Numerical analysis of the finite dimensional Ising Spin Glass model using dynamical methods

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Outline

- Introduction to Ising models and to Spin Glasses (SG)
- Dynamic techniques in Monte Carlo (MC) simulations
- Graphics Processing Units (GPUs) features and benefits
A simple model displaying a very rich physics

The Hamiltonian

$$H = - \sum_{i,k} J_{ik} S_i S_k - \sum_{i=0}^{N} h_i S_i \quad S_i \in \{-1, +1\}$$

$$Z(\beta, \{h_i, J_{ik}\}) = \sum_{\{S_i\}} e^{-\beta H[\{S_i, h_i, J_{ik}\}]} \quad \text{Partition function}$$

Free Energy density

$$f(\beta, \{h_i, J_{ik}\}) = -\frac{1}{N\beta} \log Z(\beta, \{h_i, J_{ik}\})$$
Ising Models: the ferromagnetic case in two dimensions

Isotropy assumptions: \( h_i = h, \quad \forall i \)

\[
J_{ik} = \begin{cases} 
1 & \text{closest neighbours} \\
0 & \text{otherwise}
\end{cases}
\]

\[
H = - \sum_{\langle i,k \rangle} S_i S_k - h \sum_{i=1}^{N} S_i
\]

Phase Transition

Order Parameter

\[
m_D = \frac{1}{N} \sum_{i=0}^{N} S_i
\]

\[
m_S = - \frac{\partial f}{\partial h} = \frac{1}{N} \sum_{i=0}^{N} \langle S_i \rangle
\]

Magnetization in Onsager’s solution
Ising Models: the phase transition in the ferromagnetic case

Without external field $H$ is even in $S_i$: we expect $\langle S_i \rangle = 0$; how $\langle S_i \rangle \neq 0$?

Spontaneous symmetry breaking

External Field
- External field $|h| \ll 1$: the thermodynamic limit $L \to \infty$ is well defined
- Above the transition temperature $T > T_c$: $h \to 0^\pm$, $\Rightarrow m = 0$
- Below the transition temperature $T < T_c$: nonanalyticity and spontaneous magnetization

$$h \to 0^- \Rightarrow m^- = -m^*(T), \quad h \to 0^+ \Rightarrow m^+ = +m^*(T)$$

Boundary Conditions
- Homogeneous boundary conditions: $S_i = +1$ at the boundary
- Below the critical temperature $T < T_c$: for $L \to \infty$ we have $m = m^*(T)$
**Key Features**

- $J_{ik} = 1$: the system is ferromagnetic
- A phase transition occurs involving magnetic long range order
- Analytical solution only for 2D model at $h = 0$: Onsager
- MC simulations fully under control: thermalization easily reachable
Ising Models: the Spin Glass case

What's the difference?

- Disorder: couplings chosen according to a probability distribution
  
  \[ P(J_{ik}) = \frac{1}{2} [\delta_K (1 - J_{ik}) + \delta_K (1 + J_{ik})] \Rightarrow \text{anisotropy} \]

- Frustration: couplings have opposite signs ⇒ degenerate ground states may appear

\[
\begin{align*}
-S_1S_2 \\
S_4S_1 \\
-S_2S_3 \\
-S_3S_4
\end{align*}
\]

\[
\begin{array}{c}
\Box = J_{12}J_{23}J_{34}J_{41} \\
\Box = +1 \quad \text{not frustrated} \\
\Box = -1 \quad \text{frustrated}
\end{array}
\]
Ising Models: the Spin Glass case

We need to introduce the *disorder* average: two choices

### Annealed average
- Couplings treated on the same footing of spins

\[
\langle S_b \rangle_{\text{ann}} = \frac{\sum_{\{S,J\}} S_b \{ P(J) \exp[-\beta H] \}}{\sum_{\{S,J\}} P(J) \exp[-\beta H]}
\]

### Quenched average
- Disorder is *frozen* during thermal average
- Physically meaningful for real spin glasses

\[
\langle S_b \rangle_{\text{quen}} = \sum_{\{J\}} P(J) \frac{\sum_{\{S\}} S_b \exp[-\beta H]}{\sum_{\{S\}} \exp[-\beta H]} = \langle S_b \rangle
\]

We will use quenched averages
Thermodynamic properties computed for the average sample

- Disorder average alongside thermal average
- A phase transition occurs: no long range magnetic order involved
- It is not possible to select the state with a uniform external field
- The order parameter is defined using many systems with the same disorder realizations which are called *replicas*

\[
q^{\alpha \beta} = \frac{1}{N} \sum_{i=1}^{N} S_i^\alpha S_i^\beta \\
|q^{\alpha \beta}| \leq 1
\]

Why are they called ‘Glasses’? Because their low $T$ dynamics gets *stuck*
Mean-field models:
- Sound analytic control on mean-field models
- Paramagnetic phase \( q^{\alpha\beta} = 0 \) for high \( T \)
- Exponential number of metastable states \( q^{\alpha\beta} \neq 0 \) at low \( T \) organized according to the Replica Symmetry Breaking (RSB) scheme

Finite dimensional models:
- Transition at a finite temperature
- Uncertain nature of the low \( T \) phase (RSB?)
- Exceptionally long times for MC thermalization on large systems
- Strong finite-size effects in equilibrium MC simulation
Our Aims

We wish to study in the most accurate way

- The paramagnetic-glassy transition
- The nature of the low $T$ phase
- The role of a magnetic field and the Almeida-Thouless transition

These analyses will be performed using

- Renormalization Group (RG) for dynamic critical phenomena
- Off-Equilibrium simulations: $t_{MC} \to \infty \iff L \to \infty$
- MultiSpin coding techniques
- GPUs acceleration
Dynamic Methods

- MC simulations of SG systems very slow near the transition
- Thermalization time strongly dependent on disorder realization

**Off-Equilibrium dynamics:**

- No need for thermalization
- Possibility to simulate large size systems
- Infinite-volume behaviour as long as $\xi \ll L$
Critical behaviour: dynamics and statics

- A new critical exponent: dynamic exponent $z$
- Static critical exponents independent from the dynamics
- $z$ depends at the critical point on the chosen dynamic: dynamic universality class
- Critical exponents computed in off-equilibrium MC simulations coincide with the static ones

Infinite volume: \[ \chi \sim (\beta - \beta_c)^{-\gamma}, \quad \beta \neq \beta_c, \quad L \gg \xi, \quad t_{\text{MC}} \gg 1 \]

Finite Size scaling: \[ \chi \sim L^{\gamma/\nu}, \quad \beta = \beta_c, \quad L \simeq \xi, \quad t_{\text{MC}} \gg 1 \]

Finite Time Scaling: \[ \chi \sim t^{\gamma/z\nu}, \quad \beta = \beta_c, \quad L \gg \xi, \quad t_{\text{MC}} \text{ finite} \]
NVIDIA GPUs: Fermi and CUDA

Fermi

- latest GPU chipset with 512 cores
- GPU composed of 16 Streaming Multimprocesors (SMs) each composed of 32 cores with 64KB of configurable L1 cache and Shared Memory
- Each core has one floating point unit (FPU) and one arithmetic logic unit (ALU)
- Each core performs one operation on the FPU or ALU per clock
CUDA

- hardware and software architecture
- GPU programming unit: *kernel*
- A GPU program is run through parallel *threads*
- One thread executes an instance of the kernel
- Threads organized in *blocks* which are organized in *grids*
- Each SM schedules groups of 32 parallel threads called *warp*
GPU acceleration in MC simulations

From a first work, for a microcanonical algorithm implementation: GPU runs 10 times faster than an Intel Core i7


In a more refined work implementing the Wolff single cluster algorithm: for the 2D Ising model with $L = 4096$ at the critical temperature GPU is 5.60 times faster; for 3D Ising model for $L = 256$ GPU is 7.9 times faster