

MONTE CARLO - **THEN**,
AND
MONTE CARLO - **NOW**

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Talk at the
GARUDA-NKN Partners Meet,
Bengaluru, 20 July 2012
20 July 2012

Acknowledgements:

- Thanks to Subrata Chattopadhyay, for the invitation
AIM
- the aim of this talk is to find **where we were** in the context of Monte Carlo simulation and **where we are likely to be** in the coming years;
- to identify **challenging problems** that would require collaboration in terms of sharing of computing resources, data and algorithms.

Monte Carlo : general blah ... blah

- Consider a closed system in equilibrium at temperature $T = 1/k_B\beta$.
 - k_B is the Boltzmann constant. in units of $k_B T$
- Aim is to simulate the system employing Monte Carlo methods.
- How do we do that ?
- generate a large number of micro states belonging to an equilibrium ensemble.
- Call this a Monte Carlo ensemble;

more of blah ... blah

- a Monte Carlo ensemble is a subset of a canonical ensemble
- Let the size of the ensemble be N
- In general, for a given thermodynamic property, there corresponds, in statistical mechanics, a random variable
- random because the value of the property fluctuates from one micro state to another.
- in a sense we are looking at a **private** property of a micro state. *e.g.*
 - energy,
 - magnetization of a micro state of an Ising spin system

- Estimate the thermodynamic property of the system by taking a simple arithmetic average over a Monte Carlo ensemble
- Exception to the above rule are thermal quantities like **entropy** and **free energy**
- **Entropy** is not defined for a microstate.
- entropy is not a private property of micro state
- it is a social or collective property
- To estimate entropy we need
 - to count the number of micro states of a micro canonical ensemble or
 - to sum the quantity $p_i \ln p_i$ over micro states (i) of a closed system

Monte Carlo Then and Monte Carlo Now

- to this end we need special techniques for calculating entropy and free energy
- This provides us with a natural categorization of Monte Carlo methods as:
- **Monte Carlo - Then :**
 - Boltzmann Monte Carlo methods
 - Methods that help sample from canonical ensemble
 - Boltzmann ensembles are physical

● Monte Carlo - Now :

- Non-Boltzmann Monte Carlo
- Methods that help sample from an entropic ensemble
- Non-Boltzmann ensembles are not physical ensembles
- however physical quantities can be calculated by suitable un-weighting-re-weighting techniques

Monte Carlo error bars

- The *Law of Large Numbers* guarantees that asymptotically ($N \rightarrow \infty$) the Monte Carlo estimate converges (statistically) to the true value.
- In fact the **Central Limit Theorem** helps us quantify this convergence in terms of statistical error ϵ
- ϵ = one-sigma confidence interval
- ϵ is given by the standard deviation calculated from the Monte Carlo ensemble divided by square root of the size of the Monte Carlo ensemble.
- Such error estimates are valid only
 - when the elements of the Monte Carlo ensemble are independent of each other and
 - the property under investigation has a finite variance

Critical Slowing Down

- for systems close to second order phase transition successive micostates sampled are correlated;
- the dynamics become extremely slow
- the convergence of the Monte Carlo results take prohibitively long times
- Called **critical slowing down**
- Cluster algorithms help overcome problems of critical slowing down
- near first order phase transition we have problems of large **energy barriers**
- the phase space splits into two regions separated by the energy barrier

Super-critical slowing down

- for all practical purposes these two regions do not communicate with each other: Non-ergodic
- the dynamics slows down - super-critical slowing down
- in glassy systems the phase splits into several non ergodic regions
- entropic sampling overcomes **super-critical slowing down**
- what about **entropy** barriers ?
- a few studies like Frontier sampling and JSM techniques have been proposed;
- these are however ad-hoc;
- overcoming entropy barriers remains still an open problem

MONTE CARLO - THEN : Metropolis Rejection

- Markov Chain Monte Carlo : Metropolis Algorithm
- start with an initial microstate C_0 and generate a Markov chain of microstates:

$$C_0 \rightarrow C_1 \rightarrow C_2 \rightarrow \dots \rightarrow C_n \dots$$

as described below

- Let the current microstate be C_i and its energy E_i
- Carry out local changes in C_i and construct a trial microstate C_t ;
- let the energy of the trial microstate be E_t
- If $E_t \leq E_i$ then accept the trial state and set $C_{i+1} = C_t$

Metropolis Rejection

- if $E_t > E_i$, calculate

$$p = P(C_T)/P(C_i) = \exp[-\beta(E_t - E_i)]$$

- then

$$C_{i+1} = \begin{cases} C_t & \text{with probability } p \\ C_i & \text{with probability } 1 - p \end{cases}$$

- the asymptotic part of the Markov chain contains microstates belonging to canonical ensemble at the chosen temperature
- Generate a large Monte Carlo sample of microstates taken from the end of the Markov chain

Monte Carlo estimates of mean and its statistical error

- Let N be the size of the Monte Carlo ensemble and
- O denote the property of interest
- Monte Carlo estimate of the average of O and the associated statistical error are given by

$$\bar{O}_N = \frac{1}{N} \sum_{i=1}^N O(C_i) \pm \frac{1}{\sqrt{N}} \sqrt{\frac{1}{N} \sum_{i=1}^N O^2(C_i) - \left(\frac{1}{N} \sum_{i=1}^N O(C_i) \right)^2}$$

Metropolis, balance and detailed balance

- Metropolis algorithm obeys **balance** condition:
 - this guarantees asymptotic convergence to equilibrium
- In fact Metropolis algorithm obeys a stricter **detailed balance** condition:
 - this assures asymptotic convergence to the desired equilibrium canonical ensemble at the prescribed temperature
- More importantly Metropolis algorithm generates (asymptotically) **reversible Markov chain**
 - equilibrium state does not recognize forward time from its reverse
 - equilibrium state is time reversal invariant

Monte Carlo - Now : the g ensemble

- **Entropic sampling**: Let $g(E) \geq 0 \forall E$ be a given function of energy
- we take the probability of a micro state as

$$P(C) \propto \frac{1}{g(E(C))}$$

- Let C_i of energy E_i be the current microstate and C_t of energy E_t be the trial microstate constructed by making local changes in C_i .
- if $g(E_t) \leq g(E_i)$ accept the trial state and set $C_{i+1} = C_t$

- otherwise calculate

$$\begin{aligned} p &= \frac{P(C_t)}{P(C_i)} \\ &= \frac{g(E_i)}{g(E_t)} \end{aligned}$$

Then

$$C_{i+1} = \begin{cases} C_t & \text{with probability } p \\ C_i & \text{with probability } 1 - p \end{cases}$$

- the asymptotic part of the chain would contain microstates that belong to what we call as g -ensemble.

Entropic Sampling

- $1/g(E)$ plays the role of Boltzmann weight;
- Notice : $g(E)$ is independent of temperature.
- in a sense the g -ensemble is multi canonical
- Canonical partition function can be written as

$$Q(\beta) = \int dE D(E) \exp(-\beta E)$$

where $D(E)$ is the density of (energy) states.

- Replace the Boltzmann factor $\exp(-\beta E)$ by $1/g(E)$.
We get,

$$Q_g = \int dE \frac{D(E)}{g(E)}$$

entropic sampling: flat histogram

- If $g(E) = D(E)$ then the probability is same for all energies.
- the ensemble that results from this choice of $g(E)$ is called entropic ensemble
- all energy regions are equally represented in the entropic ensemble of micro states
- The histogram of energy of visited microstates is flat.
- there are no energy barriers
- the system does a simple random walk in the energy space
- But note: **we do not know $D(E)$ before hand**

convergence of g to D

- In entropic sampling the following strategy is employed
 - start with a guess of $g(E)$;
 - if you know nothing of $D(E)$, assume $g(E) = 1 \forall E$
 - generate a certain number of microstates and build a histogram $h(E)$.
 - update $g(E)$ for all E as follows.
 - $g(E) = g(E) \times h(E)$ if $h(E) \neq 0$.
 - If $h(E) = 0$ then do not change $g(E)$
 - employ the updated $g(E)$ in the next stage, during which a fresh histogram is built.
 - after a few stages of iteration $g(E)$ would converge to $D(E)$.
 - The convergence can be monitored by looking at the flatness of the histogram.

Wang - Landau algorithm

- A Variant of entropic sampling is the Wang-Landau algorithm
- $g(E)$ is updated continuously.
- when the visited micro state is of energy E then $g(E) = g(E) \times \alpha$ where α is the Wang-Landau factor
- $\alpha = e$ in the first iteration; in the second iteration it is taken as the square root of e ;
- this square root rule is applied to successive iterations.
- Asymptotically $\alpha \rightarrow 1$ when there occurs no change in $g(E)$.
- $g(E)$ converges to the $D(E)$

Wang - Landau algorithm

- the converged $g(E)$ gives the microcanonical entropy from which all the required thermodynamics properties can be obtained
- alternately the converged $g(E)$ is used in a production run; an entropic ensemble is generated; the required properties at any temperature can be calculated by suitable un-weighting -cum-re-weighting techniques.

$$\langle \mathcal{O}(\beta) \rangle = \frac{1}{N} \sum_{i=1}^N \mathcal{O}(C_i) g(E(C_i)) \exp[-\beta E(C_i)]$$

Free Energy

Landau Free energy in Statistical Thermodynamics

$$F(T) = -k_B T \ln \left[\sum_C \exp(-\beta E(C)) \right]$$

- In the above the sum runs over all micro states of the closed system at T .
- For an equilibrium system, the sum is overwhelmingly dominated by the contributions from the micro states of energy $E = \langle E \rangle = U(T)$.
- The contributions from micro states having energies $E \neq U(T)$ are negligibly small.

- Hence we can write,

$$F(T) = -k_B T \ln \left[\sum_C \delta(E(C) - U(T)) \exp(-\beta E(C)) \right]$$

where the Krobecker δ - function is given by

$$\Delta(\eta) = \begin{cases} 1 & \text{if } \eta = 0 \\ 0 & \text{if } \eta \neq 0 \end{cases}$$

- the sum is taken over those micro states having energy $U(T)$

- then we have

$$F(T) = -k_B T \ln \left[\hat{\Omega}(U) \exp(-\beta E(C)) \right],$$

where $\hat{\Omega}(U)$ is the number of micro states of the closed system with energy $U(T)$.

- $F(T) = -T (k_B \ln \hat{\Omega}) + (-k_B T) (-\beta U) = U - TS$
- this is indeed a familiar expression for free energy from thermodynamics

Landau - Free energy

- Landau generalized the above expression for free energy to non-equilibrium systems by writing

$$F(T, E) = -k_B T \ln \sum_C \delta(E(C) - E) \exp[-\beta E(C)]$$

- In the above if we choose $E = U(T)$ we get equilibrium free energy;
- If we choose $E \neq U(T)$ we get Landau (non-equilibrium) free energy at the chosen energy.
- Thus the non-equilibrium Landau free energy is independently a function of energy and temperature.

Free energy - Thermodynamics

Landau-Free energy : Thermodynamics Point of View:

- the free energy of a closed system is given by

$$F(T, \dots) = U(S, \dots) - T(S, \dots)S$$
$$T(S, \dots) = \left. \frac{\partial U}{\partial S} \right|_{\dots}$$

- Thus F is a function of T .
- We can define microcanonical free energy, relevant for an isolated system and express F as a function of U .

$$F(U) = U - T(S(U))S(U)$$

- But F can not be expressed as a function of both T and U independently for an equilibrium system
- If you specify U then T is automatically fixed. If you specify T then U gets fixed automatically.

Landau and Landau - Ginzberg free energy

- Landau asked: what is the penalty in terms of excess free energy we require to invest if we want to keep the system in a "non-equilibrium state" at a given T with energy different from equilibrium energy $U(T)$.
- Such a "non-equilibrium free energy" is called Landau or Landau-Ginzberg Free energy

$$F(T, E) = E - TS(E)$$

where $S(E)$ is microcanonical entropy:

$S(E) = k_B \ln D(E)$. Here $D(E)$ is the density of energy states.

- If $E = U(T)$ we get the equilibrium free energy of the closed system

Landau free energy from Wang-Landau algorithm

- Wang-Landau Monte Carlo gives directly the density of states, logarithm of which is proportional to microcanonical entropy.
- Hence these techniques permit calculation of Landau-free energy directly

$$F(T, E) = E - T k_B \ln g(E)$$

- When $E = \langle E \rangle = U(T)$ we get equilibrium free energy at the given temperature
- When $E \neq \langle E \rangle = U(T)$ we get non-equilibrium Landau-free energy
- We illustrate this by considering Potts spins on a two dimensional square lattice

Potts Spin model

- each Potts spin interacts with its four nearest neighbours;
- we impose periodic boundary conditions
- the interaction energy of a pair of Potts spins at nearest neighbour sites i and j is given by

$$E_{i,j} = -J \delta(S_i, S_j)$$

- $S_i = 1, 2, \dots, q$ for a q -state Potts spin model.
- $\delta(S_i, S_j)$ is the usual Kronecker delta which equals 1 when $S_i = S_j$ and zero otherwise.

$q = 8$: Potts spin model : First order Phase Transition

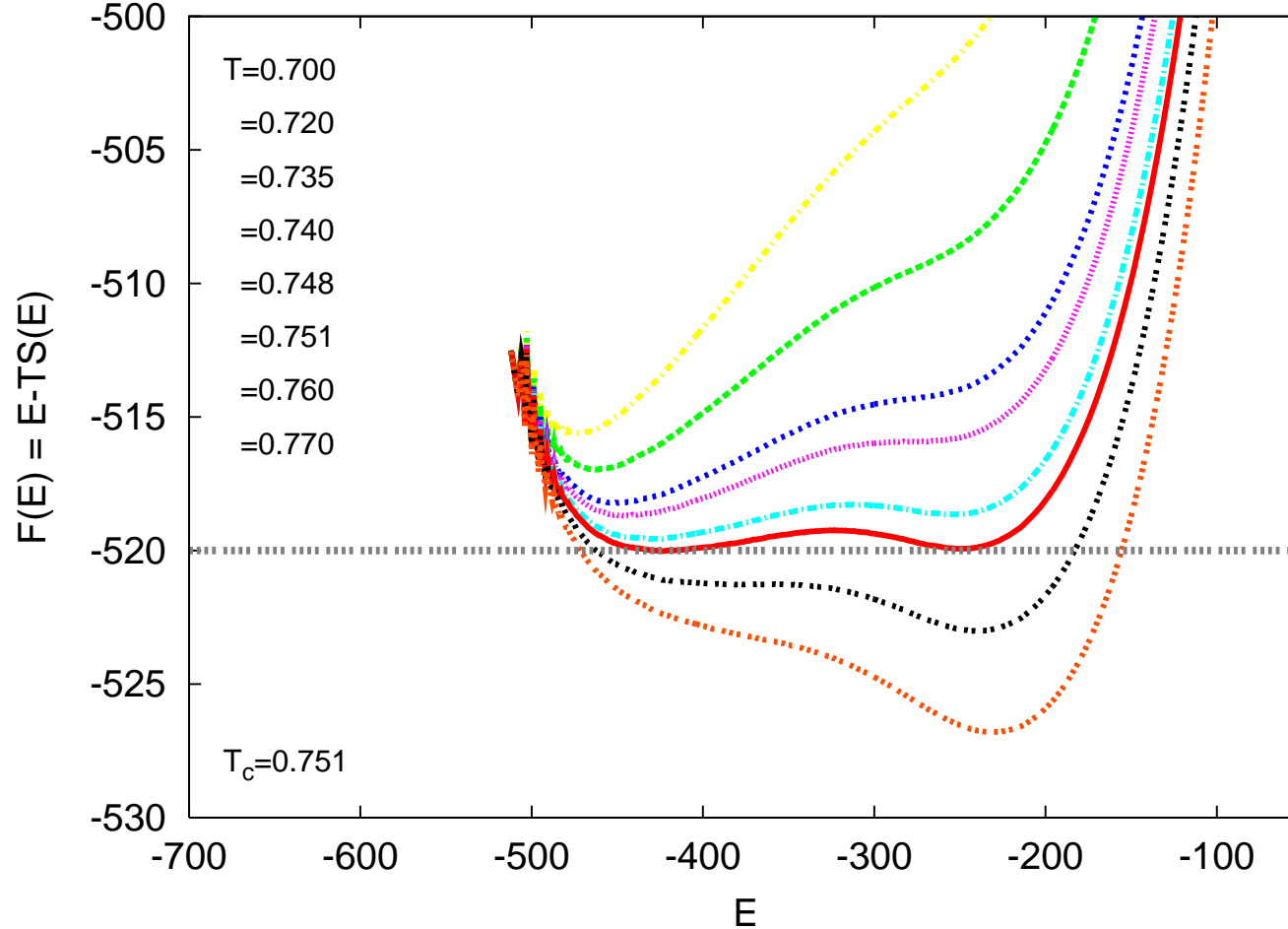


Figure 1: F versus E for various T . 16×16 square lattice: Transition is first order

$q = 3$: Potts spin model: Second order Phase Transition

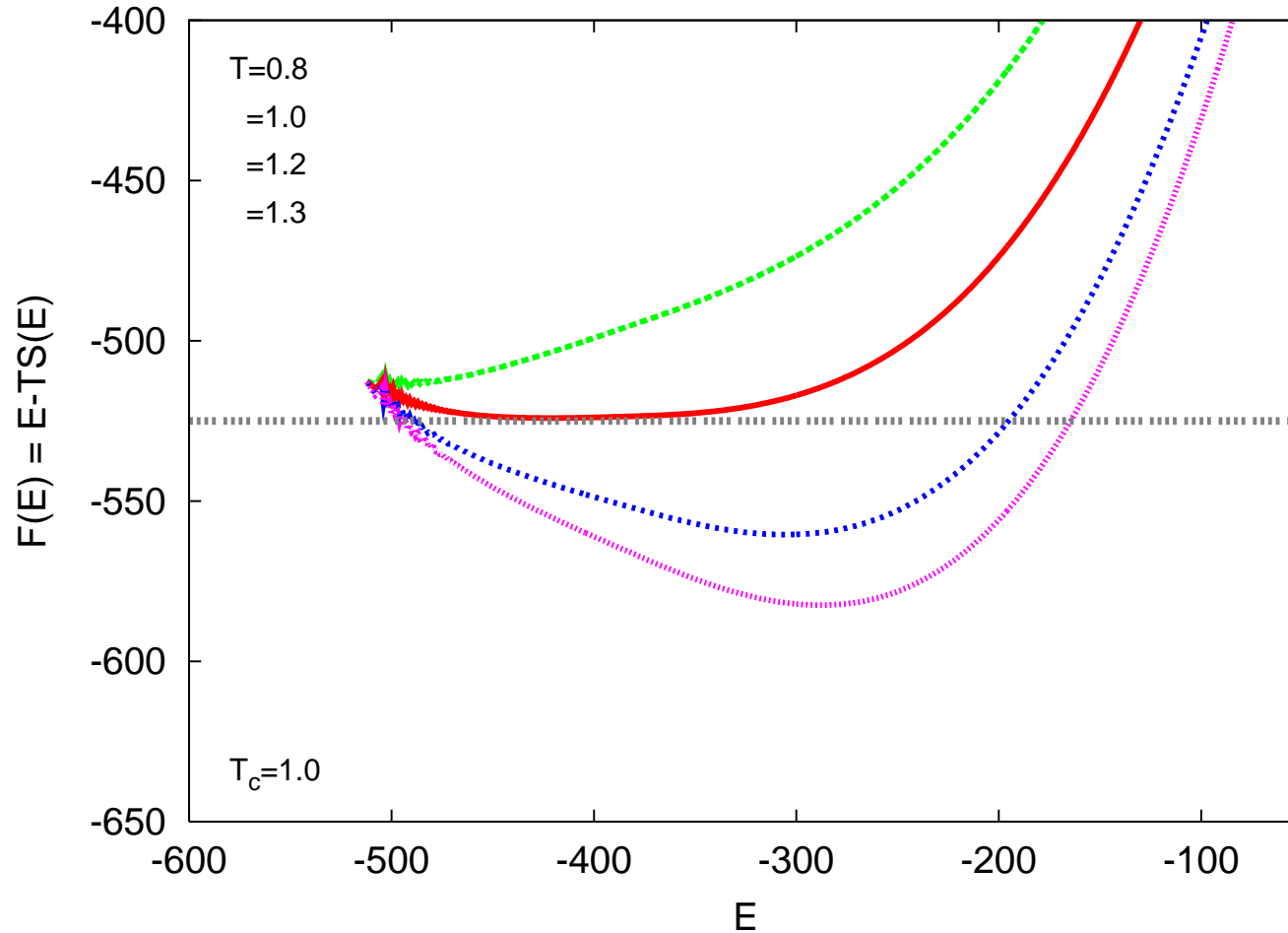


Figure 2: F versus E for various T 16×16 square lattice: Transition is second order

Good bye then

and ...

Thanks