Physics and Complexity

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Physics

Dictionary definition:

Branch of science concerned with the nature and properties of matter and energy

But today I want to use it as

a mind-set with valuable methodologies

and to show application

to complex systems in many different arenas

Complexity

- Many body systems

- Cooperative behaviour complex
  - not simply anticipatable from microscopics
    - occurs even with simple individual units and simple interaction rules
  - but with surprising conceptual similarities
    - among superficially different systems

Aim today

Illustrate use of statistical physics methodology
to understand complexity and its ubiquity
via simple models, pictures
and comparisons

Give flavour of concepts

Typical approach

- Essentials?
  - Minimal models
  - Comparisons/checks: e.g. simulation/expt.
  - Analysis: maths & ansätze
- Important consequences?
- Transfers, similarities & differences?

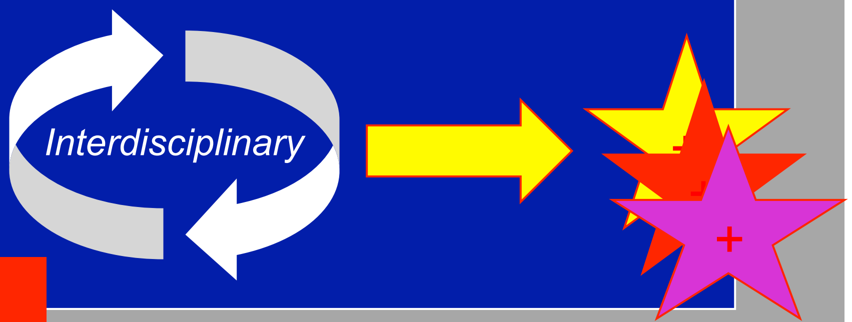
Build → • Conceptualization

Lead to → • Generalization

• Application

Methodology
Symbiosis

- Theoretical physics
  - Minimalist modelling
  - Sophisticated mathematical analysis
  - Conceptualization
- Computer simulation
  - Compare models with (more complicated) real world
  - Experiments for which no real analogue
- Real experiment



But only a broad brush picture today

Key ingredients

Frustration

Conflicts

Disorder

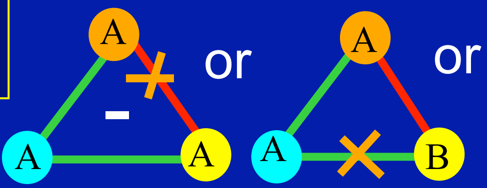
Frozen / self-induced / time-dependent

The Dean's Problem

- Dean to allocate *N* students to two dorms

- Some students like one another; prefer same dorm
- Others dislike one another; prefer different dorms

- Cannot satisfy all → **Frustration**



- Best compromise for whole student body?

The Dean's Problem as combinatorial optimization

Maximise+ a Happiness function*

$$\widetilde{H} = +\sum_{(ij)} J_{ij} S_i S_j$$

Students, *i,j*

$S_i = +/- 1$

Dorm A/B

J: Inter-student friendship: +/-

+ w.r.t. the choice of $\{S_i\}$

* alias "fitness"

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J: Inter-student friendship: +/-

N students: *N* large

Very difficult for general {*J*} with both positive & negative J_{ij} ; 2^N choices; NP-complete

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RANDOM DEAN'S PROBLEM: Characterize by probability distribution *P*(*J*)

Typical statistical physics

- Large N limit
- Disorder chosen randomly and independently from intensive distribution
- Interest in typical behaviour
  - Often self-averaging
  - But not always
    - Complex systems show non-self-averaging in some observables

Dean's model equivalent to Range-free Spin Glass Model (SK)

Dean's problem	Unhappiness	Friendship	Dorm allocation
Spin glass	Hamiltonian	Exchange interactions	Spin orientation

$$H = -\sum_{(ij)} J_{ij} S_i S_j$$

$S_i = \pm 1$; A / B

$$P(\{J\})$$

Note: physicists minimize energies, biologists maximize fitnesses

Equivalent through minus sign!

Spin glasses

- Experiment: e.g. **Au**Fe

$$H = -\sum_{ij} c_i c_j J(R_{ij}) \vec{S}_i . \vec{S}_j; \quad c_i = 0,1; \; J(R) \text{ sign osc.}$$

- Edwards-Anderson: Not exactly soluble

$$H = -\sum_{(ij)} J_{ij} \vec{S}_i . \vec{S}_j; \quad \text{finite-range } P_{sep}(J_{ij})$$

- SK: $H = -\sum_{(ij)} J_{ij} \sigma_i \sigma_j; \; \sigma = \pm 1; \; P_{\infty}(J_{ij})$

Dean's Problem/Spin Glass Model

$$H = -\sum_{(ij)} J_{ij} S_i S_j$$

$S_i = \pm 1;$ ↑ A ↓ B

Statistical physics: equilibrium

$$P_{\{J\}}(\{S\}) \sim \exp(-H_{\{J\}}(\{S\}) / T)$$

T= temperature or Dean's impatience

Paradigmic cartoon for complex many body system

Rugged Landscape

Many metastable states

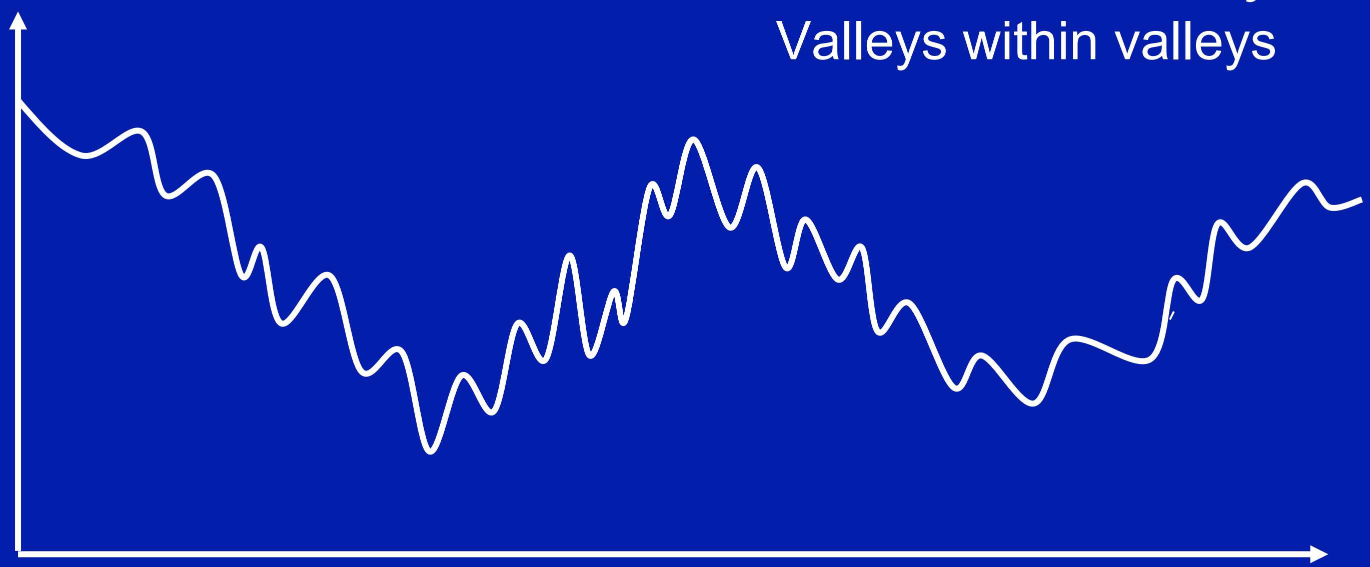
Hierarchy

Valleys within valleys

Cost
to minimise

c.f.
Fitness
to maximise

Simple algorithms
Smooth local motion

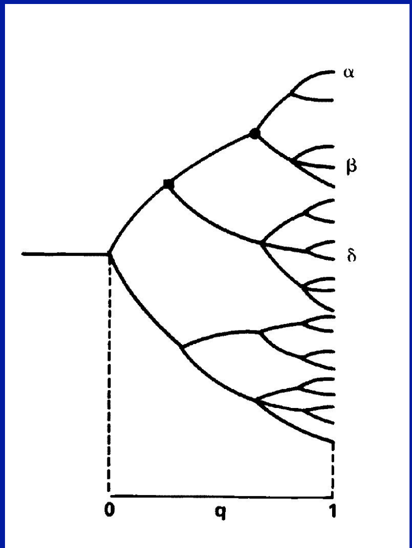


Microscopic coordinates

Hard to minimise/maximize: sticks: glassy

Where does this cartoon come from?

Simulations, analytic calculations, anzätze



e.g. SK: ultrametric
phylogenetic tree

$$q^{\alpha\delta} = q^{\beta\delta} \le q^{\beta\delta}$$

Overlap

$$q^{SS'} = N^{-1}\sum_i \langle\sigma_i\rangle^S \langle\sigma_i\rangle^{S'}$$

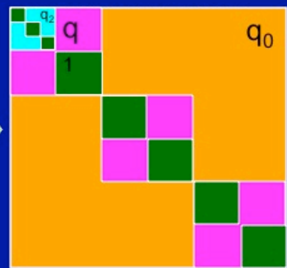
Overlap distribution

$$P(q) = \sum_{SS'} W_S W_{S'} \delta(q - q^{SS'})$$

Conventional system: single δ fn
Complex system: structure

Hierarchy

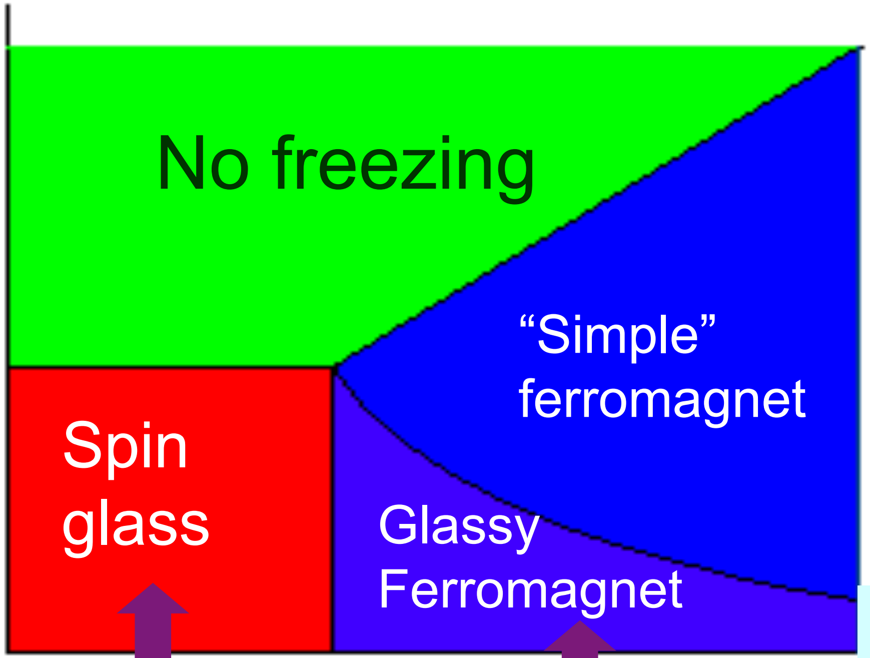
Parisi ansatz



Phase diagrams

Dean's problem/spin glass

Temperature/noise/uncertainty/Dean's impatience



Ergodic/
Easy to equilibrate

Non-ergodic/
Hard to equilibrate

Attractive bias

Many metastable states

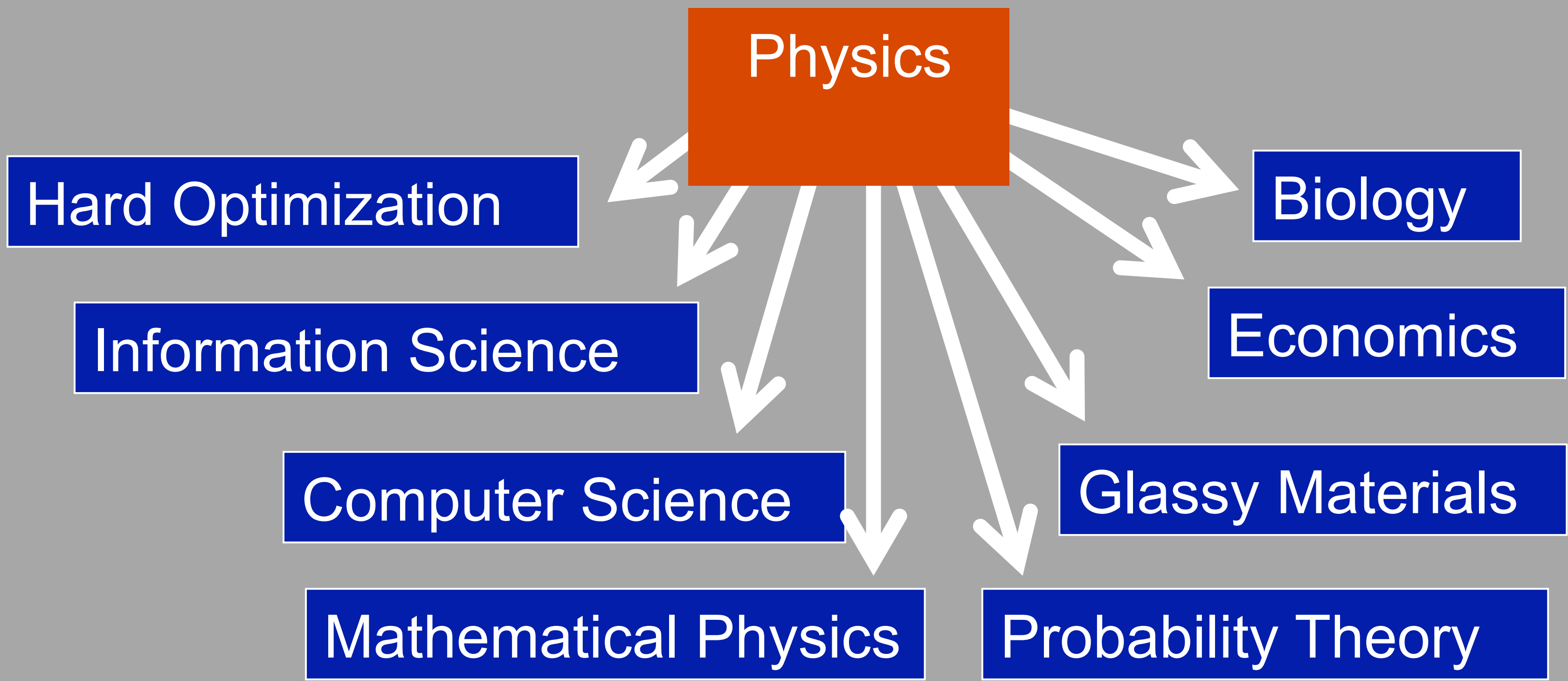
'Rugged' landscape, slow dynamics, non-ergodic

Many further results and subtleties

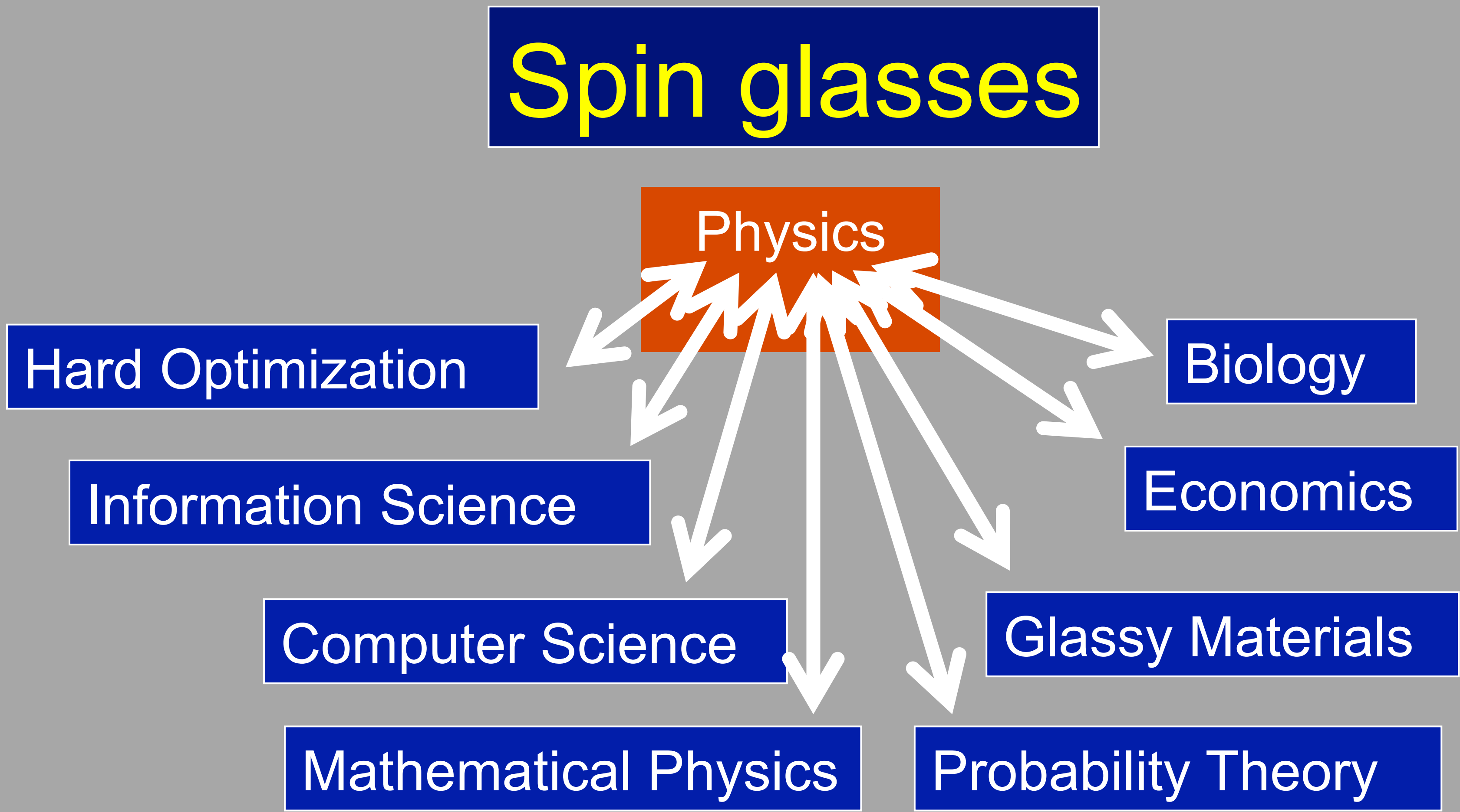
- But probably not time today
- Rather, I shall concentrate on transfers between apparently physically different systems
  - Technical and conceptual

Transfers/extensions

Spin glasses



Two-way


Spin glasses
Physics
Hard Optimization
Information Science
Computer Science
Mathematical Physics
Probability Theory
Glassy Materials
Economics
Biology

General theoretical structure

Control functions

$$F(\{J_{ij\ldots k}\},\{S_{ij..}\},\{T\})$$

Statics: Fixed (variable) Variable

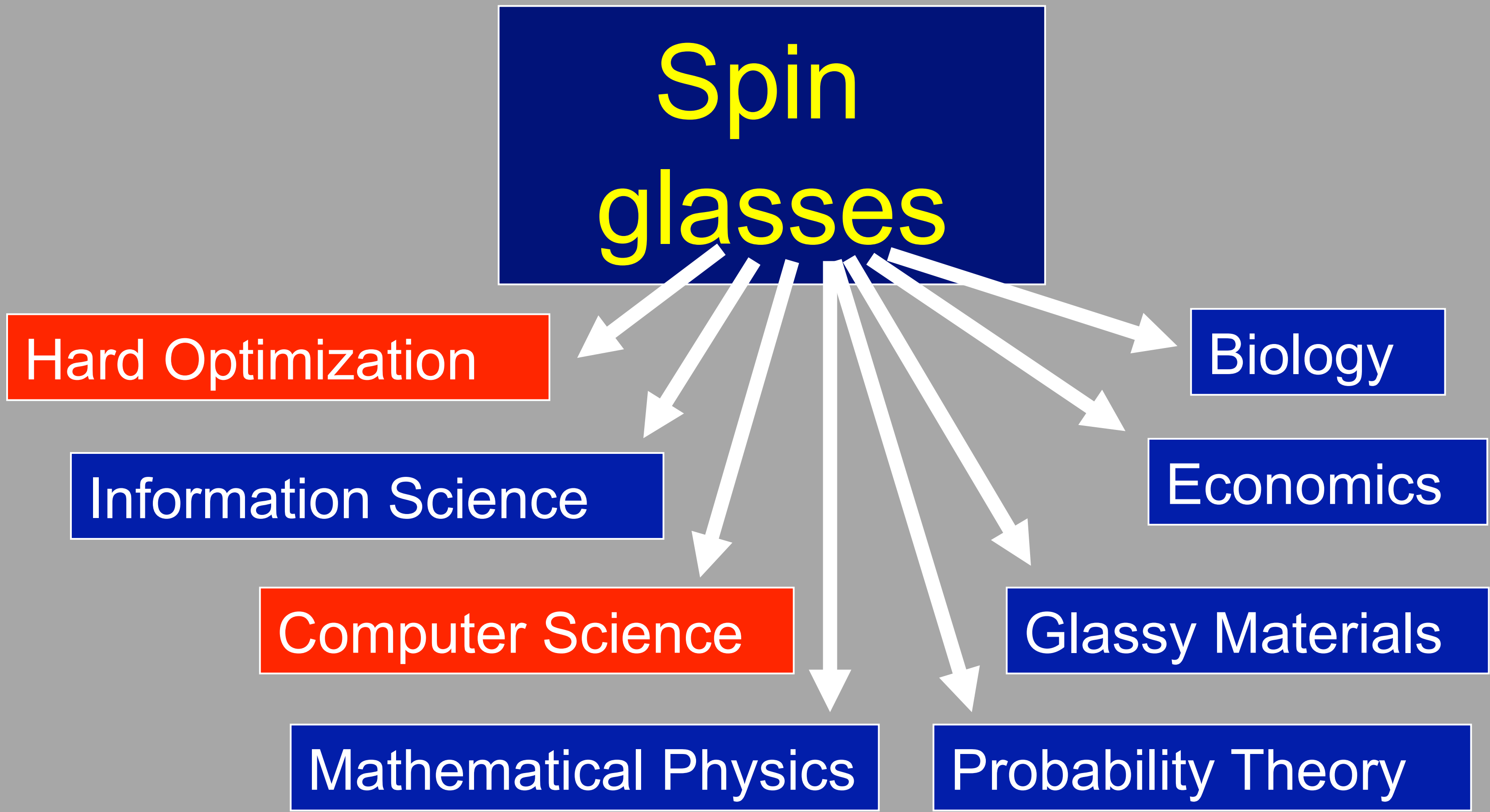
Dynamics: Slow Fast

External influences/
Intensive control parameters

Control functions, but who controls?

- Physics: nature/physical laws
- Biology: nature but not necess. equilibrium
- Hard optimization: we choose algorithms
- Information science: we have choice
- Markets: supervisors, government bodies
- Society: governments can change rules

Examples


Spin glasses
Hard Optimization
Information Science
Computer Science
Mathematical Physics
Probability Theory
Glassy Materials
Economics
Biology

Examples

- Minimizing a cost
  - *e.g.* distribution of tasks
- Satisfiability
  - Simultaneous satisfaction of ‘clauses’
- Error correcting codes
  - Capacity and accuracy

Two issues

- What is achievable in principle?
  - Analogue in stat. physics:
    - thermodynamics (“statics”)/equilibrium
    - e.g. Dean’s best expected happiness
- How to achieve it?
  - Needs algorithms ~ dynamics
    - But glassiness can badly hinder efficacy
    - Equilibrium may not be practically achievable

Two issues

- What is achievable in principle?
  - Analogue in stat. physics:
    - thermodynamics (“statics”)/equilibrium
    - May still be hard to find
- How to achieve it?
  - Needs algorithms ~ dynamics
    - But glassiness can badly hinder efficacy
    - Equilibrium may not be practically achievable

Optimization

1. Dean's problem = SK spin glass

2. Graph equi-partitioning: cost to minimise

$$C = -\sum_{(ij)} J_{ij}\sigma_i\sigma_j;\ \sum_i \sigma_i = 0;\ J_{ij} = 1 \text{ if edge, 0 otherwise}$$

Examples:

Erdos-Renyi graph = Viana-Bray spin glass

Random graph with uniform local valence/connectivity

(generalizable to distribution of nodes of different valence)

Aside

- Usually interesting (for theoretical physicist) to employ as few parameters as possible to specify a system, including disorder

- Sometimes easy analytically and simulationally
- Sometimes not – one or other or neither
  - E.g. random graphs of fixed distribution of vertex connectivities; see Klein-Hennig & Hartmann arXiv: 1107.5734 (simulations ➔ bias)
  - Or amorphous network
    - I know of no simple analytic specification
    - ? Simulationally use Monte-Carlo at finite T with WWW (*c.f.* T1) moves ?

- Some problems difficult to pose analytically as minimization of a cost function – see your 'neighbour' Stefan Mertens + his new book with Moore

K-satisfiability

simultaneous satisfiability

of many 'clauses' of length K

$$(x_{i_1} \text{ or } x_{i_2} \text{ or.. } \overline{x_{i_K}}) \text{ and } (x_{j_1} \text{ or } \overline{x_{j_2}} \text{ or.. } x_{j_K}) \text{ and } \ldots$$

$$x = 1, \quad true$$
$$\bar{x} = 0, \; false$$

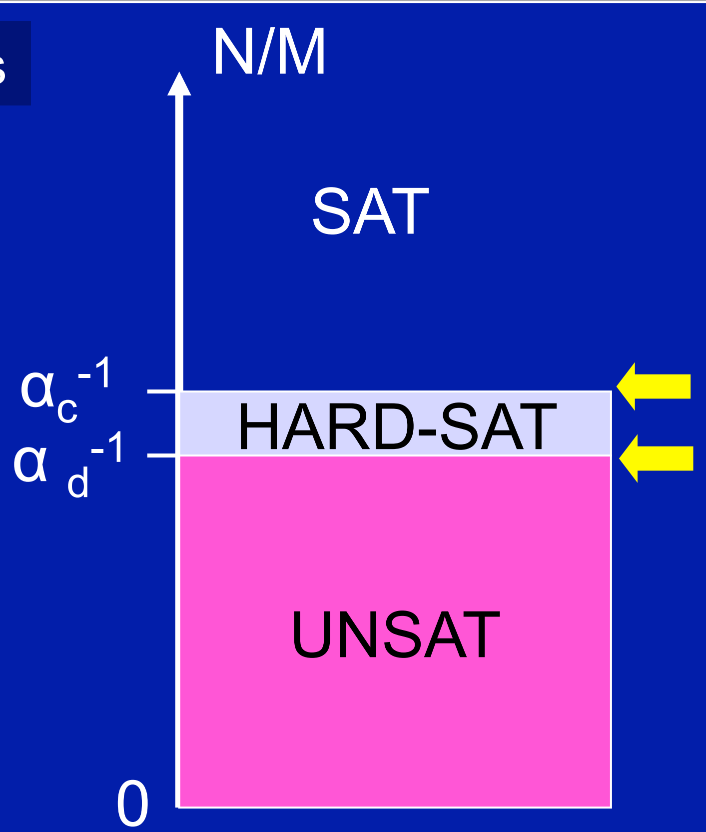
Especially
Random K-SAT

$$\alpha \equiv \frac{M}{N} = \left\{ \frac{\text{\# of clauses}}{\text{\# of variables}} \right\}$$

Phase transition(α): SAT / UNSAT

Random K-SAT

Phase transitions



Simple algorithms stick

Theoretically achievable limit

Physicists recognised this subtlety through comparison with *K-spin glass*

Where the idea came from

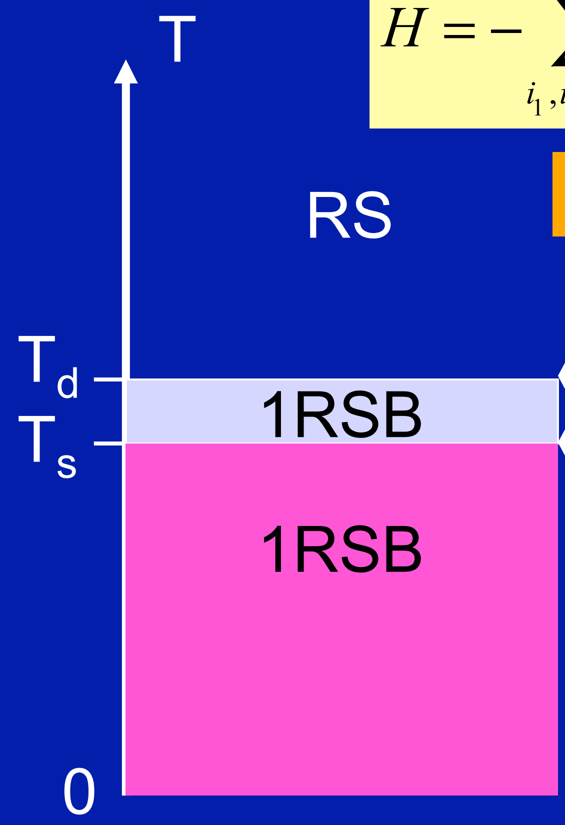
K (>2) -spin glass

Extension of SK s.g.

$$H = -\sum_{i_1, i_2 .. i_K} J_{i_1 i_2 .. i_K} S_{i_1} S_{i_2} .. S_{i_K}$$

Random

2 transitions



Dynamical transition

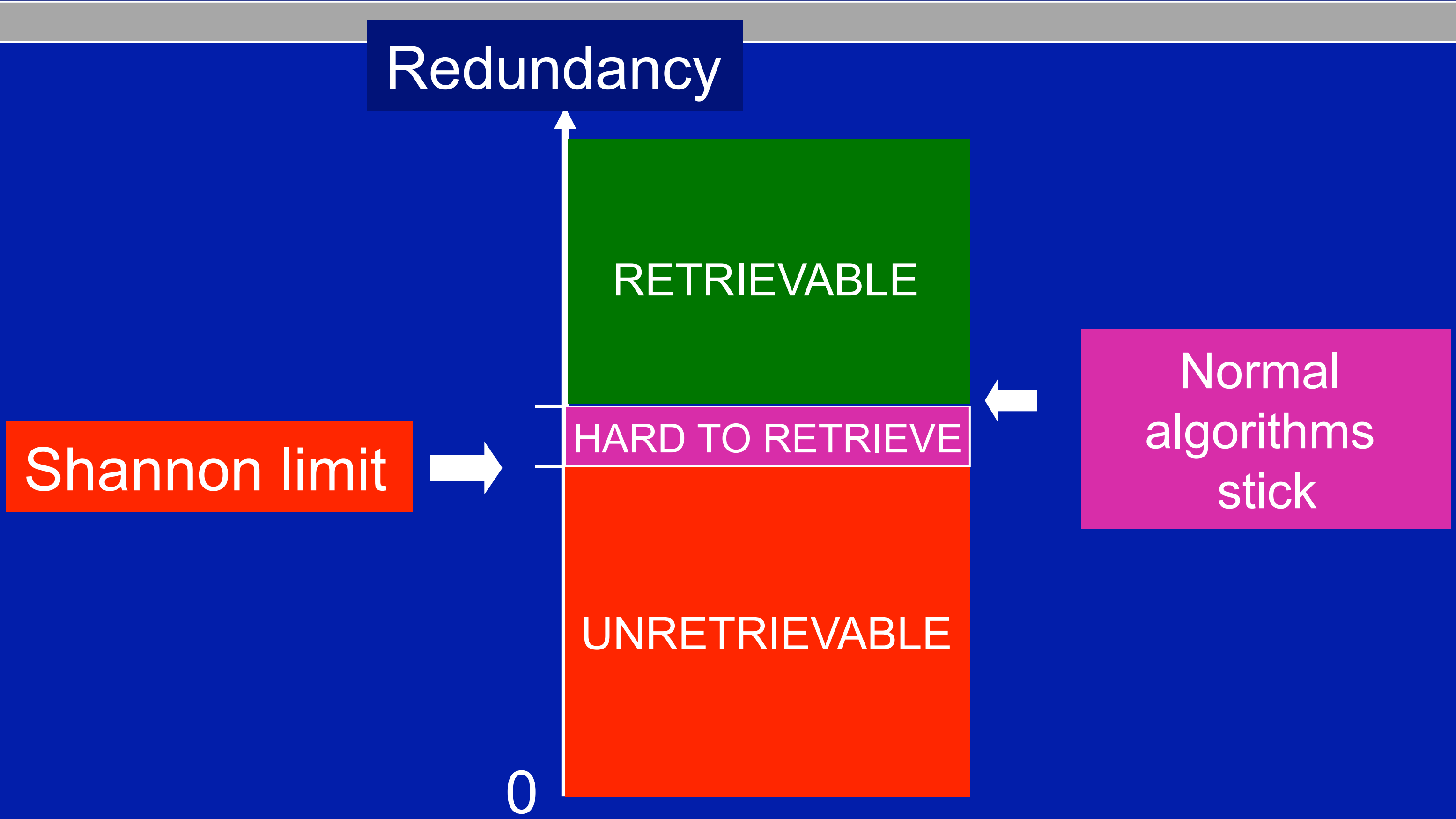
Thermodynamical transition

RSB=Glassy

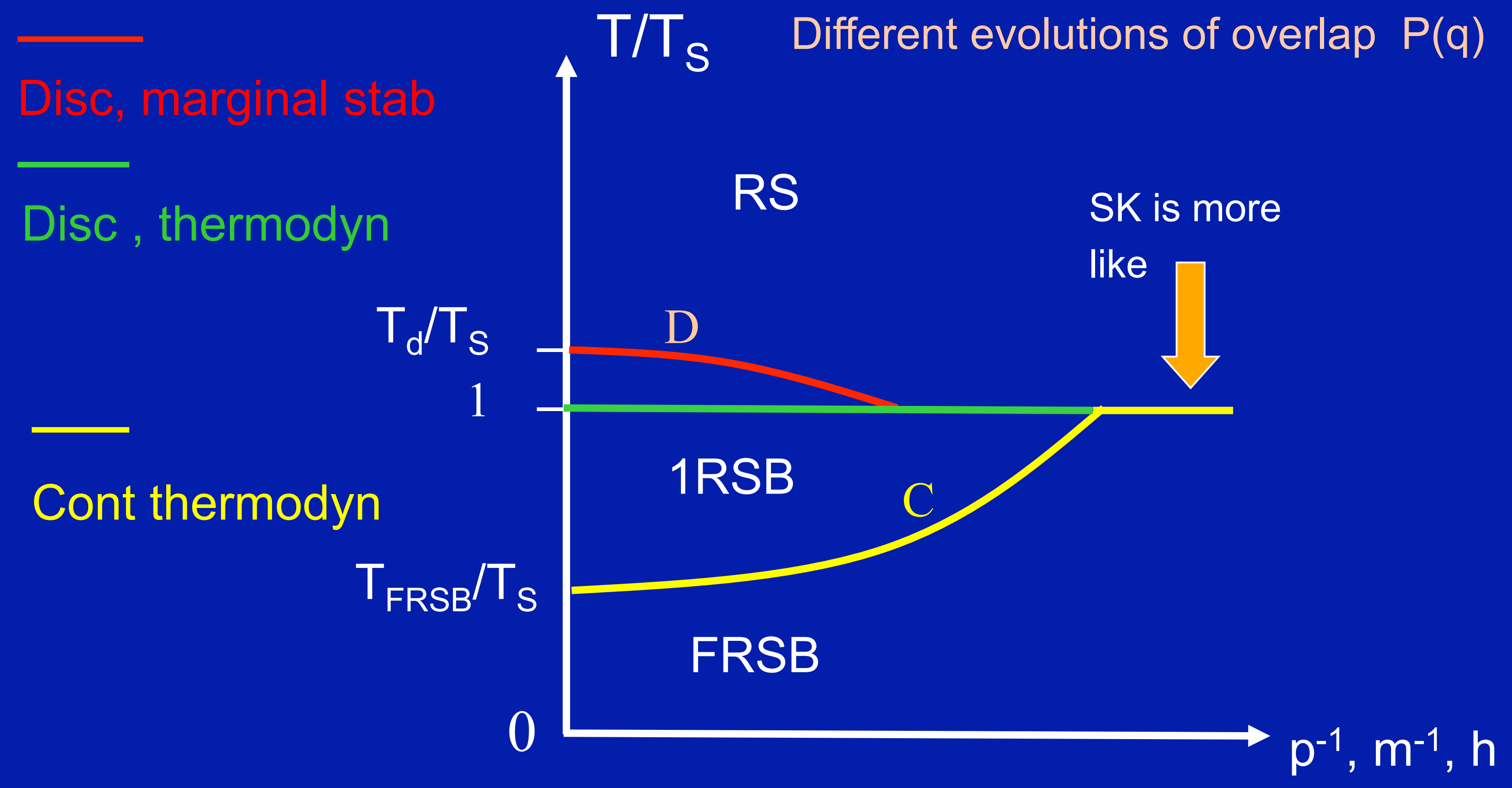
1RSB = all macrostates equally orthogonal

Originally looked at as a purely intellectually interesting extension of SK

Similarly: error-correcting codes



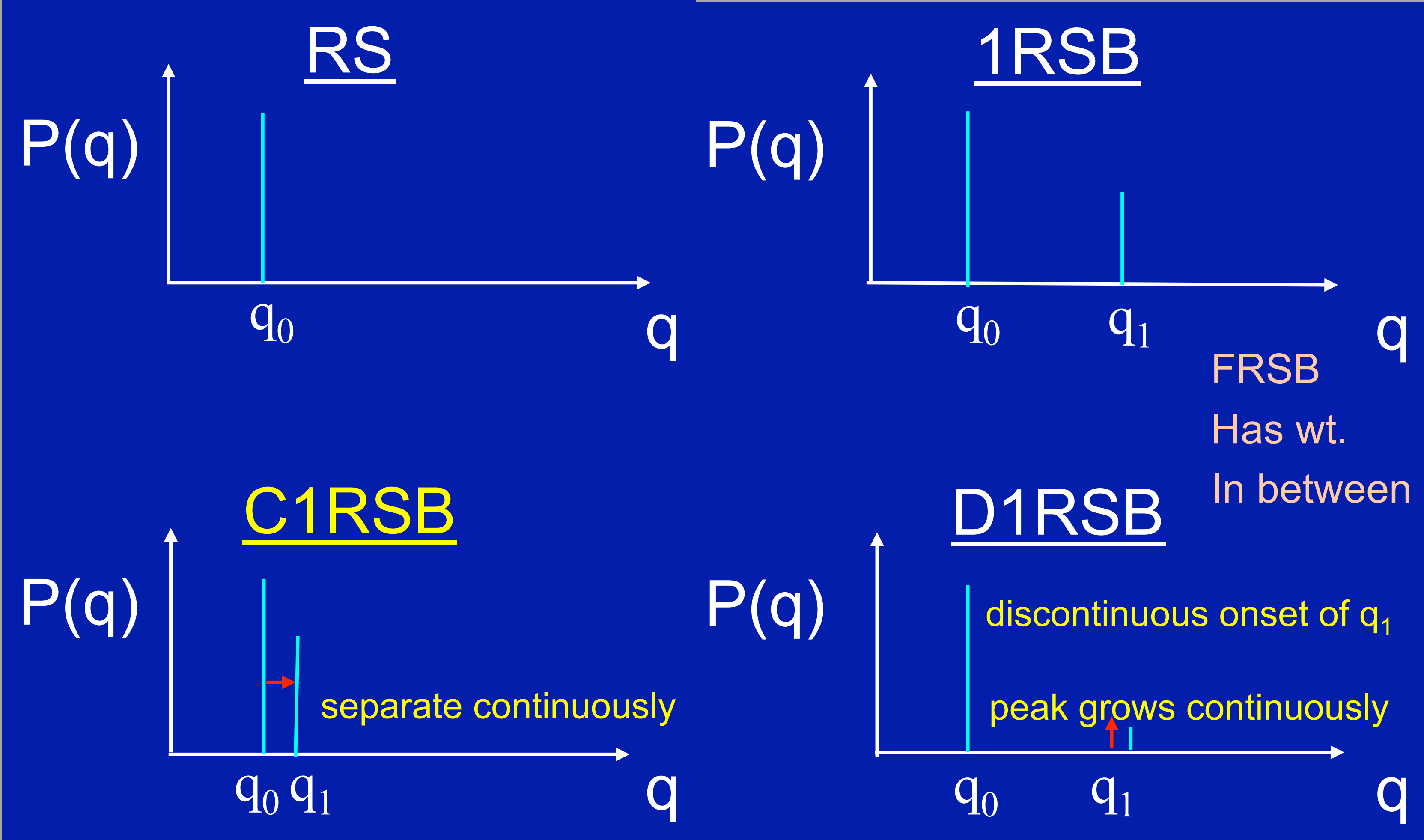
Generic phase transitions



Potts, quadrupolar, p-spin in field

RS, RSB and onset

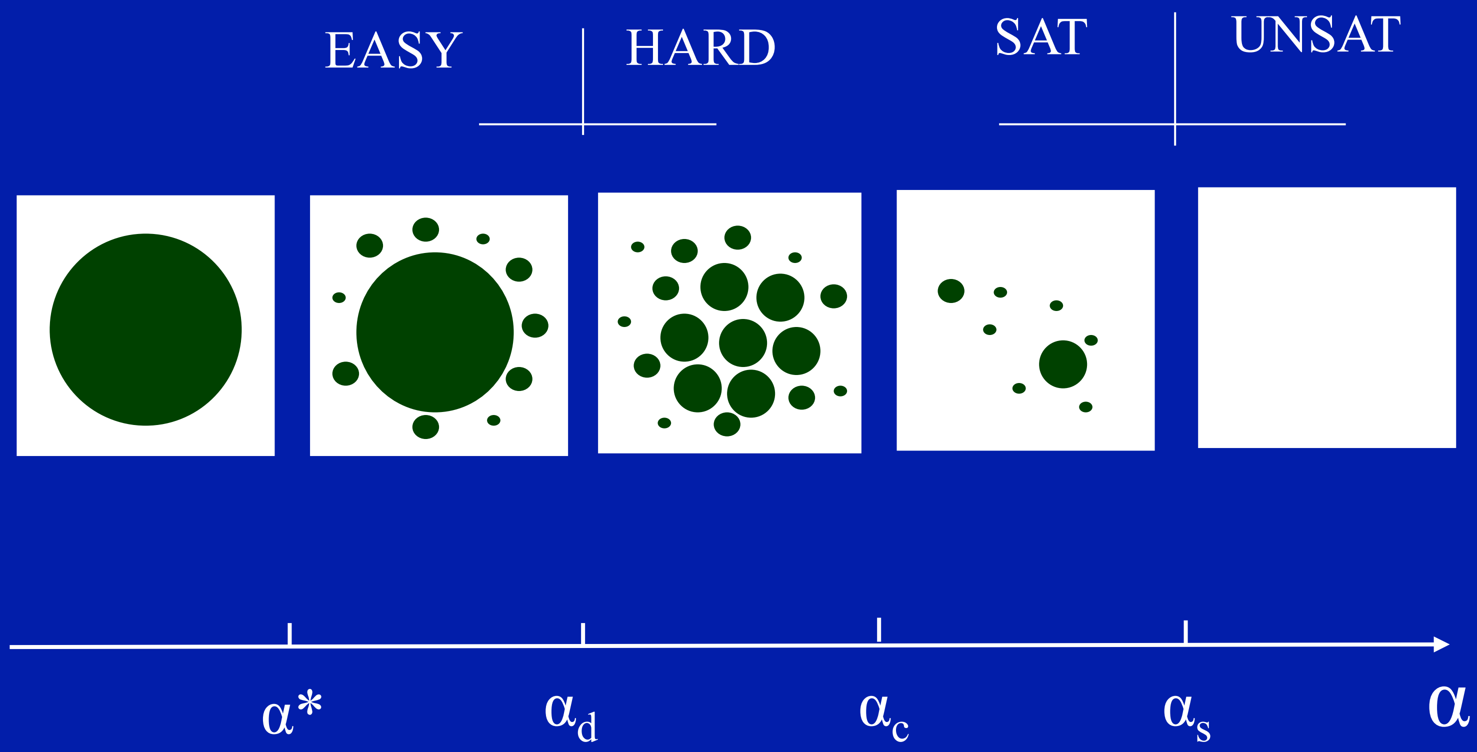
(via overlap distributions)



In fact, more regimes

Clustering: Random K-SAT

Cartoon of satistiability space



Kzakala et. al. (2007)

Understanding brings opportunities

- Normal physics
  - Nature gives dynamics
- Artificial and model systems
  - Ensemble thermal-weighting or optimization
  - We can design dynamics
  - Computational algorithms & Simulational expts.
    - Simulated annealing
    - Parallel tempering
    - Belief/survey propagation
    - Controlled systems
    - New probes

Temperature

- Natural for real physics
- Characterise stochastic noise or uncertainty also in other scenarios; e.g. Dean's impatience

- Often useful for practical optimization by algorithmic dynamics to introduce an artificial 'temperature' T_A :

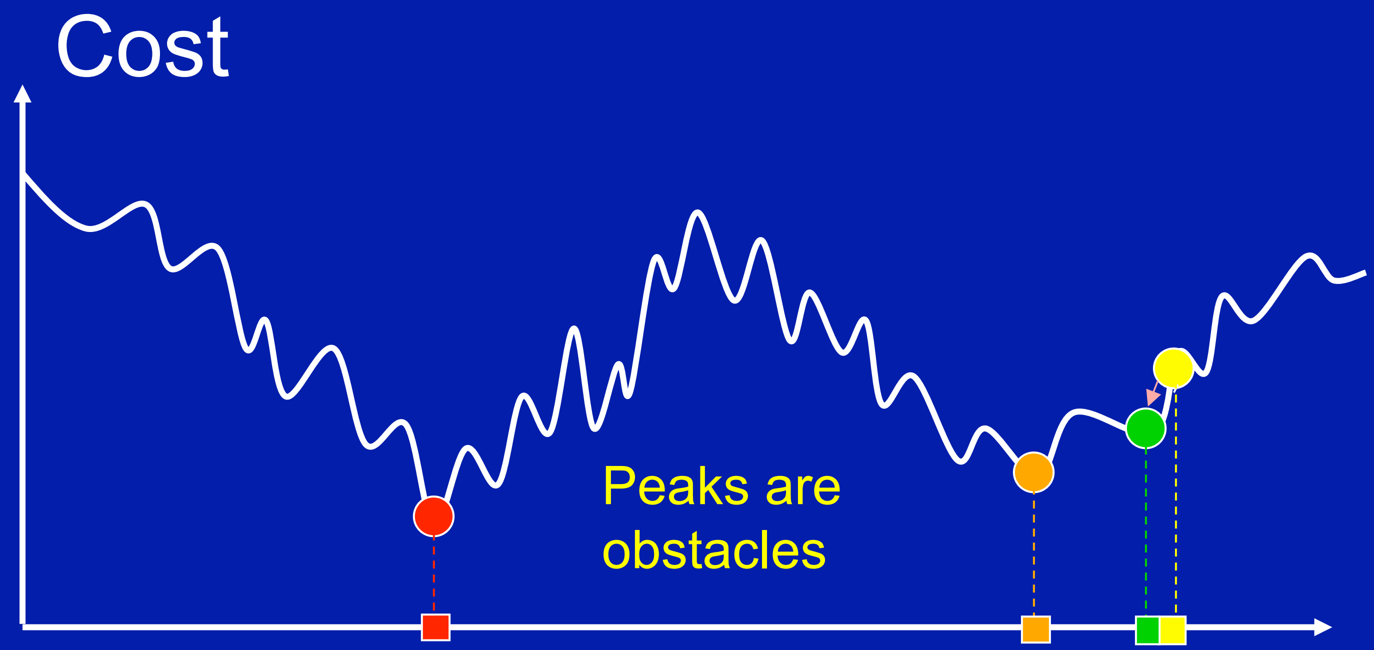
$$P(\boldsymbol{S}) \sim \exp(-H_{\{J\}}(\boldsymbol{S})/T_A)$$

and reduce slowly (simulated annealing).

Or analytic analogue: $H_{\min} = Lim_{T_A \to 0} F(T_A)$

- Other analogues in other problems

Landscape paradigm for hard optimization



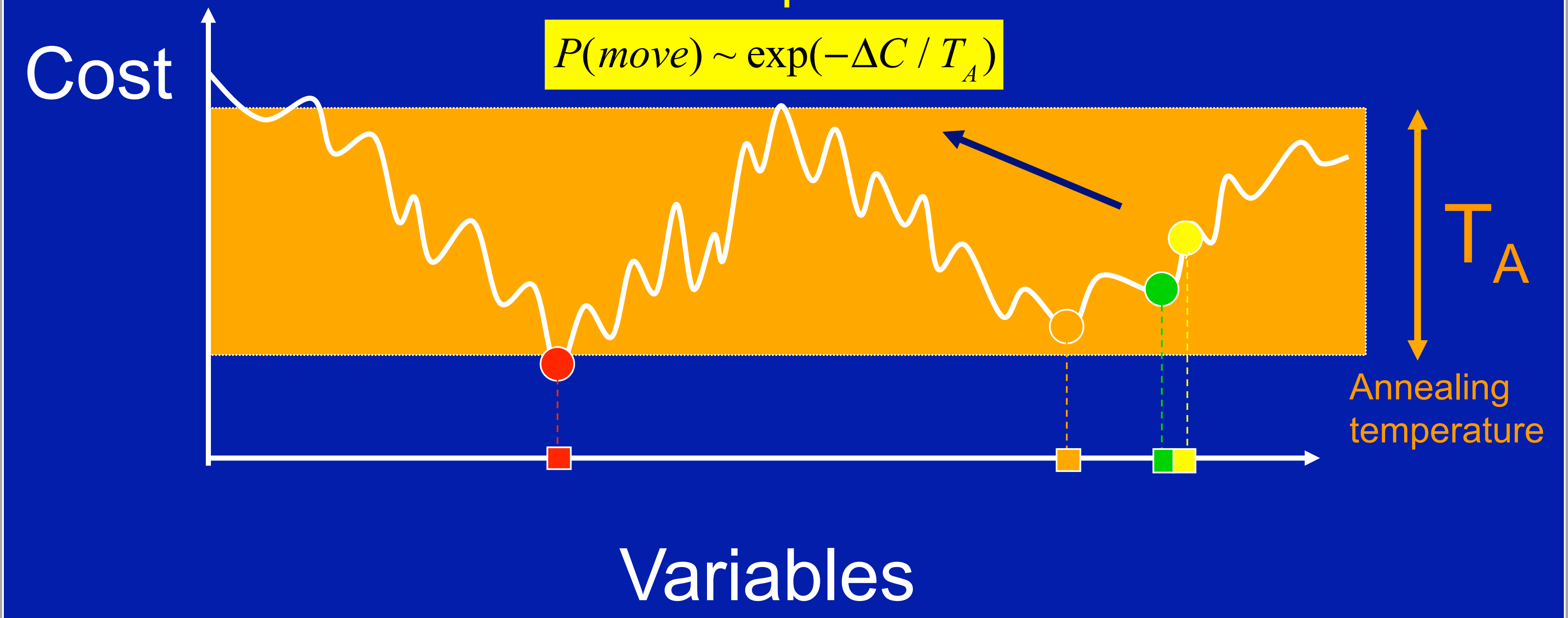
Steepest descent gets stuck

Simulated annealing

Probabilistic hill-climbing

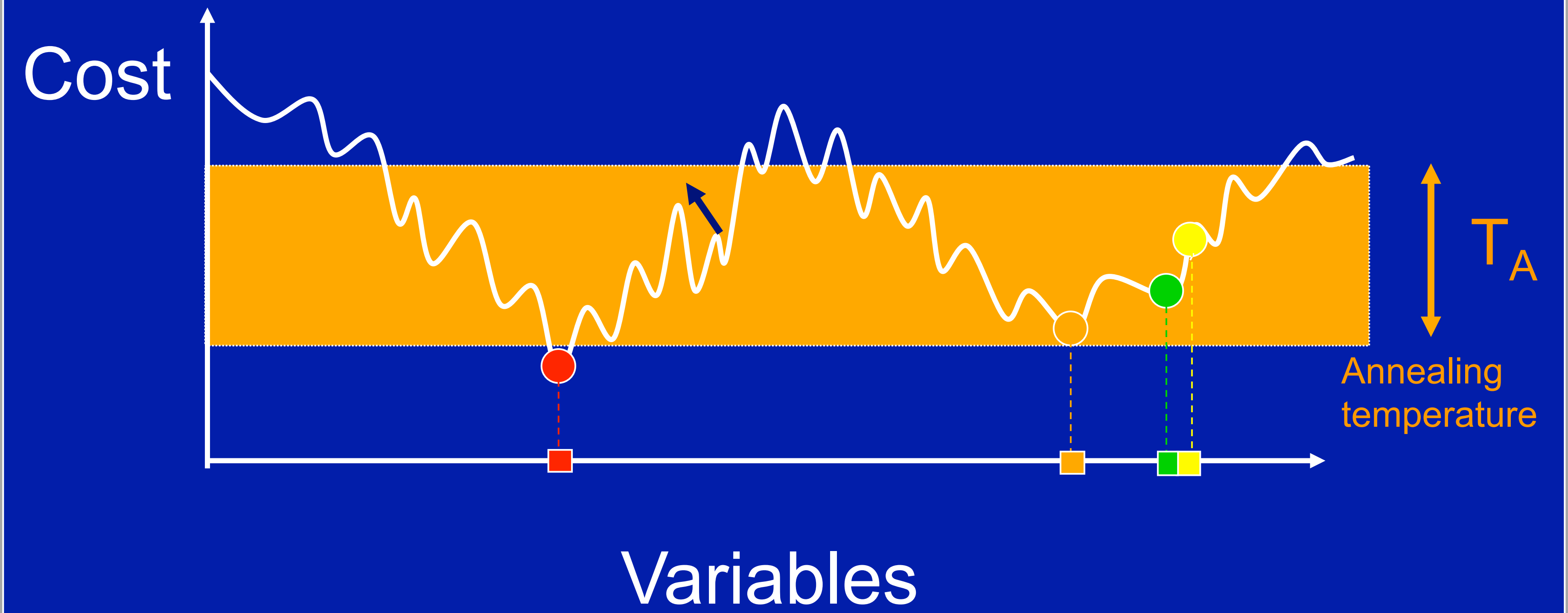
Add 'temperature'

$$P(move) \sim \exp(-\Delta C / T_A)$$



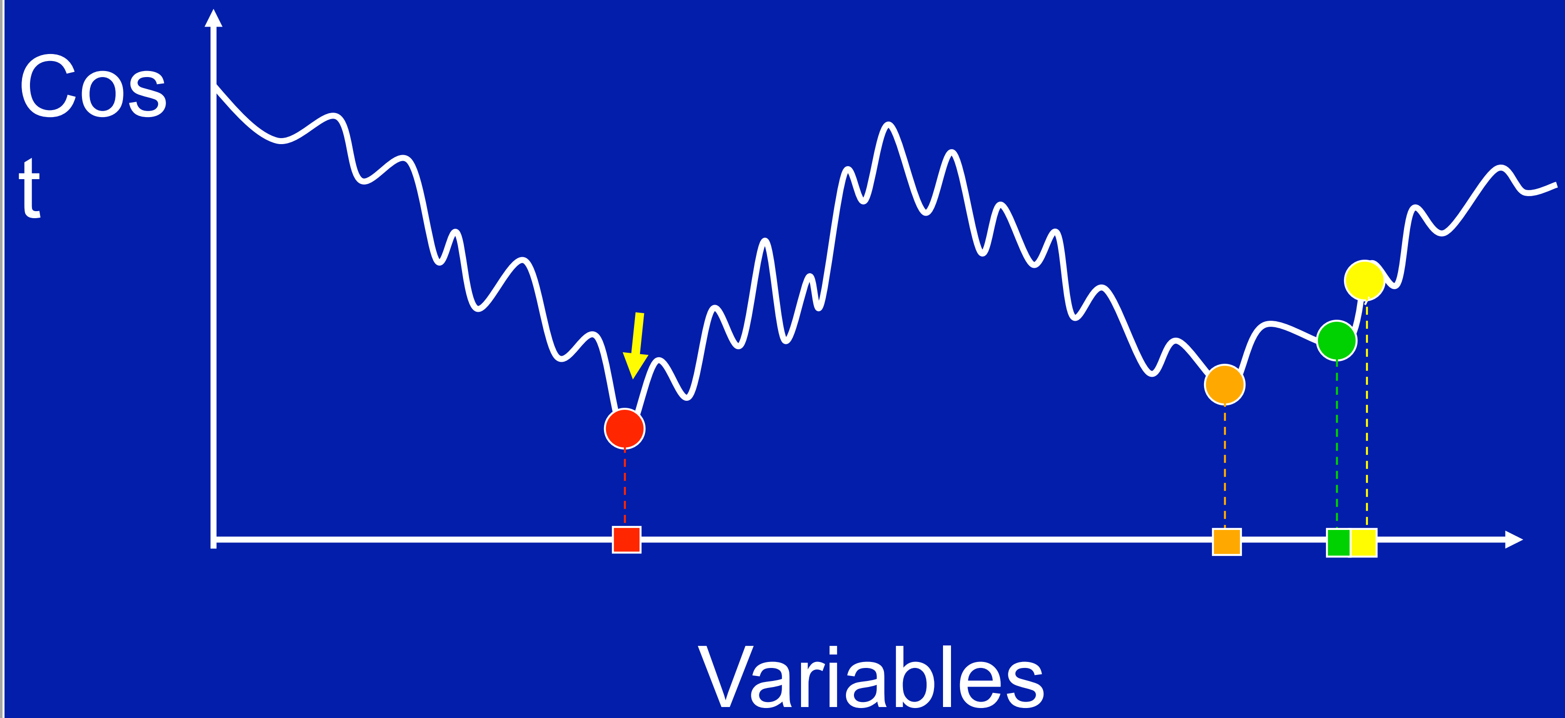
Simulated annealing

Gradually reduce T_A

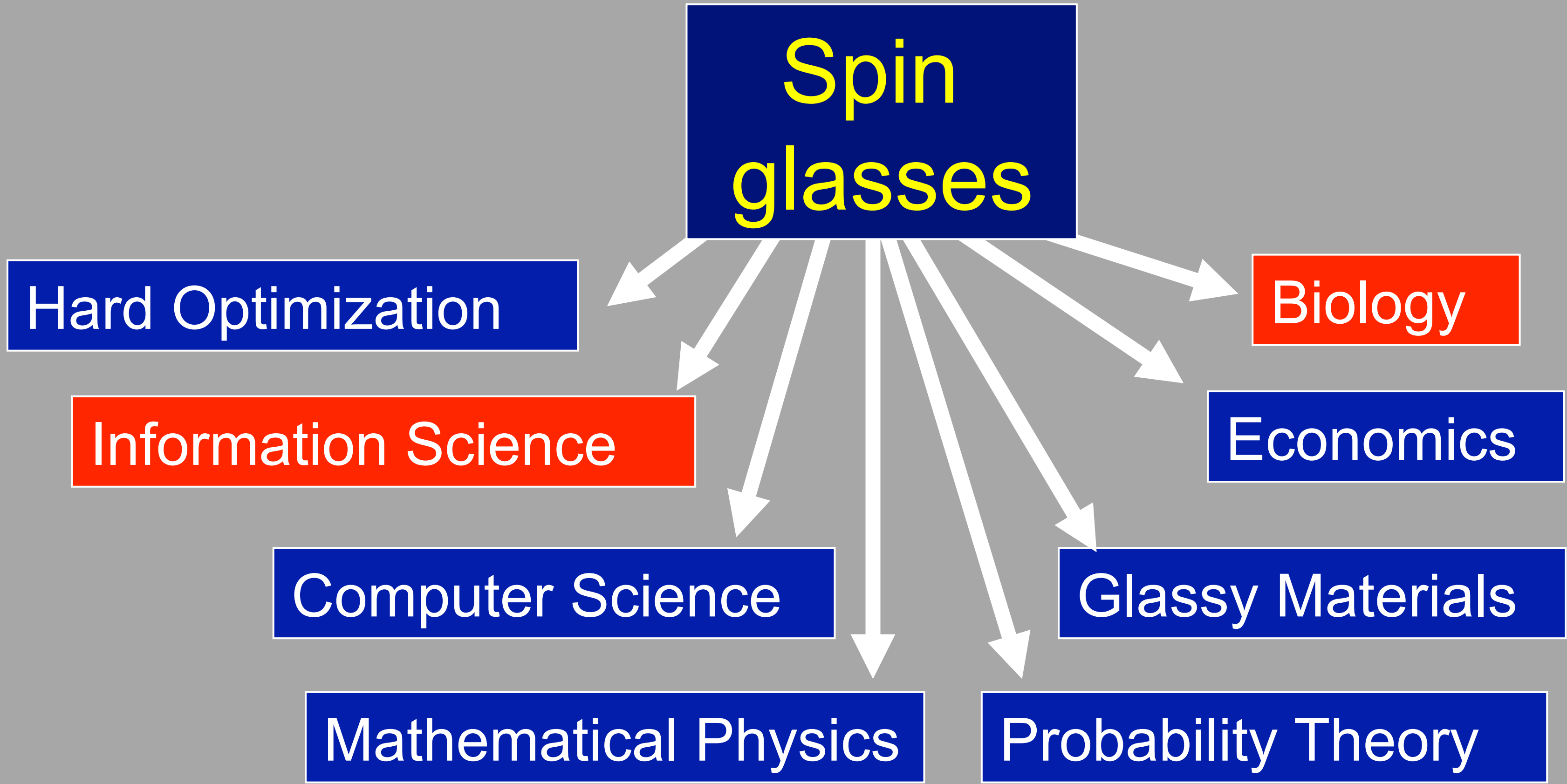


Simulated annealing

Hopefully



More examples



Neural network

Highly idealised

Neurons, rate of firing

Control function

$J_{ij} = \sum_{\mu} \xi_i^{\mu} \xi_j^{\mu}$

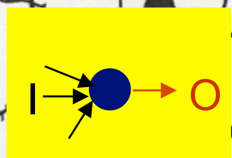
$$H = -\sum_{ij} J_{ij} S_i S_j$$

Synapses

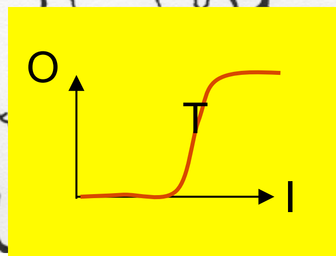
+/- ; excitatory/inhibitory

Store memories

T ~ synaptic sigmoidal response rounding



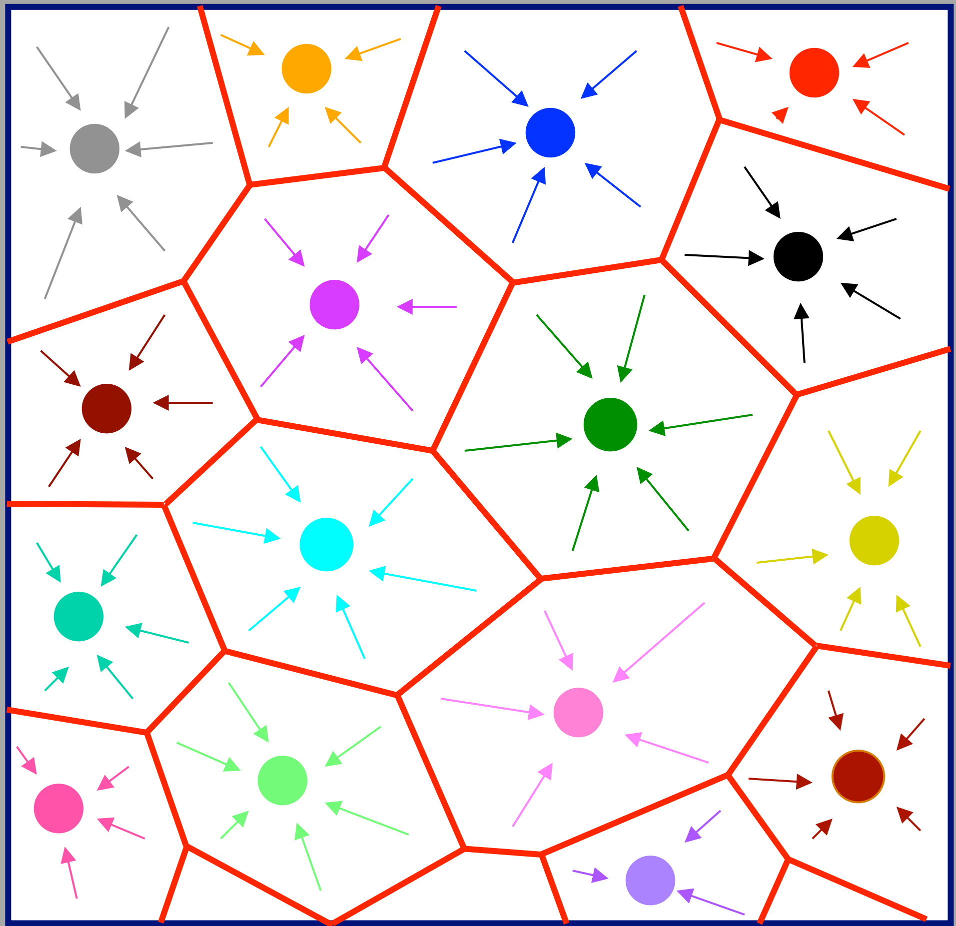
$$I_i = \sum_j J_{ij} S_j$$



Quasi-spin statistical mechanics

Attractors

Schematic illustration 1

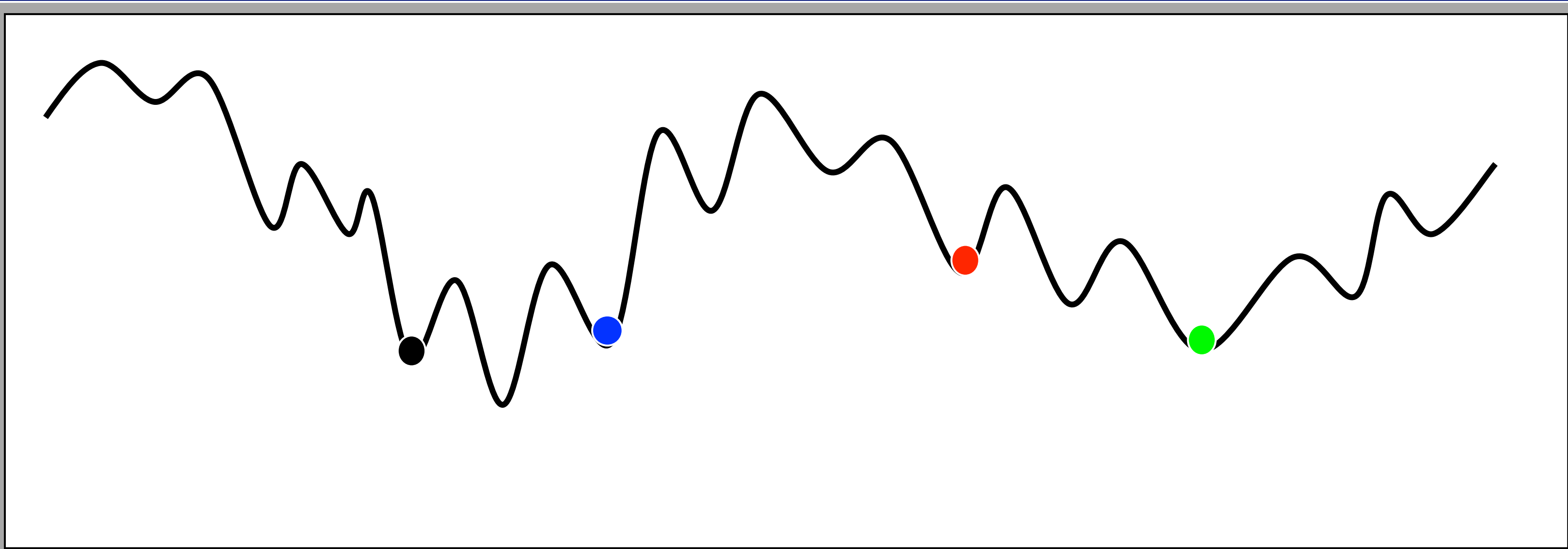


High-dimensional 'phase space' *

- Associative memory
  'attractors'
  memorized patterns
- Retrieval basins
- Many memories
  ~ many attractors
  require frustration
  Stored in {J}

Schematic illustration 2

Rugged landscape



Valleys ~ attractors   Sculpture ~ learning

$\{S_i\}$ $\{J_{ij}\}$

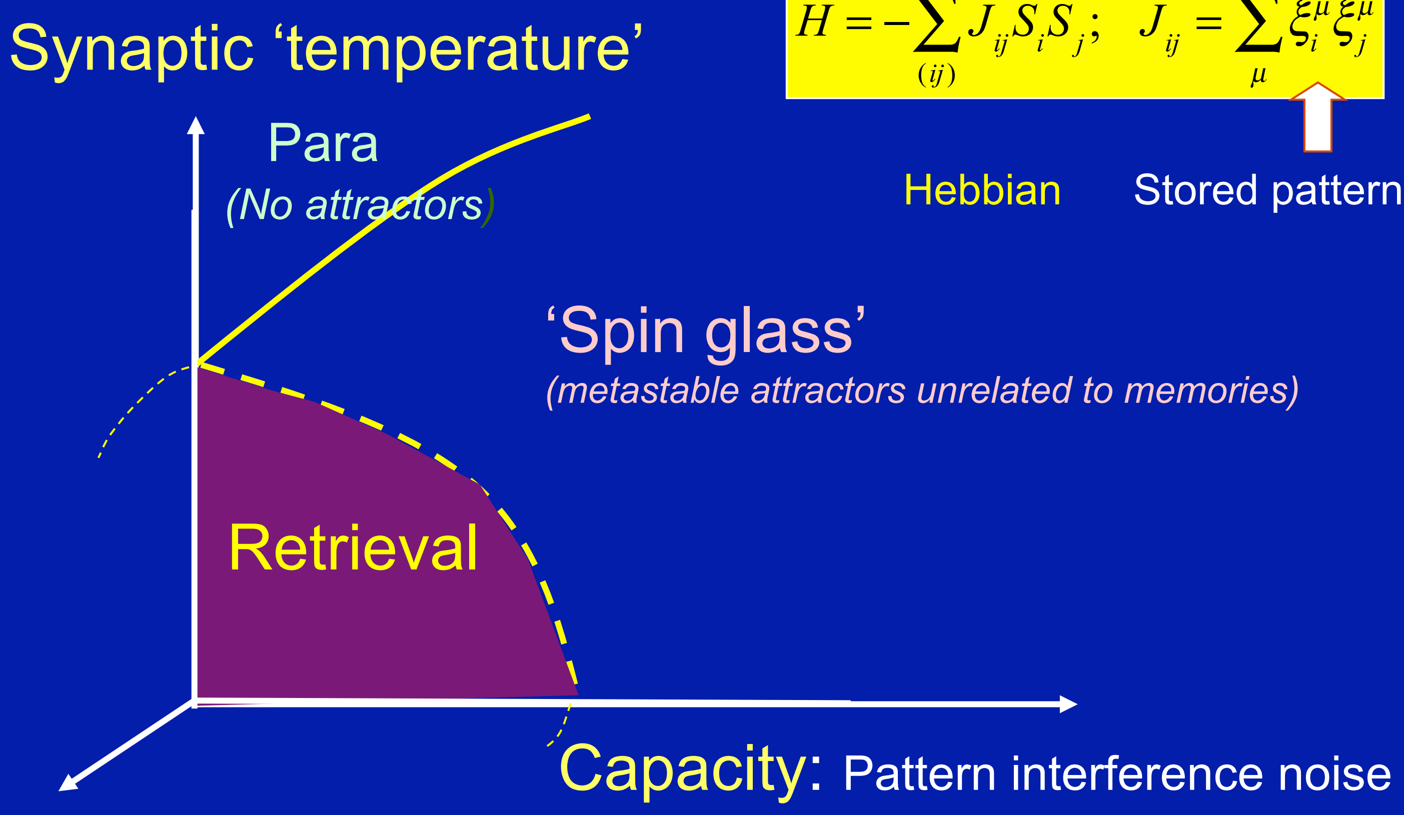
Different timescales

fast retrieval   *slow learning*

‘Phase diagram’: Hopfield model

$$H = -\sum_{(ij)} J_{ij} S_i S_j ; \quad J_{ij} = \sum_{\mu} \xi_i^{\mu} \xi_j^{\mu}$$

Hebbian Stored pattern

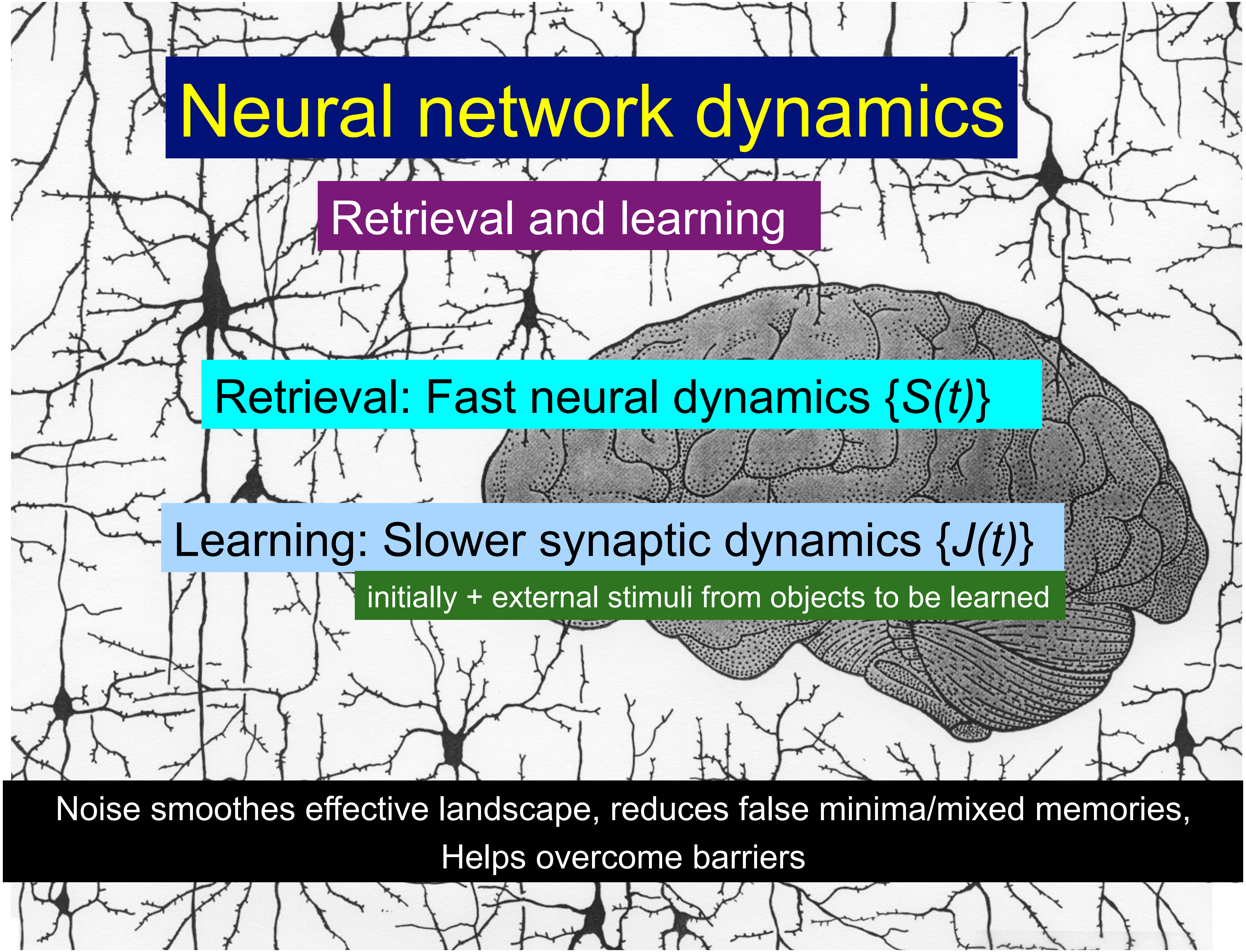


‘Temperature’/ stochastic noise

Stat. Mech.

Energy ➔ Free Energy

- Temperature smoothes free energy
  - Reduces ruggedness
- Neural networks
  - Small noise reduces false minima in effective landscape
  - Large noise prevents storage



Neural network dynamics

Retrieval and learning

Retrieval: Fast neural dynamics $\{S(t)\}$

Learning: Slower synaptic dynamics $\{J(t)\}$

initially + external stimuli from objects to be learned

Noise smoothes effective landscape, reduces false minima/mixed memories,
Helps overcome barriers

Compromise

- Many minima imply frustration
- But too much gives no useful recall
  - Many attractors unrelated to learned information
- Need compromise
  - Places limits on capacity

Minimal frustration

Proteins

Proteins: Heteropolymrers

Many amino acids

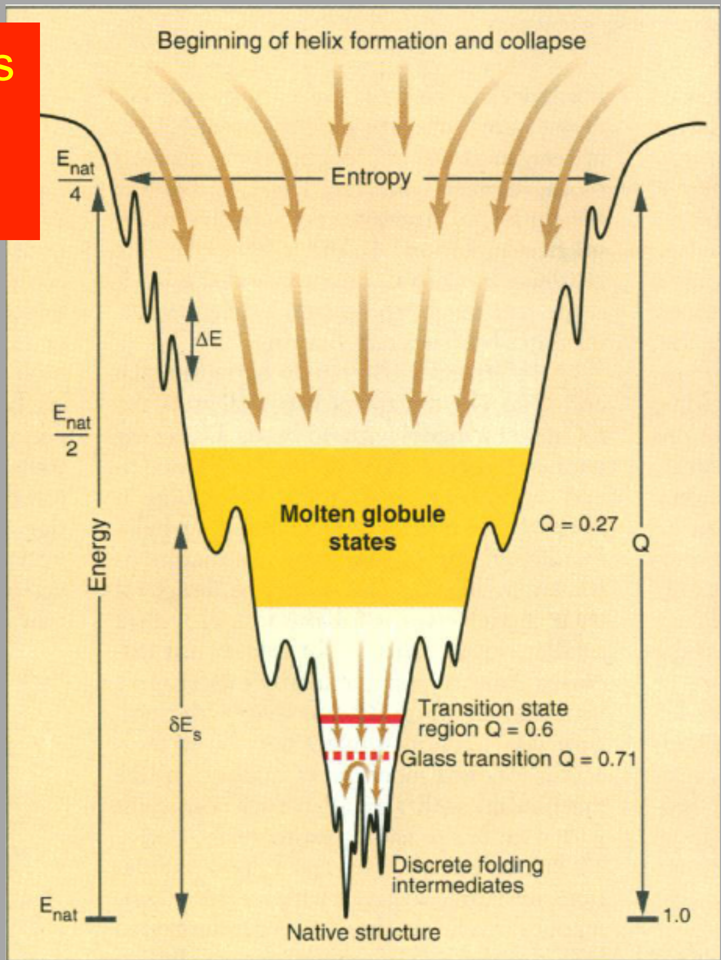
Frustrated interactions

Must fold fairly easily

Minimal frustration

Folding funnel

Wolynes et. al.



Random heteropolymers

In general, very frustrated

Fold poorly, glassy

Evolution:

Initial random soup

Fast: attempt to fold

Slower time-scale:

Reproduction/mutation

Good folders selected

Analogies

Glassy/slow	More minimal frustration/faster
Spin glass	Neural network
SK	Hopfield
Random heteropolymer	Protein
	Wolynes
Random Boolean network	Autocatalytic sets
	Kauffman
	Boolean Neural nets
	Aleksander; Wong & S
LR full occ OK	But still questions on best formulation
SR still ?	and analysis

Theoretical methodology

- Statics/thermodynamics:
  - Partition function

$$Z = Tr\{\exp[-\beta H]\}$$

  - Generating function introduce auxiliary generating fields

$$Z(\{\lambda\}) = Tr\{\exp[-\beta H - \sum_i \lambda_i \phi_i]\}$$

$$\langle \phi_i \rangle = Lim_{\lambda \to 0} \partial_{\lambda_i} \ln Z(\{\lambda\})$$

In practice often done implicitly, also spontaneous symmetry-breaking

Note: physical observables given by ln Z

Disorder: average ln Z

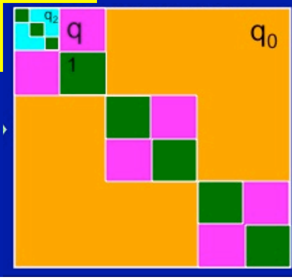
- Average {ln Tr exp .. } difficult
- Average {Tr exp ...} easier

$$\ln Z = \lim_{n\to 0} Z^n;\ n \text{ replicas}$$

- Average over quenched disorder in interactions
  - Gives effective system with extra (replica) labels on variables

$$\overline{\langle \phi_i \rangle_{\{J\}}} \equiv Lim_{n\to 0} \langle \phi_i^\alpha \rangle_{eff};\quad \overline{\langle \phi_i \rangle_{\{J\}}^2} \equiv Lim_{n\to 0} \langle \phi_i^\alpha \phi_i^\beta \rangle; \alpha \neq \beta$$

m $\qquad\qquad$ $q^{\alpha\beta}$



$$\to q(x); 0 \leq x \leq 1 \qquad \overline{P(q)} = \int dx \delta(q - q(x))$$

Theoretical methodology

- Dynamics:
  - Generating functional

$$Z(\{\lambda\}) = \int D\vec{\phi}(t)\delta(\text{microscopic eqn. of motion}^{*})\exp(\vec{\lambda}(t).\vec{\phi}(t))$$

$$\left\langle \phi_i(t))\phi_j(t') \right\rangle \sim Lim_{\{\lambda\}\to 0}\partial_{\lambda_i(t)}\partial_{\lambda_j(f')}Z(\{\lambda\}); \;\; \mathrm{Z}(\{\lambda\}=0)=1$$

    - Disorder averaging gives effective non-disordered system with interacting epochs.

* Either as given by nature, or by computer algorithm used

Theoretical methodology

- Dynamics:
  - Generating functional

$$Z(\{\lambda\}) = \int D\vec{\phi}(t)\delta(\text{microscopic eqn. of motion})\exp(\vec{\lambda}(t).\vec{\phi}(t))$$

$$\left\langle \phi_i(t))\phi_j(t')\right\rangle \sim Lim_{\{\lambda\}\to 0}\partial_{\lambda_i(t)}\partial_{\lambda_j(f')}Z(\{\lambda\}); \;\; Z(\{\lambda\}=0)=1$$

- Disorder averaging gives effective non-disordered system with interacting epochs.
  - Analyse using much exponentiation of delta functions

$$\delta(x) = \int dy \exp(ixy)$$

  - and re-parameterizations of unity

$$1 = \int dx\delta(x) = \int dx\, dy \exp(ixy)$$

→ Macrodynamics

$$Z_{eff} \sim \int DCD\tilde{C} \exp\{N\Phi(\{C(t,..,t'),\tilde{C}(t,..,t')\})$$

↑

Corr^{n} & response functions

- *Extremal domination*

  → *self-consistency eqns.*

  with memory

  not restricted to equilibrium nor stationarity

Reproduce replica results and go beyond

Another aside

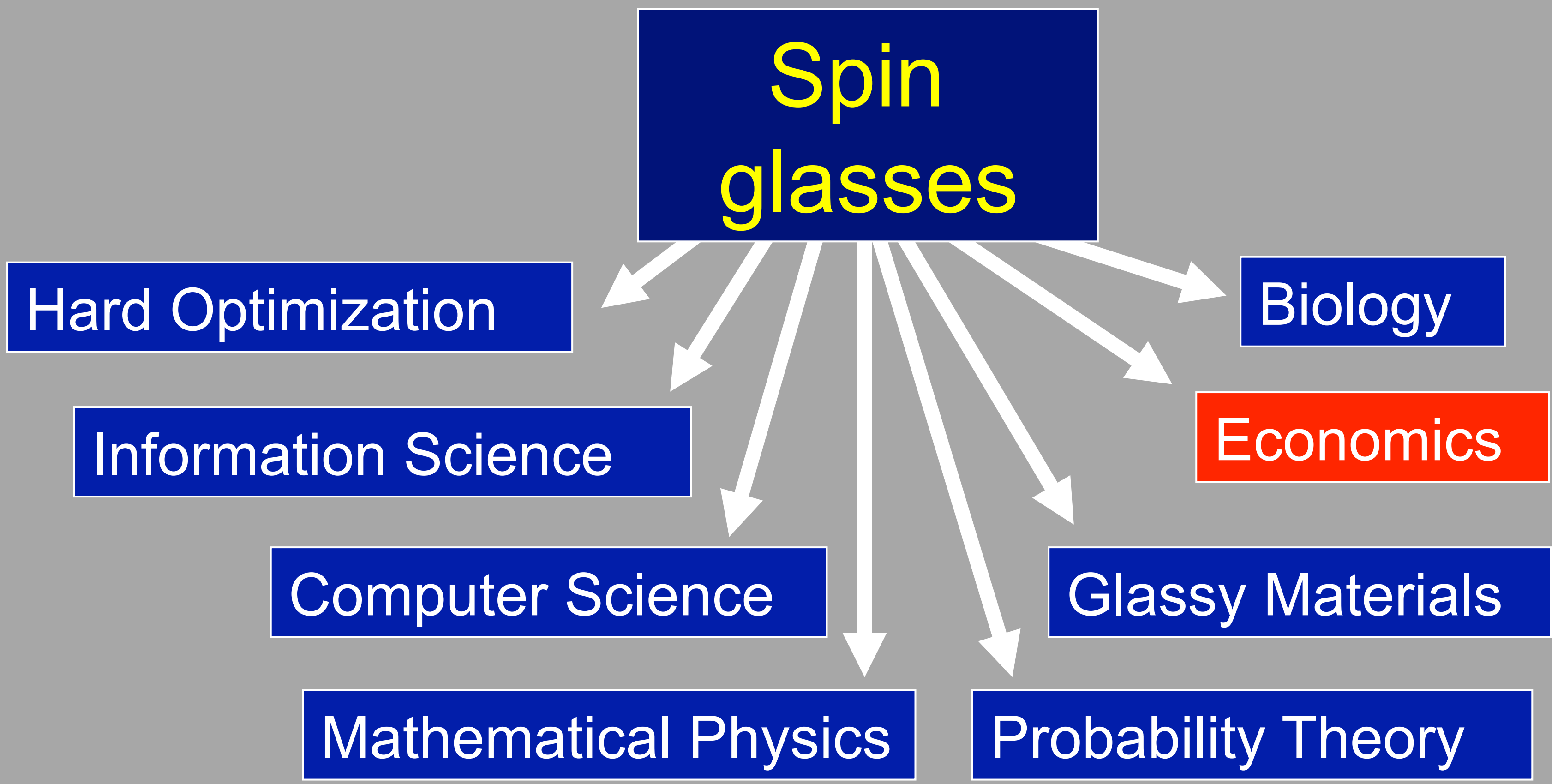
- Fast neurons (spins), slow synapses (exchange)
- Hebbian synaptic dynamics + decay

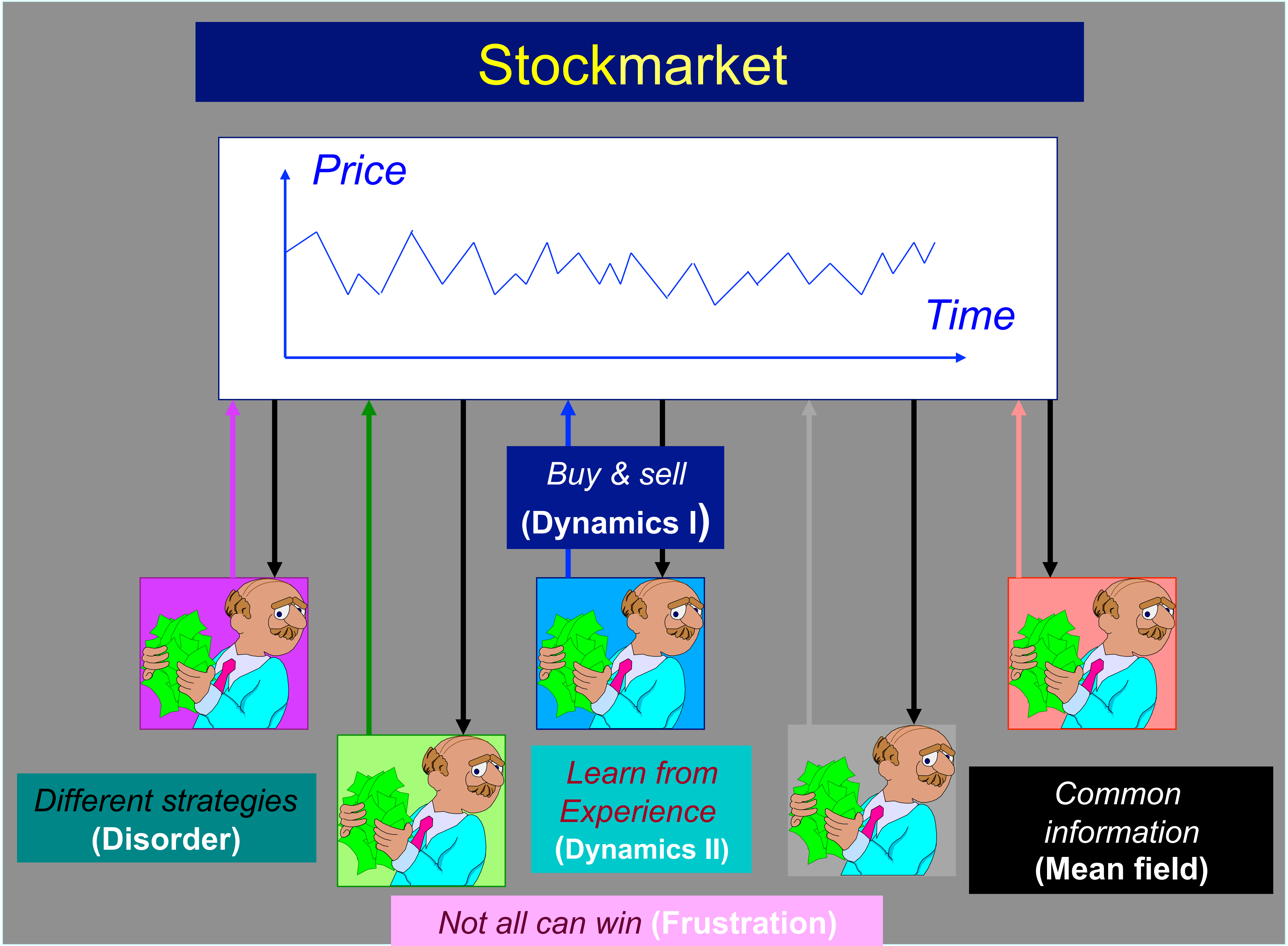
$$\tau \partial J_{ij} / \partial t = \lambda \langle S_i S_j \rangle - \mu J_{ij} + \eta_{ij}(t)$$

↑ Assume adiabaticity

- Two stochastic temperatures: $T_S, T_J;\ T_S / T_J = n$
- Behaves like replica theory but with this *n*
  - Recall that Kondor showed critical mimimum *n* for complexity.

More examples





Stockmarket
Price
Time
Buy & sell
(Dynamics I)
Different strategies
(Disorder)
Learn from Experience
(Dynamics II)
Common information
(Mean field)
Not all can win (Frustration)

Simple minimalist model

Minority game

N agents 2 choices

Aim to be in minority

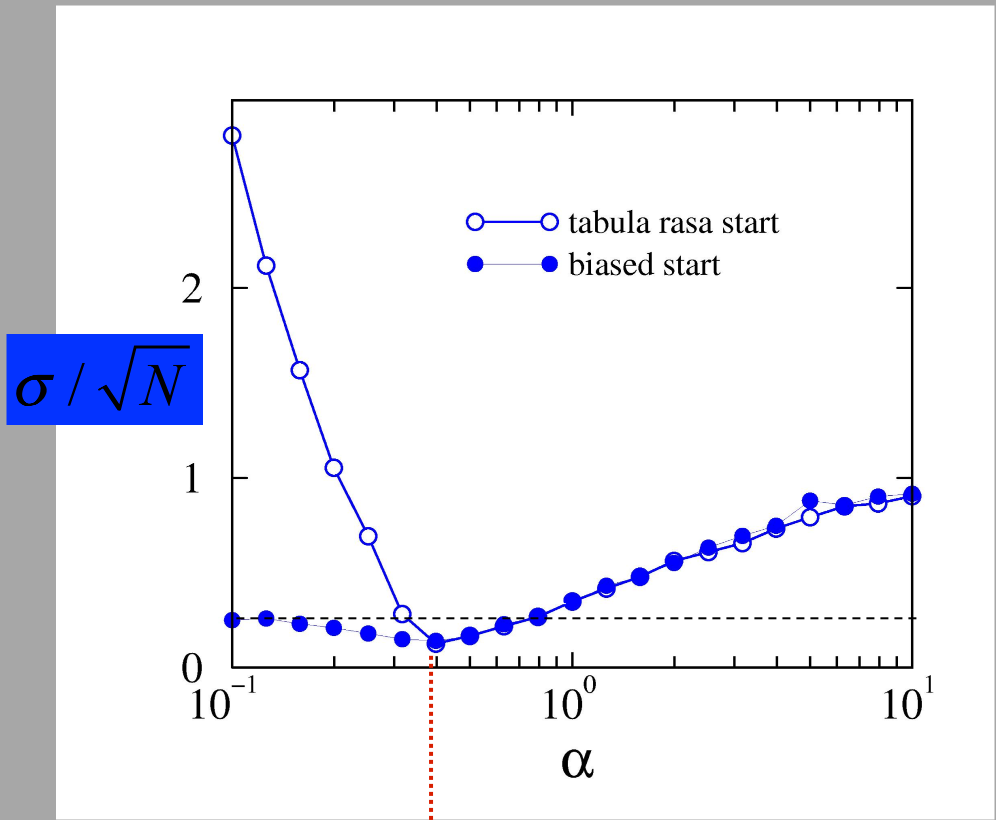
Individual strategies → Collective consequence

- act on common information (e.g. minority choice for last m steps)
- preferences modified by experience (keep point-score – use highest)

↓

Correlated behaviour & phase transition

Volatility



Non-ergodic

Ergodic

Phase transition

Minimum in volatility

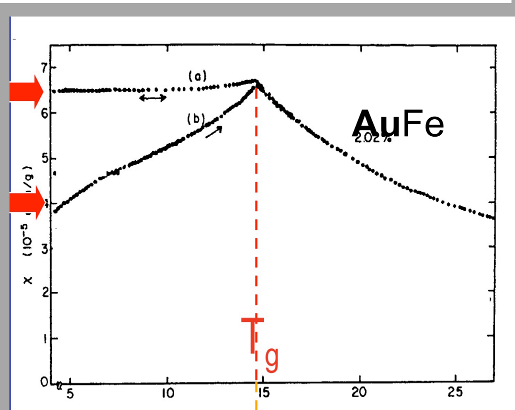
&

Ergodic/ non-ergodic

c.f. s.g. susceptibility m/h

FC

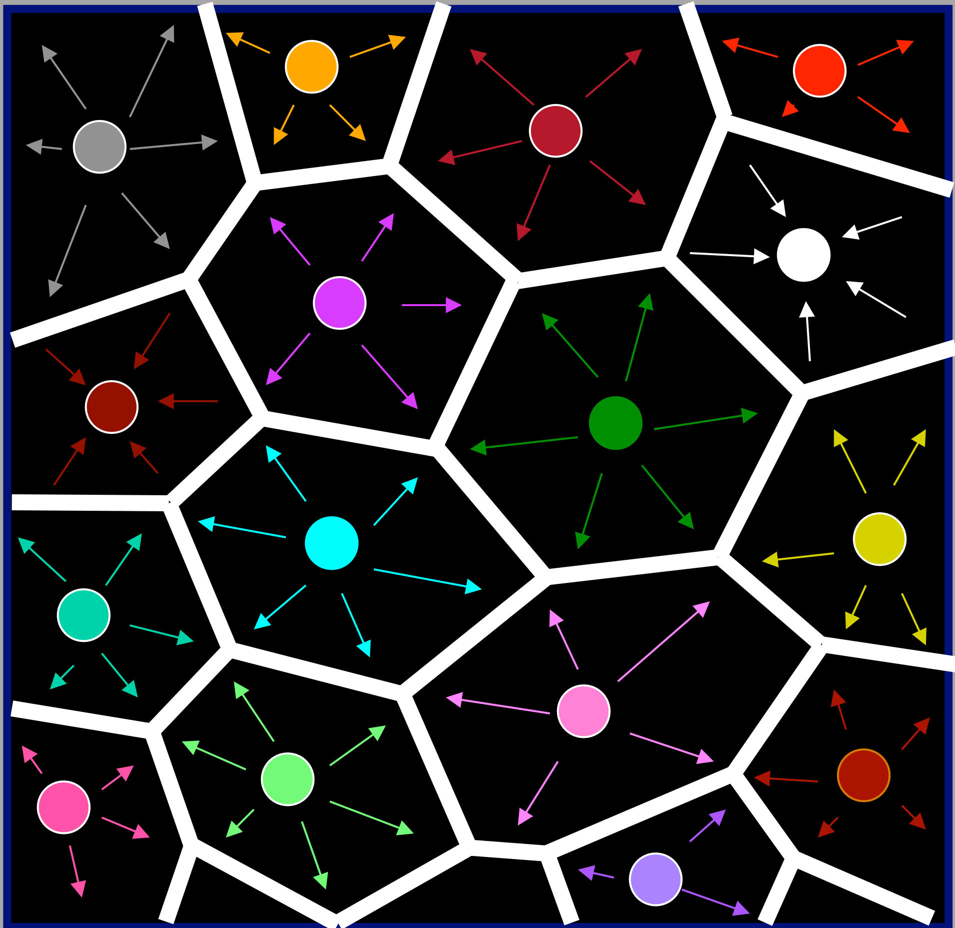
ZFC



Essentially unaltered for ‘random history’

Also analogy with Hopfield neural network but different

Minority game



•One strategy/agent, random histories

•D-dim vectors: $\{\xi_i^\mu\};\ \mu = 1,..D$

•Follow strategy instruction if point-score positive, otherwise do opposite

• Integrate out histories

$$H = +\sum_{(ij)} J_{ij} S_i S_j$$

$$J_{ij} = \sum_{\mu} \xi_i^\mu \xi_j^\mu$$

Many repellors

c.f. attractors in neural network

Two different strategies/agent gives also 'random'field term

Dynamics

after averaging, re-parametrizing, integrating out microscopic variables, extremizing etc.

Effective single-agent ensemble

Non-Markovian stochastic process

$$p(t+1) = p(t) - \alpha \sum_{t' \le t} (\mathbf{1}+\mathbf{G})^{-1}_{tt'} \operatorname{sgn} p(t') + \theta(t) + \sqrt{\alpha}\,\eta(t)$$

$$\text{where } \langle \eta(t)\eta(t')\rangle = [(\mathbf{1}+\mathbf{G})^{-1}(1+\mathbf{C})(\mathbf{1}+\mathbf{G}^{\mathrm{T}})^{-1}]_{tt'}$$

with coloured noise, memory, self-consistent correlation & response functions

$$C_{tt'} = \langle \operatorname{sgn} p(t) \operatorname{sgn} p(t')\rangle_* \equiv N^{-1}\sum_i \langle \operatorname{sgn} p_i(t) \operatorname{sgn} p_i(t')\rangle$$

$$G_{tt'} = \frac{\partial}{\partial\theta(t')}\langle \operatorname{sgn} p(t)\rangle_* \equiv N^{-1}\sum_i \frac{\partial}{\partial\theta_i(t')}\langle \operatorname{sgn} p_i(t)\rangle$$

where $< f >_*$ is an effective average involving $P_0(p(0))$, G, C

Exact but non-trivial

Simulations & iterated theory

Analytic solution via dyn. gen. fnl.

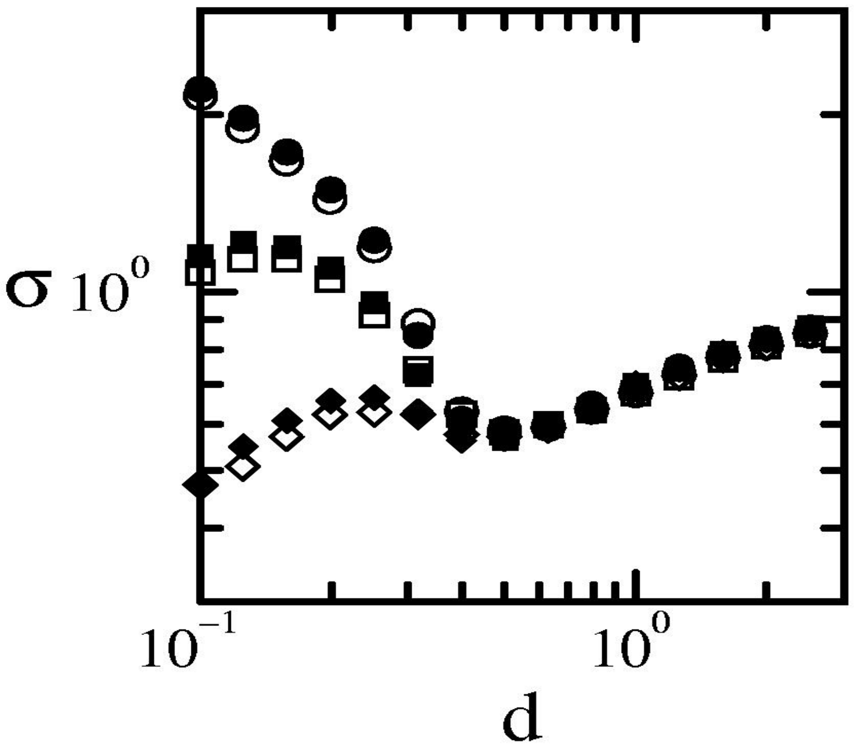
Representative agent ensemble

Initial bias

$p_i(0)=0$

$p_i(0)=0.5$

$p_i(0)=1$



These are for 2 strategies per agent.

For just one strategy/agent, followed or not, depending on point-score, there is no cusp for *tabula rasa,* but still ergodic-nonergodic

Open = simulations Solid = numerical iteration of analytic effective agent equations

Galla & S

Infinite-range/range-free?

- Not real spin glasses
- Nor probably real biology

- But realistic
  - for many hard optimization problems
  - for neural networks?
  - for systems driven by information available to all; e.g. via internet, radio, TV
    - e.g. financial markets, some human behaviour

Conclusion

- Many examples of complex systems
  - Driven by frustrated interactions and disorder
    - Sometimes indirectly generated
    - Detailed balance or fundamentally out-of-equilibrium
    - Conceptual similarities despite different appearances
    - But also differences
- Many opportunities for conceptual and mathematical transfer from physics
- Offer the physicist challenges not present in conventional dictionary-definition “physics”

Recall

Very simple microscopic entities

Very simple pairwise interactions

Rich complexity in collective behaviour

due to frustration and disorder

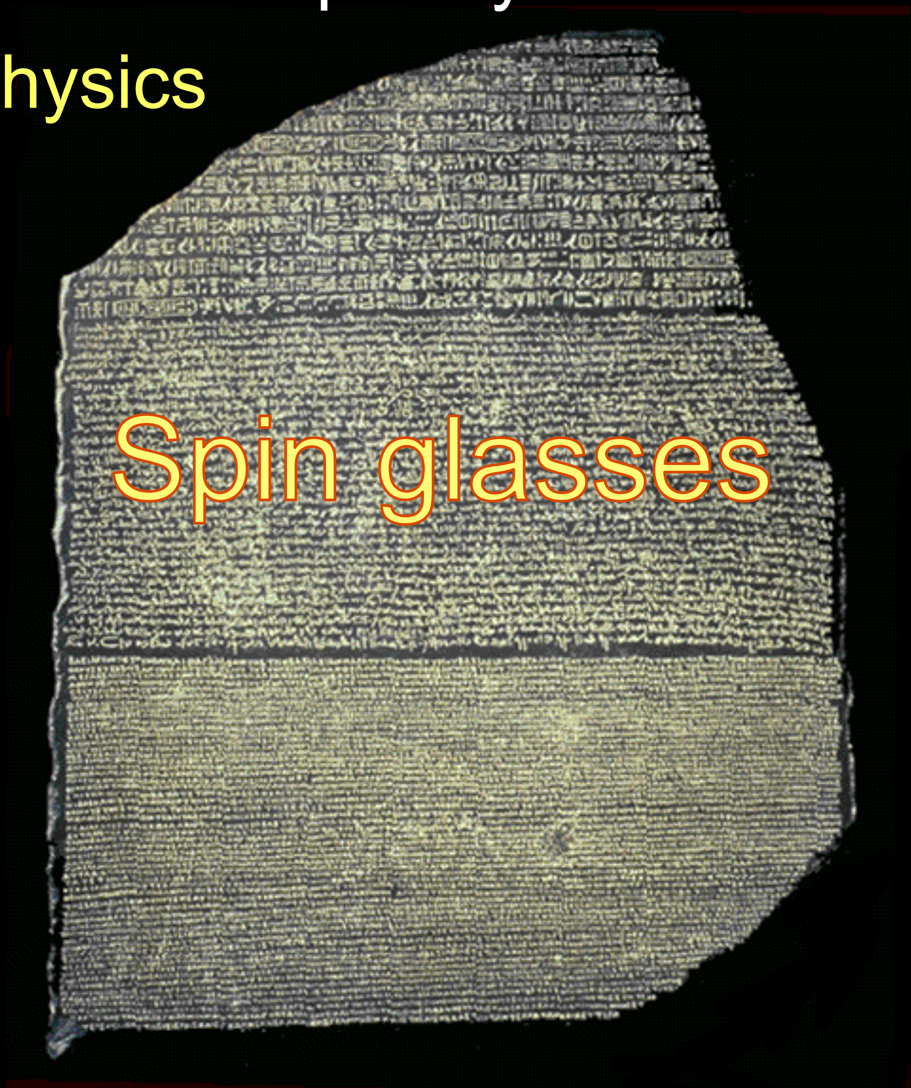
`Complex' is different from `complicated'

Conclusion

Complexity Science

Fascinating Physics

Novel maths

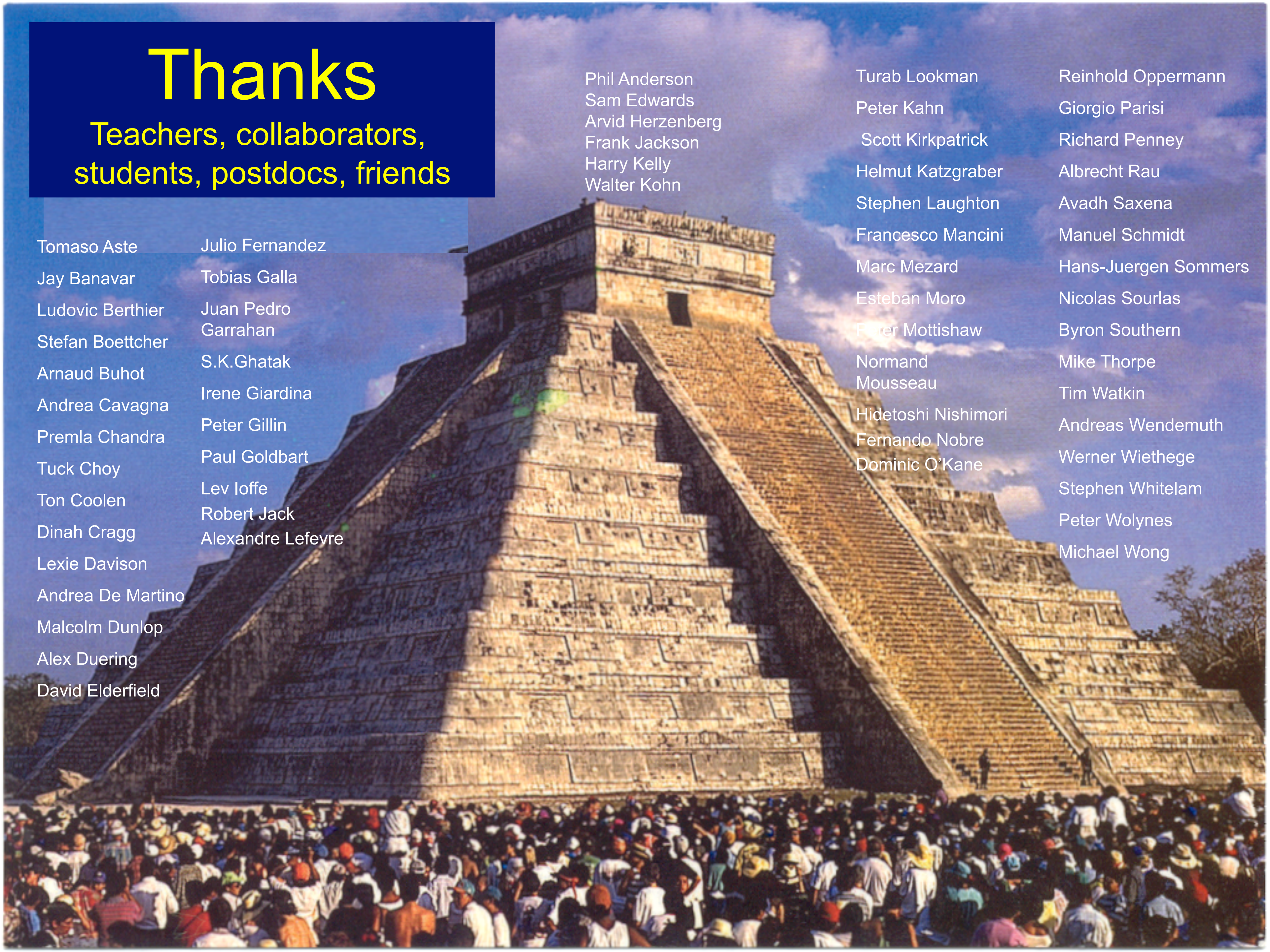


Transfers

Opportunities

Caveats & Cautions

- This was only a broadbrush illustration
  - Only range-free systems
    - Only average thermodynamic limit properties
    - There are differences as well as similarities
  - For finite-range systems
    - There is still controversy about all transfers from range-free
  - Real systems may not be equilibrium
    - And may have many complications (e.g. human society)
  - For many issues one needs new/better algorithms
  - In computer science there are many gegrees of hardness
    - ? Reflections in statistical/many-body physics?
  - Even the best ‘Rosetta Stone’ is not a full dictionary



Thanks
Teachers, collaborators, students, postdocs, friends
Tomaso Aste
Jay Banavar
Ludovic Berthier
Stefan Boettcher
Arnaud Buhot
Andrea Cavagna
Premla Chandra
Tuck Choy
Ton Coolen
Dinah Cragg
Lexie Davison
Andrea De Martino
Malcolm Dunlop
Alex Duering
David Elderfield
Julio Fernandez
Tobias Galla
Juan Pedro Garrahan
S.K.Ghatak
Irene Giardina
Peter Gillin
Paul Goldbart
Lev Ioffe
Robert Jack
Alexandre Lefevre
Phil Anderson
Sam Edwards
Arvid Herzenberg
Frank Jackson
Harry Kelly
Walter Kohn
Turab Lookman
Peter Kahn
Scott Kirkpatrick
Helmut Katzgraber
Stephen Laughton
Francesco Mancini
Marc Mezard
Esteban Moro
Peter Mottishaw
Normand Mousseau
Hidetoshi Nishimori
Fernando Nobre
Dominic O'Kane
Reinhold Oppermann
Giorgio Parisi
Richard Penney
Albrecht Rau
Avadh Saxena
Manuel Schmidt
Hans-Juergen Sommers
Nicolas Sourlas
Byron Southern
Mike Thorpe
Tim Watkin
Andreas Wendemuth
Werner Wiethege
Stephen Whitelam
Peter Wolynes
Michael Wong