Cracking the glass problem

Approaches:
Real space; Energy landscape; Dynamics
Glass problem embodies 3 big scientific issues: disorder, nonlinearity, far-from-equilibrium

Ramifications:
- Mathematical tools for other areas
- Materials science
- Networks for structure and dynamics

Implications – biology (e.g., memory, regulation, tissues), computer science (e.g., constraint satisfaction)
...

Cracking glass problem: opens up new view of matter and organization
What is a solid and why is it rigid?

Poles of rigidity

**Crystals**
- complete order
- formed by nucleation
- symmetries & defects
- mediate flow

**Glasses**
- extreme disorder
- fall from equilibrium

Challenge

*Exponential number* of competing minima:
- old tools no longer apply

Structure and dynamics *inextricably* linked:
- at glass transition (freezing)
- in solid (moving between minima through landscape)
Need unified description of amorphous matter

⇒ Loss of ergodicity in liquid: slow relaxation
transformation from liquid to solid
– is it a transition? or a crossover?

⇒ Properties of glassy solid
glassy excitations
glassy response and deformation

Unification: solid as marginally stable state
Loss of ergodicity in liquid: slow relaxation

Above glass “transition” \((T > T_g)\)

Relaxation time increases continuously:

with universal features:

- supercooled liquids
- materials above yield stress
- granular flows…

Universal features need universal explanations
Properties of glassy solid

New excitations appear:
  low temperature  
    (two-levels systems)
  intermediate temperature  
    (boson peak)
  high temperature  
    (thermal conductivity)

all different from crystalline behavior

Aging – glass continues to evolve after creation

Universal features need universal explanations
Glass situated unavoidably close to instability
Linearly stable but small perturbation can push it over barrier into new state with essentially equivalent properties
⇒ elasticity, plastic flow, avalanches

How does such behavior arise?
Appears finely tuned but is robustly present

Why ubiquitous?
Many systems have it – from glasses to satisfiability problems

Can its analysis lead to tools for calculations?

Can be seed for universal explanation
Jamming

Far-from-equilibrium way to create solids:

Instantaneous quench of frictionless spheres to $T = 0$, finite-ranged repulsive potentials

Jamming transition at $T = 0$:

*non-trivial* critical exponents same for all $d \geq 2$ (Why?)

Exponential number of minima – similar statistical properties

Low-frequency vibrations $\neq$ plane waves

At transition no length scale where elasticity emerges

Idealized model: marginal stability, epitome of disorder, essence of rigidity formation without crystallization
“Landscapes” used as metaphor from string theory to biology

⇒ glasses provide new understanding of rugged landscapes

Our landscapes no longer merely a metaphor: make **concrete calculations** for transitions & dynamics
Elizabeth Gardner transition

Gardner transition emerges out of $d = \infty$ solution
Deep within glass phase, landscape becomes fractal

Mathematical foundation for marginal stability

⇒ non-trivial high-frequency processes
⇒ general to many random constraint-satisfaction problems

Qualitatively new way to understand landscapes and behavior far from equilibrium
Selected highlights from past year
Multi-pronged attack on important issues identified in proposal

Algorithm development
(advances in simulation techniques / machine learning)

Analytic results
(Gardner transition in finite dimension / excitations)

Computational results
(test-bed for predictions / new phenomena)

New tools for exploring and understanding landscape

Leads into new research directions
“Swap” Monte Carlo method

Optimized to supercool optimized poly-disperse liquids to temperatures that even experiments cannot reach!

⇒ dynamics of fluid, Gardner transition, glassy rheology, jamming transition, …

Other approaches: vapor deposition to equilibrate generic “ultra-stable” glasses

Algorithms will be made publicly available
Machine learning $\Rightarrow$ structural signature of glassy dynamics: softness, $S$

Probability of rearrangement:  $P_R(S) = e^{\Sigma(S) - \Delta E(S)/T}$

with well-defined energy barrier $\Delta E(S)$

$P_R(S)$ and $\Delta E \Rightarrow$ heterogeneous dynamics

Aging depends only on $T$, $\rho$, $\rho$ and $S$ distribution. (Not history!)

Does $S$ apply at low $T$ obtained from Monte Carlo swaps?
Gardner transition – what persists in finite $d$?

Identified critical point for Gardner transition
Full replica-symmetry-breaking through RG analysis.
Transition brought into dimensions of interest.

Universality in 3D?
Seen in hard spheres,
but in soft potentials transition not sharp;
with localized excitations.

Breakdown of standard elasticity

Average shear moduli exist; non-linear elastic moduli diverge

Gardner transition $\Rightarrow$ basis for understanding landscape
Excitations: determine material’s behavior; window into formation

Mean-field prediction for density of vibrational states:

\[ D(\omega) \sim \begin{cases} 
\omega^{d-1} & \omega << \omega_0 \\
\omega^2 / \omega^* & \omega_0 << \omega << \omega^* \\
\text{constant} & \omega >> \omega^*
\end{cases} \]

\( \omega^2 \) does not match 3D simulations, fold-instability argument, random-matrix theory.

At what dimension, \( d \), does it agree?

Non-linear response in super-cooled liquids
- Non-standard criticality due to correlated clusters
- Signatures of non-standard RG fixed point

Excitations in frictional materials
- Responsible for hysteresis in flow
Manipulation and control: functional matter depends on nature of ground states

Principle of bond-independence of global response
Control global moduli independently
Positive or negative Poisson ratio

New directions:

Biology ⇒ glasses ⇒ biology:
Inspired by allostery in proteins
Control multiple sites in disordered network (with or without surfaces)

New edge modes for weakly-connected materials

Constraint-satisfaction:
how much control can one hope to achieve?
**Future**

**Collaborators**

**Schools & Meetings**
- Inaugural Collaboration Meeting / June 2016
- Renormalization group theory of disordered systems workshop / July 2016
- Recent advances on glass and jamming transitions workshop / January 2017
- Simons Collaboration on Cracking the glass problem Annual Meeting / March 2017
- Boulder School on Frustrated and disordered systems / July 2017

**Training the next generation**
Our journey

Extending reach of simulation techniques into unexplored areas

Translate mathematical tools broadly to other areas

Understanding glassy ground states –
Turn metaphor of rugged energy landscape into science

Implications for materials
Allows manipulation to provide new functionality
Illuminate questions in biology

Exciting and rich set of outcomes from fundamental analysis