Welcome to 3rd Annual Meeting!
Simons Foundation Collaboration
Cracking the Glass Problem
March 7, 2019
Overview of collaboration

Glassiness is universal:  *What is the glass problem?*

**Scientific goals**

*What would constitute success*

**Accomplishments**

*Science*

*Built an international community;*
  
  *train next generation of scientists*
  
  *disseminate results*

**Future plans**

*Current projects*

*Emerging directions*
Glassiness is universal!
Emerges in different contexts (not just materials)

Glass problem fully embodies:
Disorder, nonlinearity, far-from-equilibrium
(Frontiers for all science)

lava flow
foams
landslide
supercooled liquids
materials above yield stress
granular flows
Glassiness is universal!
Emerges in different contexts (not just materials)

Glass problem fully embodies:
Disorder, nonlinearity, far-from-equilibrium
(Frontiers for all science)

Repercussions

⇒ Mathematical tools for other areas
⇒ Computer science
⇒ Materials science to architecture
⇒ Biology

See talks by Vincenzo Vitelli & Marc Mézard!
Cannot perturb (add defects) $\implies$ physics of glasses

Need fundamental understanding of distinct properties of disordered state of Nature

Reality exists between extremes of order & disorder

What are new laws of disorder?
Understanding of solids based on *crystal order*

Solid is equilibrium phase of matter:
Memory of formation erased

How solids form:
Crystallization (1^{st}-order transition – nucleation)

What is solid’s free-energy landscape:
Single deep minimum

Why solids flow and deform:
Defect mediated

What are solid’s elementary excitations:
Lattice vibrations (Debye law)
Understanding of solids based on \textit{glass disorder} can be non-equilibrium.

Solid is equilibrium phase of matter:
- Memory of formation erased
- Aging, evolution and memory

How solids form:
- Crystallization (1\textsuperscript{st}-order transition — nucleation)
- Quenching (jamming), glass transition

What is solid’s free-energy landscape:
- Single deep minimum
- Number of minima: $\sim e^{AN}$

Why solids flow and deform:
- Defect mediated
- What is a defect?

What are solid’s elementary excitations:
- Lattice vibrations
- Tunneling two-level systems
  + ...
(Universal) properties of glassy solid

New excitations appear:
  low temperature
    (new set of excitations)
  intermediate temperature
    (boson peak)
  high temperature
    (thermal conductivity)

all different from crystalline behavior

Universal features need universal explanations

See talk by Frances Hellman!
(Universal) slow relaxation in liquid
Above glass “transition” ($T > T_g$)

Dramatic increase of relaxation time (divergence?):

Response:

Universal features need universal explanations
“Landscapes”: from string theory to biology

Waddington’s epigenetic landscape
Quantifying single-cell potency as balls rolling downhill: Shi

String theory landscape
Andrei Linde

Fitness landscape
Optimization of genetic code to be robust against swap of codons: Novozhilov

Disorder everywhere: computer science, biology, geophysics/ecology

Explore rough energy landscapes in glasses

Explore basin minima – linear excitations (normal modes)
Traverse barriers with temperature or forcing (rheology)
Nature of saddles & ground states:
  relaxation within and between basins
  functionality of different minima

⇒ glasses provide new understanding
Challenges

Glass transition:
- Exponential number of competing minima:
  - standard tools of statistical mechanics no longer apply
- Free-energy landscape is rough
- Statics and dynamics *inextricably* linked
  - far-from-equilibrium relaxation

Glassy phase of matter:
- Many ground states
  - how properties related?
  - what is universal?
- How does system move through landscape
  - aging

Tools we are developing now address problems and lead in new directions
Collaboration goals

Unified theory of glassy matter
  including relaxation dynamics approaching glass transition

3-pronged strategy

Bridge dimensions: \( d = \infty \rightarrow d = 3 \) using field theory, simulations
Decrease temperature from equilibrium liquid: \( \Rightarrow \) dynamics
Add temperature to jamming: \( \Rightarrow \) excitations & dynamics
Our team

- Biroli
- Kurchan
- Berthier
- Reichman
- Charbonneau
- Liu
- Corwin
- Manning
- Zamponi
- Nagel
- Franz
- Parisi
- Wyart
Our team

Glass physics (boundaries disappeared)
Selected Accomplishments

Dynamics in $d = \infty$ (mean-field limit)

Swap Algorithm

Gardner transition in finite dimensions

Rheology – traversing landscape

Metamaterials – function emerging out of disordered landscape

Tissue biology

+ …
Dynamic equations of liquids in high dimensions

Random first-order transition:

$p$-spin spin-glass is mean-field model of structural glasses

\[ H = \sum J_{i1,i2,...,ip} s_{i1} s_{i2} \cdots s_{ip} \]

Captures:

- Entropy crisis between liquid and glass
- Mode-coupling dynamics
- Goldstein’s geometrical arguments for dynamics
- Aging, effective temperatures
- Shear-thinning in response to energy input

Historic criticisms:

- Assumes quenched randomness
- No particles present (i.e., degrees of freedom of spins are discreet)
- “Never-correct approximation”
- Neglects activated processes
Exact solution for particles as $d \to \infty$

No assumption of quenched randomness
Shows particles explicitly
IS correct approximation in $d = \infty$

Small parameter from expanding in $1/d$ in limit $d \to \infty$

*Low* $d \implies$ short loops of particles in contact
*High* $d \implies$ size of loops diverges

In $d = \infty$ contacts have topology of tree
no loops: paths never return
Mean-square particle displacement in $d = \infty$

Caging and eventual freezing at critical density

Scenario: similar to Random First-Order Transition (RFOT)
New phase $\implies$ breakup of landscape structure (Gardner phase)
Activation exponentially small in $d = \infty$

(hints how to include such effects)

Relevance to $d = 3$? Some extrapolations appear smooth

Success! Correct theory in $d = \infty$
Swap Monte-Carlo algorithm

Swap Monte-Carlo
Allow exchange of two particles of different sizes
Tune distribution and interaction potentials to accept many moves.

Standard

\[ \varphi = 0.85 \]

As density increases \( \Rightarrow \) liquid sluggish

Swap

BUT

Swap sampling efficiency remains very high
How good is Swap Monte-Carlo algorithm

It is incredibly efficient (> 10 orders of magnitude better)!
Shatters experimental and computational glass ceilings in 2 & 3 dimensions!
Obtain configurational entropy
Surpasses even experiment!

Rarefaction of metastable states compatible with existence of ideal, thermodynamic glass transition

Length scales consistent with experiments from linear response and new non-linear experiments

Kauzmann temperature (i.e., entropy crisis) extrapolation vanishes in $d = 2$
Swap: major new tool

Allowed studies of:
- vapor deposition vs. slow liquid cooling yielding transitions
- low-energy excitations
- jamming transitions of very stable glasses
- investigation of supercooled liquids in low dimension

Success! Major algorithmic advance

See talk by Mark Ediger!
Detailed mean-field \((d = \infty)\) calculations:

Phase transition into new marginally-stable amorphous phase

- Density of states is changed
- Elasticity is changed
- Rheology is changed
- Low-temperature transport is changed

Unifies real-space and mean-field descriptions of jamming and glasses with emergence of collective glassy excitations
Gardner physics in low-dimensions

Exponents same as for jamming in \( d = 2, 3 \)

RG studies

Numerical studies using swap:
- rapid growth of relaxation time, susceptibility, and correlation length
- 3-\( d \) data for hard spheres consistent with Gardner transition
- As particles become softer, transition disappears

Know where and why Gardner transition exists
and in what glassy material it is physically relevant

Success! Correct understanding in low dimensions
Rheology (navigating rough landscape)

**Rheology:** Traverse landscape by shear stress or compression

**Mean field:**

Linear response:

Density of vibrational modes at low $\omega$: $D(\omega) \propto \omega^2$

At increased stress:

1$^{\text{st}}$ order transition to yielding, entire system yields at once

**Success!** Understand mean-field limit

**Next:** extend to low dimension where modes and rearrangements are localized
Rheology: traverse landscape by global shear stress or compression

Can also explore landscape via microscopic alterations – pruning individual bonds

Far-from-equilibrium systems store memories – directed aging

Malleable rough energy landscapes – not possible with order

Successfully opens new directions!

See talk by Andrea Liu!
Confluent (i.e., space-filling) tissue rigidity transition

Experiment:
Rigidity is function of cell shape
Cells dense like solid yet flow as fluid
Biological function needs tunable moduli ratio: G/B

Vertex model: $E_{cell} = k_A (A - A_0)^2 + k_P (P - P_0)^2$
Preferred shape: target perimeter to (area)$^{1/2}$
Like jamming: G/B increases continuously

Structural order parameter: confirmed in lung cells

Successful important application!
Creation of community

2 KITP programs (w/ 3 associated conferences)
  Memory formation in matter
  Rough high-dimensional landscape

2 summer schools:
  Boulder, CO: Frustrated and disordered systems
  Beg Rohu, France: Glasses and jamming (2019)

14 additional workshops:
  Glass and jamming problems (kickoff meeting)
  RG theory of disordered systems
  Advances on glass and jamming transitions
  New results from collaboration (NY annual meeting)
  From disordered systems to black holes
  New results from the collaboration (Royaumont meeting)
  Yielding of amorphous solids
  Beyond mean-field theory: glassy and disordered systems
  Gardner transition
  New results from the collaboration (NY annual meeting)
  High-dimensional dynamics
  Yielding and depinning in disordered systems
  New results from the collaboration (Royaumont meeting)
  Dynamical equations for dense liquids
International affiliates

Gerard Ben Arous
Carolina Brito
Chiara Cammarota
Atsushi Ikeda
Edan Lerner
Kunimasa Miyazaki
Markus Müller
Tommaso Rizzo
Srikanth Sastry
Grzegorz Szamel
Gilles Tarjus
Hajime Yoshino
Students and postdocs

Congratulations to Camille Scalliet
Awarded “For Women and Science Program” of L’Oréal Foundation, UNESCO

Congratulations to Valentina Ros
Winner of EPS Statistical and Nonlinear Physics Early Career Prize
Future

Dynamical mean-field theory
  Activated dynamics: from mean field to real space
Defects, flow, and low-temperature glasses
  How does mean field break down? Localized excitations
  Dynamics: Identify localized events from structure
  Origin of "universal" low-temperature excitations in glasses

Our new tools make these possible!

New interdisciplinary directions
Functional disordered materials
Biological relevance – solidify significance
Memories and learning in matter
  Novel exotic forms of memory

Our new understanding opens these possibilities!
Our journey
Glassy physics universal: extends broadly throughout science

Why so prevalent, why so universal?
Underlying exact mean-field description

How we make contact with $d = 3$?
New tools, algorithms

New directions
Implications apparent in many areas

Now is the time!
Exciting outcomes from fundamental analysis
Many successes! Opens many new directions!
Organization

Director
Nagel

Executive Committee
Biroli
Charbonneau
Liu
Parisi

External Advisory Committee
Cristopher Moore
James Sethna
Wim van Saarloos

Dynamics
Biroli - Liaison

Energy landscape
Charbonneau - Liaison

Real space
Liu - Liaison

Tool transfer:
Applied math; CS
Parisi - Liaison

Workshops
Kurchan; Reichman

Computer Facilities
Berthier; Corwin

Shared Postdoc
Reichman; Wyart

Seeds / affiliates
Manning; Zamponi

Community Outreach
Franz; Manning

Robust organization plan