Disordered materials

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Master IFCP – Paris, October 8, 2019

SIMONS FOUNDATION

What is it about?

- High energy physics vs. low-energy physics.

- Quantum effects (‘hard’ condensed matter) versus classical physics (‘soft’ condensed matter).

- Microscopic approach versus large scale behaviour (turbulence, non-linear physics).

KEYWORDS: Soft condensed matter, complex fluids, non-equilibrium statistical mechanics, material properties, chemical physics, fluids and disordered solid materials, contact with experiments.

TECHNIQUES: advanced statistical mechanics, exactly soluble models, computer simulations (molecular dynamics and Monte Carlo methods), kinetic theory & nonequilibrium processes, random matrices, field theory & renormalisation group, replica technique.

Simons Collaboration

- Medium-scale team (13 PIs) to ‘Crack the glass problem’: `https://scglass.uchicago.edu/`
- Generous support: $16M in 2016-23, giving us freedom and visibility.
- Headquarter in Chicago (Sid Nagel).
- Financial support from Simons Foundation (New York).
- Collaborators: Paris, Orsay, Montpellier, Lausanne, Rome, New York, Philadelphia, Chicago, Oregon, Duke, Syracuse, Tokyo, Kyoto, Bangalore, Amsterdam, London...

Cracking the sailing problem

[Beg Rohu Summer School, July 2019]

APS News, Sep. 2019

MEMBERSHIP UNIT PROFILE

APS Membership Unit Profile: The Division of Soft Matter

BY ABIGAIL DOVE

The APS Division of Soft Matter (DSOFT) is concerned with dense, many-body systems in which quantum effects do not play a primary role. This encompasses a staggering variety of materials from the everyday to the exotic, including polymers such as plastics, rubbers, textiles, and biological materials like nucleic acids and proteins; colloids, a suspension of solid particles such as fogs, smokes, foams, gels, and emulsions; liquid crystals like those found in electronic displays; surfactant systems, which involve networks of amphiphilic particles with distinct hydrophobic and hydrophilic domains; and granular materials.

Perhaps counterintuitively, many forms of soft matter like window glass and "oobleck" (a non-Newtonian fluid like water and cornstarch) can be surprisingly hard. What makes soft materials "soft" is their ultra-responsiveness to external fields and therefore high susceptibility to deformation and falling out of equilibrium. These materials tend to be disordered at the molecular scale and homogeneous at the macroscopic scale, whereas the mesoscopic scale shows unexpected order and dynamics. It is the physics of these systems that occupies the minds of the approximately two thousand researchers in DSOFT.

Doug Durian

According to DSOFT chair Doug Durian (University of Pennsylvania), the field of soft matter is an ecosystem where each researcher establishes their own unique niche of research problems—in contrast to some

DSOFT CONTINUED ON PAGE 6

STRATEGIC PLAN

APS Innovation Fund: Inaugural Winners Selected

BY DAVID VOSS

The APS Innovation Fund (IF) was launched in early 2019 to encourage APS members to develop fresh approaches to serving the physics community (*APS News*, March 2019) in line with the Society's new Strategic Plan. Applicants were encouraged to think big, from advancing global engagement to fostering equity and inclusion in physics.

More than a hundred pre-proposals were received by mid-March, of which 10 full proposals were considered by the selection committee. Four of these were ultimately selected for funding at levels between $50,000 and $100,000 per year for two years, with a fifth proposal still under consideration.

"It was surprising that we received over a hundred proposals in a six-week time period," said APS President David Gross, co-chair of the selection committee. "I take that as an indication of the enthusiasm of APS members and staff for this initiative. I'm also very pleased that APS has been able to respond and launch the project so quickly."

Funded projects need to align with the APS Strategic Plan that was rolled out earlier this year and funds will not be used to support existing projects. "The Innovation Fund is a new initiative," explains APS Director of Project Development Theodore Hodapp, co-chair of the selection committee. "It is inspired by the APS Strategic Plan and will capture thoughtful and forward-looking

FUND CONTINUED ON PAGE 7

APS physics **2019** GENERAL ELECTION

The results are in! Congratulations to these newly elected members of APS leadership:

VICE PRESIDENT
Frances Hellman
University of California, Berkeley

INTERNATIONAL COUNCILOR
Ursula Keller
ETH Zurich

GENERAL COUNCILOR
Robert McKeown
Jefferson Laboratory; College of William & Mary

CHAIR-ELECT, NOMINATING COMMITTEE
Maria Spiropulu
California Institute of Technology

Thank you to all who voted, and special thanks to our election candidates. More info: aps.org/about/governance/election/

物理科学雑誌

parity

パリティ

2019
03

PHYSICS TODAY 提携

素粒子を用いた地球物理 | 多角的にみたガラス物理

物理に女性が少ないのはなぜか | 家庭の物理学

実験室で模擬する宇宙磁場の起源と進化 | イカはいかにして球形レンズを工学実現したのか | 衣服にも貼れる超薄型有機太陽電池

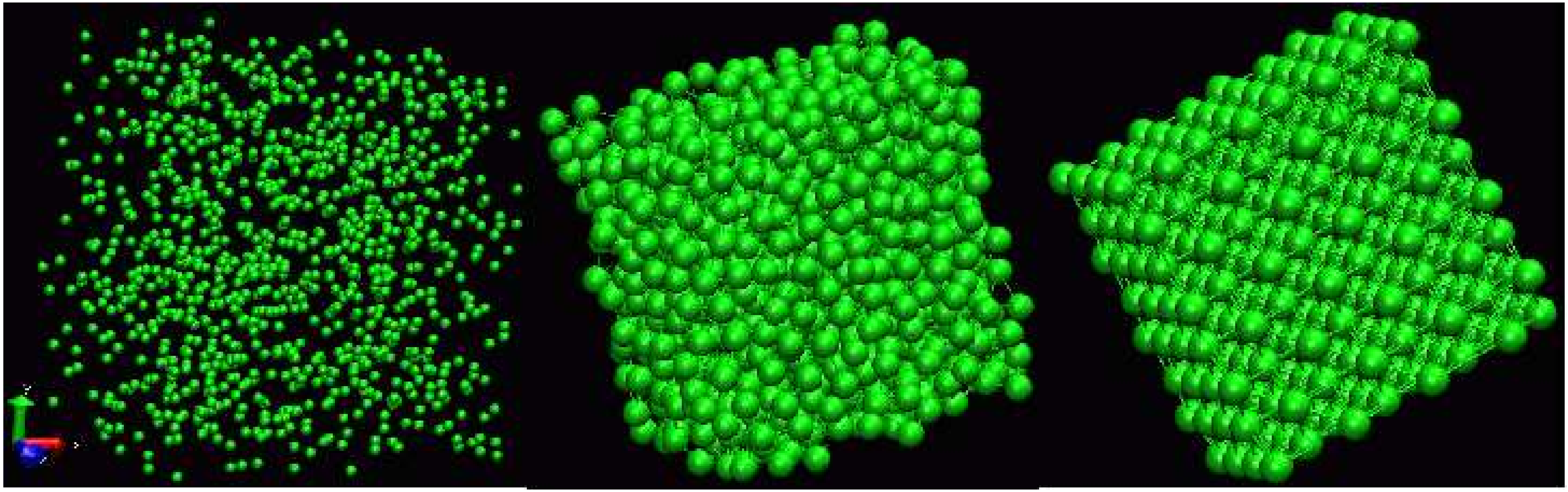
物理の雑誌

MARUZEN

[From ‘Facets of glass physics’, Physics Today 2016]

Statistical mechanics

- Statistical mechanics: understanding the different states of matter, starting from microscopic interactions between elementary units.

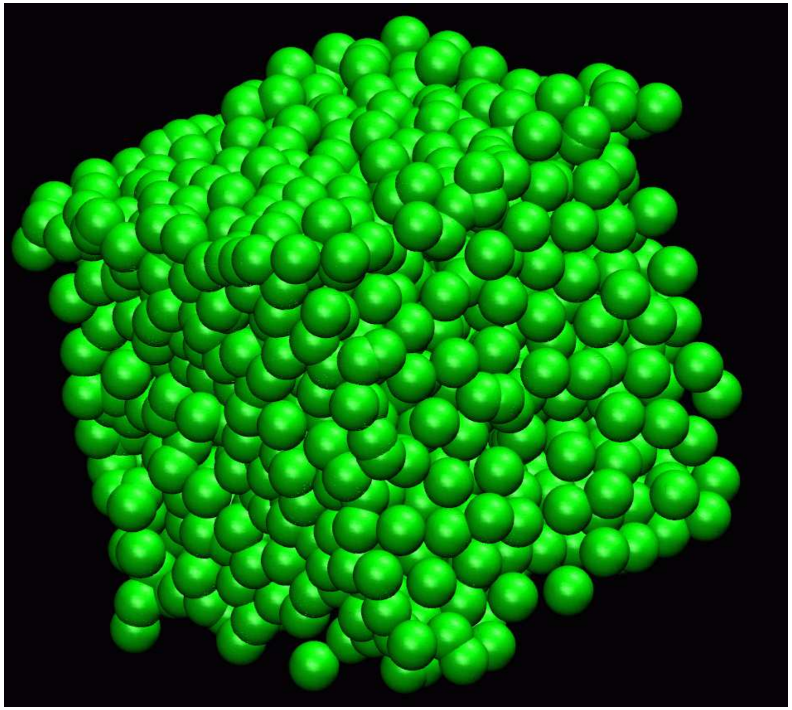


- Simple states of matter: gas, liquid, crystal.

[Tabor, CUP]

- Disordered materials? Where are glasses, foams, gels, sandpiles, mayonnaise, shampoo, chocolate, but also skin tissues?

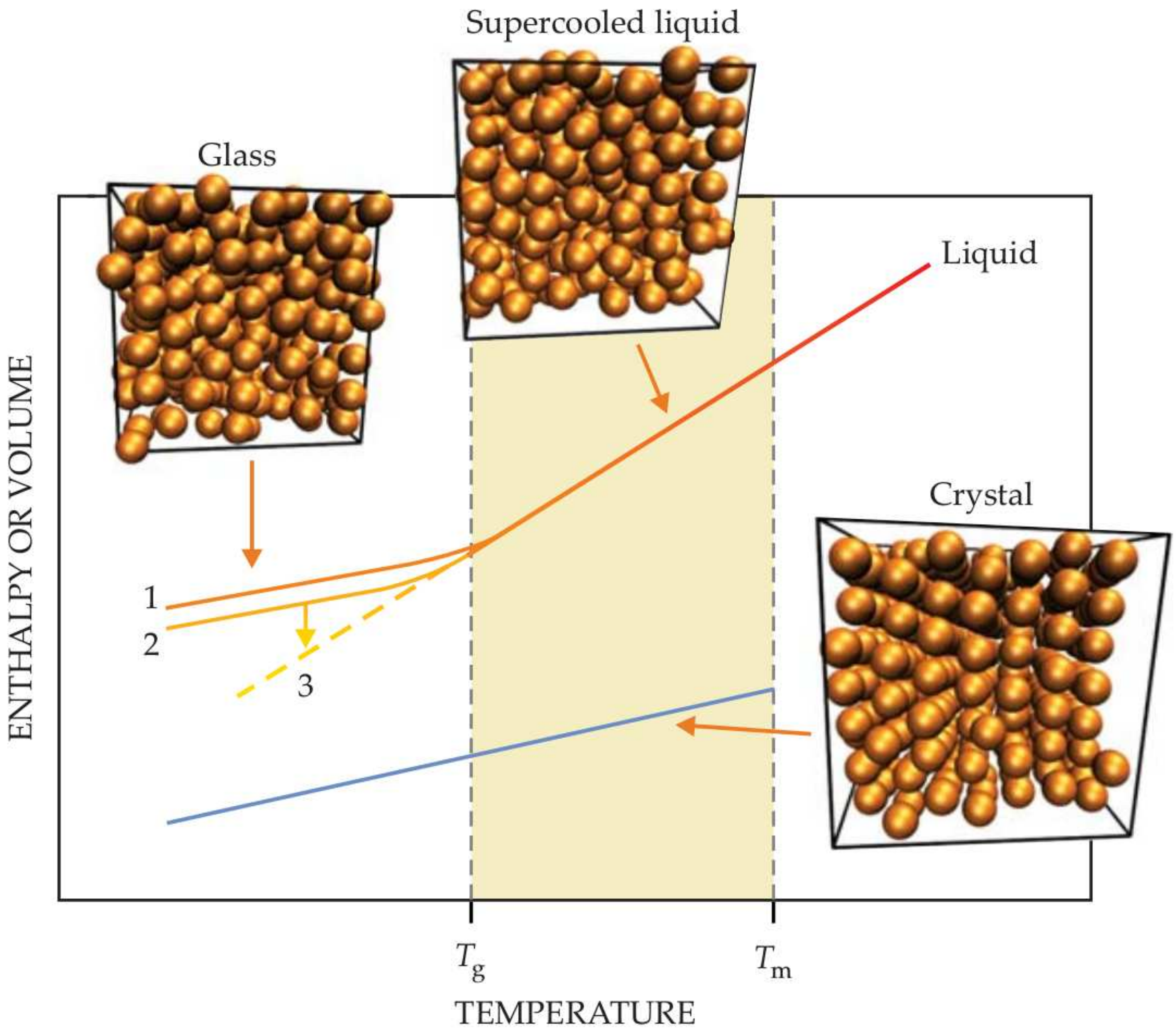
Simplest ‘complex’ solid: Glass



- Glasses have the apparent structure of liquids, but the rigidity of crystals: window glasses, plastics, organic glasses in electronic devices, etc.

- Essential crystal property: $C_p \sim T^3$ (Debye) does not hold for glasses where $C_P \sim T$. Basic glassy excitations are not fully understood.

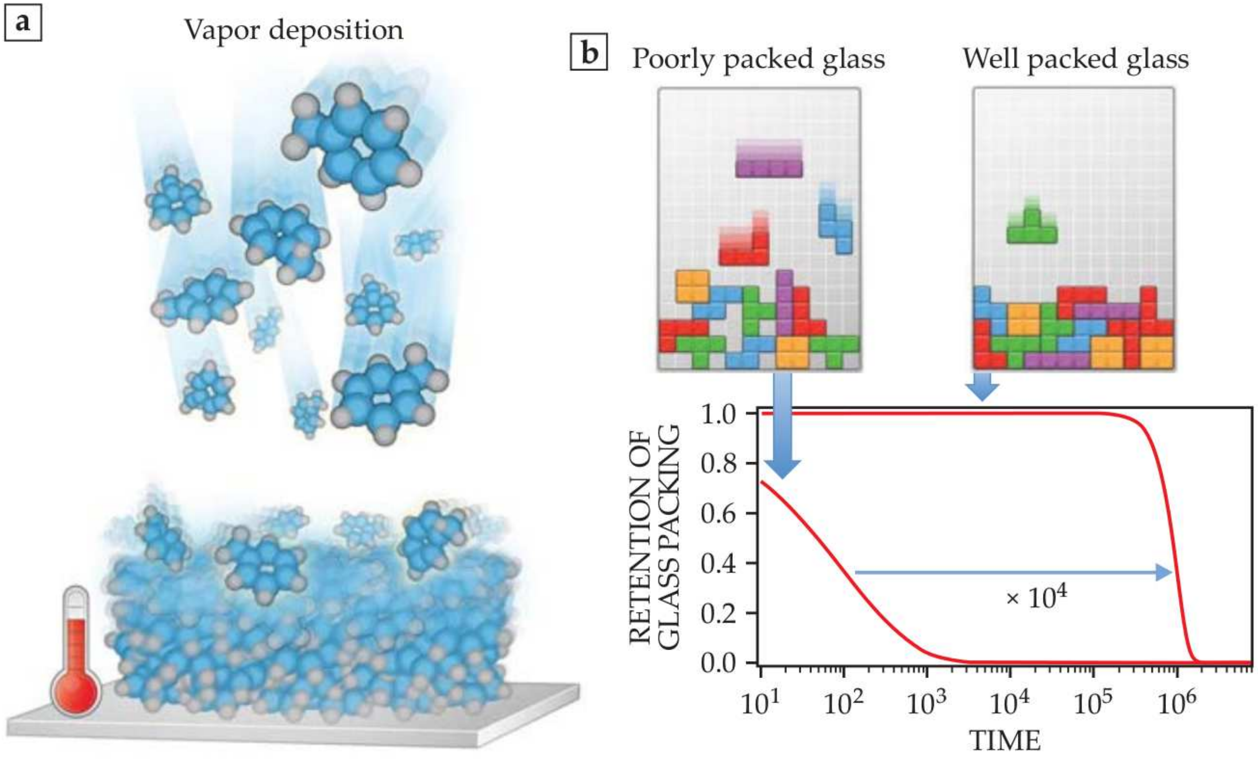
How to create glasses? Cool



[Berthier & Ediger, Physics today ’16]

Ultrastable glasses – Assemble

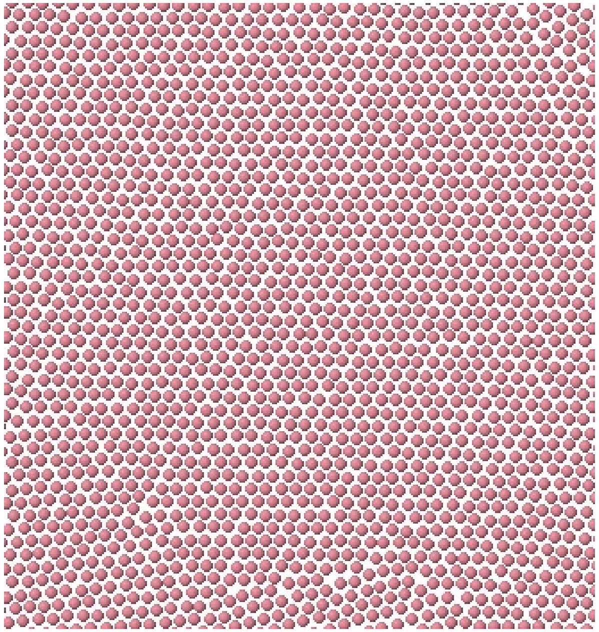
- Direct production of the material layer-by-layer. Vapor deposited glasses seem to produce non-conventional ultrastable glasses. [Mark Ediger, 2007]



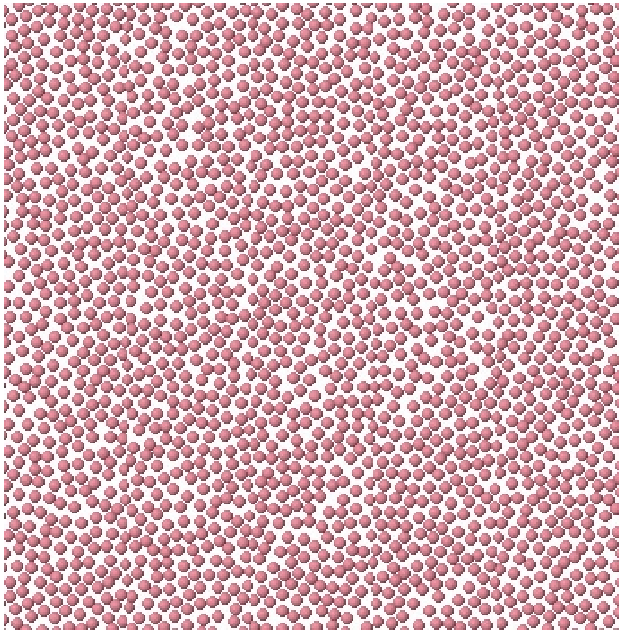
- These new materials behave as million-year old glasses. They make better materials for applications (pharmaceuticals, electronics).

Complex disordered systems

- Perfection is unique, but there are so many ways to be imperfect...



Crystal

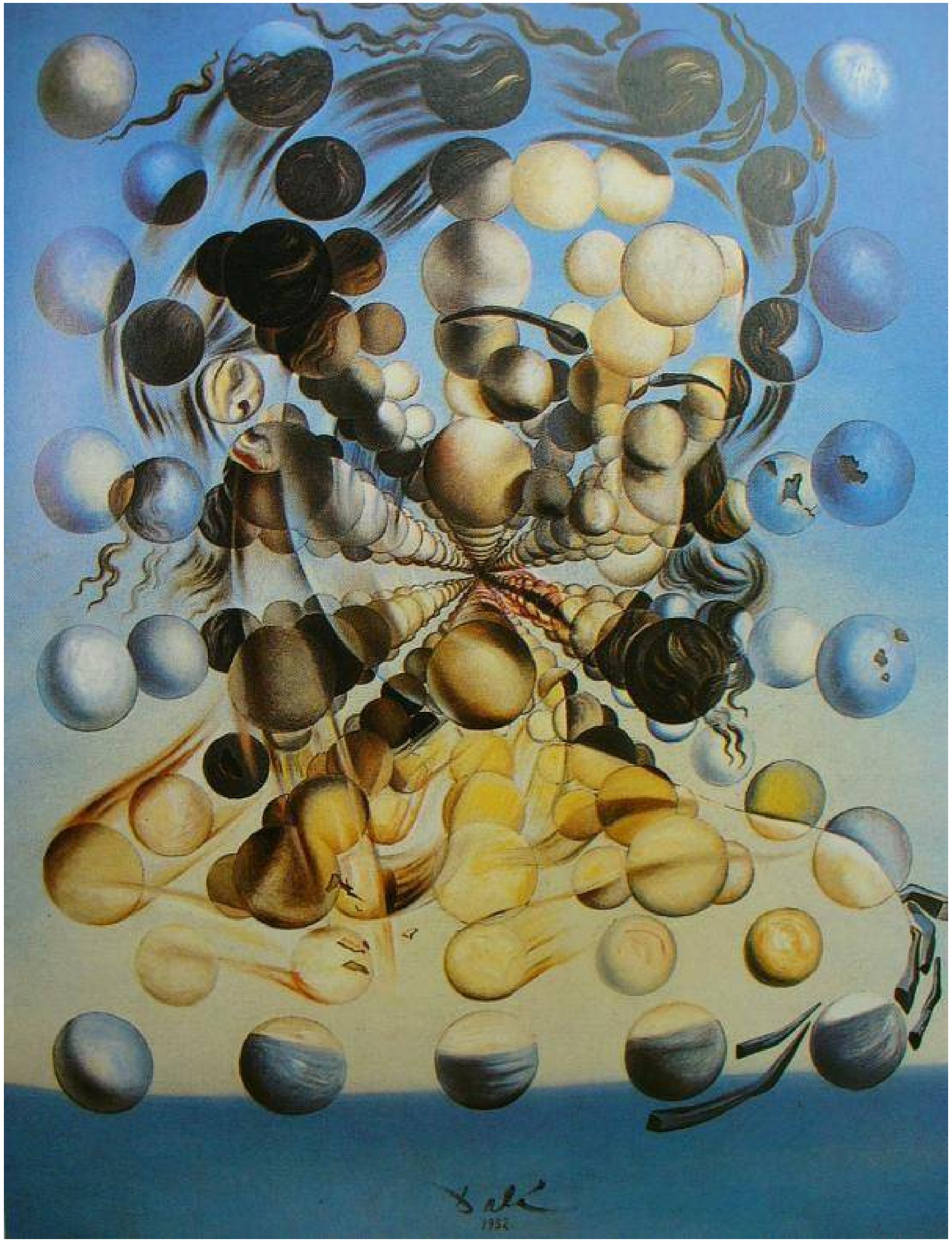


Glass

"*Have no fear of perfection - you'll never reach it.*" – Salvador Dalì.

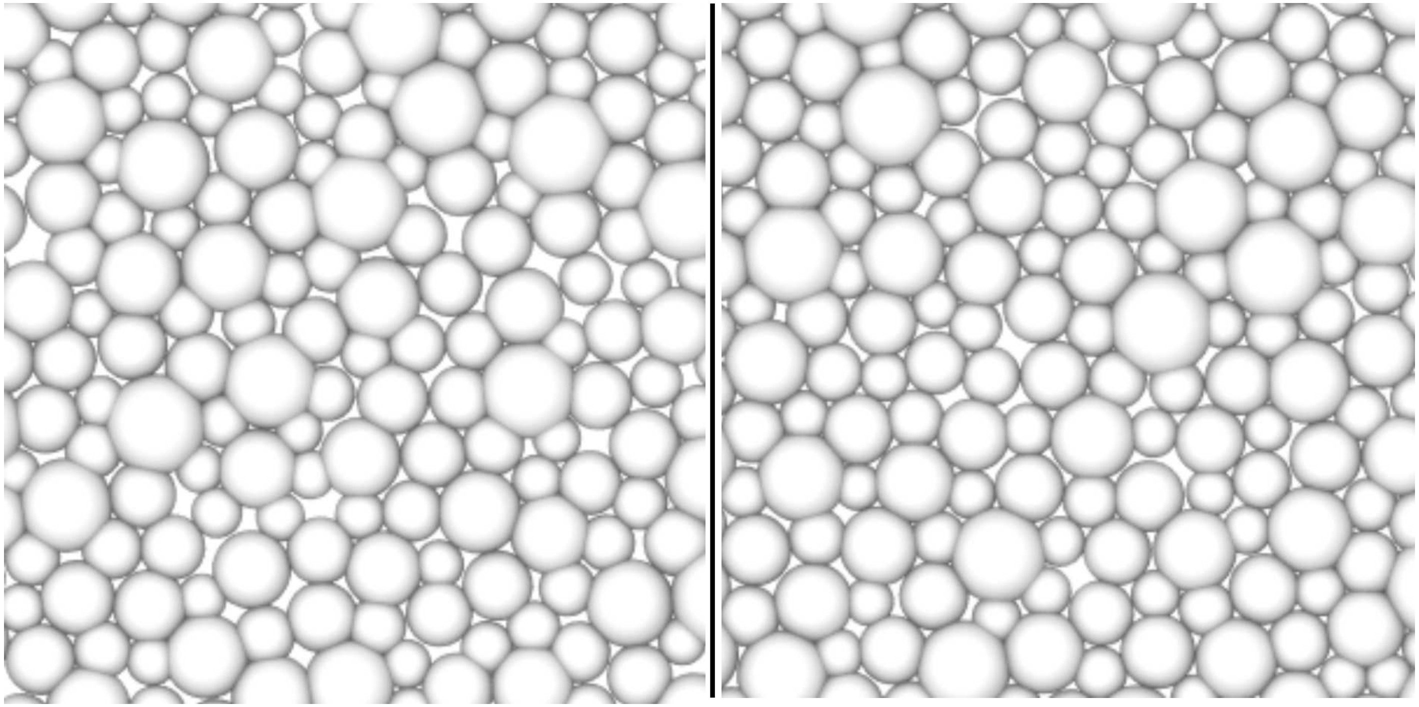
- Glasses can exist in many different forms, in fact: $\log \mathcal{N}_{\text{glass}} \propto N$ (entropy, or 'complexity'...).

[S. Dalì, Harmony of spheres, 1978]



[S. Dalì, Galatea of spheres, 1952]

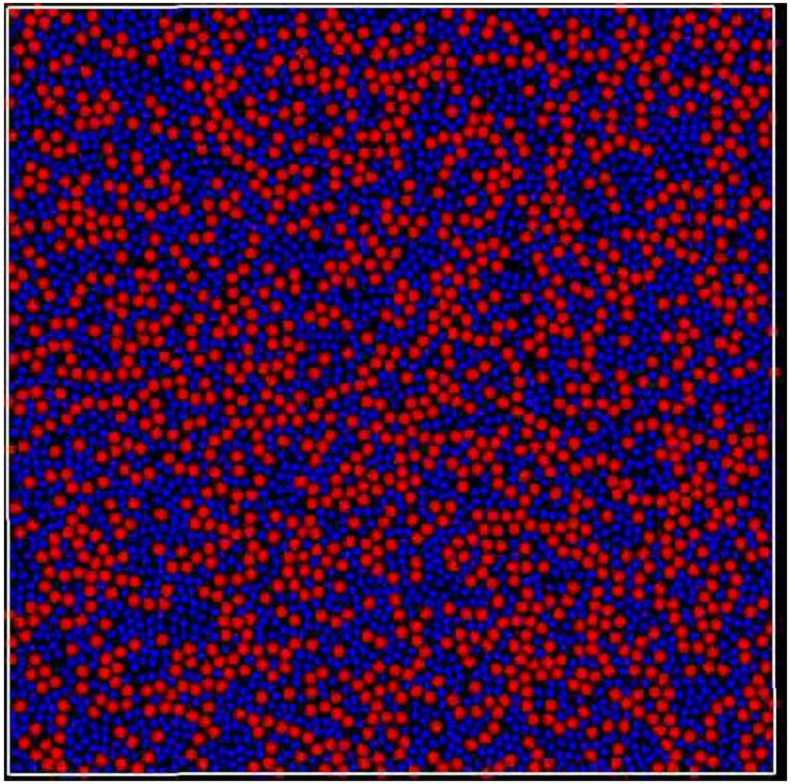
Why is it difficult?



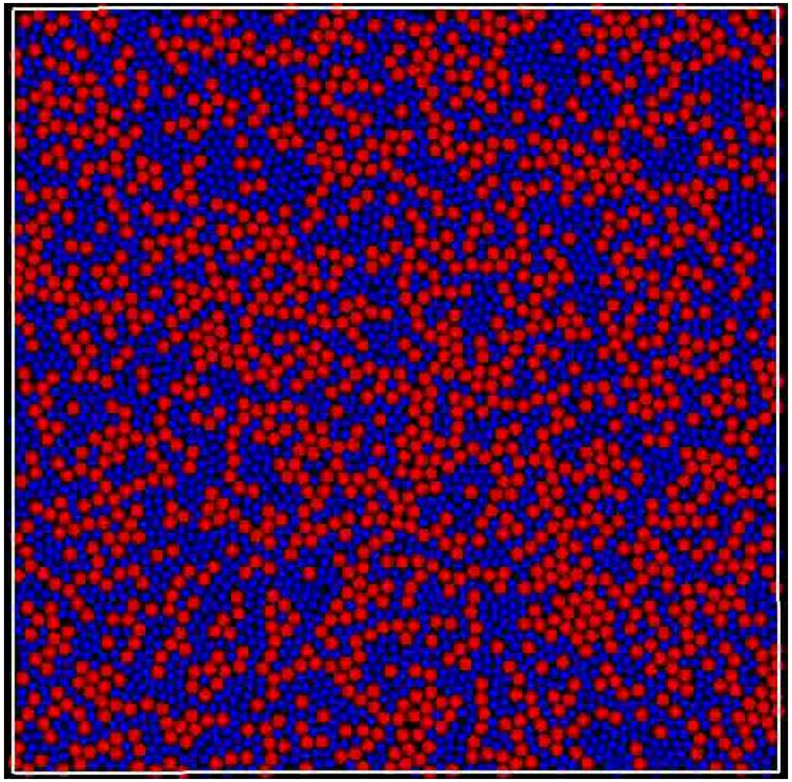
- Liquid configuration on the right relaxes 10^{10} times slower than left one (from 1 sec → 300 years).

- The ‘structure’ of the fluid barely changes across glass transitions–unlike most known phase transitions.

What happens, then?



Fluid

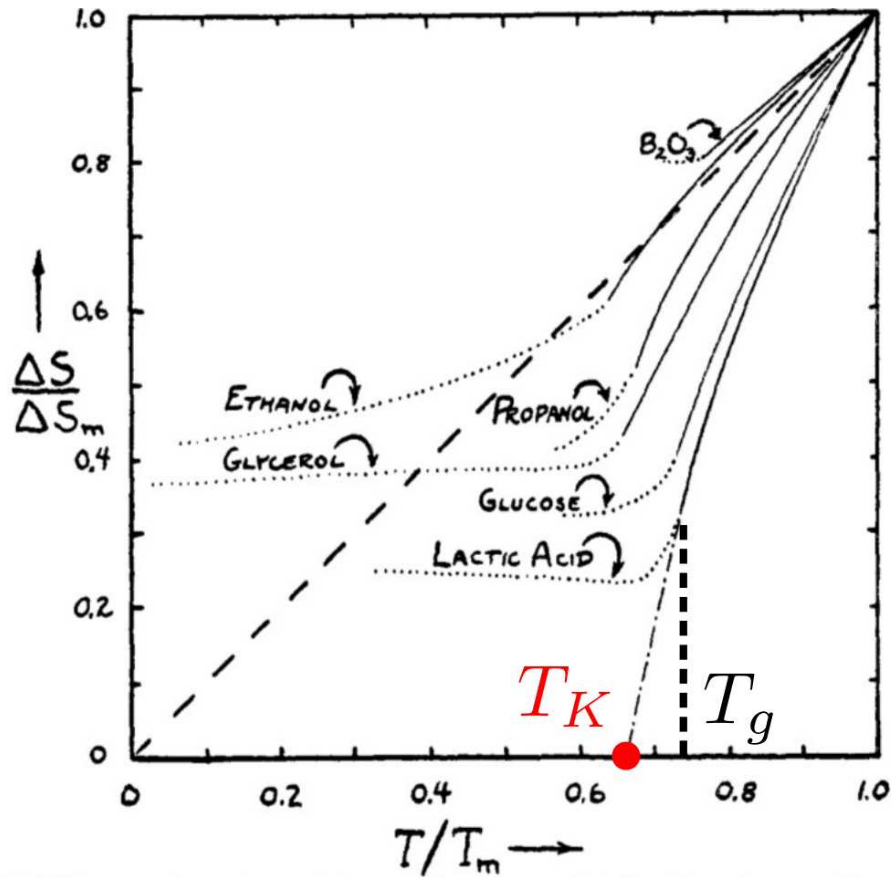


Glass

- Dynamics get arrested as temperature decreases, with no sign of any underlying singularity.

- Two well-known phases of matter are in fact not separated by any phase transition. In fact, they are the same phase.

Configurational entropy



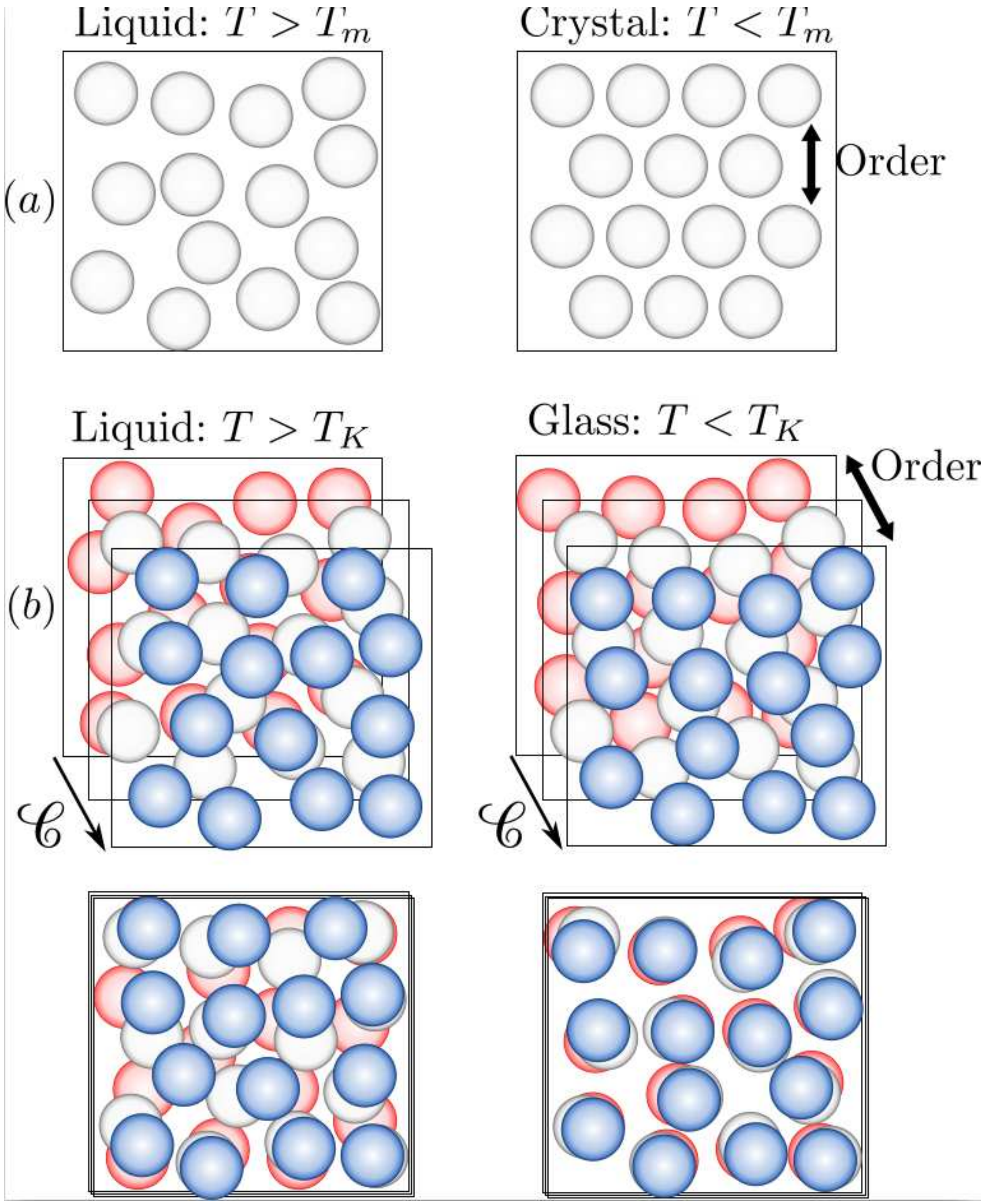
- In 1948, Kauzmann defined a “configurational entropy”, $S_{\rm conf} = S_{\rm liq} - S_{\rm xtal}$, which decreases steeply.

- Extrapolation to lower T suggests an ‘entropy crisis’, or ‘paradox’.

- Suggests a possible thermodynamic phase transition at some $T_K > 0$.

- The observed phenomenon at T_g might be due to a real phase transition which cannot be studied in equilibrium conditions.

Why entropy?



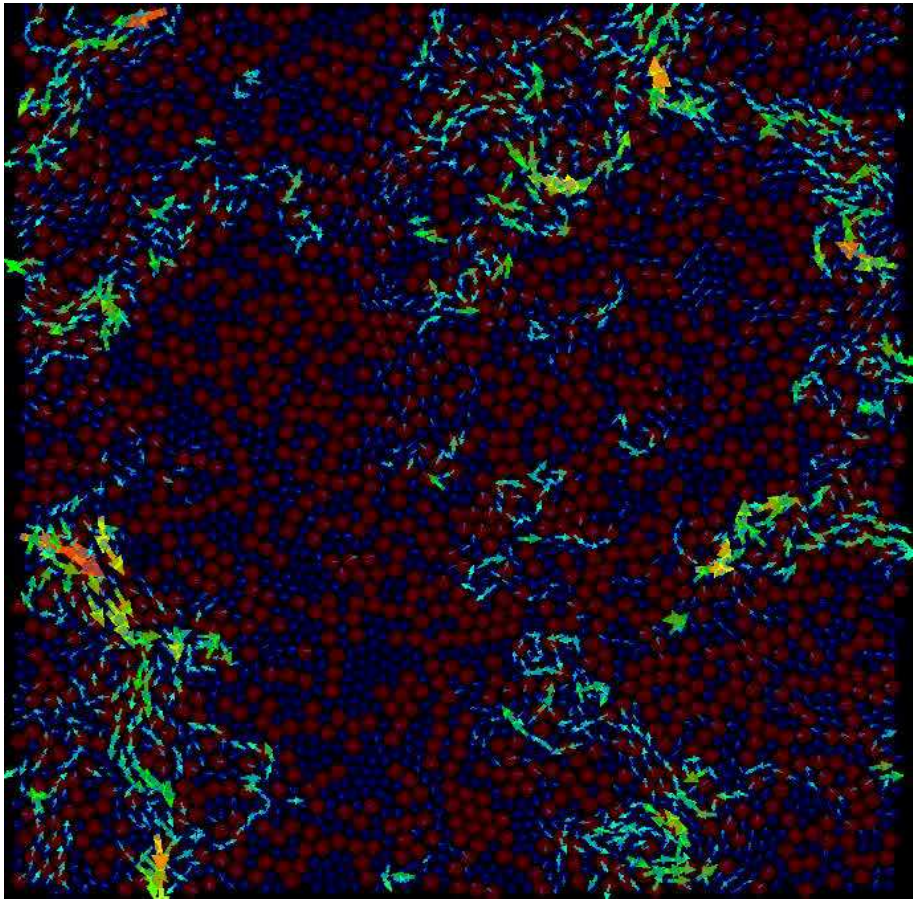
- Structure of single configurations is not the relevant quantity.

- Wrong question: How do packings look like? (They all look disordered!)

- Better question: How many different packings are there?

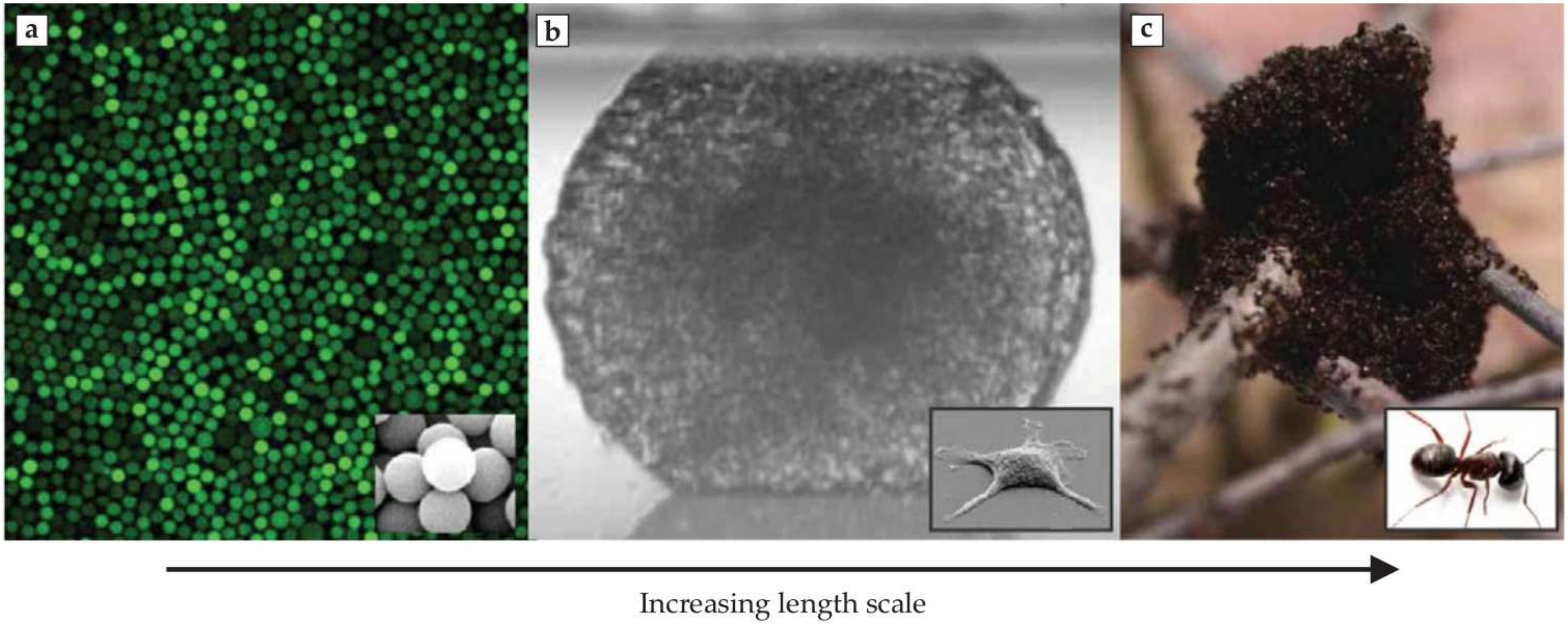
- Complex systems can exist in a large number of states: this is what makes them interesting/difficult: new methods needed.

Dynamics?



- Conventional statistical mechanics does not care about dynamics: but dynamics is slow, complex and a relevant part of the physics in disordered materials: new methods needed.

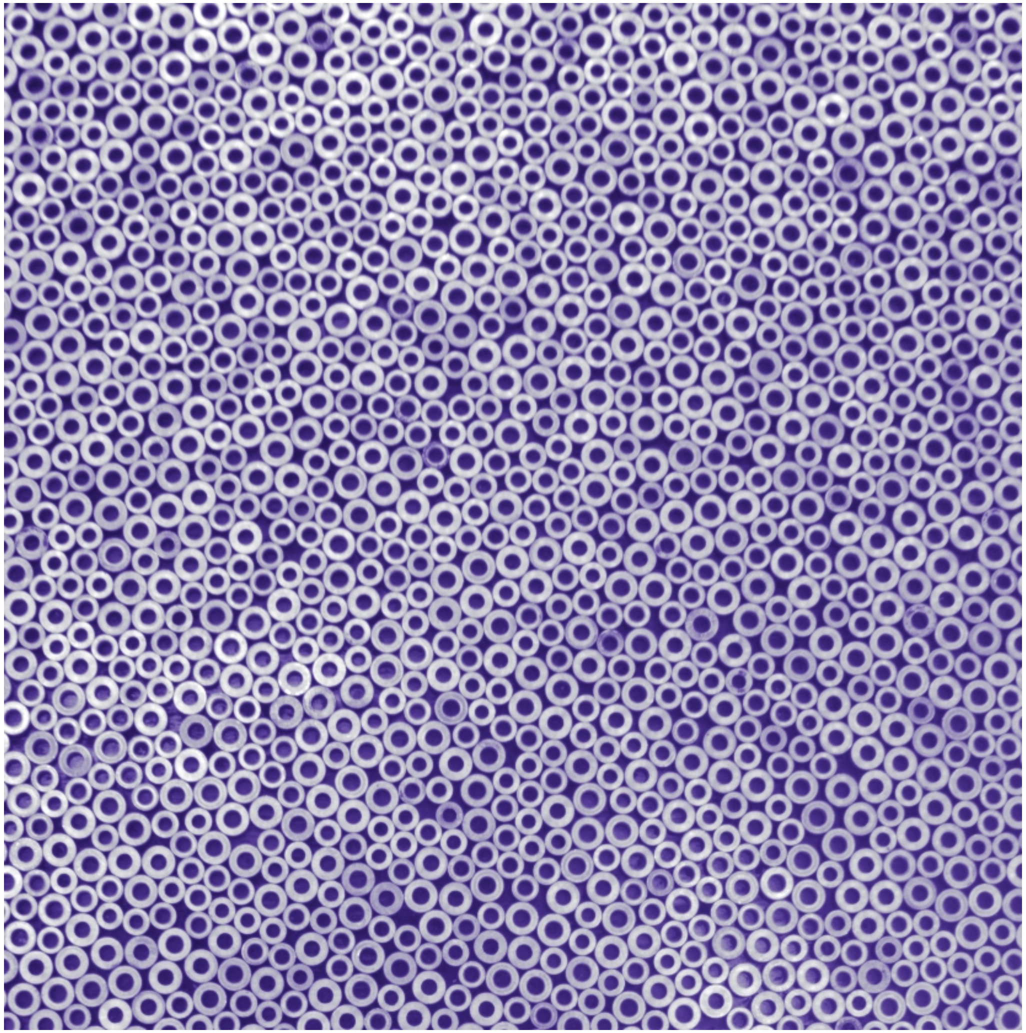
More complex glasses



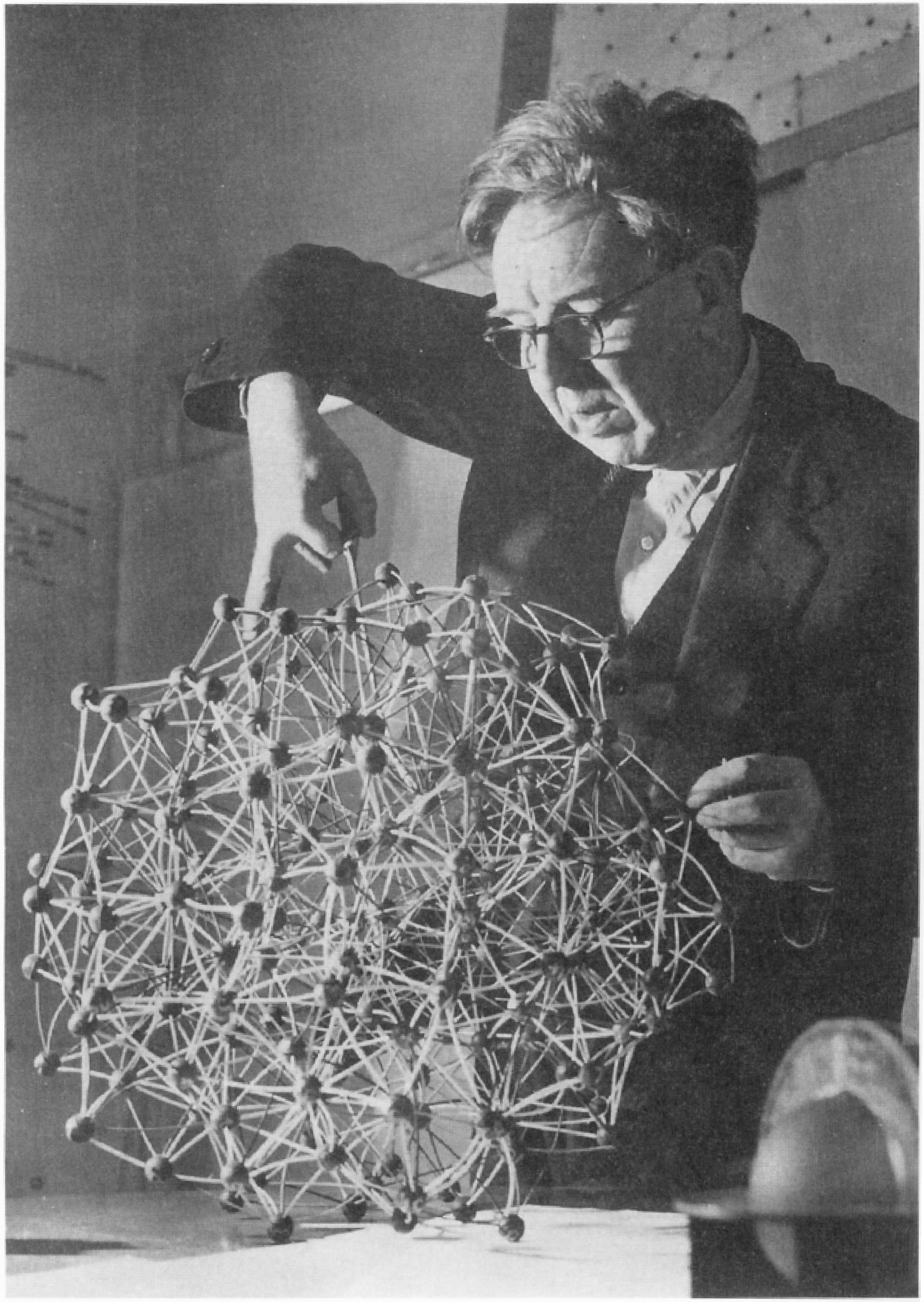
- Fundamental problem for statistical mechanics of disordered materials, condensed matter and chemical physics, with many applications anywhere from molecular liquids, colloids, to grains and biophysical systems.

- Glassy transitions also relevant for computer science and statistical inference: constrained optimisation problems are glassy problems.

Amorphous macroscopic packings



[Courtesy rue Mouffetard / O. Dauchot]



27. Sage constructs his first ball-and-spoke model of liquid structure, confident that he will be interrupted every few minutes so that the model would be disordered

J. D. Bernal

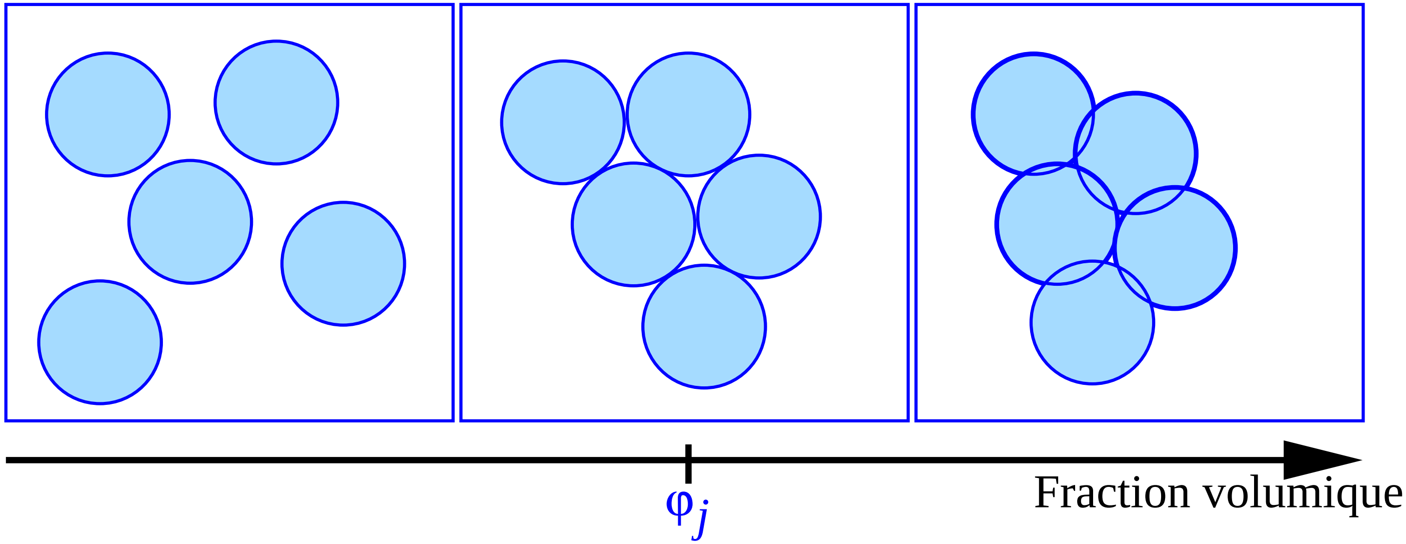
"*This theory treats liquids as homogeneous, coherent and irregular assemblages of molecules containing no crystalline regions or holes.*"

- Theory of liquids as a random packing problem.
- Experiments with grains, computer simulation.

[J. D. Bernal, "*A geometrical approach to the structure of liquids*", Nature (1959)]

The 'jamming' transition: 2000's

- Athermal packing of soft repulsive spheres, e.g. $V(r < \sigma) = \epsilon(1 - r/\sigma)^2$.



Low φ: no overlap, fluid *Large φ: overlaps, solid*

- Describes non-Brownian suspensions (below), sandpiles (at), foams and emulsions of large droplets (above).

- A geometric phase transition: how to attack the problem using statistical mechanics? No thermal fluctuations, disorder, many states.

Theoretical challenges

- We want to understand & predict the physical properties of amorphous solids, from glasses to sandpiles, from a microscopic perspective.

- At the theoretical level, it is difficult to treat:

–disorder: materials with impurities;

–here the disorder is 'self-induced' since all particles and interactions are equivalent (no 'defects').

–materials that are not in thermal equilibrium: ergodicity is broken in glasses when dynamics gets arrested.

–dynamical phenomenon of a collective nature.

–complex systems with very many equilibrium states.

–systems where dynamics is not governed by thermal fluctuations (granular matter, tissues, ants: field of active matter), as dynamics is the only theoretical route.

Computer simulations

- Lattice models are unconvincing.

- Classical pair potentials for simple polydisperse fluids, using Molecular Dynamics, Brownian dynamics, or Monte Carlo simulations.

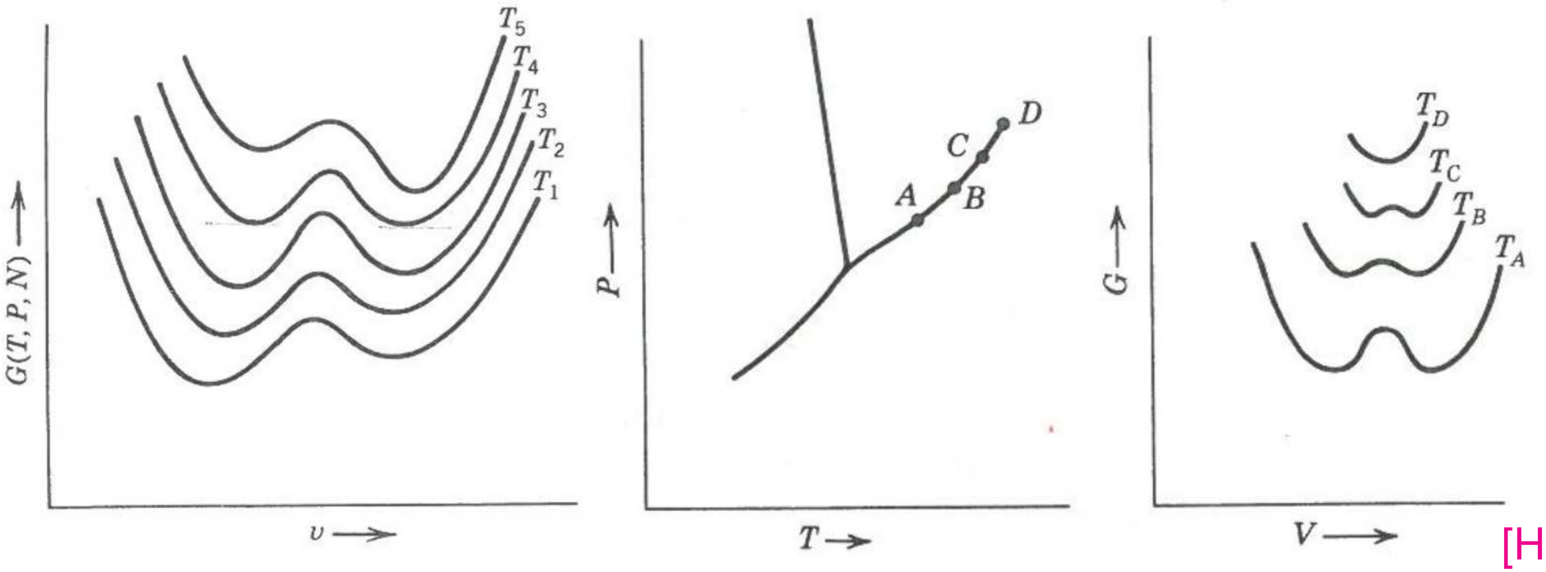
- 'Simplest' glass model: off-lattice hard spherical particles (in reality: complex molecules).

- In 2017, a simple Monte Carlo algorithm to produce ultrastable computer glasses was developed, with a computational speedup larger than 11 orders of magnitude (3000 years $\rightarrow$ 1 sec).

- Unlike experiments, computer simulations can measure almost anything: they are a key tool to connect theory to experiments.

Lessons from simpler problems

- Liquid-gas transition: First-order transition ending at a critical point.



[H. Callen]

- Van der Waals (1873): Mean-field equation of state predicts nature of phase transition, and a simple “landscape” with (only) 2 states.

- Missing in mean-field theory: Nucleation (’30-’60) and critical fluctuations (’75).

- Mean-field theory valid in large enough dimension, $d \geq 4$, non-trivial fluctuations in $d < 4$.

Introducing disorder

- Random field Ising model (Imry-Ma ’75): $H = -J\sum_{ij} S_i S_j - \sum_i h_i S_i$.

- Ferromagnetic phase transition in mean-field limit.

- Lower critical dimension incorrectly predicted by perturbative RG & supersymmetry yielding dimensional reduction (’76-’79).

- Rigorous methods (mathematical physics methods, ’84-’89) establish $d_l = 2$.

- Non-perturbative RG treatment needed for $d < 6$ because of proliferation of metastable states [Tarjus-Tissier, 2004-...]

- Lesson: The simplest disorder variation in the Ising model is enough to make the physics analytically extremely difficult.

Spin glasses

- Edwards-Anderson model ('75): $H = -\sum_{ij} J_{ij} S_i S_j$.

- Mean-field model has a (novel) spin glass phase transition (SK '75).

- Mean-field solution for spin glass phase using replica symmetry breaking [Parisi '79-'83], encoding hierarchical free energy landscape.

- Mean-field solution valid for $d \geq 6$ (using replica field theory, '90's).

- In $d = 3$ the existence of a phase transition is now widely accepted.

- The nature of the low-temperature phase in $d = 3$ is not understood. It is unclear whether (the mathematically complex) mean-field theory is relevant to describe the physics in finite dimensions.

Glasses made of particles

- Off-lattice hard spheres as the simplest glass model.

- Mean-field thermodynamic solution, $d \to \infty$, established in 2013. The theory has an underlying phase transition where the entropy associated to the number of glassy states vanishes. [Kurchan, Parisi, Zamponi '13]

- Universality class of $d = \infty$ hard spheres is the same as some spin glass models, such as p-spin model: $H = -\sum_{i_1 \cdots i_p} J_{i_1 \cdots i_p} S_{i_1} \cdots S_{i_p}$.

- Dynamics of the dense fluid in mean-field limit is being studied analytically as we speak (in this building). [Zamponi, Kurchan]

- The theory [and the lessons learnt from simpler models] show that new physics must emerge in $d < \infty$, so this is only a solid starting point.

- The field is wide open to study analytically the role of finite d fluctuations in model glasses, analytically and numerically. [Franz, Biroli, Tarjus, Parisi]

Some big questions

- Does any of this construction survive in physical dimensions, in particular $d = 2$ and $d = 3$?

- Can one show/disprove that an entropy crisis takes place?

- Does the decrease of entropy drive glass formation?

- Are there important lengthscales that emerge in $d < \infty$?

- Are there key features ignored by mean-field theory?

- This is what we do in the Simons Collaboration, and in the glass community at large. Three final examples...

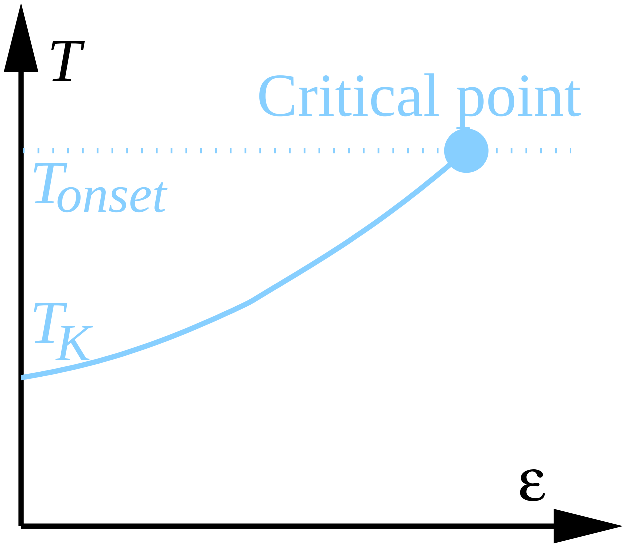
The 'hidden' phase transition

- Mean-field theory: Close to thermodynamic glass transition, the glass phase is metastable with respect to the fluid.

- Just as in van der Waals theory for fluids, this predicts the existence of a line of first-order transitions, ending at second order critical point.

- Glass transition at T_K cannot be analysed directly.

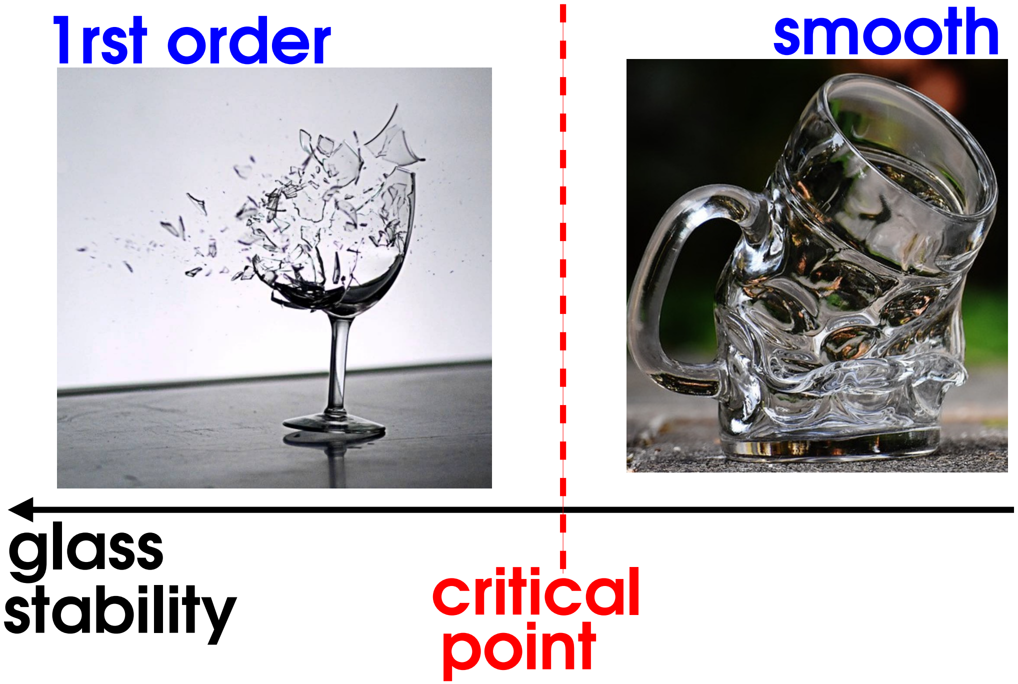
- First order transition and critical end-point are currently being studied numerically and analytically.



- We think we are able to establish the existence of the critical point in $d = 3$ liquids, with same universality class as RFIM.

Mechanical properties of glasses

- New algorithm to prepare glasses of different stability allows us to understand better the mechanical response of amorphous solids.



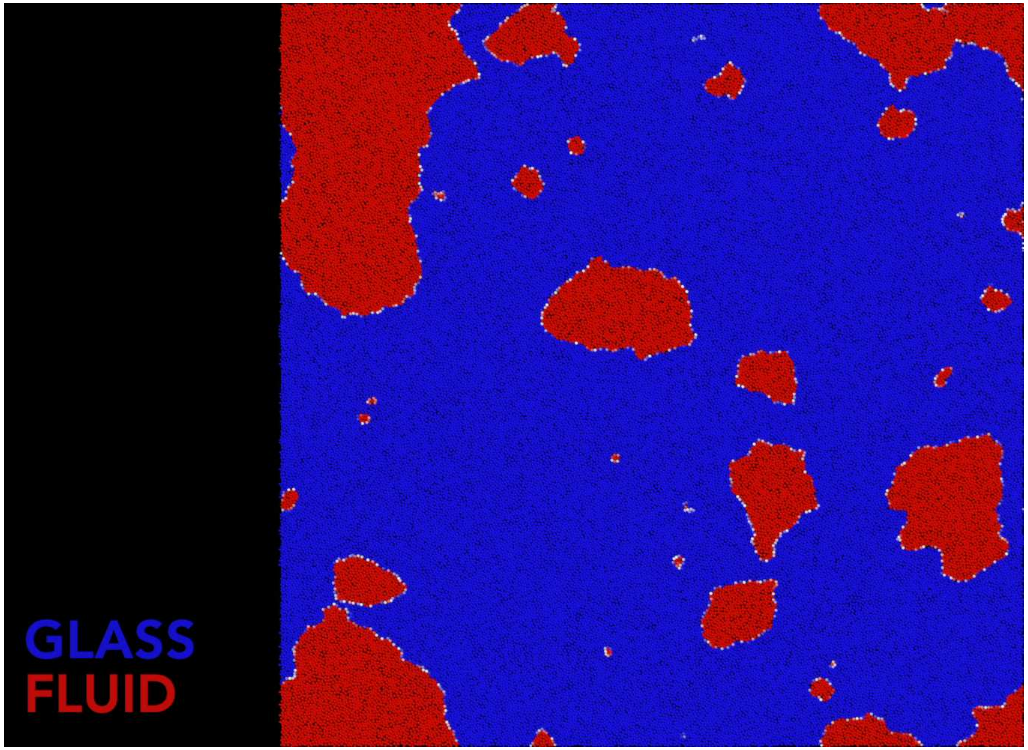
[Ozawa, this building]

- We find that ‘ordinary’ glasses deform homogeneously whereas stable glasses break abruptly. We are using the language of phase transitions to describe the rheology of glasses.

How ultrastable glasses melt

- Mark Ediger studies how his ultrastable glasses melt when heated, but he can’t see directly inside the sample.

- We are starting computer simulations to understand that non-eq. process with atomistic resolution.



- This week with Mark, we started to understand how this happens.

Conclusions

- Glass problem: an open problem in classical physics, with exciting theoretical, conceptual, computational, and practical ramifications.

- This is an exciting moment: mean-field theory is well-understood, finite d fluctuations need to be studied, novel computational methods are available.

[Cambridge University]

- An excellent level of funding within an active world-wide collaboration.

- Come and visit and work with us!