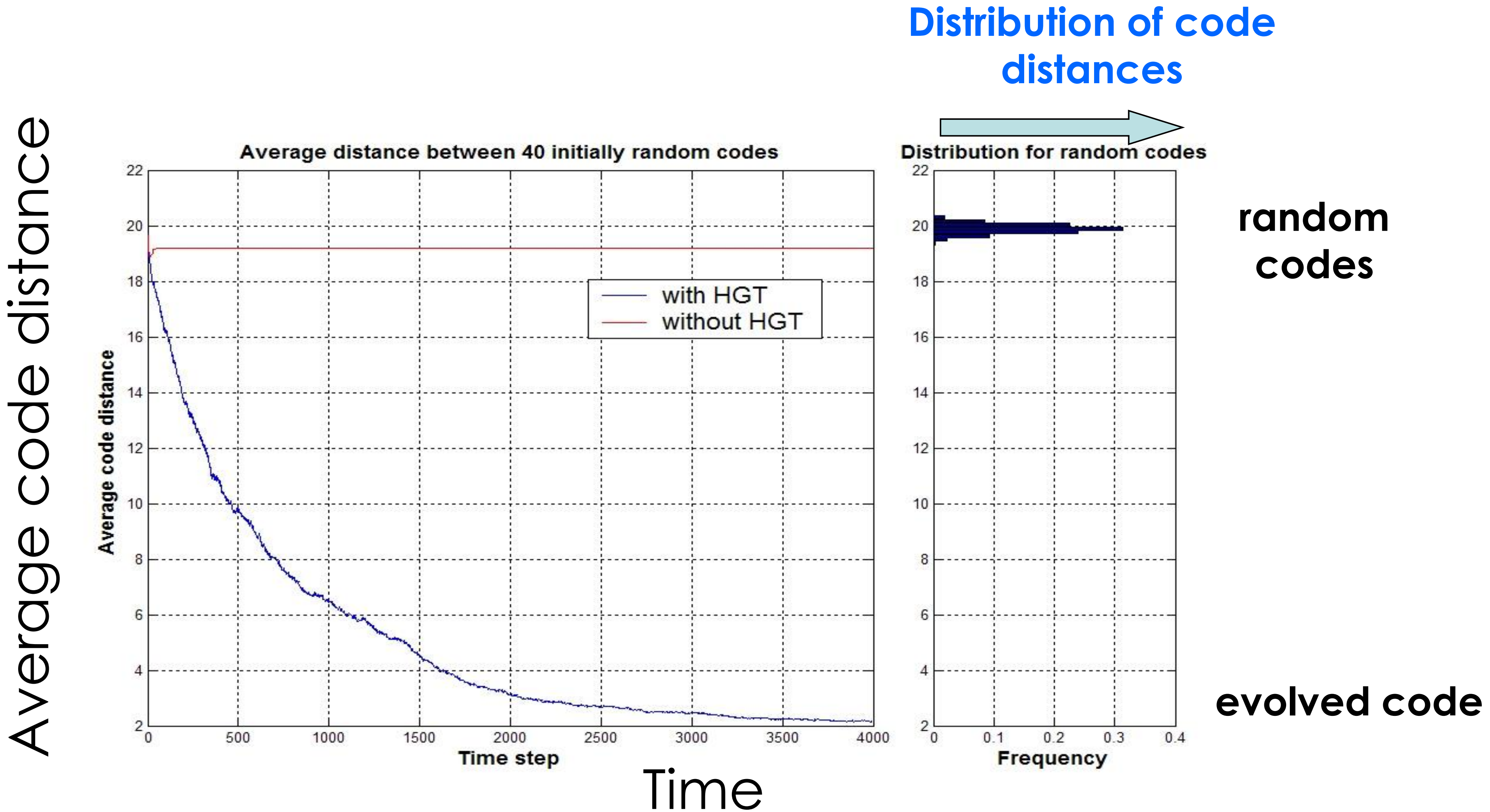
Evolution of code quality



Vetsigian et al. PNAS (2006)

HGT leads to optimality

Evolution of code distances



HGT leads to universality

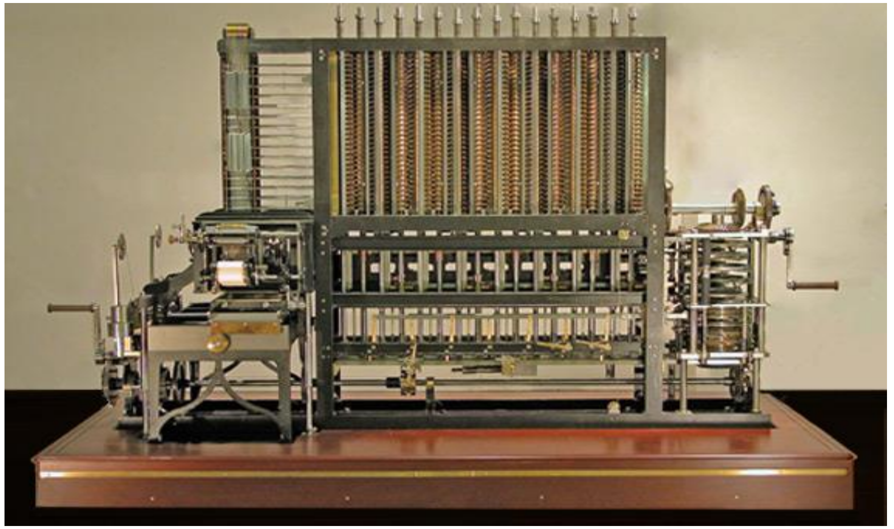
Vetsigian et al. PNAS (2006)

Universal Biology

Universal Computation

Universal Computation

Universal Computation



Universal Computation

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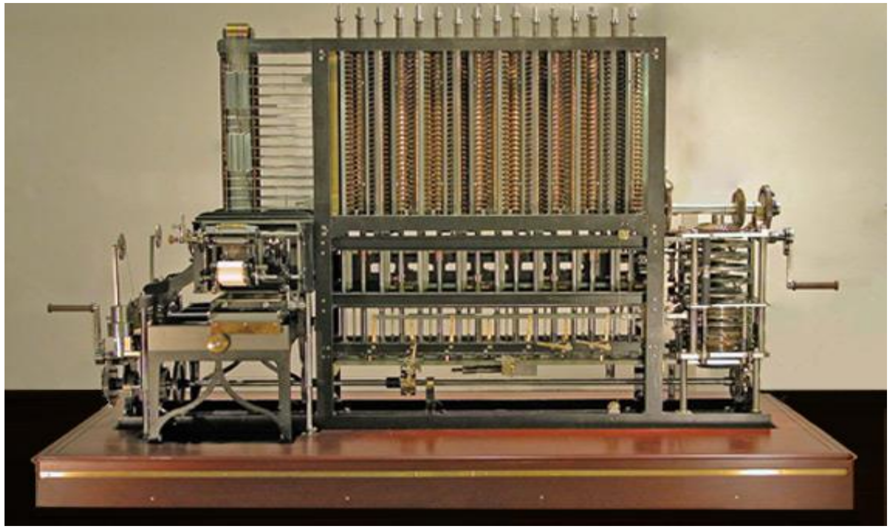

Universal Computation

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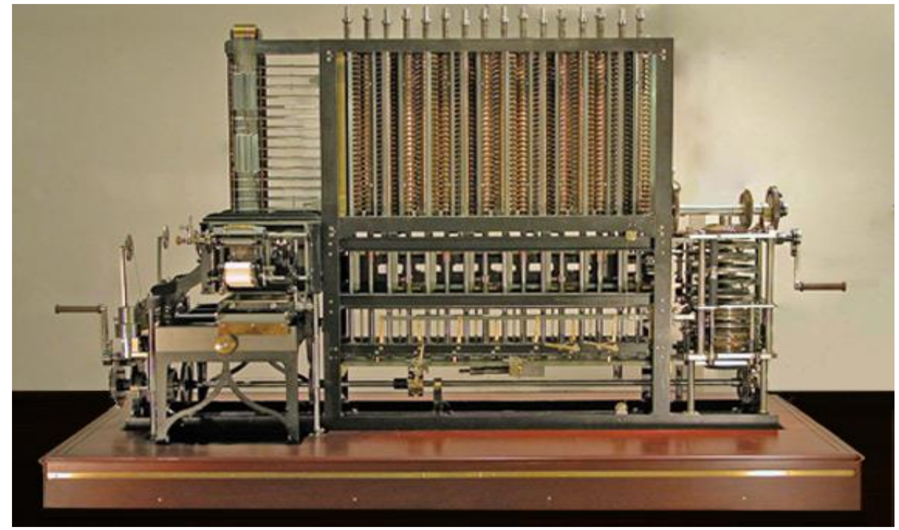


- **A computer is neither a shiny chunk of glass, plastic and silicon not a bunch of cog wheels, springs and levers.**
- **It is an abstract concept (Turing machine with a von Neumann architecture etc.) that can be instantiated in many ways.**

Universal Biology: new physical laws?

- Schrodinger, Delbruck, … earliest physicists to work in biology
  - Partial motivation was to find new physical laws!
- Where would such laws lie?
  - Our answer: emergence and existence of life itself
  - How does matter self-organize hierarchically to create replicating, evolvable structures?
  - How do molecules come to life?
- To understand biology in the same sense that we understand physical phenomena, we need to understand EXISTENCE and not just SPECIFIC REALIZATION
  - Dynamics of systems that can reprogram themselves

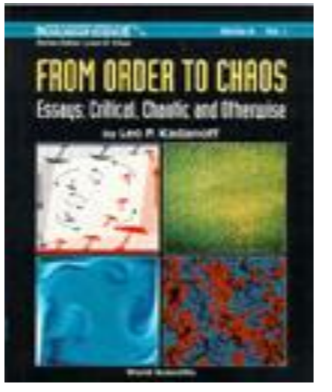
Exploiting emergence …

We can understand nature using minimal models

Purpose of computer simulation

- **At that time there was a great national push toward understanding the dynamics of urban development. Jay Forrester of MIT had developed a computer model of urban change, which took a very simplified view of a urban society … and then used the output of that model to prescribe social policy. I did not like the policy prescribed.**
- **Consequently, I set out to use the modeling tools that Forrester had developed to reach conclusions which were more to my liking. … Our first result was that while not changing the model at all, we could reach opposite conclusions from that of the Forrester group.**
- **We went on to build other models which more accurately recorded our own prejudices and points of view. But after a while, the point we had made began to sink in. If these models really represented little more than we could say in words, why not leave out the computer?**
- **The construction of this sort of computer model seemed to be a rather pointless endeavor. For this reason, and others, I moved away from urban studies.**

Leo P. Kadanoff 1993



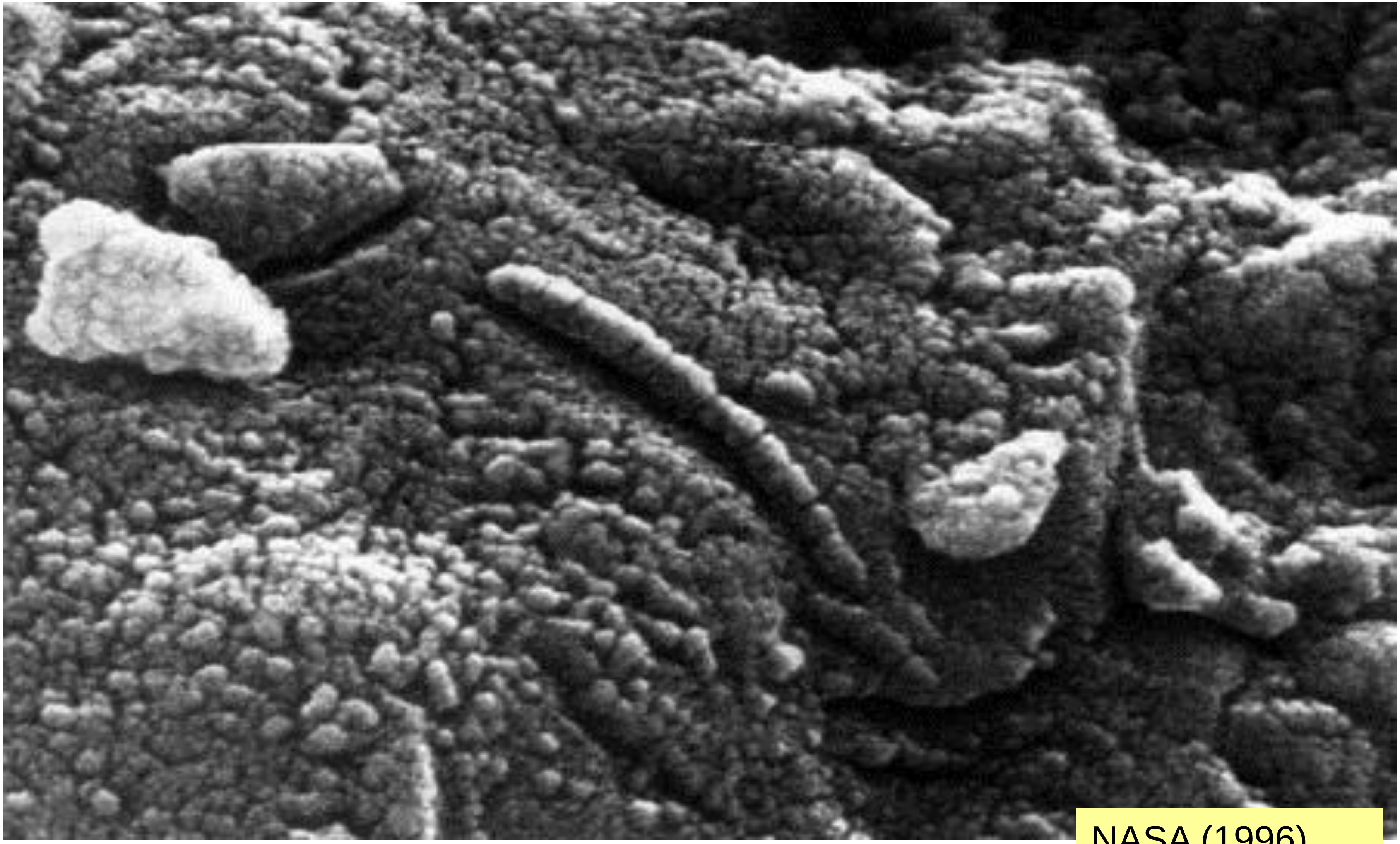
Purpose of computer simulation

- **Moral of this story:**
  - Either compute to get numerical information that verbal arguments cannot address
  - Or compute to find emergent phenomena: an outcome of the dynamics that is not mandatory, and usually collective
    - Example: the Hamiltonian of a fluid and a solid are identical, but only for low temperatures, can there be a non-zero shear modulus

Exploiting emergence to model complex pattern formation

Farewell to excessive realism

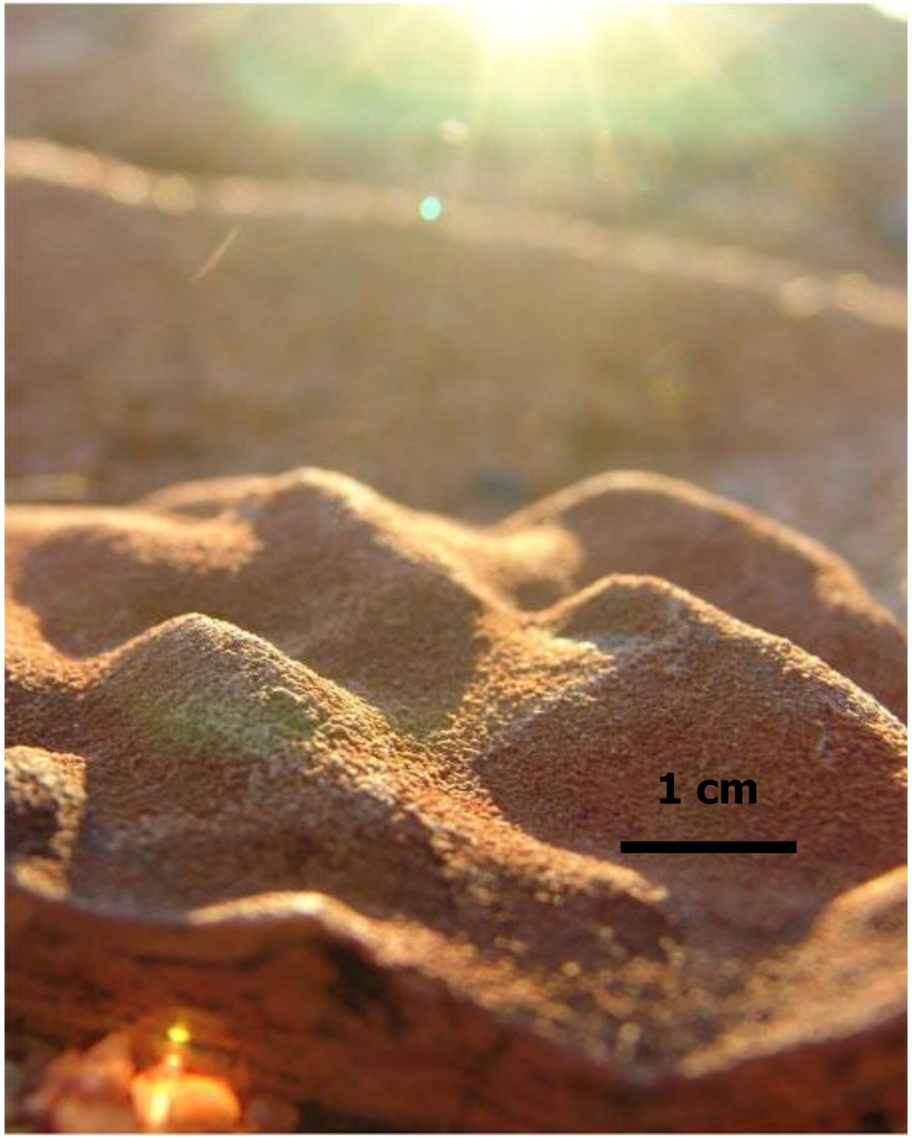
ALH84001 – Life on Mars?



NASA (1996)

Life on Earth?

- **Did microbes on Earth 3.43 Billion years ago make these stromatolites?**
- **What makes the patterns and structures we see around us?**



Credit: Abigail Allwood

Travertine terraces at geothermal hot springs

Mammoth Springs at Yellowstone

Photo by Larry Ulrich

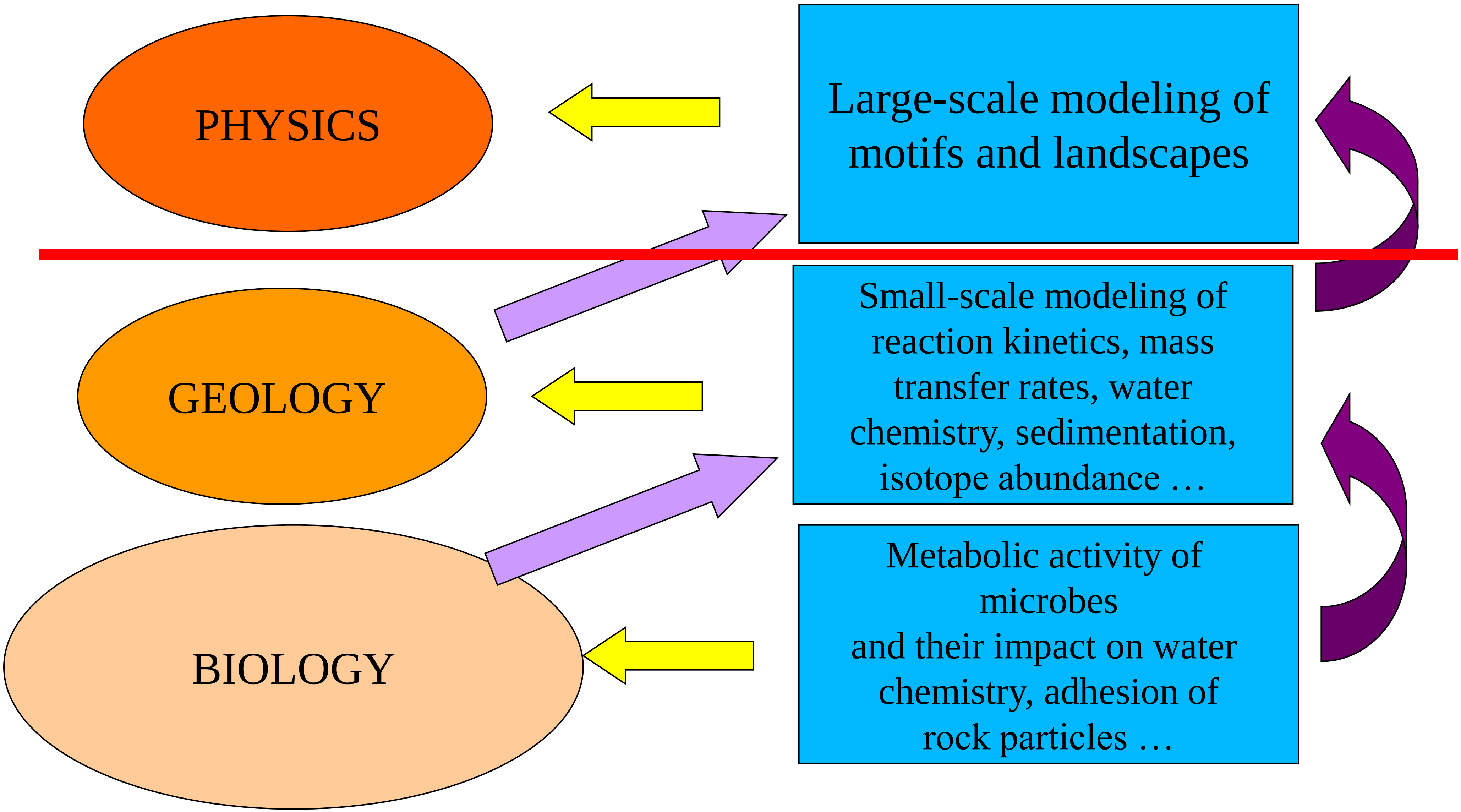
The challenge:
Identify the origins of geological structures

Terraces and ponds formed by calcium carbonate deposition at
Mammoth Hot Springs, Yellowstone National Park, USA

The challenge?

- Natural landscapes form beautiful patterns with repeated motifs:
  - Stalactites
  - Ponds and terraces
  - Icicles
  - Snowflakes
  - Hexagonal crazing patterns
- How do these motifs form, apparently spontaneously?
- How are these motifs arranged to form the landscape we see?
- How can we quantify and predict the properties of geophysical landscapes?
- Is there a meaningful distinction between biotic and abiotic origin?

But it’s not just geology …

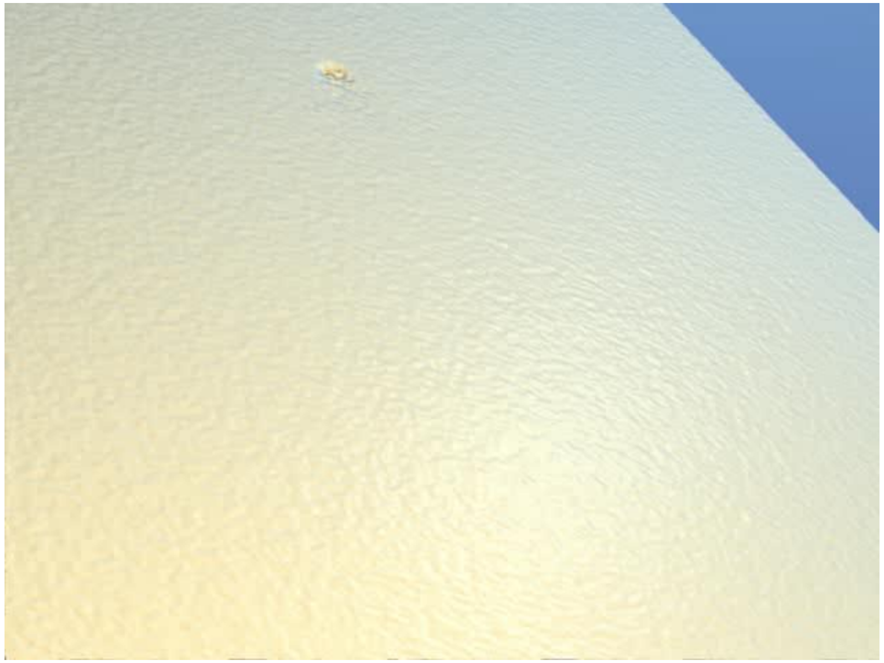


What’s new?

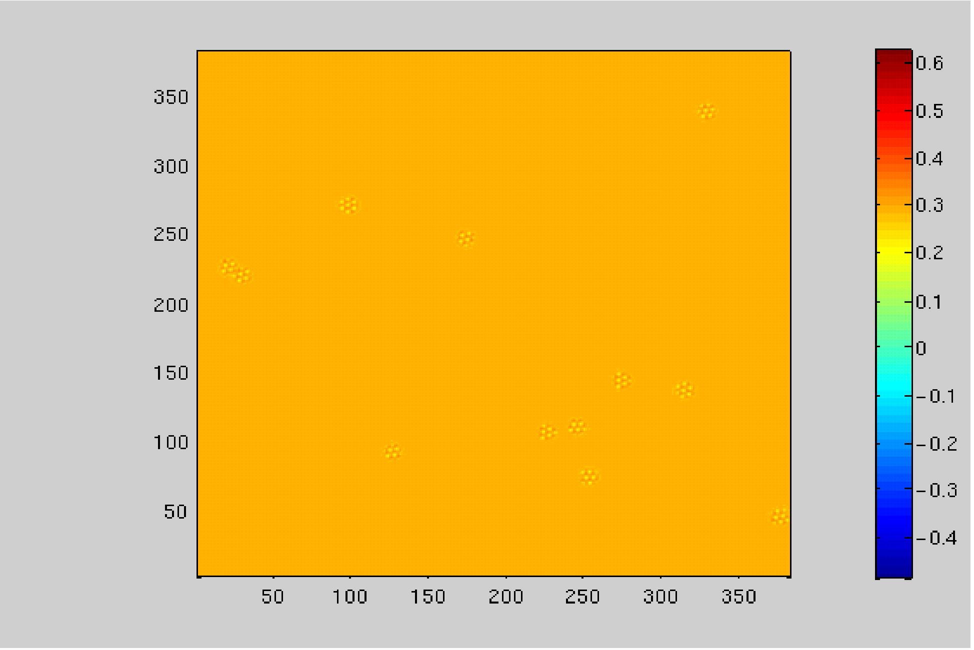
- **Physics models focus on large-scale phenomena**
    - **Approach applicable when the patterns are generic and do not depend sensitively on the mineralogy, crystallography, fabrics and textures of underlying rocks**
    - **Can predict shapes and statistical properties of landscapes**
    - **Can predict modes of growth and potentially inform debates about the origin of geological features**
  - **Can make laboratory analogues of geological pattern formation on time-scales millions of times faster than geological processes**

- **Geology important at small scales**

Computer simulations of emergent order



Emergent order in geophysics – formation of terraces and ponds at a geothermal hot spring



Emergent order in condensed matter physics – formation of a polycrystalline film

Summary

- Emergence arises in large systems due to strong interactions between constituents
- Collective state exhibits novel response characteristics, and loses memory of underlying level of description
- Onset accompanied by a phase transition (smooth or discontinuous)
- Emergent rigidity in equilibrium systems. Non-equilibrium?
- Scaling phenomena near onset if the phase transition is smooth
- Emergence leads to new abstractions, such as the genetic code
- Emergence can be exploited for purpose of modeling.