Large scale simulations of spin glasses

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Plan of the talk:

- The definition of spin glasses.
- Why simulations in spin glasses are challening.
- The physics of spin glasses.
- Algorithmic tricks: annealing and temperings.
- The Janus computers.
- Off-equilibrium Fluctuation Dissipation Relations.

Spin glasses Let us consider for example a cubic lattice in D dimension.

- $U(i,\mu) = \pm 1$ is a Z_2 gauge field on the lattice at infinite temperature:
- $\sigma_i = \pm 1$ is a Z_2 matter field,.
- The Hamiltionian is

$$H_U(\sigma) = -\sum_{i,\mu} \sigma(i) U(i+\mu) \sigma(i+\mu) - \sum_i h\sigma(i)$$

  In the nutshell we have non-linear sigma model of the Z_2 in presence of a symmetry breaking field h.

Comments:

- We are interested to compute the quenched free energy

$$F(\beta) = \beta^{-1} \overline{\ln(Z_U(\beta))} \qquad Z_U(\beta) = \sum_{\{\sigma\}} \exp(-\beta H_U(\sigma))$$

- At $h = 0$ to find the minimum of $H_U(\sigma)$ is equal to find the Landau gauge, σ being the gauge fixing (usually denoted with g.
- Gribov ambiguity $\Longleftrightarrow$ many minima of $H_U(\sigma)$.

Find the minimum of $H_J(\sigma)$ is computational difficult: it is an NP complete problem.

In $D = 3$ there are algorithms that take a time proportional to

$$2^L$$

for a system with L^3 spins.

At low temperature, the thermalization time, measured in Montecarlo sweep, increases roughly as

$$L^{10}$$

(We denote by J the quenched gauge field: not U as before.)

This model (Edwards Anderson model) describes schematically what happens in real materials (e.g. metallic alloys). The name spin glass comes from the very slow *glassy* relaxation of spins.

In the limit where the space dimensions D goes to infinity, the model is soluble at equilibrium (mean field theory and we have good information on non-equilibrium properties.

The typical spins flip time is 10^{-12}. Many experiments are seeing time relaxations of hours (i.e 10^{16} spin flip times).

For a given sample the control parameters that can be changed during experiments are the temperature and magnetic field.

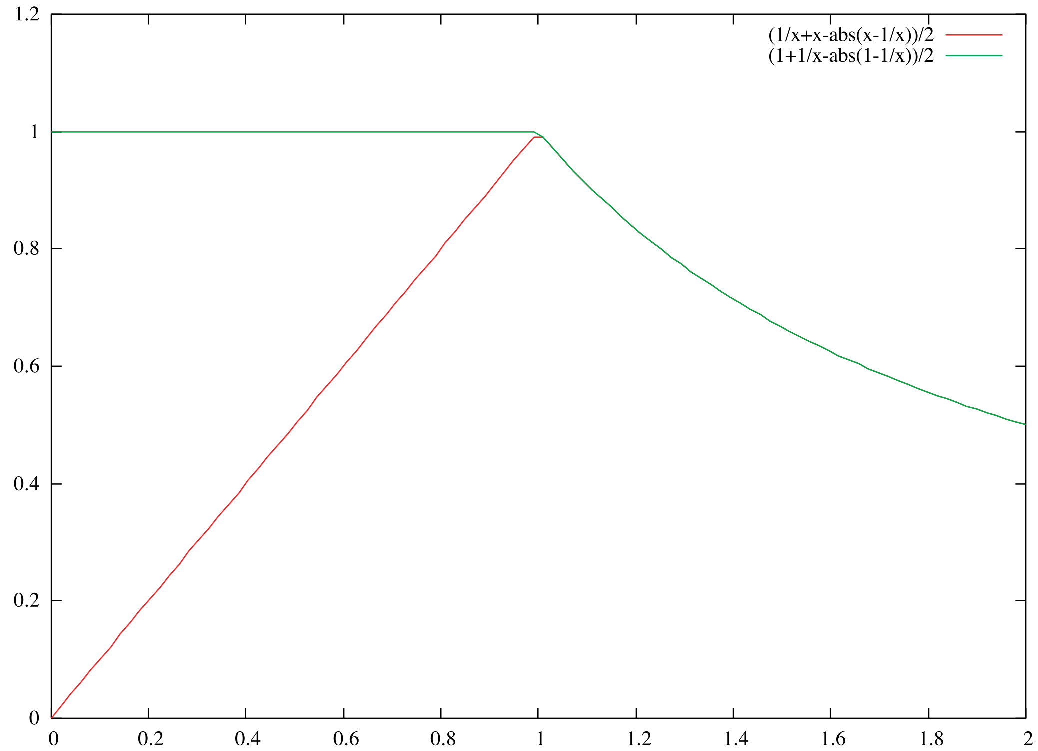
The most popular observable is the magnetization, that can be measured quite accurately with a SQUID.

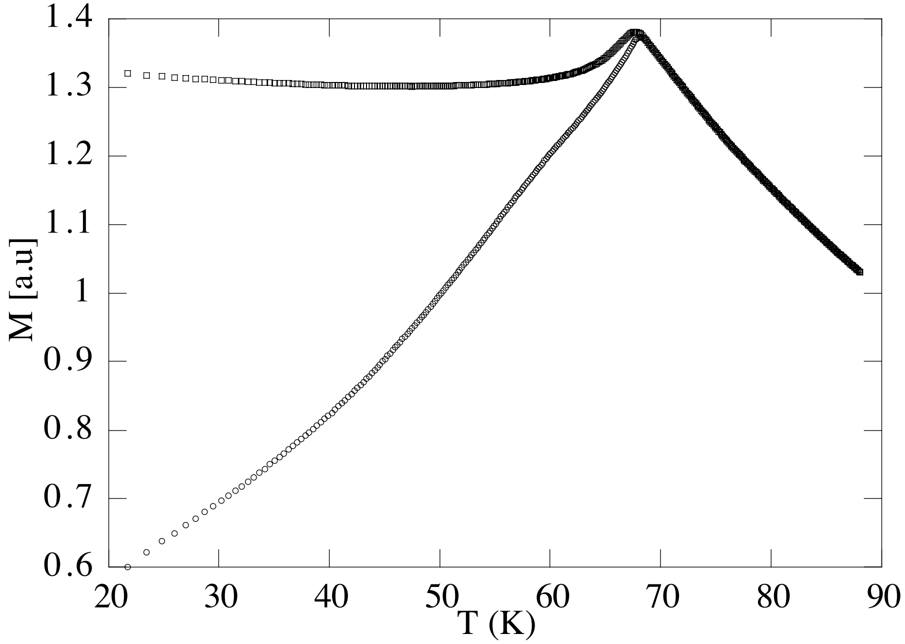
We can define two physically relevant magnetic susceptibilities.

χ_{LR}, i.e. the magnetic response within a state, that is observable when one changes the magnetic field at fixed temperature and one does not wait too much.

χ_{eq}, the true equilibrium magneticsusceptibility, that is very near to χ_{FC}, the field cooled susceptibility, where one cools the system in presence of a field.

The difference between the two susceptibilities is the hallmark of very slow relaxation replica symmetry breaking.





At the left we show the results in mean field, at the right we have the experimental data on metallic spin glasses. The similarities among the two are striking.

Using gauge invariance, the susceptibility is given by

$$\chi = \beta(1 - \langle m^2 \rangle) \qquad \langle m^2 \rangle = \frac{1}{V} \sum_i m(i)^2$$

.

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According to mean field theory the system may stay in different states labeled by α, with a probability given by w_α. Each state has a different local magnetization

$$\langle \sigma(i) \rangle_\alpha = m(i)_\alpha \qquad q_{EA} \equiv \frac{1}{V} \sum_i m(i)_\alpha^2$$

$$d_{\alpha,\gamma} = \frac{1}{V} \sum_i (m(i)_\alpha - m(i)_\gamma)^2 = 2(q_{EA} - q_{\alpha,\gamma}) \qquad q_{\alpha,\gamma} = \frac{1}{V} \sum_i m(i)_\alpha m(i)_\gamma$$

In the experimental available times, the system is confined in one state the average squared magnetization is high $\chi = \beta(1 - q_{EA})$.

When we average over all these regions, the average magnetization is much smaller; $\chi = \beta(1 - \overline{q})$:

$$\overline{q} = \sum_{\alpha,\gamma} w_\alpha w_\gamma q_{\alpha,\gamma}$$

The onset of irreversibility is a *bona fide* critical point for a second order phase transition. We can write for the total magnetization density $m(h)$

$$m(h) = \chi h + \chi_3 h^3 + \chi_5 h^5 + \dots$$

The non-linear susceptibility χ_3, the correlations length ξ and the relaxation time τ diverge as

$$\chi_3(T) \propto \frac{1}{(T-T_c)^\gamma} \qquad \xi(T) \propto \frac{1}{(T-T_c)^\nu} \qquad \tau(T) \propto \frac{1}{(T-T_c)^{z\nu}}$$

The values of the exponents are peculiar:

$$\gamma = 6.1 \pm 0.1 \quad \nu = 2.56 \pm 0.04 \quad z = 6.8 \pm 0.1$$

How to thermalize below T_c?

Think of a gauge theory: the free energy depends on the number of instantons.

If transitions among different topological sectors are exponentially depressed at large β, how to get the right distribution of instantons?

- Annealing: slow cooling from above T_c. Not good: it goes into a random state!
- Simulating tempering. The temperature is a dynamic quantity. Let us put $\beta = 1$ in the probability distribution and use an effective Hamiltonian

$$\beta_n H_J[\sigma] + g_n$$

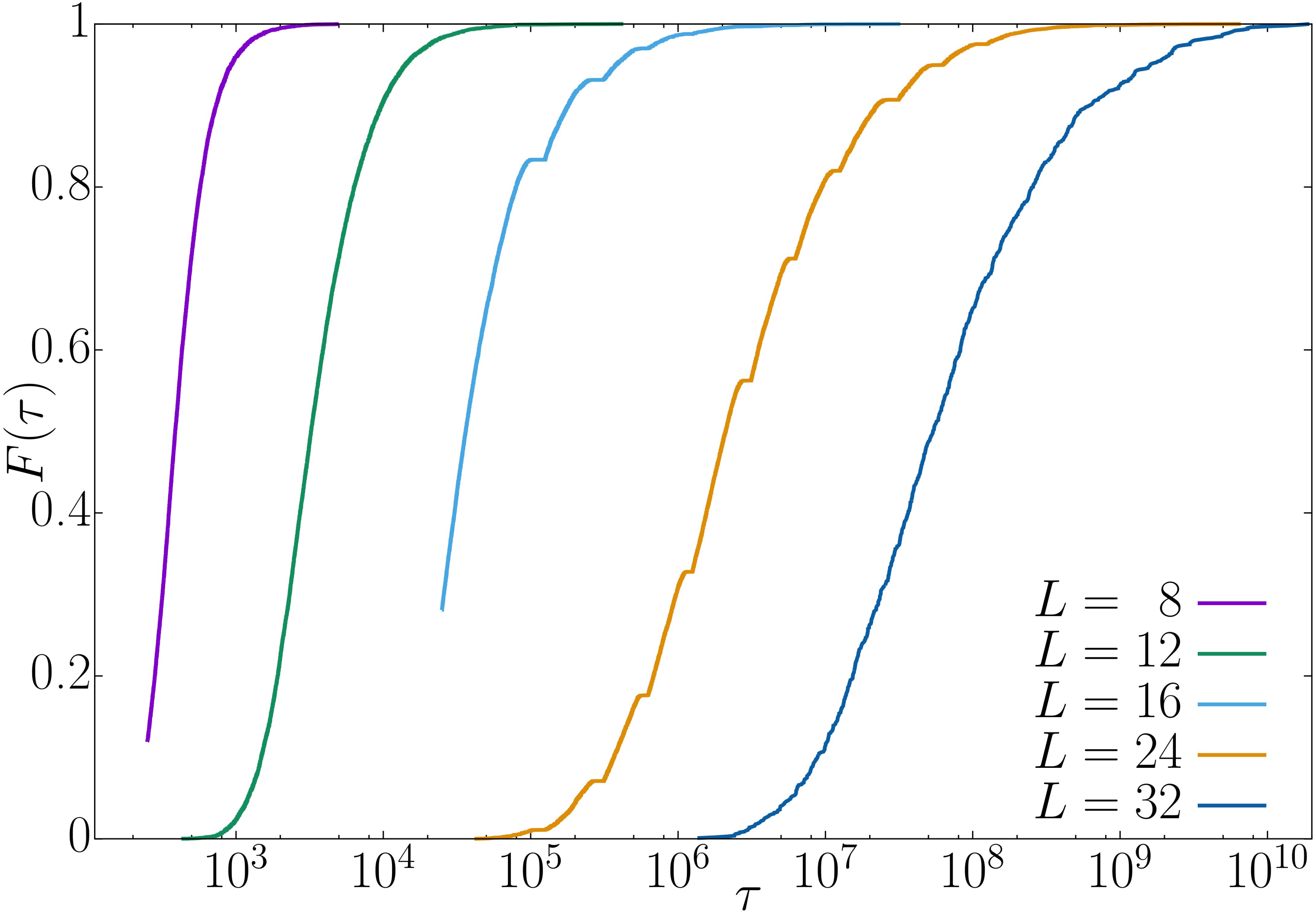
where g_n are tuned in such a way that the systems make a random walk in temperature. OK but we have to tune g_n.

- Parallel tempering. We introduce K copies of the system. The effective Hamiltonian is

$$\sum_{n=1,K} \beta_n H_J[\sigma_n]$$

We add a **swap** move $\sigma_n \Longleftrightarrow \sigma_{n+1}$

$$\Delta H = (\beta_n - \beta_{n+1})(H_J[\sigma_n] - H_J[\sigma_{n+1}])$$



Decorrelation time in units of Montecarlo sweep for different values of L in $D = 3$.

Fast computers: Janus I and Janus II.

JANUS uses a dedicated processor architecture and uses Field Programmable Gate Arrays (FPGA) as the enabling technology to implement that architecture. FPGAs are integrated circuits that can be configured at will after they have been assembled in an electronic system.

The selected FPGA has some 485000 logic cells and includes $\sim$ 32 Mbit embedded memory. We embed within each FPGA about than 2000 spin-flip engines, each updating one spin in one clock cycle. This corresponds to an average update rate of 1 spin every 2.5 ps for each spin-flip engine.

A set of 16 SPs are mounted onto a *Processing Board*. All SPs belonging to each PB are directly connected and controlled by a Control Processor (CP). The CP is a full-fledged computer, running the Linux operating system. We have a system with 16 Processing Boards, installed at BIFI in Zaragoza.

At the end: about 10^{14} spin flips per second.

About 10^{14} spin flip per second.

We are interested in systems of size up to $160^3 \approx 10^7$ spins in order not to have finite size effects. Target total time of 10^{11} Montecarlo sweep, roughly speaking 0.1 seconds.

We need to average over many systems to get high statistics: we are interested to the magnetization at small magnetic field h: the signal is proportional to h and the noise is independent on h.

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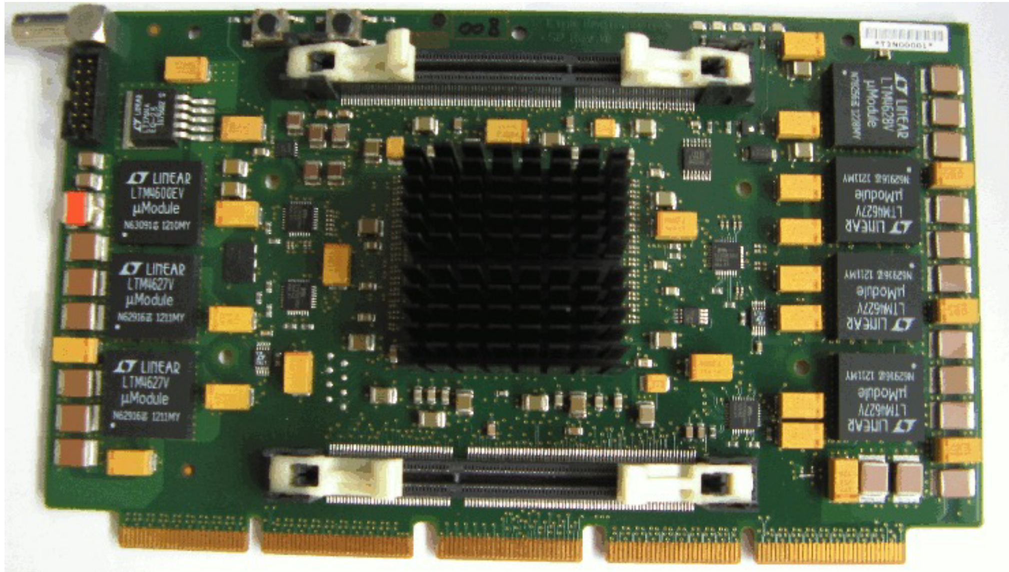
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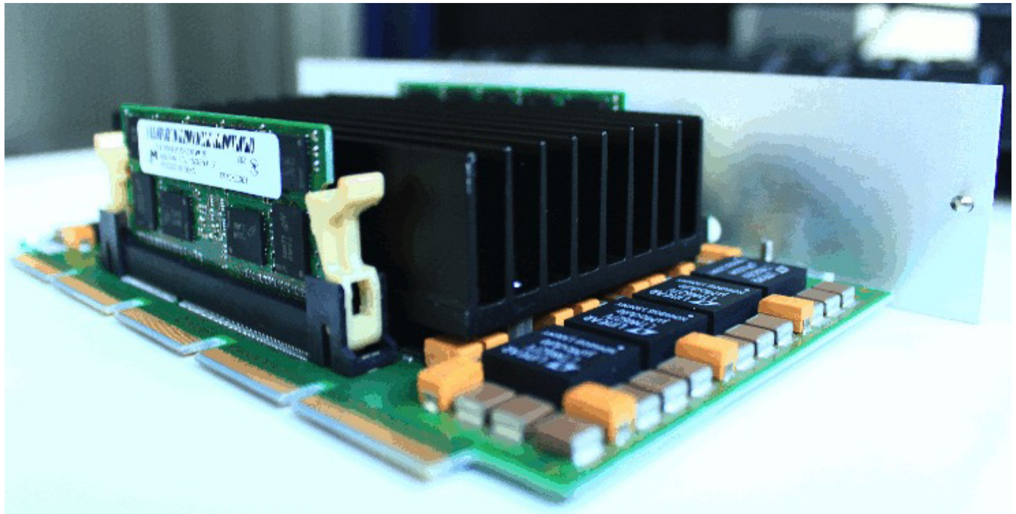


Off-equilibrium observables

We suddenly cool a three-dimensional spin-glass sample from high temperature to the working temperature at the initial time $t_{\mathrm{w}} = 0$.

During the non-equilibrium relaxation a coherence length $\xi(t_{\mathrm{w}})$ grows, which is representative of the size of the spin-glass domains.

Then, from the waiting time t_{w} on, we place the system under a magnetic field of strength H, and consider the response function at atime $t + t_{\mathrm{w}}$

$$\chi(t + t_w, t_{\mathrm{w}}) = \left. \frac{\partial m(t + t_{\mathrm{w}})}{\partial H} \right|_{H=0}$$

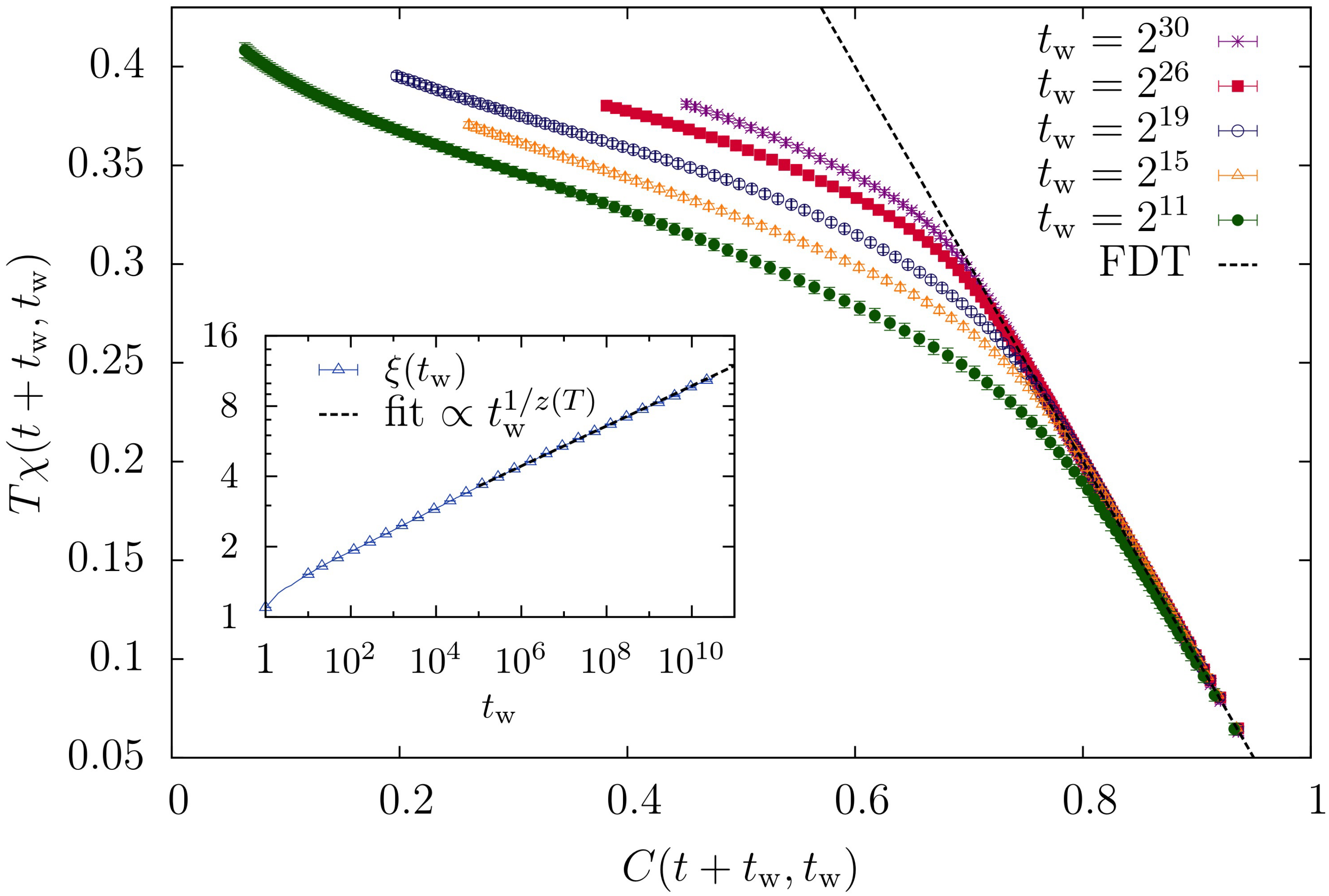
where $m(t + t_{\mathrm{w}})$ is the magnetization density.

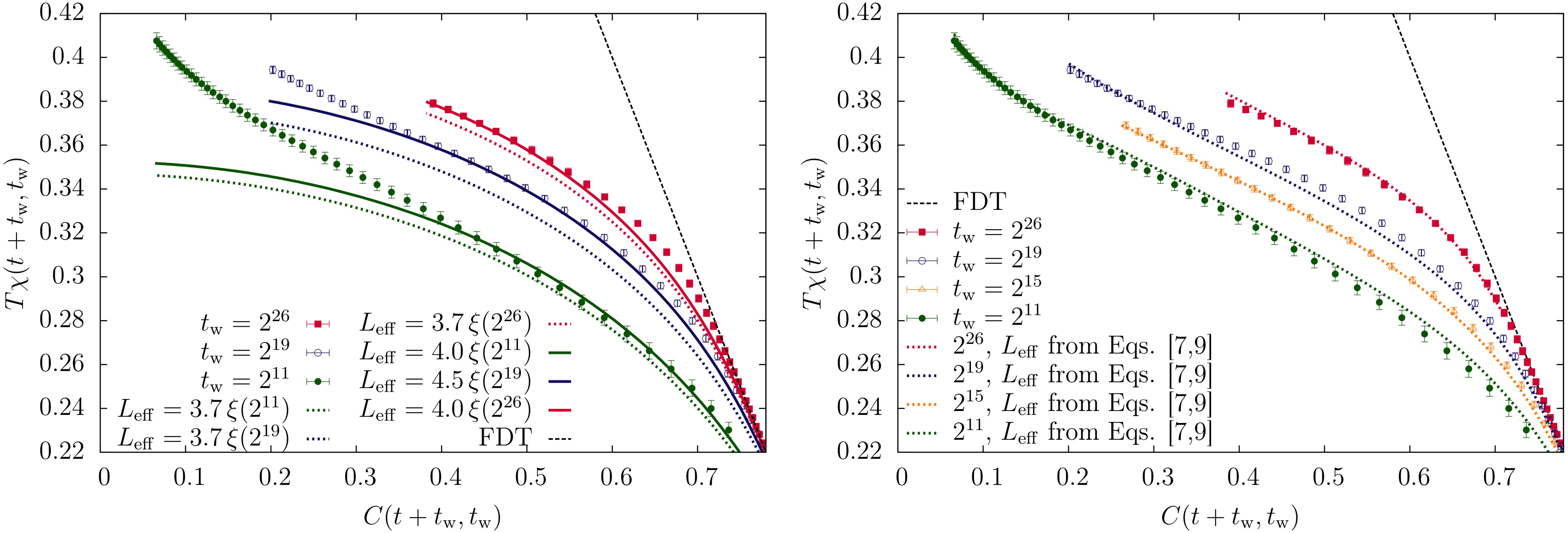
The correlation function $C(t + t_w, t_{\mathrm{w}})$ is defined as

$$C(t + t_w, t_{\mathrm{w}}) = \frac{1}{V} \sum_i \sigma_i(t)\sigma_i(t_w)$$

$$\chi(t + t_w, t_\mathrm{w}) = X(C(t + t_w, t_\mathrm{w}))$$

Naive prediction: the function X can be computed from equilibrium simulations





$T\chi(t+t_\mathrm{w},t_\mathrm{w})$
$C(t+t_\mathrm{w},t_\mathrm{w})$
$t_\mathrm{w}=2^{26}$
$t_\mathrm{w}=2^{19}$
$t_\mathrm{w}=2^{11}$
$L_\mathrm{eff}=3.7\,\xi(2^{11})$
$L_\mathrm{eff}=3.7\,\xi(2^{19})$
$L_\mathrm{eff}=3.7\,\xi(2^{26})$
$L_\mathrm{eff}=4.0\,\xi(2^{11})$
$L_\mathrm{eff}=4.5\,\xi(2^{19})$
$L_\mathrm{eff}=4.0\,\xi(2^{26})$
FDT
$T\chi(t+t_\mathrm{w},t_\mathrm{w})$
$C(t+t_\mathrm{w},t_\mathrm{w})$
FDT
$t_\mathrm{w}=2^{26}$
$t_\mathrm{w}=2^{19}$
$t_\mathrm{w}=2^{15}$
$t_\mathrm{w}=2^{11}$
2^{26}, L_eff from Eqs. [7,9]
2^{19}, L_eff from Eqs. [7,9]
2^{15}, L_eff from Eqs. [7,9]
2^{11}, L_eff from Eqs. [7,9]

Wishing list

- Faster algorithms (we use algorithms more than 20 years old).
- Faster hardware and maybe flexible:

  Janus III?

  Special purpose processor?

  GPU clusters?
- New theoretical predictions for new observables.