

History, power and perspectives

of numerical simulations of spin glasses

Enzo Marinari

(*Sapienza*, Rome, Italy)

Bengaluru, India (sadly from the internet), December 2021

Spin glasses are (very) complex systems. When trying to get a theoretical control over them numerical analysis is crucial.

Parisi solution is the exact solution of mean field, and exposes Replica Symmetry Breaking (RSB), i.e. a many state equilibrium structure.

Relation to finite dimensional systems.

Transition in a non zero magnetic field.

Field theory helps, but very difficult, and many results are not easy to disambiguate.

In such a difficult situation the use of **effective, appropriate algorithms** is mandatory.

A very good algorithm is the one that **uses as much as possible of the knowledge** you have about the system.

There is a long tradition of discussing new algorithms for effective numerical simulations, starting from particle physics, where in any case some of this starts.

Pseudofermions, for simulations of lattice QCD with fermions. *A Proposal for Monte Carlo Simulations of Fermionic Systems*, F. Fucito, E. Marinari, G. Parisi and C. Rebbi, Nucl. Phys. **B180** (1981) 369.

$SU(2)$ embedding in $SU(3)$ matrices, for lattice QCD, *A New Method for Updating $SU(N)$ Matrices in Computer Simulations of Gauge Theories*, N. Cabibbo and E. Marinari, Phys. Lett. **119B** (1982) 387.

And in **quantitative biology**, description of the metabolic behavior of bacteria. **Flux Balance Analysis:**

Constrained Allocation Flux Balance Analysis,

Matteo Mori, Terry Hwa, Olivier Martin, Andrea De Martino and Enzo Marinari,

PLoS Comput Biol 12(6): e1004913.

Plan of the talk.

- **Optimized Monte Carlo Methods**
- **Dedicated Computers:** APE and Janus
- An old, interesting, paradigmatic story: numerical simulations determining a **correlation length ξ** inspired experiments.
- A few and selected results among the most **recent numerical analysis**, based on very large scale simulations (mainly from the Janus collaboration).

A very partial selection of recent results from the **Janus collaboration**. Mainly to give you a first view about the main ideas. Raffaele Tripiccione, who has been one of the most crucial researchers in the Janus Collaboration, is not with us anymore, and we all miss him immensely.

- *Non-equilibrium spin glass dynamics from picoseconds to a tenth of a second*, Phys. Rev. Lett. **101** (2008) 157201.
- *A statics-dynamics equivalence through the fluctuation-dissipation ratio provides a window into the spin-glass phase from non-equilibrium measurements*, PNAS 114 (2017) 1838.
- *Matching microscopic and macroscopic responses in glasses*, Phys. Rev. Lett. 118 (2017) 157202.
- *Aging rate of spin glasses from simulations matches experiments*, Phys. Rev. Lett. **120** (2018) 267203.

- *The Mpemba effect in spin glasses is a persistent memory effect*, PNAS 116 (2019) 15350-15355.
- *Scaling law describes the spin-glass response in theory, experiments and simulations*. Physical Review Letters 125 (2020) 237202 (with R. Orbach group).
- *Temperature chaos is present in off-equilibrium spin-glass dynamics*. Communication Physics 4, 74 (2021).
- I. Paga, Q. Zhai et al., *Spin-glass dynamics in the presence of a magnetic field: exploration of microscopic properties*, J. Stat. Mech. (2021) 033301 (with R. Orbach group).
- A comprehensive summary of the most recent developments: *From glassy bulk systems to spin glass films: simulations meet experiments*, Ilaria Paga, PhD Thesis (June 2021).

It is appropriate to quote a few more results.

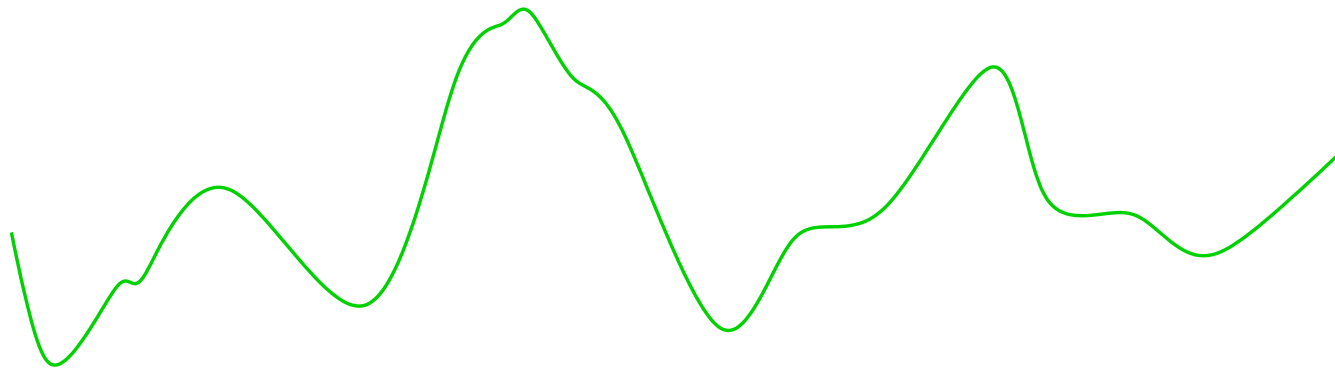
- *Spontaneous energy-barrier formation in an entropy-driven glassy dynamics*, C. Cammarota and E. Marinari, Phys. Rev. E **92** (2015) 010301(R).
- *Numerical Evidences of Universal Trap-Like Aging Dynamics*, C. Cammarota and E. Marinari, J. Stat. Mech. (2018) 043303.
- *An experiment-oriented analysis of 2D spin-glass dynamics: a twelve time-decades scaling study*, L. A. Fernandez, E. Marinari, V. Martin-Mayor, G. Parisi and J. J. Ruiz-Lorenzo, J. Phys. A: Math. Theor. **52** (2019) 224002.
- *Dimensional crossover in the aging dynamics of spin glasses in a film geometry*, L. A. Fernandez, E. Marinari, V. Martin-Mayor, I. Paga and J.J. Ruiz-Lorenzo Phys. Rev. B **100** (2019) 184412.

Optimized Monte Carlo Methods: Parallel Tempering

For Tempering and Parallel Tempering see: EM and Parisi 1992, Tesi et al. 1995; Geuer and Thompson 1994; Hukushima et al. 1995.

Free Energy Barriers

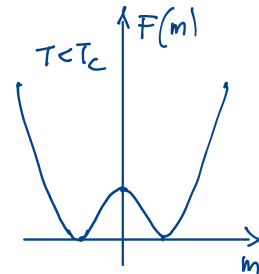
This is a **Complex** Free Energy landscape



Normal Monte Carlo cannot and does not work.

Difficult to cross. Crucial to cross.

Also for Ising model we have a problem of this kind, but symmetry helps us.



Inspecting half of the phase space gives us most of the information we really need about the system.

If we **change T free energy barriers change**. When T **increases** barriers become **smoother** and smoother. When T reaches T_c the landscape has been flattened.

Idea: let the system **walk in temperature space**, going down to the low, interesting T value, and up all the way, through a chain of **intermediate T values** up to $T \gg T_c$. (A bit like annealing, but **always** at thermal equilibrium: **tempering is annealing for free energy**).

Generic class of methods where you modify the probability distribution π :

$$\int \pi O \sim \int \nu O' , \quad \text{where } \nu = \frac{\pi}{\rho} , \quad O' = \rho O$$

density scaling or umbrella sampling

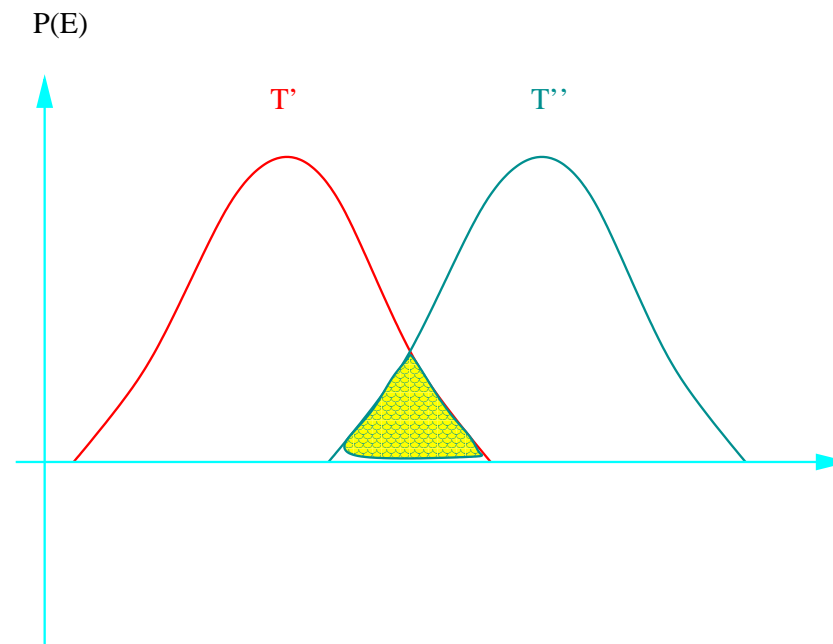
Here the method is very simple since you have **exactly the Boltzmann distribution at each T value** (no reconstruction is needed: just select data at the correct T value). **The method:**

- **select** a discrete set of T values, $T_{(\alpha)} : \alpha = 0, 1, 2, \dots, M$. Here $T_0 = T_{\min}$ (typically smaller than T_c) and $T_M = T_{\max}$ (typically larger than T_c).
- **Clone** your system M times, i.e. consider M configurations C_α of your system.
- **start by assigning** $T(C_0) = T_0, T(C_1) = T_1, \dots, T(C_M) = T_M$.

Eventually you can go ahead with Monte Carlo sweeps.

Two parts of Monte Carlo sweep:

- Usual MC sweeps on all copies of the system at fixed temperature.
- Swap two values of T . Consider $C(T_0)$ and $C(T_1)$. Propose to the two copies to swap their values of the temperature.



Selection of T values range and spreading is the freedom of the method. If equidistributed T values and T_{\min} is fixed free physics parameters are N_T and ΔT .

Use Metropolis to swap the values of the temperature among two copies of the system

$$\Delta S \equiv S' - S = (\beta' E + \beta E) - (\beta E + \beta' E')$$

do previous point for all configuration couples $C(T_1)$ and $C(T_2)$, $C(T_2)$ and $C(T_3)$ and so on ...

Choice of

- T_{\min} : interesting physics + reasonable CPU time.
- T_{\max} : “ \gg ” T_c .
- N_T : keep high acceptance factor for tempering swap.

Check thermalization

- Symmetry of $P_J(q)$ (here this is not as a strong check as in normal Monte Carlo: spin flip is not the slowest mode anymore).
- Check convergence of observables on logarithmic time scale.
- Check that acceptance rate for tempering has been kept high (see earlier).
- Each of the N_T copies of the system must have covered the $T_{(\alpha)}$ space with “many visits”.

Parallel Tempering can be used as an optimization scheme. Search for ground state. Similar to annealing.

Potential advantages of parallel tempering: built in schedule. Could be of help.

Cluster like, Swendsen–Wang and Wolf like methods do not work for spin glasses. Fortuin-Kasteleyn like cluster already percolate at T_c .

Many things have been tried but nothing really works very well.

Finding a very effective cluster method for spin glasses would be a remarkable achievement.

Multicanonical methods (B. Berg et al.) can deal with a number of general situations, since you can change in a complex way the a priori probability distribution (control for example first order phase transitions).

For spin glasses multicanonical methods have probably a slightly lesser performance than parallel tempering.

Replica MC algorithm by Swendsen and Wang: comparable to PT in many situations.

Quantum annealing (Finnila et al., Chem. Phys. Lett. 1994, Car, Martonak, Santoro and Car, Science 2002) for example for Traveling Salesman Problem.

Quantum annealing: use quantum mechanical tunneling to overcome barriers in a more effective way. Can work better than simple SA.

We do reconstruct **equilibrium**, i.e. **long times probability distribution** P_{eq} , thanks to optimized Monte Carlo methods.

Usual Monte Carlo, local in space and in time, is needed for studying the (long time) dynamical behavior of the system.

In the most cases real **experiments look indeed at out of equilibrium, dynamical behavior** of the system.

Cugliandolo-Kurchan findings, and the suggestion of using correlation functions as a well behaved proxy of physical time, are very relevant here.

In the following in many cases we will discuss about **usual, local** Monte Carlo dynamics.

Optimized Computers: from APE to Janus.

Such an intense program of numerical simulations requires **dedicated, powerful tools**.

First with Lattice QCD studies Nicola Cabibbo and Giorgio Parisi have launched the design and the construction of the **APE Computers**.

This has continued in a Spanish-Italian collaboration with **Janus and Janus-2, born for spin glass physics**.

Many ideas introduced in this process have been important and still have a relevance.

Dedicated computers for us started with the **APE project** (a SIMD computer oriented to Lattice Gauge Theories simulations, but ready for much more).

Group directed by Nicola Cabibbo and Giorgio Parisi. Nicola was more attracted by the hardware, Giorgio from the software (always a very critical part).

At that time there was a **window of opportunity**, using specific features of our problem.

Our background: **1982, synchronous MPP** in Edinburgh (David Wallace, Peter Higgs). **1982-1984 Cray** in Paris (vector machine, **too sophisticated** for our “simple” needs).

Crucial ideas (product of 3 times 3 matrices):

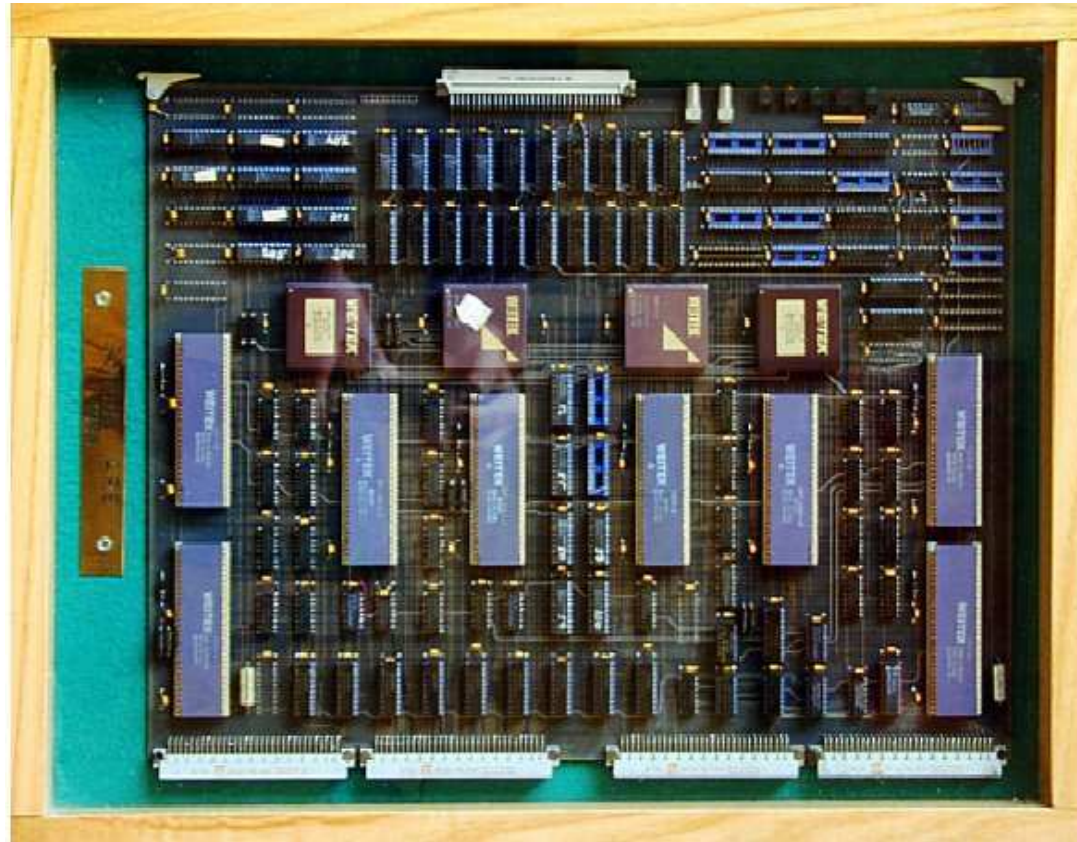
- **Synchronous.** (the APE, not so clever indeed, but very powerful).
- **Data reusal.**
- **Fast registers.**

256Mflops and later *1Gflops*. And this was a leader in the world.

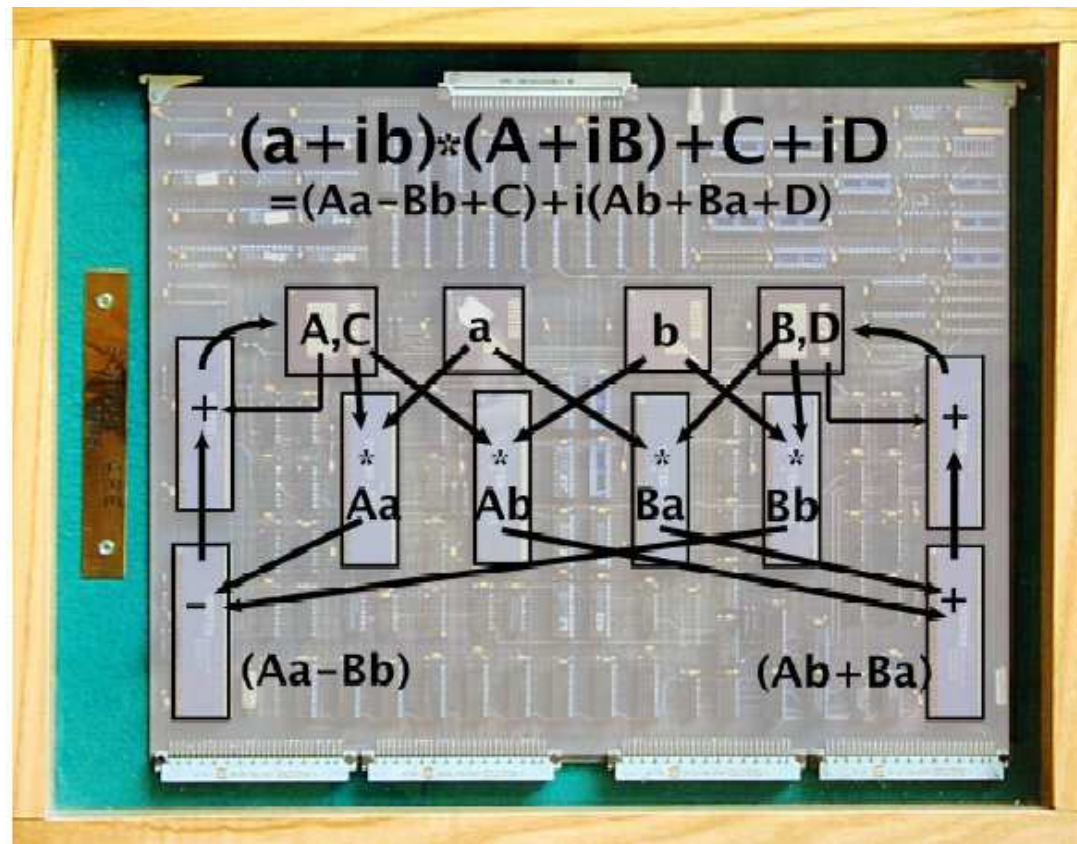
iPhone X, close to 600 Gflop.

Later on: APEcento, APEmille (1 Tflop for LGT in 2000), APEnext.

We developed the high level APESE language.



An APE node.



For complex arithmetic (as needed in $SU(3)$ computations).

Competition on LGT specialized computers: Christ@Columbia (1Gflop), Weingarten@IBM (ten Gflop a few years later).

Many computers specialized for different problems.

RTN@Zaragoza 1992 and SUE@Zaragoza 2001, SUE: A. Cruz, J. Pech, A. Tarancón, P. Téllez, C. L. Ullod and C. Ungil

Janus comes from these paths, and goes very far with spin glasses. Simulations on physical time scales, of the order of one second.

Just a few words about the home built, **Janus and Janus II** super-computers, from a collaboration of Spanish and Italian groups.

The Janus super computers are dedicated to the study of spin glass systems, and allows very large scale simulations of systems with binary spins.

The Janus supercomputers are FPGA-based (field-programmable gate array) massively parallel spin-glass number crunchers.

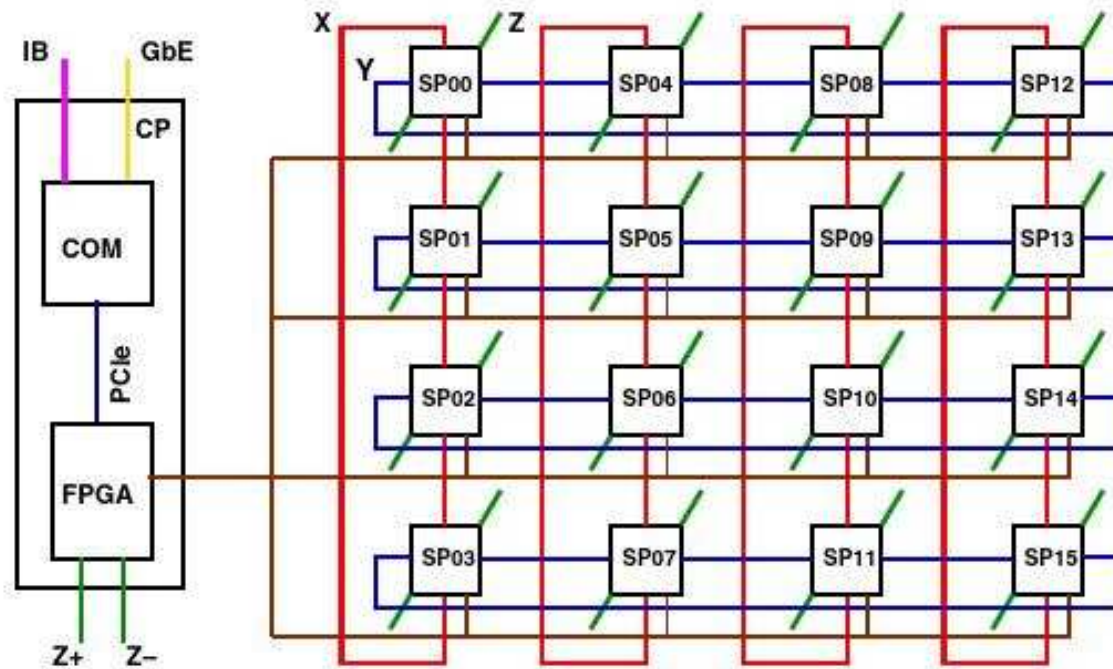
Bi-programmable (you configure the FPGA hardware and you run codes on it).

How it looks

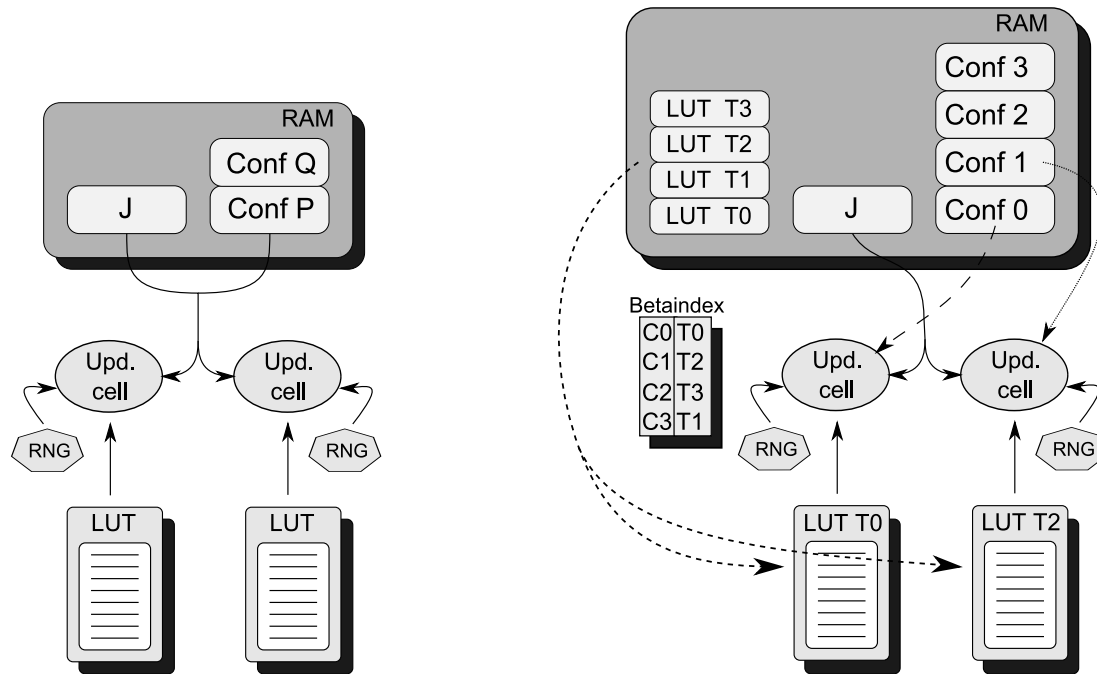


The Janus 2 connectivity.

M. Baity-Jesi et al. / Computer Physics Communications 185 (2014) 550–559



MC, PT and look up tables.



And now we discuss an important numerical result from 1995...

E. Marinari, G. Parisi, F. Ritort and J. Ruiz-Lorenzo, *Numerical Evidence for Spontaneously Broken Replica Symmetry in 3D Spin Glasses.*, Phys Rev. Lett. 1996

A very ambitious title, but this is not at all our point today...

$D = 3$ Edwards Anderson spin glass. A computation on the APE, lattice QCD super-computer: some of the hardware we had built was indeed dedicated to studying spin glass physics. APE was very effective for this.

Both static analysis (with parallel tempering), that we will not discuss here, and dynamical analysis.

We look numerically at **overlap overlap correlation functions** restricted to those pairs of configurations which have a small value of q . This is what you get when you do a dynamical analysis on large lattices starting from different configurations.

Consider a system of side L and define the **equilibrium correlation function** as

$$C(x, L) = V^{-1} \overline{\left\langle \sum_i \sigma_{i+x} \tau_{i+x} \sigma_i \tau_i \right\rangle},$$

brackets are for the thermal average.

RSB: you expect $C(x, \infty) \propto |x|^{-\lambda}$, where λ is an appropriate exponent which has been estimated analytically in less than 6 dimensions for the $q = 0$ correlation functions (de Dominicis, Kondor and Temesvari 1995).

Consider large systems, with $L = 64$. Very far from equilibrium.

Numerical simulations starting from two independent random configurations (and take some average over couplings). q^2 stays small in the whole run: $q \approx 0$. So this is a way to study numerically systems with small overlap.

In order to do that we consider the **time dependent equal time correlation function at time t**

$$G(x, t) = V^{-1} \overline{\sum_i \langle \sigma_{i+x} \tau_{i+x} \sigma_i \tau_i \rangle_t} .$$

Average is done at time t , i.e. after t Monte Carlo cycles after the random start. For large times t the correlation function $G(x, t)$ is essentially different from zero for distances not too larger than a **dynamic correlation length $\xi(t)$ which increases (and maybe diverges) with time.**

Our numerical data are well represented with the functional form

$$G(x, t) = \frac{A(T)}{x^\alpha} \exp\left\{-\left(\frac{x}{\xi(T, t)}\right)^\delta\right\},$$

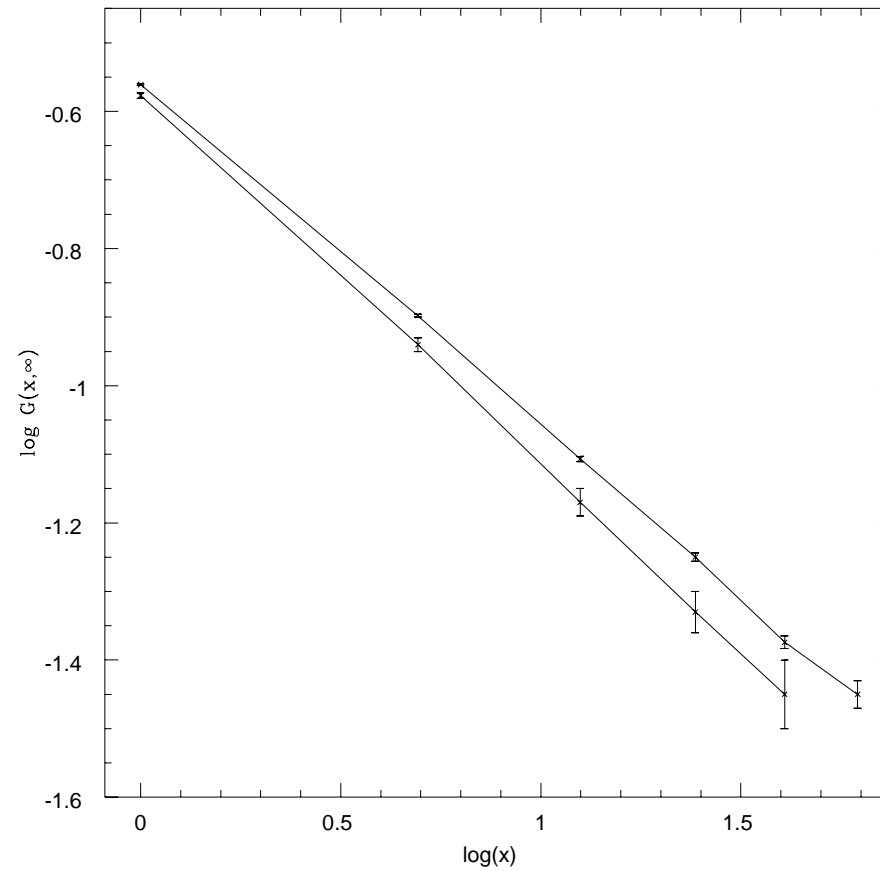
where $\xi(T, t) \equiv B(T) t^{\lambda(T)}$.

We get good fits. The exponents α and δ are only weakly dependent on T .

The correlation length exponent $\lambda(T)$ is approximately given by $0.16T$ (see also Kiesker et al. 1996).

For going at $t \rightarrow \infty$ we fit at fixed distance:

$$G(x, t) = G(x, \infty) \exp\left\{-A(x) t^{-\lambda(T)}\right\}.$$



Here $T \sim 0.7 T_c$. Lower line is from the dynamics we have described.
Power law $x^{-\alpha}$ with $\alpha = 0.50 \pm .03$, as predicted by RSB.

We have determined numerically a temperature dependent correlation function in a $D = 3$ system, and we have shown it scales like one would expect from Parisi theory.

We have now a problem that is quite frequent. What can be easily determined in numerical experiments is not always easy to determine in real experiments, and the other way around.

Obtaining a reasonably direct determination of a correlation function in experiments is not easy.

Luckily our results prompted a team of experimental groups to analyze the problem, and to obtain a remarkable breakthrough.

Y.G. Joh, R. Orbach, G.G. Wood, J. Hammann and E. Vincent,
Extraction of the Spin Glass Correlation Length, Phys Rev. Lett.
1999.

Let us see right ahead what they did, by following the very clear abstract of the paper.

The peak of the spin glass relaxation rate,

$$S(t) = d[-M_{TRM}(t, t_w)/H]/d \log t$$

is directly related to the typical value of the free energy barrier which can be explored over experimental time scales.

A change in magnetic field H generates an energy $E_z = N_s \chi_{fc} H^2$ by which the barrier heights are reduced. χ_{fc} is the field cooled susceptibility per spin, and N_s is the number of correlated spins.

The shift of the peak of $S(t)$ gives E_z , generating the correlation length, $\xi(t, T)$.

Fits to power law dynamics, $\xi(t, T) \propto t^{\alpha(T)}$ and activated dynamics $\xi(t, T) \propto (\log t)^{1/\psi}$ compare well with simulation fits, but possess too small a prefactor for activated dynamics.

The authors first discuss our overlap-overlap, time dependent $q = 0$ correlation function, and its large time limit.

Their measurements: cool a sample in a magnetic field through the glass temperature T_g to the measuring temperature T , waiting a time t_w ,

then cut the field to zero and measure the decay of the magnetization.

This generates the response function,

$$S(t) = d \left[\frac{-M_{TRM}(t, t_w)}{H} \right] / d \log t$$

where $M_{TRM}(t, t_w)$ is the thermo-remanent magnetization at time t .

Barrier heights surmounted during aging are reduced upon a change in magnetic field by E_z , a quantity related to the change in Zeeman energy (scaling laws by Vincent, Bouchaud, Dean and Hamman).

Assumption: barriers $\Delta < E_z$ in the initial state (before the magnetic field is changed) are quenched.

Population of occupied states transitions to states of lowest energy corresponding to the new value of the magnetic field.

At small magnetic field changes, barrier height corresponding to the waiting time t_w ,

$$\Delta(t_w, T) = k_B T (\log t_w - \log \tau_0).$$

Local equilibration on a time scale of the order of t_w .

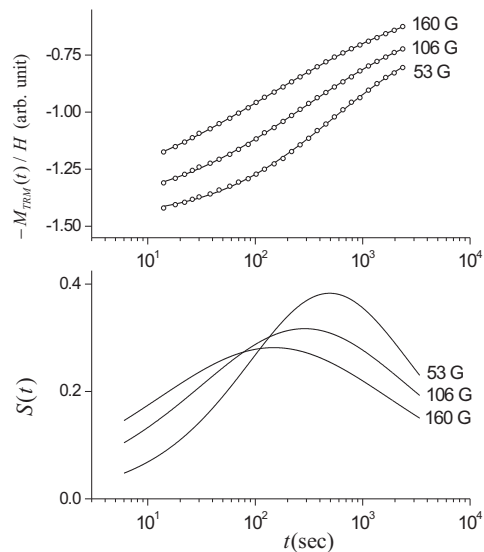
This causes a peak in the response function $S(t)$ for measurement times t close to the waiting time t_w .

When the magnetic field change is increased, E_z increases. The effective barrier height is $\Delta(t_w, T) - E_z$.

This implies a reduction of the measuring time at which $S(t)$ peaks.

The peak in $S(t)$ is associated with an effective waiting time, t_w^{eff} , and

$$\Delta(t_w, T) - E_z = k_B T (\log t_w^{\text{eff}} - \log \tau_0)$$



Results from experiments on thiospinel and on CuMn 6%.

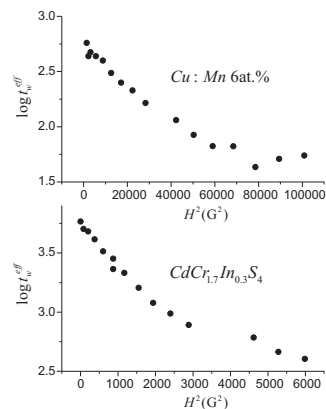
E_z magnetic energy associated with a change in magnetic field.

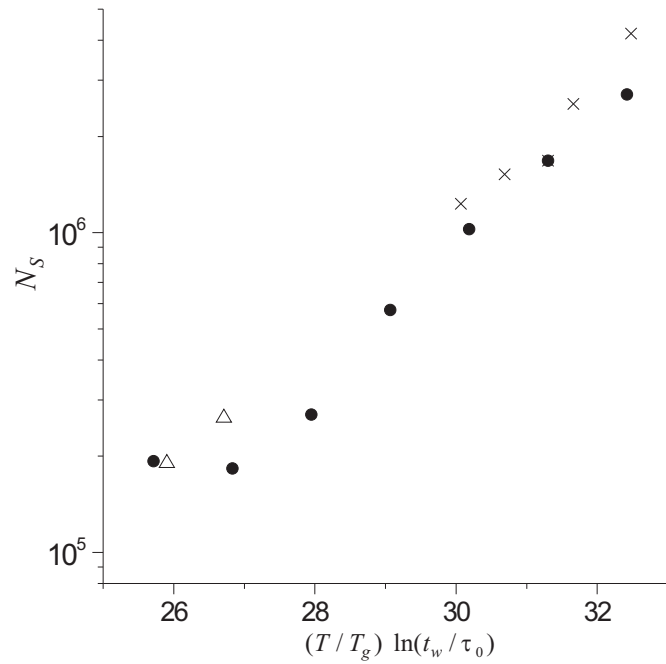
Number of spins participating in barrier hopping can be derived from,

$$E_z = N_s \chi_{fc} H^2 .$$

N_s defines a volume over which the spins are effectively locked.

It defines the radius of this region as the spin glass correlation length ξ . If N_s was the sum of small clusters the activation energy would be connected to small barriers, and $S(t)$ would not shift its peak.





N_S versus $\log t_w$ in log log scale.

A comparison of experimental and numerical results is really good.

Experiments find

$$\xi(t_w, T) = 0.653(t_w/\tau_0)^{0.169T/T_g}$$

to be compared with a prefactor of order one and an exponent estimated as $0.16T/T_g$ from our numerical simulations.

Also, the fact that this has built an experimental setting where a correlation length can be estimated is of very large importance.

Twenty years later...

(we know who D'Artagnan is, since the author, Alexandre Dumas, explains very well he eventually turned out to be a Nobel Laureate..)

Two joint paper among the Janus Collaboration and the Texas experimental group,

New computational and experimental facilities allowed us to push our understanding further.

From the Janus Collaboration + Texas:

Scaling law describes the spin-glass response in theory, experiments and simulations. Physical Review Letters 125 (2020) 237202.

Spin-glass dynamics in the presence of a magnetic field: exploration of microscopic properties, J. Stat. Mech. (2021) 033301 (with R. Orbach group).

Parallel study of non-equilibrium spin-glass dynamics both in an experiment in a CuMn single crystal and in a large-scale simulation of the EA model carried out on Janus 2.

Zero-field-cooled protocol: the spin glass is suddenly quenched from a temperature well above T_g down to the working temperature $T_m < T_g$ and is then left to relax for a time t_w .

The growth of the correlation length $\xi(t_w)$ is unbounded for $T < T_g$, but very slow.

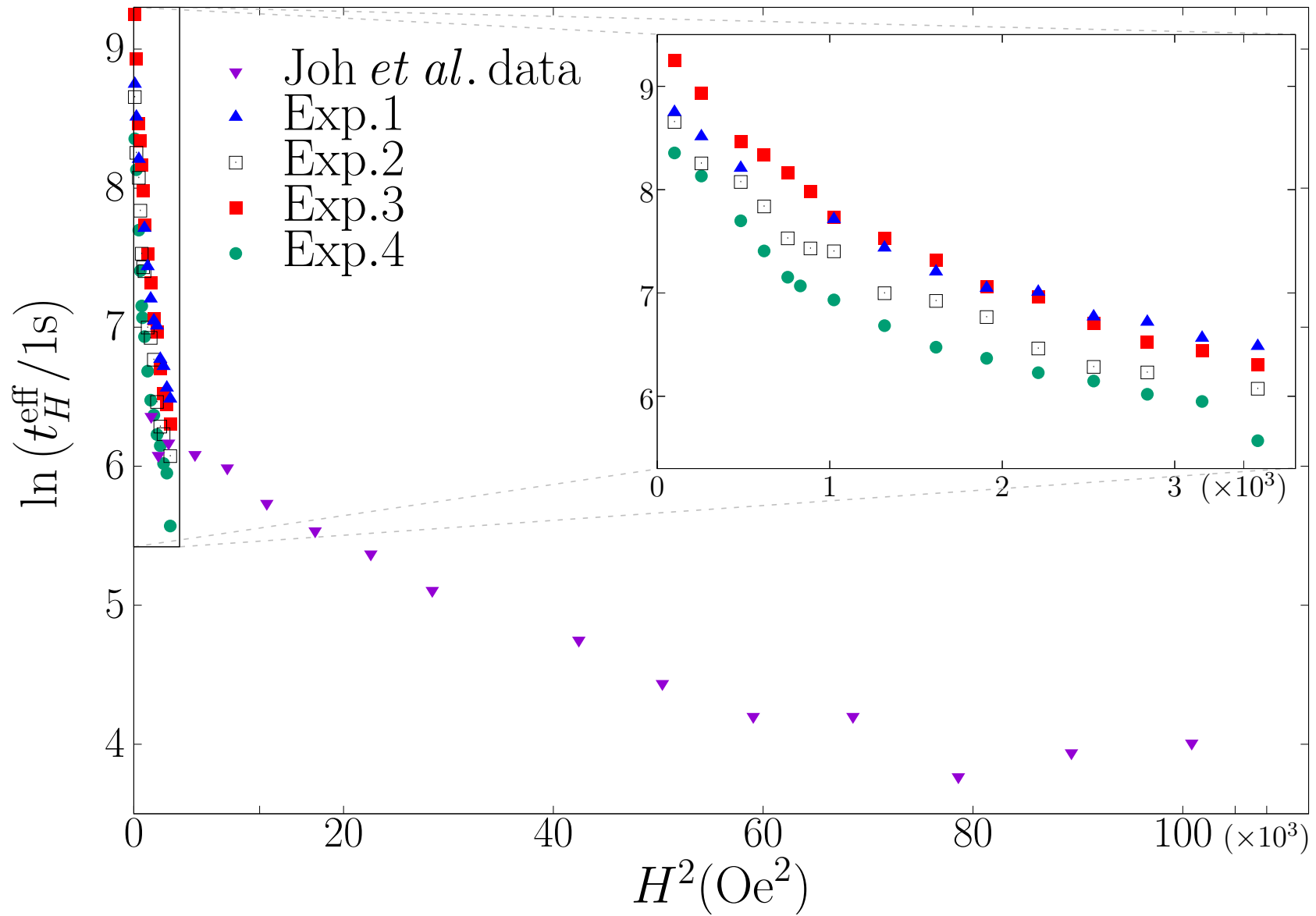
At time t_w , a magnetic field H is applied and the growing magnetization $M(t, t_w; H)$ is recorded up to time $t + t_w$ (the t_w dependence is included because spin glasses perennially age at $T < T_g$, slowly approaching equilibrium but never reaching it).

The maximum of the relaxation function $d(M/H)/d \log t$ defines a time t_H^{eff} directly related to the height of the free-energy barriers that the system encounters.

In a magnetic field, the Zeeman effect lowers these barriers by an amount proportional to H^2 and to the number of spins in a glassy cluster.

Therefore, an Arrhenius law would predict a linear behavior of $\log t_H^{\text{eff}}$ with H^2 .

Yet departures from a straight line are observed for large values of H^2 .



Experiments: measurements in a single CuMn crystal. The single crystal is important because the growth of $\xi(t_w)$ is not limited like in a poly-crystal with grain boundaries.

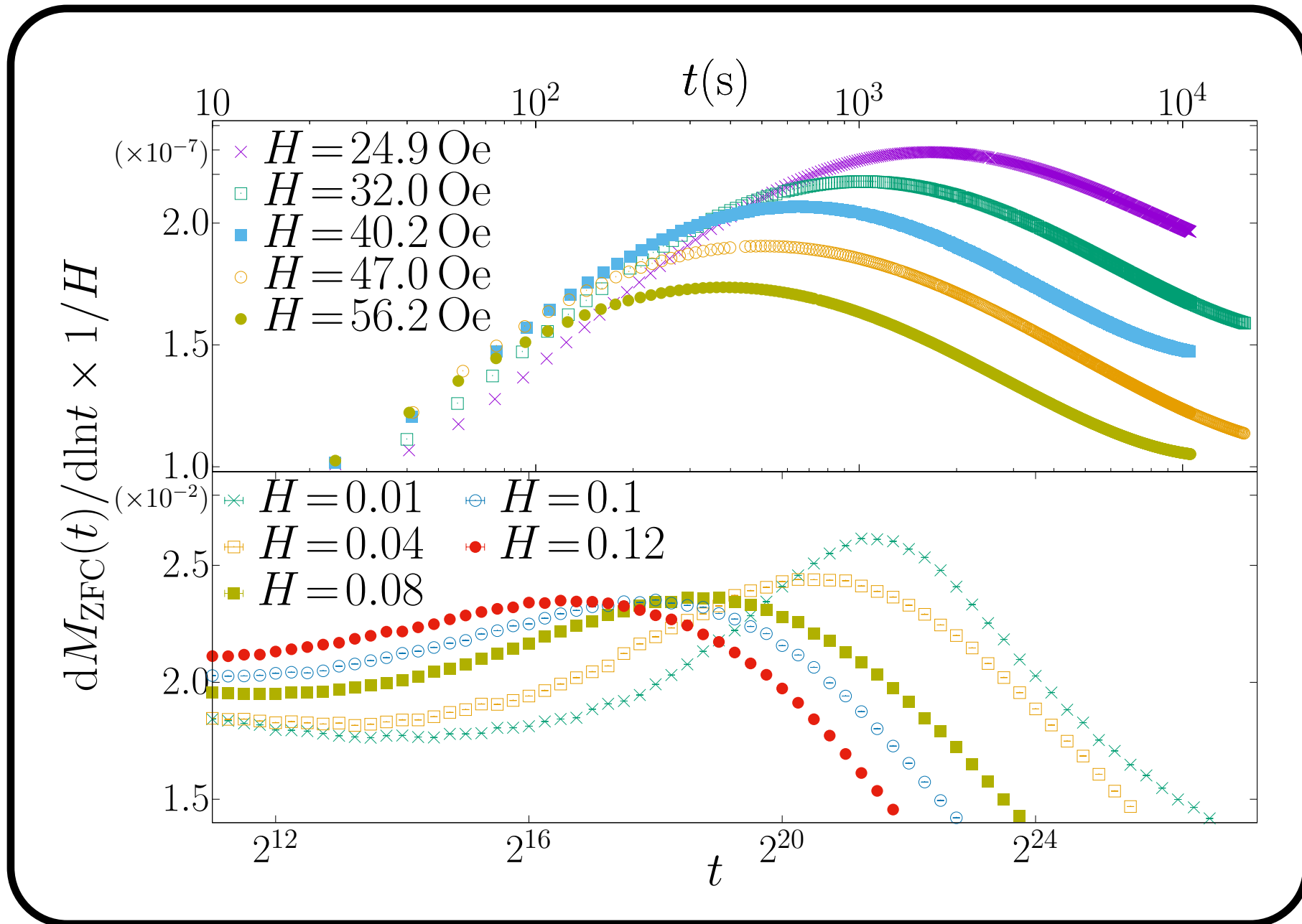
These detailed experimental data will allow us to derive and verify a **scaling law for the response to the magnetic field** that is still valid for large fields and close to T_g .

$$\ln \frac{t_H^{\text{eff}}}{t_{H \rightarrow 0^+}^{\text{eff}}} = \frac{\hat{S}}{T} \xi^{D - \frac{\theta}{2}} H^2 + \xi^{-\theta/2} \mathcal{G}(\xi^{D - \frac{\theta}{2}} H^2; T).$$

ξ is a function of t_w , \hat{S} is a constant, θ stands for the replicon exponent.

For small values of x the scaling function behaves as $\mathcal{G}(x) \sim x^2$ ($x = \xi^{D-\frac{\theta}{2}} H^2$): \mathcal{G} is of order H^4 for small values of the magnetic field and, if ξ is small (the typical case well below T_g), the contribution of \mathcal{G} can be neglected for small H .

Before this work it was typically only possible to test the H^2 term. We find here, however, that for larger fields, or larger correlation lengths (which are found only close to T_g), \mathcal{G} is the dominant contribution. This analysis offers a unified framework that rationalizes the entire range of experiment and simulations.



New Janus II numerics:

In order to **mimic the experimental setup** in the simulations an initial random spin configuration is placed instantaneously at the working temperature T_m

and left to relax for a time t_w , with $H = 0$.

At time t_w , the external magnetic field is turned on

and we record the magnetization $M(t, t_w; H)$ and the correlation function

$$C(t, t_w; H) = \sum_{\mathbf{x}} s_{\mathbf{x}}(t_w; H = 0) s_{\mathbf{x}}(t + t_w; H) / V ,$$

where $V = 160^3$.

Mismatch of experimental and numerical scales. A common issue. Normally for example the time you can reach in a numerical simulation is far smaller of the one you can reach in experiments.

Experimental range (16 Oe to 59 Oe) corresponds to $0.0003 \lesssim H \lesssim 0.0012$ in the IEA model,

but the signal-to-noise ratio limited our simulations to $H \geq 0.005$.

We used two main ideas to match these scales.

1. we can use dimensional analysis. Reduced temperature:

$$\hat{t} = (T_g - T)/T_g$$

$$\hat{t}_{\text{num}} \approx \hat{t}_{\text{exp}} \left(\frac{H_{\text{num}}}{H_{\text{exp}}} \right)^{\frac{4}{\nu(5-\eta)}},$$

where $\nu = 2.56(4)$ and $\eta = -0.390(4)$ are $H = 0$ critical exponents.

We have selected $T_m = 0.9$ and $T_m = 1.0$.

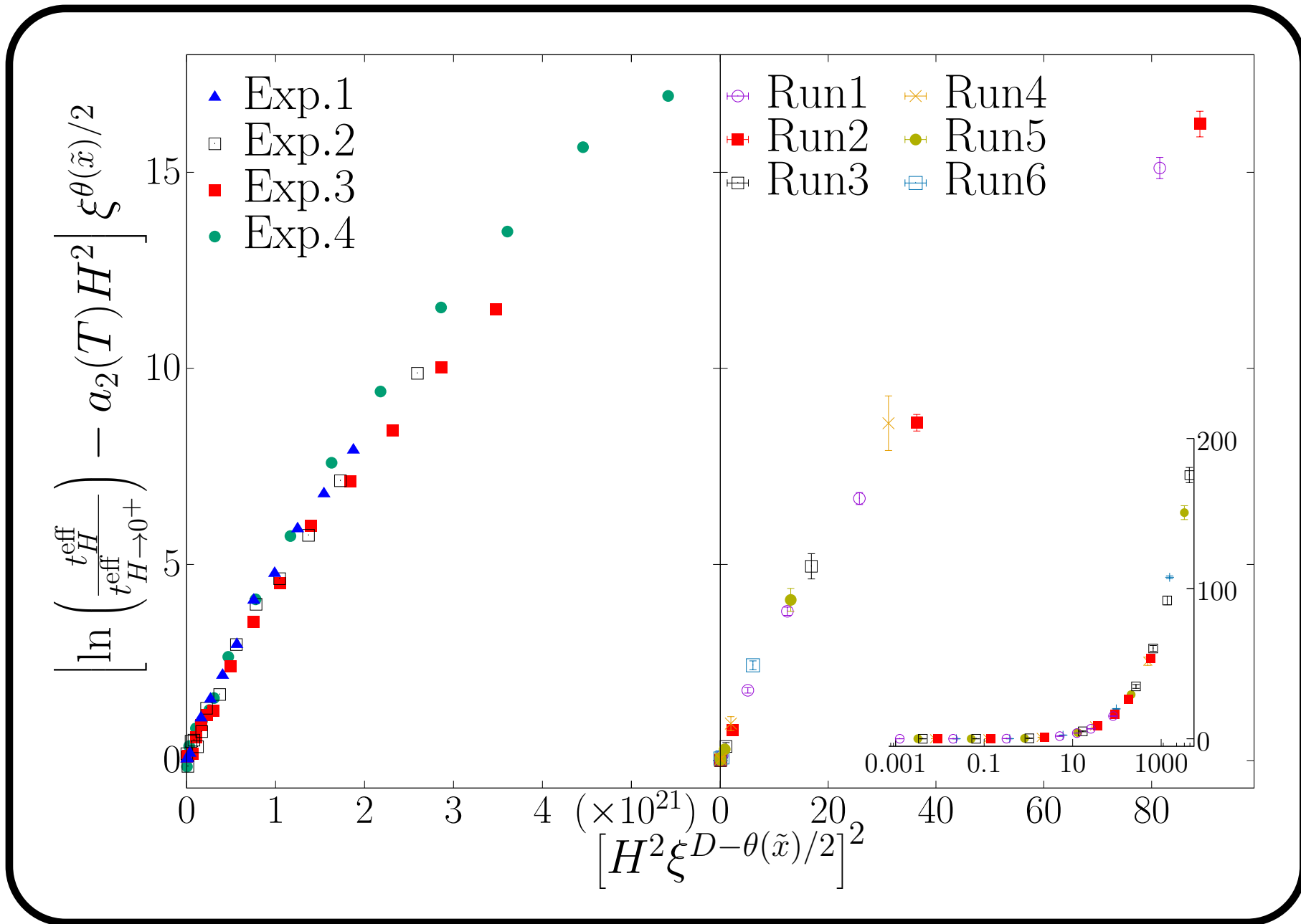
2. Use the correlation function as time scale. (connected to Cugliandolo Kurchan ideas).

When $H \rightarrow 0$, $C(t, t_w; H) \rightarrow C_{\text{peak}}$ which suggests estimating t_H^{eff} in the simulations from

$$C(t_H^{\text{eff}}, t_w; H) = C_{\text{peak}} .$$

As we can see in the figure in next slide **the scaling law is perfectly verified both for numerical and for experimental data.**

There is consistency of experimental data and RSB theory for a very large spectrum of values of the magnetic field.



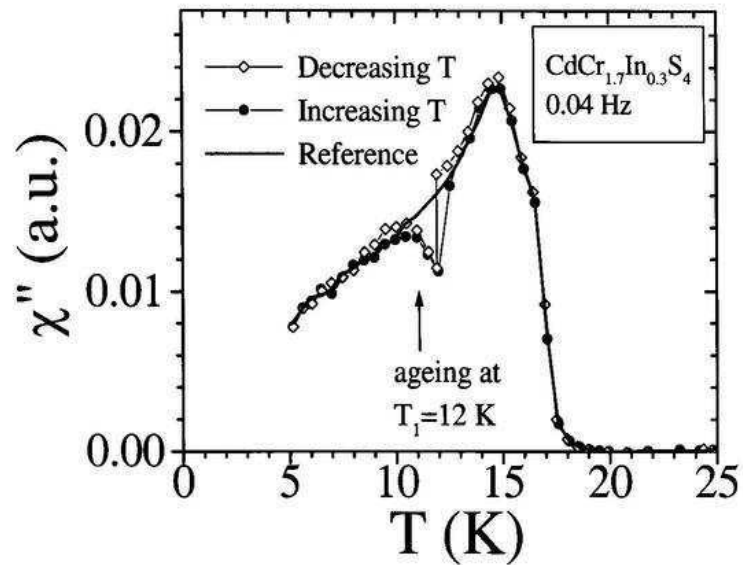
What is next?

A lot...

I gave a few details about what is going on in the last years at the start of the talk.

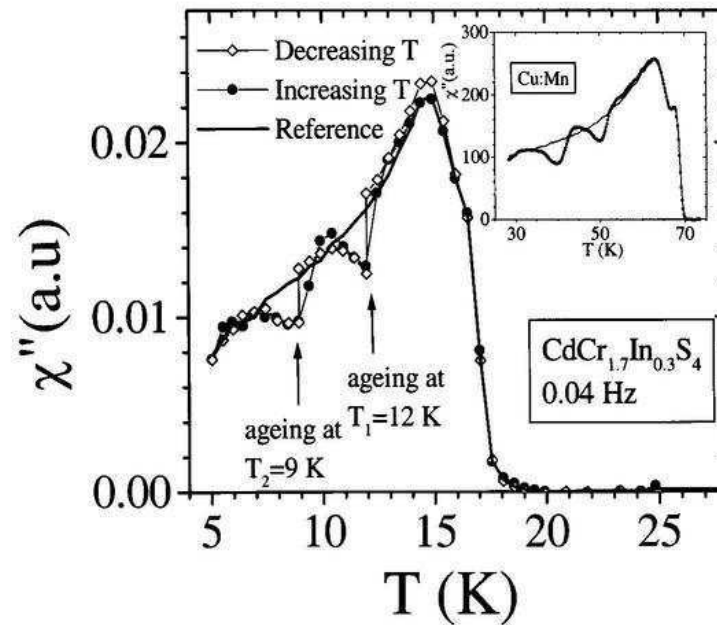
Now I only want to stress **Temperature Chaos** (a very crucial phenomenon, that can teach us a lot about the structure of the stable states of the system) and **Memory**.

In both these cases new numerical experiments are giving new information and hopefully paving new roads.



PRL 81(1998)3243 FIG. 1

K. Jonason, E. Vincent, J. Hammann, J.P. Bouchaud, P. Nordblad,
Memory and Chaos Effects in Spin Glasses, PRL 1998.



PRL 81 (1998) 3263 FIG. 2

K. Jonason, E. Vincent, J. Hammann, J.P. Bouchaud, P. Nordblad,
 Memory and Chaos Effects in Spin Glasses, PRL 1998.

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