NUMERICAL SIMULATION OF THE 
EDWARDS-ANDERSON MODEL 
WITH THE MULTI-OVERLAP ALGORITHM

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Ising model with random (nn) quenched couplings. (hyper-) cubic lattice

\[ Z_J = \sum_{\{s\}} \exp(-\beta H_J(\{s\})) \]

\[ H_J(\{s\}) = -\sum_{\langle i,k \rangle} J_{i,k} s_i s_k - h \sum_i s_i \]

Realization: \( J = \{ J_{i,k} \} \). The \( J_{i,k} \) are independent random variables.

\[ \mathcal{P}(J_{i,k}) = \frac{1}{\sqrt{2\pi}} \exp(-J_{i,k}^2/2) \quad \text{or} \quad \frac{1}{2} \left( \delta(J_{i,k} - 1) + \delta(J_{i,k} + 1) \right) \]
Interested in disorder averaged extensive quantities, like

\[ f = -\frac{1}{\beta V} \ln Z_J = -\frac{1}{\beta V} \sum_J \mathcal{P}(J) \ln Z_J \]

Simple model for spin-glasses: materials with a “glassy” low temperature phase

- Without periodic order \( (\langle \frac{1}{V} \sum e^{-\vec{k}_i \vec{r}_i s_i} \rangle = 0, \quad \langle s_i \rangle \neq 0) \)
- With an extremely slow dynamics, aging, memory effects, …

Example: Ag Mn, Cu Mn, Cu Fe

Random magnetic “quenched” impurities with RKKY interaction \( \propto \cos 2K_F r / r^3 \) (Ruderman, Kittel, Kasuya and Yosida)
The infinite range version of the model (Sherrington-Kirkpatrick model) is well understood with mean field theory.

\[ H_J(\{s\}) = - \sum_{i<k} J_{i,k} s_i s_k - h \sum_i s_i \]

\[ P(J_{i,k}) = \sqrt{\frac{N}{2\pi}} \exp(-J_{i,k}^2/2N) \]

First perform average over the disorder. Consider \( n \) independent replica (uncoupled copies with same \( J \)).

\[ -\frac{1}{\beta N} \ln Z_J = - \lim_{n \to 0} \frac{1}{\beta N n} ((Z_J)^n - 1) \]

\[ f = - \lim_{n \to 0} \frac{1}{\beta N n} ((Z_J)^n - 1) \]

\[ (Z_J)^n = \sum_{\{s\}} \exp \left( \frac{\beta^2}{2N} \sum_{i<k} (\sum_{a=1}^n s_i^a s_k^a)^2 + \beta h \sum_{i} \sum_{a=1}^n s_i^a \right) \]

Mean Field equations. Parisi ansatz.
The order parameter is a function $q(x)$, $x \in [0, 1], q \in [0, 1]$

Two phases in zero magnetic field:
- Paramagnetic
- Glassy

Infinite number of equilibrium states. Ultrametric structure.

...
**What about the original physical model** (Edwards-Anderson) ?

Twenty years of controversy.

“One has to turn a triple somersault in order to claim that the mean field limit is not a good starting point to study the case of finite D dimensional models, with D lower than the upper critical dimension and higher than the lower critical dimension” (Enzo Marinari, Giorgio Parisi, Juan J. Ruiz-Lorenzo)

“Studying the SK model is pointless as it gives such a misleading picture of spin glasses” (Mike Moore)

Major impact of numerical simulations

- Existence of two phases ( \( d > d_l \geq 2 \) ) ?
- Nature of the low temperature phase
**Pure states, overlap between states, function** $P(q)$

Ising $T < T_c$: in the thermodynamical limit. Two (pure) states separated by a potential barrier $\propto \exp(2\sigma_{o,o}L^{d-1})$

For a state invariant by translation

$$<O> = p <O>_{+} + (1-p) <O>_{-} \quad p \in [0, 1]$$

($p = 1/2$ if p.b.c. and $h = 0$)

$$P(s) \propto p \left( e^{-\frac{(s-m)^2 L^d}{2\chi_0}} + (1-p) e^{-\frac{(s+m)^2 L^d}{2\chi_0}} \right)$$

Symmetry breaking $\iff$ several pure states

Note: This does not contradict either

- Concavity of the entropy $P(s) \propto \exp(-\beta E L^d) \exp(S(s))$

$$S(s) + S(s') \leq 2S\left(\frac{s + s'}{2}\right) \quad \frac{\partial^2 S}{\partial s^2} \leq 0$$

- Concavity of the free energy

$$\frac{\partial^2 F}{\partial h^2} = -L^d \chi \leq 0$$
Sherrington Kirkpatrick

\[ \langle O \rangle = \sum_{\alpha} w_{\alpha} \langle O \rangle_{\alpha} \]

\[ \sum_{\alpha} w_{\alpha} = 1 \quad w_{\alpha} \geq 0 \]

\[ q_{\alpha,\beta} = \frac{1}{N} \sum_{i} \langle S_{i} \rangle_{\alpha} \langle S_{i} \rangle_{\beta} \]

Ising \( T < T_{c} \): \( q_{++} = q_{--} = m^{2} \), \( q_{+-} = q_{-+} = -m^{2} \)

\[ P_{J}(q) = \sum_{\alpha,\beta} w_{\alpha} w_{\beta} \delta(q - q_{\alpha,\beta}) \]

\[ P(q) = \overline{P_{J}(q)} \]

Ising: \( P(q) = \frac{1}{2}(\delta(q - m^{2}) + \delta(q + m^{2})) \)

Sherrington-Kirkpatrick: \( P(q) \) is related to the order parameter of Parisi solution \( q(x) \)

\[ P(q) = \frac{1}{dq(x)} \quad q \geq 0 \quad (\text{to be symetrized}) \]

Replica symmetry breaking \( \Longleftrightarrow \) Non triviality of \( P(q) \)
\( P(q) \) can be measured by numerical simulation

\[
P_J(q) = \frac{1}{(Z_J)^2} \sum_{\{s\},\{t\}} e^{-\beta\left(H_J(\{s\})+H_J(\{t\})\right)} \delta(q - \frac{1}{N} \sum_i s_i t_i)
\]

\[
P(q) = \overline{P_J(q)}
\]

One simulates two uncoupled systems, with the same \( J \) (two real replica), and accumulates the histogram of the instantaneous values of \( q \), the overlap between the two real replica (not between two pure states). \( P_J(q) \) is determined without knowing the pure states.

Expectation for finite volume.
Monte Carlo

This model is extremely difficult to simulate, due to its extremely slow dynamics, and the need to average over a large number of realizations \( J \) (no “self-averaging”)

Way out: non local artificial dynamics

• “Multiple Markov chain” (Tesi, Van Rensburg, Orlandini and Whittington) “exchange Monte Carlo” (Hukushima and Nemoto) “parallel tempering”

One simulates \( p \) copies of the system at temperatures \( T_1, T_2, \ldots, T_p \). New Monte Carlo move: exchange of two copies. Potential barriers are avoided

• “Multi-Overlap Algorithm”

Derived from the multi-canonical algorithm (“Umbrella sampling”) used very successfully in the past to simulate the neighborhood of first order phase transitions.

One simulates an unphysical Hamiltonian designed specifically to suppress the potential barriers.
Temperature driven phase transitions: In the neighborhood of $T_t$ the energy probability distribution $P(E)$ is dominated by two gaussian peaks centered around $E = E_o$ and $E = E_d$ ($P(E_o) \approx P(E_d)$)

Very slow dynamics

$$\tau \approx \frac{P_{E,\text{max}}}{P_{E,\text{min}}}$$

More precisely

$$\tau \propto L^{d/2} \exp(2\sigma_{o,d} L^{d-1})$$

Algorithm: unphysical Hamiltonian $G_L(E)$ designed in such a way that $P^{(G_L)}(E)$ has little variation inside $[E_o, E_d]$

One generates $N_{\text{conf}}$ configurations with the Metropolis algorithm, then

$$P^{(G_L)}(E) \propto \exp(-\beta G_L(E) + S(E))$$

and estimates (reweighting)

$$<O> \approx \frac{\sum_{t=1}^{N_{\text{conf}}} O_t \exp(-\beta L^d E_t + \beta G_L(E_t))}{\sum_{t=1}^{N_{\text{conf}}} \exp(-\beta L^d E_t + \beta G_L(E_t))}$$

This is exact, and the re-weighting makes sense.
Tunneling time: number of sweeps needed for $E_o \leftrightarrow E_d$

Expect $\tau \propto V$ ($\tau \propto L^z$ with $z = d$)

Plus: Exponential sampling improvement for $E \approx (E_o + E_f)/2$

● Systems are simulated in increasing order of lattice size.
● For each lattice size:
  ● An approximation of $P(E)$: $\hat{P}(E)$ is determined. (e.g. extrapolating from a smaller lattice)

$$G_L(E) = L^dE + \frac{1}{\beta} \ln\left(\frac{\hat{P}(E)}{\hat{P}(E_o)}\right) \quad E \in [E_o, E_d]$$

$$G_L(E) = L^dE \quad \text{otherwise}$$

● Simulation is done with $G_L(E)$
● Expectation values are computed by re-weighting

**Potts 2d:**

$\tau \propto V^{1.3}, z \sim 2.6$

Was $\tau \propto exp(2\sigma_{o,d}L^{d-1})$
Interface tension of the 2d Potts model

\[ 2\sigma_{o,d} = \sigma_{o,o} = 1/\xi_d = \frac{1}{4} \sum_{n=0}^{\infty} \ln \left[ \frac{1 + w_n}{1 - w_n} \right] \]

with \( w_n = \left[ \sqrt{2} \cosh((n + \frac{1}{2}) \frac{\pi^2}{2} v) \right]^{-1} \),

\[ v = \ln \left( \frac{1}{2} (\sqrt{q + 2} + \sqrt{q - 2}) \right) \]


\[ \sqrt{\frac{P_{L_{\text{max},o}} P_{L_{\text{max},d}}}{P_{L_{\text{min}}}}} \bigg|_{\beta = \beta_t} \propto L^{-p+d/2} \exp(2\sigma_{o,d} L^{d-1}) \]

\[ F(L) = \frac{1}{2L^{d-1}} \ln \left[ \frac{P_{L_{\text{max},o}} P_{L_{\text{max},d}}}{(P_{L_{\text{min}}})^2} \right] \bigg|_{\beta = \beta_t} \]

\[ F(L) = 2\sigma_{o,d} + \frac{a_1}{L^{d-1}} + \left( -p + \frac{d}{2} \right) \frac{\ln(L)}{L^{d-1}} + \frac{a_2}{L^d} + \frac{a_3}{L^{d+1}} + \ldots \]
$F(L)$  

$q=10$ Potts model  

infinite volume theory  

FIG. 10
Table 1: Comparison between the analytical and Monte Carlo results for the order-disorder surface tension of the 2-d Potts model.

<table>
<thead>
<tr>
<th>q</th>
<th>$\xi_d$</th>
<th>$\sigma_{o,d}$</th>
<th>Analytical</th>
<th>Monte Carlo</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>10.56</td>
<td>0.094701</td>
<td>0.09781(75)</td>
<td>Berg Neuhaus</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.10</td>
<td>Janke</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.0950 (5)</td>
<td>Billoire Neuhaus Berg</td>
</tr>
<tr>
<td>20</td>
<td>2.70</td>
<td>0.370988</td>
<td>0.3714 (13)</td>
<td>Billoire Neuhaus Berg</td>
</tr>
</tbody>
</table>


Application to the Edwards Anderson model

Same strategy applied to $P_J(q)$

Two uncoupled replica

One adds a coupling $S_J(q)$ between the two replica, designed in such a way that $P_J^{(S_J)}(q)$ is nearly flat in the whole interval $q \in [-1, 1]$

Results for the original (uncoupled replica) system are obtained by re-weighting

*Recursive stochastic estimate of $S(q)$*

Request at least $n_{\text{start}}$ tunneling events of the form (We use $n_{\text{start}} = (4), 10, 20, 40$)

\[ q = 0 \leftrightarrow |q| = 1 \]

*Equilibration*

*Production: At least $n_{\text{prod}}$ tunneling events of the same form. We use $n_{\text{prod}} = 20, (80)$. Keep 65536 measurements in time series.*
Simulation: 288 (375 Mhz) processor CRAY T3E at CEA Grenoble (T3E at NIC Juelich (HLRZ) and ZIB Berlin) and FSU work stations.

\[ J_{i,k} = \pm 1 \] (No constraint)

- \( 4^3, 6^3, 8^3, 12^3 \) lattices , \( T = 1.0 (T_c = 1.11(4)) \)
- \( 2 \times 4096 \) realizations (but \( 12^3 (512+128) \))
- \( 4^4, 6^4, 8^4 \) \( T = 1.666 (T_c = 2.02(3)) \)
- 4096 realizations (but \( 8^4 (1024) \))

Ranmar: Marsaglia, Zaman. Period \( \sim 2 \times 10^{43} \) Portable

Ranlux: Marsaglia, Zaman. Period \( \sim 5.2 \times 10^{171} \) using every 389 number (Martin Lüscher) Portable

Ranf: Period \( 2^{46} \)

- Trivial parallelism (SHMEM)

Run with \( N \) processors, \( M \) realizations not (yet) completed \( (N \leq M) \)

The first \( N \) not completed realizations are given to the \( N \) processors.

At the end of the job \( M' \leq M \) realizations are still not completed

Next job is submitted with \( \min\{N, M'\} \) processors
Same (f90) source code with cpp directives contains both work-station and CRAY T3E versions

On a 375 Mhz T3E

0.50\mu s second / site update (d=3 Ranmar)

0.73\mu s second / site update (d=4 Ranmar)
if(my_pe().eq.0) then
  i_task0=0
  open(unit=10,file='input.dat',status='old',form='formatted')
  read(10,107) n_task
  print *, 'Run with ',n$pes,' processors'
  do i=1,n_task
    read(10,107) ntab(i)
  enddo
endif

call barrier

call shmem_get(n_task,n_task,1,0)
call shmem_set_lock(lock)
call shmem_get(i_task,i_task0,1,0)
i_task=i_task+1
call shmem_put(i_task0,i_task,1,0)
call shmem_get(nra,ntab(i_task),1,0) ! get nr
call shmem_clear_lock(lock)
**Figure 12^3**

- icprod scatter plots \((4^3, 6^3, 8^3)\). We had to restart some \(12^3\) and \(8^4\) realizations

**Figure icprod**

Choice of \(\{N_{\text{replica}}, n_{\text{start}}, n_{\text{prod}}\}\)

\(8^3\): Increasing \(n_{\text{prod}}\) \(20 \to 80\) does not help

We used \(n_{\text{start}} = (4), 10, 20, 40\)

- Tunneling time
  \[ q = 0 \leftrightarrow |q| = 1 \]

\[ \ln \langle \tau \rangle = a_1 + a_2 \ln V \quad (\text{expects } a_2 = 1) \]

\(a_2 \approx 2\) \(\quad d = 3\) and \(d = 4\)

- \(P(q)\), FSS

\[ P(q) = L^{\beta/\nu}F(qL^{\beta/\nu}, (T - T_c)L^{1/\nu}) \]

- \(P_J(q)\)

We have precise determinations of the \(P_J(q)\). What can we learn from it?
Symmetrized, canonically reweighted q-histogram

'rq00001.qcsh'
Original q-histogram

25
Symmetrized, canonically reweighted q-histogram

're00003.qcsh'
Symmetrized, canonically reweighted q-histogram

'\texttt{r00007.qcsh}'
Symmetrized, canonically reweighted q-histogram

'\texttt{r00013.qcsh}'
Symmetrized, canonically reweighted q-histogram
\[
\ln (\tau) = a_1 + a_2 \ln (V)
\]

- \(a_1 = -2.72 \pm 0.030\)
- \(a_2 = 2.32 \pm 0.037\)

Goodness of fit \(Q = 5 \times 10^{-20}\)

\[\exp \text{ fit } Q = 3 \times 10^{-159}\]
\( \ln (\tau) = a_1 + a_2 \ln (V) \)

- \( a_1 = -2.894 \pm 0.082 \)
- \( a_2 = 1.937 \pm 0.015 \)

Goodness of fit \( Q = 8E-15 \)

Exponential fit \( Q = 0.05 \)
$P(q) / L^{\beta/\nu}$

- $L$
- $4$
- $6$
- $8$
- $12$

$T = 1$

$\beta/\nu = 0.255$
Try to connect to the Metropolis dynamics:

Consider the following 1-d dynamics that would lead to the observed $P_J(q)$,

$T_{i,j}$ is the probability to jump from $q_j = j/V$ to $q_i = i/V$, $i, j \in [-V, -V + 2, \ldots V - 2, V]$

$$T = \begin{pmatrix}
1 - w_{2,1} & w_{1,2} & 0 & \cdots \\
w_{2,1} & 1 - w_{1,2} - w_{3,2} & w_{2,3} & \cdots \\
0 & w_{3,2} & 1 - w_{2,3} - w_{4,3} & \cdots \\
0 & 0 & w_{4,3} & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix}$$

$$w_{i,j} = \frac{1}{2} \min\left(1, \frac{P_J(q_i)}{P_J(q_j)}\right)$$

Let $\lambda_i$ be the eigenvalues of $T$ ($\lambda_1$ the second largest eigenvalue) $|\lambda_i| \leq 1$, $\lambda_i$ real (tridiagonal sign symmetric)

$$\lambda_i^n \sim e^{-n(1 - \lambda)}$$

The autocorrelation time is

$$\tau = \frac{1}{V(1 - \lambda_1)}$$

Distribution function $F(X)$: Probability that $\tau < X$

$F(1/2)$ is the median $\tau$
3d cumulative distribution function of tau

L=4
L=6
L=8
L=12
4d cumulative distribution function of tau

- $L=4$
- $L=6$
- $L=8$
Conclusions

- Spin Glasses, EA, SK
- Multicanonical algorithm
- Multioverlap algorithm
  
  Lattices up to $12^3 / 8^4$ ($T < \approx T_c$)
  
  $\tau \propto V^{\approx 2}$
  
  Precise $P_J(q), P(q)$ for $q \in [-1, 1]$
  
  Barriers ?