

Quantum versus Thermal annealing, the role of Temperature Chaos

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Janus Collaboration

In collaboration with Itay Hen (Information Sciences Institute, USC).

CPRCS 2014, Capri, September 10 2014.

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Is **quantum computing** our breakthrough?

- 1 Desperate problem, desperate solutions: the **Janus** computer.
- 2 The **temperature chaos** algorithmic wall.
- 3 A more conventional approach to temperature chaos.
- 4 **D-wave**, the chimera lattice and temperature chaos.

The Janus Collaboration

Team from 5 universities in Spain and Italy:

- **Universidad Complutense de Madrid:**
M. Baity-Jesi, L.A. Fernandez, V. Martin-Mayor, A. Muñoz Sudupe
- **Universidad de Extremadura:**
A. Gordillo-Guerrero, J.J. Ruiz-Lorenzo
- **Università di Ferrara:**
M. Pivanti, S.F. Schifano, R. Tripiccone
- **La Sapienza Università di Roma:**
A. Maiorano, E. Marinari, G. Parisi, F. Ricci-Tersenghi, D. Yllanes, B. Seoane
- **Universidad de Zaragoza:**
R.A. Baños, A. Cruz, J.M. Gil-Narvión, M. Guidetti, D. Iñiguez, J. Monforte-Garcia, D. Navarro, S. Perez-Gavero, A. Tarancon, P. Tellez.



Physicists and engineers dedicated to the design and exploitation of special-purpose computers, optimised for Monte Carlo simulations in condensed matter physics.

Desperate problems, desperate solutions: Janus (I)

Even with binary spins, simulation of spin-glasses is heavy in **two respects**:

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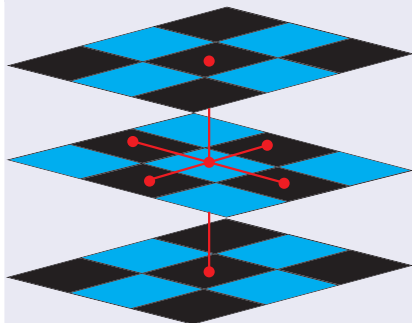
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Modern architectures (GPU, Xeon, Xeon- ϕ) efficient **only for larger N**
 \rightarrow astronomical number of updates ($\sim e^{cN}$, probably).

Desperate problems, desperate solutions: Janus (II)

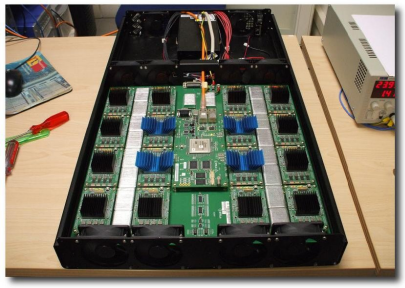
Parallelizable problem



- Parallelise within each instance
- We divide the lattice in a checkerboard scheme, all sites of the same colour can be updated simultaneously
- Memory bandwidth: 13 bits to update one bit! Only solution: Memory **“local to the processor”**.

Desperate problems, desperate solutions: Janus (II)

Parallelizable problem



FPGA opportunity window:

- Large on-chip memory (several Mbits).
- Huge bandwidth on-chip “distributed” memory (~ 10000 bits in and out per clock cycle).
- Large amount of logic \rightarrow 1024 Spin-Update Engines.

Janus 1 (2008): $\times 1000$ boost in spin-glasses simulations.

Green computer: $\times 0.001$ energy consumption per update.

Janus 2: **Fall 2014**

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- ...
- **Temperature chaos**

Temperature chaos: the showstopper (I)

Increasing computing speed $\times 1000$, not such a big deal

- Pre-Janus era: up to $N = 16^3$ spins.
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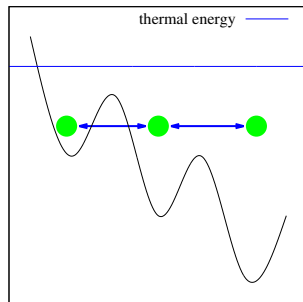
- Simulating at **fixed** temperature, simply not enough.
- **Temperature** needs to become **dynamic**.

Temperature chaos: the showstopper (II)

Simulated Annealing

Simplest protocol:

- 1 High T : easy exploration

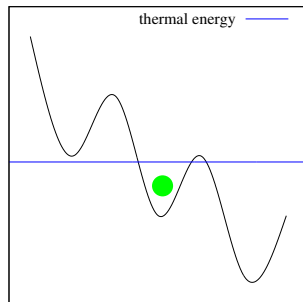


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Trapped at nearby local minimum.



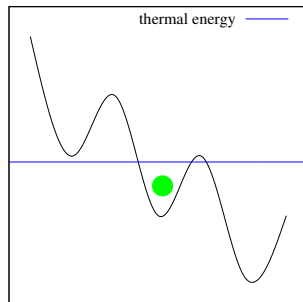
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Outdated algorithm.

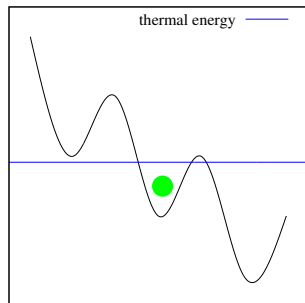


Temperature chaos: the showstopper (III)

Parallel Tempering

T raised or lowered:

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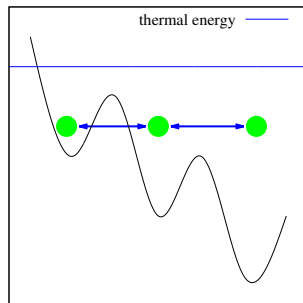


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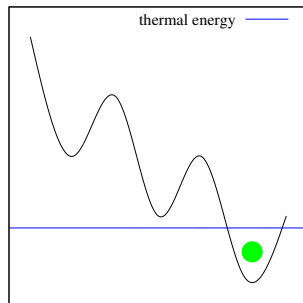


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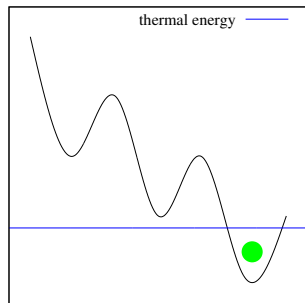


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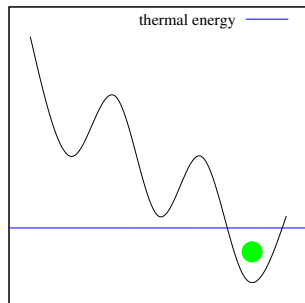
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- N_T temperatures: simultaneous simulation of N_T clones (one at each temperature).
- Periodically, clones attempt to exchange their temperature. The rule preserves detailed balance.

Temperature chaos: the showstopper (IV)

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Each clone performs a temperature Random Walk.

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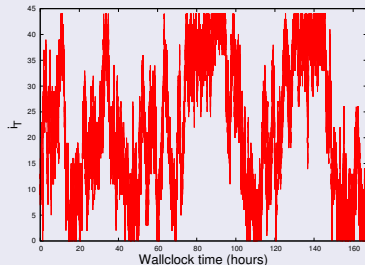
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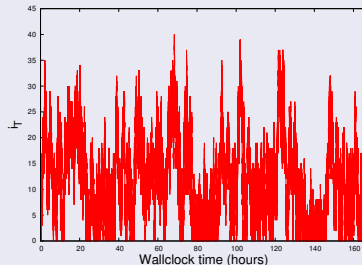
The simulation is *long enough* if all the clones visited all the temperatures several times. Mixing time: τ .

Random Walk in temperatures of a clone

A mixing Random Walk

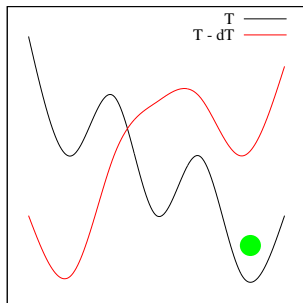


A stuck Random Walk



Temperature chaos: the showstopper (V)

Temperature chaos: Relevant minima, completely different at nearby temperatures. T -random walk refuses to go across.

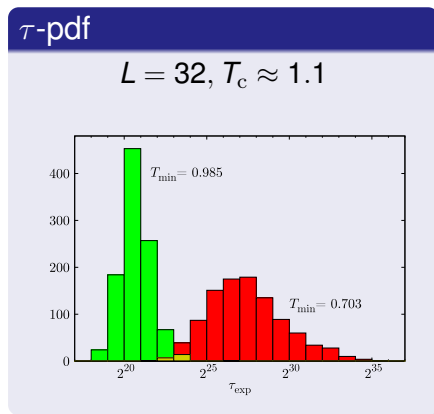


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\mathcal{T} : Operational definition of Temperature chaos.

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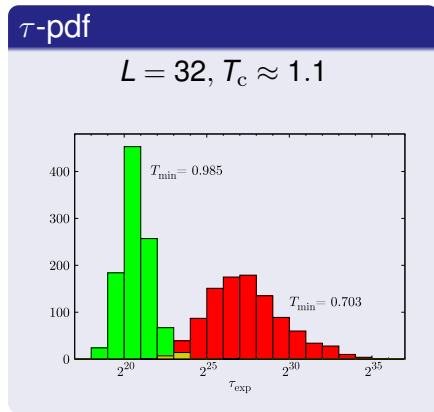
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- Extreme sample-to-sample fluctuations.

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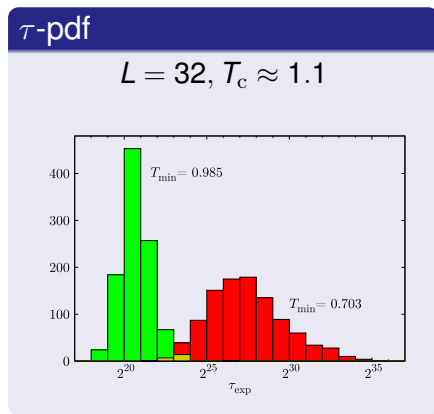
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- Extreme sample-to-sample fluctuations.
- L and T sensitivity.

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τ : Operational definition of Temperature chaos.



- Extreme sample-to-sample fluctuations.
- L and T sensitivity.
- At variance with standard T -chaos studies, it is **easy** to observe the effect.

Contacting with conventional approach (I)

Defining T -chaos through a Markov MC dynamics is:

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- Unsatisfying: T -chaos is supposed to be a **static** effect!

However, it provides a **useful** definition. Instead, the static approach:

- Hard for some analytically tractable models.
Sherrington-Kirkpatrick: Rizzo-Crisanti (2003)
Migdal-Kadanoff: McKay, Nihat-Berker, Kirkpatrick, (1982).
- Numerically, very hard to identify. Scaling laws barely known
(Katzgraber & Krzakala, 2007).
- We still lack predictions relevant for experiments.

Contacting with conventional approach (II)

Our main ingredients (Fernandez, V.M.-M,Parisi,Seoane, 2013)

- **Janus data base** (2010): $\mathcal{O}(10^3)$ samples, $L \leq 32$, well thermalized at low temperatures.
- Wash-out thermal fluctuations (Ney-Nifle and Young, 1997)
- Look at whole distribution (not only average!)
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Consistency checks:

- Must correlate with dynamic approach
- Previously *subtle* effects should become visible.

Washing-out thermal fluctuations

Useful technicality: the **chaotic parameter**

$$X_{T_1, T_2}^J = \frac{\langle q_{T_1, T_2}^2 \rangle_J}{\sqrt{\langle q_{T_1, T_1}^2 \rangle_J \langle q_{T_2, T_2}^2 \rangle_J}}$$

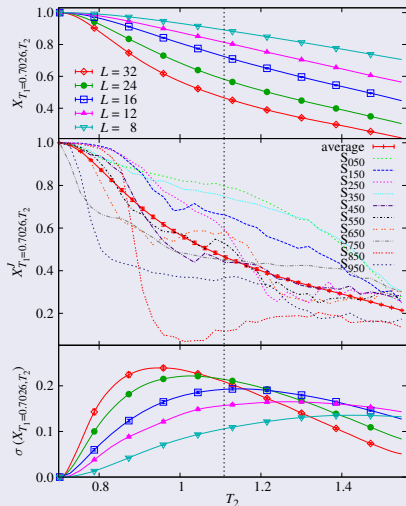
$X^J = 1 \rightarrow$ no chaos; $X^J = 0 \rightarrow$ strong chaos.

Mind that, for $T_1, T_2 < T_c$ and large L , one expects

$$X_{T_1, T_2}^J \sim \langle q_{T_1, T_2}^2 \rangle_J$$
$$\langle q_{T_1, T_1}^2 \rangle_J \sim \langle q_{T_2, T_2}^2 \rangle_J \sim 1.$$

Contacting with conventional approach (IV)

Average or full distribution?



- **Expectations:**

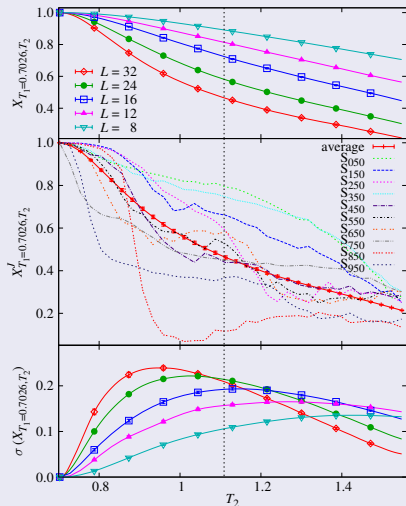
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- $T_2 > T_c$: nothing happens.

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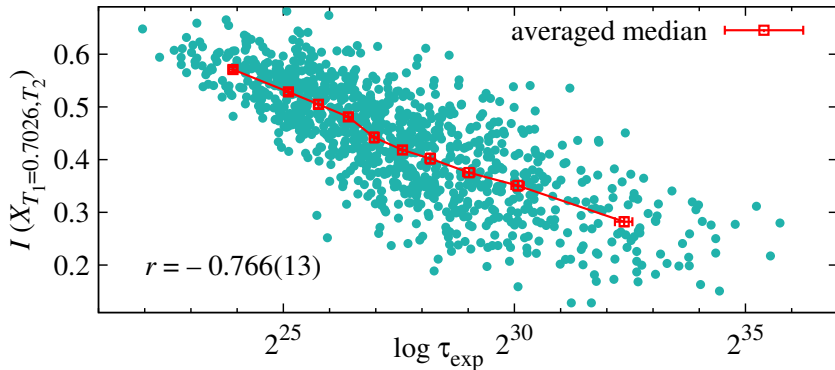
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- In the **slowest samples** we identify **chaotic** events (\sim level-crossings in Quantum Mechanics).

$$I_J = \int_{T_{\min}}^{T_{\max}} dT_2 X_{T_{\min}, T_2}^J$$

Contacting with conventional approach (V)

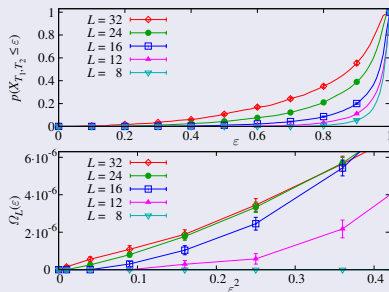
I_J **correlates** with τ ! We are on the right track...



Contacting with conventional approach (VI)

Large deviations functional

3D, $T_1 = 0.7$, $T_2 = 0.84$, ($T_c = 1.1$).



$$\Omega_L(\epsilon, T_1, T_2)$$

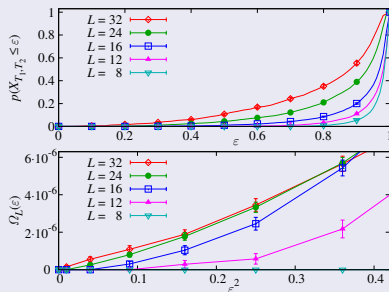
$$\text{Probability}[X_{T_1, T_2}^J > \epsilon] = e^{-L^D \Omega_L(\epsilon)}$$

- $\Omega > 0 \rightarrow$ **chaos!**

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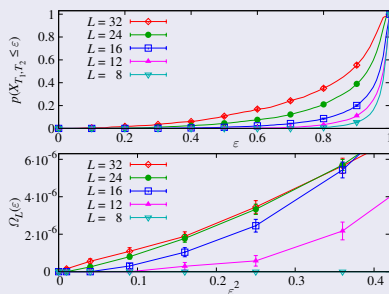
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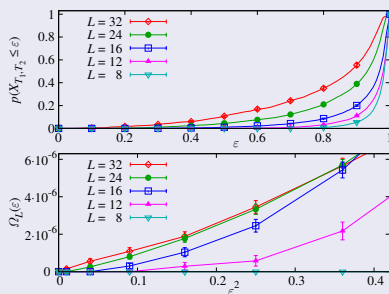
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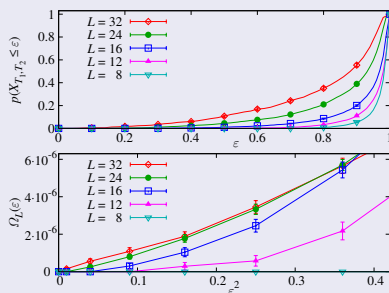
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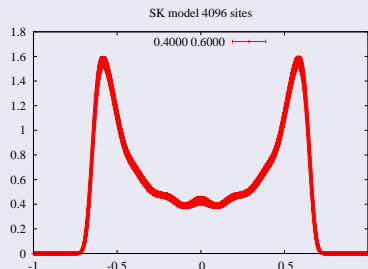
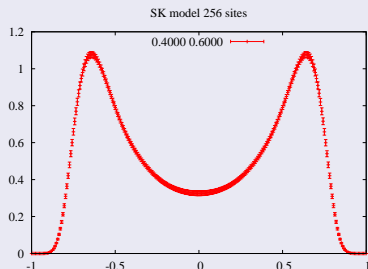
Weak-chaos scaling (Katzgraber & Krzakala, 2007) explained: $\zeta = D/b = 1.07(2)$

Chaos length: $\xi_C = L^a$ unless $\beta = 1$.

Contacting with conventional approach (VII)

SK finally yields to numerics (Billoire 2014)

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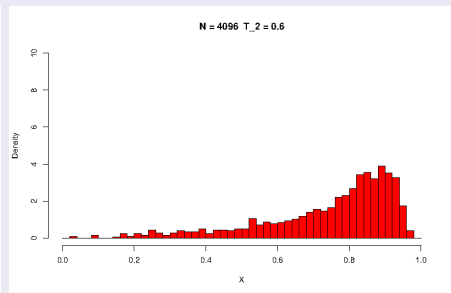
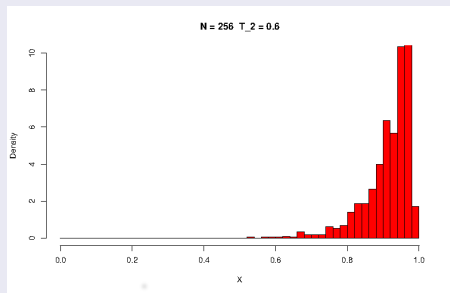


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But $\Omega(X_{T_1, T_2}^J > \epsilon) \gg \tilde{\Omega}(q_{T_1, T_2})$ (see also Rizzo 2014)



Take-home messages

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- Dynamic methods might be preferable in real calculations.
- **Three** (rather than 2) scaling variables: N , ΔT and ϵ .
- Temperature chaos is **generic** for large problem size N .
- In practice, specially for small N :
 - 1 The large majority of problem instances are *easy* (small τ).
 - 2 For some of them, though, τ inordinately large.
 - 3 The larger is N , the more frequently missbehaving instances appear \rightarrow difficult to assess algorithmic scaling with N .

Is quantum-computing our breakthrough? (I)

From an impressive insight (Richard P. Feynman, 1982)

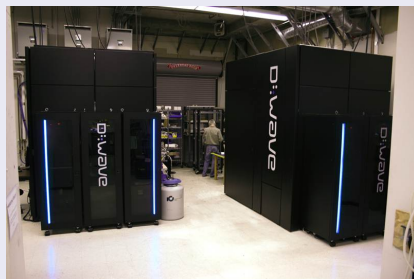


NP-problems, specially simulation of **quantum** systems: best solved on **quantum computers**...

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... to (possibly) quantum-computing objects (2014).

D-wave Two



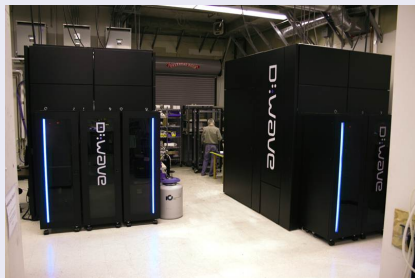
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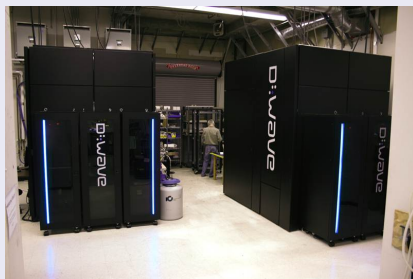
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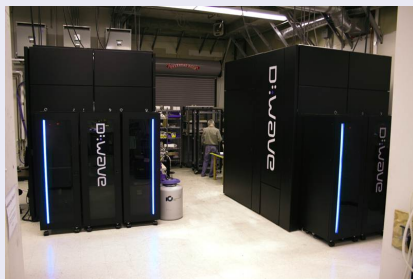
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All requirements met? \rightarrow global minimum.

D-wave Two



Is quantum-computing our breakthrough? (II)

D-wave solves a **toy problem**:

- Small problems $N = 512$ (actually, $N = 503$ in USC).

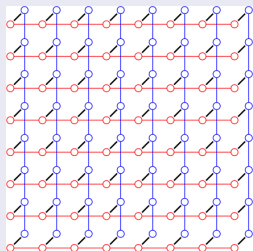
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Chimera



Each blob: 8 q-bits

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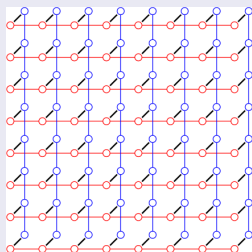
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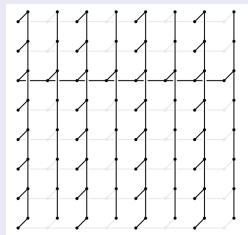
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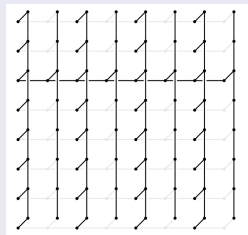
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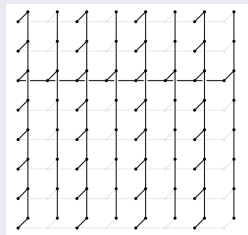
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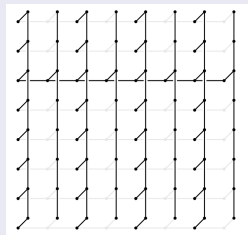
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Are we learning something?

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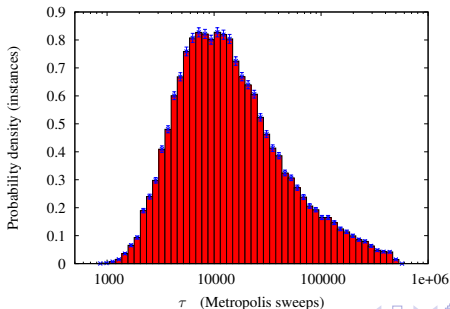
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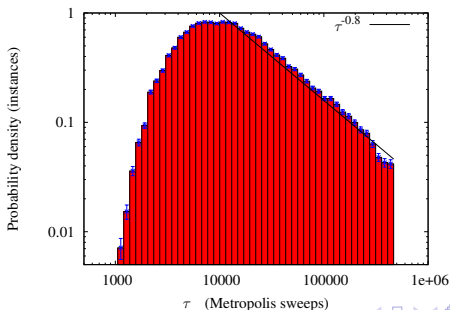
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Not at first sight... But look at that **fat tail!**

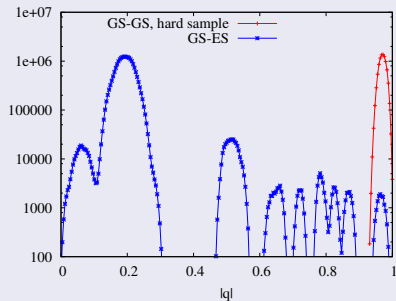
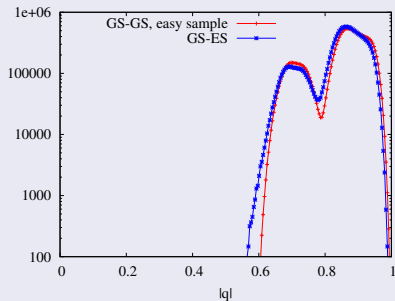
2 in 10^4 instances: $\tau \gg 10^7$.



Is quantum-computing our breakthrough? (IV)

As usual, τ pinpoints peculiar samples...

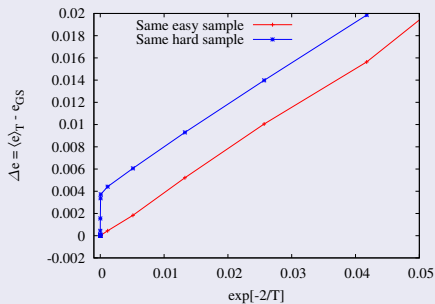
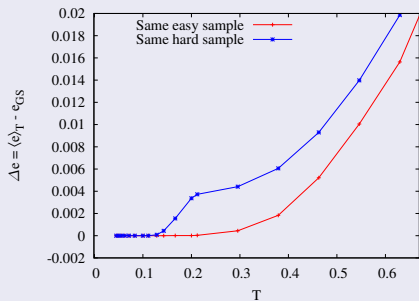
Overlap between Ground-State and 1st Excited-State...



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... or energy-dependence with T .



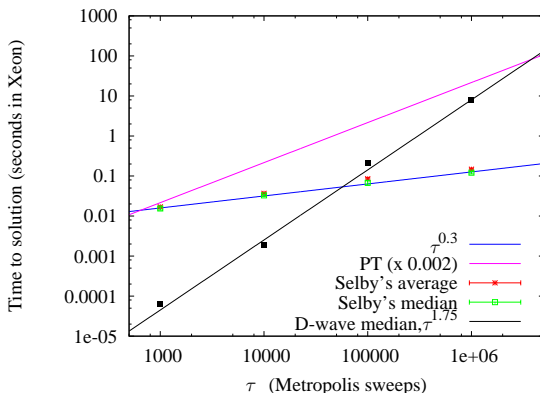
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Meaningful algorithmic classification at fixed N : τ -scaling.

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Parallel-Tempering: τ^1 , Selby heuristics (2D!): $\tau^{b \approx 0.3}$, D-wave: $\tau^{a \approx 1.75}$.



Conclusions

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- Not everything in Spin-Glasses Physics is self-averaging. Temperature chaos is a clear example.
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 - Reasons for failure intrinsic? Current investigation.

Many thanks to...

- The Janus collaboration,
- Alain Billoire,
- Itay Hen,
- The meeting organizers,
- ... and to you (the audience), for your attention!