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# Parallel simulations in ferromagnetic spin systems

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**Abstract.** We study the thermodynamical limits that are obtained from a parallel updating of ferromagnetic spins on a lattice. We investigate the relationships existing between the parallel model and the sequential model. We compare both of their free energy functions. A long-range model for which the mean-field theory is correct is also studied. The last part of the article indicates how parallel updating can be efficiently used in short-range model simulations.

## 1. Introduction

Monte Carlo simulations of interacting particle systems are traditionally carried out by using a sequential updating of the spins called *Glauber dynamics* (see Liggett, 1985). The interacting environment of a spin is held fixed while a decision is made about whether or not to flip it. The neighbours are treated after the spin is updated. Although this algorithm is easy to implement on sequential computers, it is rather slow and not well adapted to parallel machines. Many authors have proposed the same simplification of this algorithm but for different purposes. The simplification consists of simultaneously flipping all spins using the environment which exists before the spins are flipped. In this new algorithm, all decisions are made independently given the environment.

Such dynamics have been considered by Dawson (1975) who proved that the parallel algorithm does not always converge in distribution to the probability measure obtained in the sequential case.

Koslov and Vasiliev (1980) gave a necessary and sufficient condition for a simultaneous updating of spins on the $d$-dimensional lattice ($d \geqslant 1$) to be reversible. A reversible probability distribution exists if and only if the local dynamics is the Glauber dynamics associated to a pair potential on the lattice. The authors also gave a characterization of the set of all invariant probability distributions when the interactions are translation invariant.

In the neural networks terminology, parallel Glauber dynamics associated to a pair potential is often called *Little dynamics*. It was studied by Peretto (1984) for associative memories and by Azencott (1996), François *et al* (1992) for Boltzmann machines. Parallelized versions of the simulated annealing algorithm have also been investigated by Trouvé (1988) and Ferrari *et al* (1993).

In statistical physics, simultaneous updating of spins was suggested by Neumann and Derrida (1988) to simulate the corresponding Gibbs states on a lattice. They applied their approach to Ising spins and spin glasses in two dimensions. Using informal arguments, they concluded that at least the first moment of various thermodynamical quantities were correctly reproduced. Monte Carlo simulations indicate that the algorithm gives a correct critical temperature for the square lattice Ising model (see Landau and Stauffer, 1989).

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In this article, we shall study some properties of the free energy function of the Gibbs states associated to the parallel updating of ferromagnets. In section 3, we shall consider a model for which the mean-field arguments are exact. This long-range model will be analogous to the Curie–Weiss model in statistical mechanics (see Ellis, 1985). The relationships between the parallel mean-field model and the Curie–Weiss model (which is the sequential mean-field model) will be investigated.

In section 4, we shall consider ferromagnetic models on the $d$-dimensional lattice and theoretically justify the existence of the free energy function and the magnetization. We shall give some examples of short-range models for which the magnetization is the same in both sequential and parallel algorithms.

Although a parallel simulation does not always produce the desired Gibbs states, we shall show that it can be efficiently used to simulate Ising models on particular lattices by significantly reducing the size of the lattice.

## 2. Parallel dynamics

This section is devoted to the definition of the *parallel Glauber dynamics* on a finite subset, $\Lambda$, of the $d$-dimensional lattice $\mathbb{Z}^d$, $d \geqslant 1$. A point $x \in \Lambda$ is viewed as a site on which a spin with value $\eta(x) = +1$ or $\eta(x) = -1$ is placed. The interaction between the sites is described by a ferromagnetic potential

$$\forall x, y \in \mathbb{Z}^d \qquad J_{\{x,y\}} \geqslant 0 \tag{1}$$

which is translation invariant, i.e.

$$J_{\{x,y\}} = J(x - y) \tag{2}$$

where $J$ is a function of $\mathbb{Z}^d$ satisfying

$$\mathcal{J} = \sum_{x \in \mathbb{Z}^d} J(x) < \infty. \tag{3}$$

The model depends on two parameters: the inverse temperature $\beta > 0$ and the external field $h \in \mathbb{R}$. We define the parallel Glauber dynamics as the discrete time Markov chain $\eta_\Lambda^t$ ($t \in \mathbb{N}$) on $X_\Lambda = \{-1, +1\}^\Lambda$ for which the transition probabilities are given by

$$\forall \zeta, \xi \in X_\Lambda \qquad \mathrm{P}(\eta_\Lambda^{t+1} = \zeta | \eta_\Lambda^t = \xi) = \prod_{x \in \Lambda} q_x(\xi, \zeta(x)) \tag{4}$$

with

$$q_x(\xi, \zeta(x)) = \frac{\exp(\zeta(x)\beta(\sum_{y \in \Lambda} J(x-y)\xi(y) + h))}{Z_x(\xi)} \tag{5}$$

and

$$Z_x(\xi) = \exp\left(\beta\left(\sum_{y \in \Lambda} J(x-y)\xi(y) + h\right)\right) + \exp\left(-\beta\left(\sum_{y \in \Lambda} J(x-y)\xi(y) + h\right)\right). \tag{6}$$

As noticed by the authors cited in the introduction, the previous dynamics is time-reversible and ergodic. The parallel algorithm converges to a unique probability distribution which is given by the following formula

$$\forall \eta \in X_\Lambda \qquad \pi_{\Lambda,\beta,h}^{\mathrm{par}}(\eta) = \frac{\exp(-\beta H_{\Lambda,\beta,h}^{\mathrm{par}}(\eta))}{Z^{\mathrm{par}}(\Lambda, \beta, h)} \tag{7}$$

where

$$H^{\mathrm{par}}_{\Lambda,\beta,h}(\eta) = -\frac{1}{\beta}\sum_{x\in\Lambda}\ln 2\cosh\beta\left(\sum_{y\in\Lambda}J(x-y)\eta(y)+h\right) - h\sum_{x\in\Lambda}\eta(x) \quad (8)$$

and

$$Z^{\mathrm{par}}(\Lambda,\beta,h) = \sum_{\eta\in X_\Lambda}\exp(-\beta H^{\mathrm{par}}_{\Lambda,\beta,h}(\eta)). \quad (9)$$

Throughout this article, we shall try to compare the result produced by a parallel updating of spins with the result produced by the classical sequential procedure. We recall that a sequential algorithm updates a single site at a time and converges to the Gibbs state which is associated to the following Hamiltonian

$$\forall\eta\in X_\Lambda \qquad H^{\mathrm{seq}}_{\Lambda,h}(\eta) = -\tfrac{1}{2}\sum_{x,y\in\Lambda}J(x-y)\eta(x)\eta(y) - h\sum_{x\in\Lambda}\eta(x). \quad (10)$$

We shall focus on the relationships existing between the thermodynamical quantities of both models.

We shall denote by $\langle.\rangle_\Lambda$ the mathematical expectation taken with respect to the Gibbs measure, $\pi_\Lambda$, on the configuration set $X_\Lambda$. When necessary, we shall add a superscript to distinguish between the parallel and sequential quantities. The finite volume magnetization in $\Lambda$ is

$$M(\Lambda,\beta,h) = \sum_{x\in\Lambda}\langle\eta(x)\rangle \quad (11)$$

and the free energy is

$$\Psi(\Lambda,\beta,h) = -\frac{1}{\beta}\ln Z(\Lambda,\beta,h). \quad (12)$$

In the sequential case, the thermodynamical limits

$$m^{\mathrm{seq}}(\beta,h) = \lim_{\Lambda\uparrow\mathbb{Z}^d}\frac{1}{|\Lambda|}M^{\mathrm{seq}}(\Lambda,\beta,h) \qquad \text{and} \qquad \psi^{\mathrm{seq}}(\beta,h) = \lim_{\Lambda\uparrow\mathbb{Z}^d}\frac{1}{|\Lambda|}\Psi^{\mathrm{seq}}(\Lambda,\beta,h) \quad (13)$$

exist for all $\beta>0$, $h\neq 0$ and are related by the following formula

$$\forall\beta>0, h\neq 0 \qquad m^{\mathrm{seq}}(\beta,h) = -\frac{\partial}{\partial h}\psi^{\mathrm{seq}}(\beta,h). \quad (14)$$

In section 4, we shall justify the existence of such limits in the parallel case. To do so, we shall exploit the *dedoubling* argument which is stated in the next lemma.

*Lemma 2.1.* The finite volume Gibbs state $\pi^{\mathrm{par}}_{\Lambda,\beta,h}$ is the projection on $X_\Lambda$ of the Gibbs state on $X_\Lambda\times X_\Lambda$ associated with the Hamiltonian

$$\forall(\eta,\zeta)\in X_\Lambda\times X_\Lambda \qquad H^{(2)}_{\Lambda,h}(\eta,\zeta) = -\sum_{x,y\in\Lambda}J(x-y)\eta(x)\zeta(y) - h\sum_{x\in\Lambda}(\eta(x)+\zeta(x)). \quad (15)$$

*Proof.* Let $\eta \in X_\Lambda$. We develop the expression of $\pi^{\mathrm{par}}_{\Lambda,\beta,h}(\eta)$ to obtain

$$\pi^{\mathrm{par}}_{\Lambda,\beta,h}(\eta) = \frac{2^{|\Lambda|}}{Z^{\mathrm{par}}(\Lambda,\beta,h)} \prod_{x\in\Lambda} \cosh\left(\beta\left(\sum_{y\in\Lambda} J(x-y)\eta(y) + h\right)\right) \exp -\beta h \sum_{x\in\Lambda} \eta(x)$$
$$= \frac{1}{Z^{\mathrm{par}}(\Lambda,\beta,h)} \sum_{\zeta\in X_\Lambda} \exp(-\beta H^{(2)}_{\Lambda,h}(\eta,\zeta)).$$

□

For a finite set $\Lambda \subset \mathbb{Z}^d$, the configuration space $X_\Lambda \times X_\Lambda$ can be identified to the set $X_{\Lambda\cup\Lambda'}$ where $\Lambda'$ is a (distinct) copy of $\Lambda$. Thus, we can think of the set of spins $\Lambda$ as being dedoubled. The interactions on $\Lambda$ induce a new potential on the doubled set $\Lambda \cup \Lambda'$. For the doubled model, the graph of interactions is bipartite: the spins in $\Lambda$ only interact with those of $\Lambda'$.

## 3. Mean-field models

In this section, we shall present mean-field models for the Gibbs states that are obtained from a parallel simulation of ferromagnetic spins. Mean-field models are non-rigorous approximations of original models. In a mean-field approximation, one usually considers the spins as being independent. One replaces the interaction between spins by an interaction with a collective mean value $-1 \leqslant m \leqslant +1$. For the parallel algorithm, the approximation consists of replacing the doubled Hamiltonian, $H^{(2)}_{\Lambda,h}$, defined in equation (15) by

$$\forall(\eta,\zeta) \in X_\Lambda \times X_\Lambda$$
$$H^{mf}_{\Lambda,h}(\eta,\zeta) = -\sum_{x,y\in\Lambda} J(x-y)(\eta(x)m + m\zeta(y)) - h\sum_{x\in\Lambda}(\eta(x)+\zeta(x))$$
$$= -(m\mathcal{J}+h)\sum_{x\in\Lambda}(\eta(x)+\zeta(x)). \tag{16}$$

Then, the partition function $Z^{\mathrm{par}}_{mf}(\Lambda,\beta,h)$ can be explicitly computed

$$Z^{\mathrm{par}}_{mf}(\Lambda,\beta,h) = \sum_{\eta\in X_\Lambda}\sum_{\zeta\in X_\Lambda} \exp\left(-\beta H^{mf}_{\Lambda,h}(\eta,\zeta)\right)$$
$$= (2\cosh\beta(\mathcal{J}m+h))^{2|\Lambda|}. \tag{17}$$

Since $m$ must be the mean value of the spin $\eta(x)$, we have

$$m = \langle\eta(x)\rangle^{mf}_\Lambda = \tanh\beta(\mathcal{J}m+h). \tag{18}$$

The parallel partition function is exactly the square of the sequential mean-field partition function. Both models have the same magnetization, $m$. We shall now develop some results concerning a long-range model for which the mean-field approximation is exact.

Let $n$ be a positive integer and $\Lambda_n = \{-n,+n\}^d \subset \mathbb{Z}^d$. We denote the set $X_{\Lambda_n}$ by $X_n$. We study the specific free energy of the *parallel Curie–Weiss model* which is described by the following finite volume Gibbs state

$$\forall\eta\in X_n \qquad \pi^{\mathrm{par}}_{n,\beta,h}(\eta) = \frac{1}{Z^{\mathrm{par}}(n,\beta,h)} \sum_{\zeta\in X_n} \exp(-\beta H^{\mathrm{cw}}_{n,h}(\eta,\zeta)) \tag{19}$$

where

$$H^{\text{cw}}_{n,h}(\eta,\zeta) = -\sum_{x,y\in\Lambda} \frac{\mathcal{J}}{|\Lambda_n|}\eta(x)\zeta(y) - \frac{h}{|\Lambda_n|}\sum_{x\in\Lambda}(\eta(x)+\zeta(x)). \tag{20}$$

This model is similar to the classical Curie–Weiss model which can be considered as the sequential model (see Ellis, 1985). For the Curie–Weiss model, we recall that the finite volume Gibbs state is associated to the Hamiltonian

$$\forall \eta \in X_n \qquad H^{\text{cw}}_{n,h}(\eta) = -\frac{1}{2}\sum_{x,y\in\Lambda} \frac{\mathcal{J}}{|\Lambda_n|}\eta(x)\eta(y) - \frac{h}{|\Lambda_n|}\sum_{x\in\Lambda}\eta(x). \tag{21}$$

The specific free energy $\psi^{\text{seq}}_{\text{cw}}(\beta,h)$ can be computed as the solution to the following variational problem

$$-\beta\psi^{\text{seq}}_{\text{cw}}(\beta,h) = \lim_{n\to\infty}\frac{1}{|\Lambda_n|}\ln Z^{\text{seq}}_{\text{cw}}(n,\beta,h) = \sup_{a\in\mathbb{R}}\{\beta\tfrac{1}{2}(\mathcal{J}a^2+ha) - I(a)\} \tag{22}$$

with

$$I(a) = \begin{cases} \dfrac{1}{2}((1-a)\ln(1-a)+(1+a)\ln(1+a)) & \text{if } |a|<1 \\ \infty & \text{if } |a|\geqslant 1. \end{cases} \tag{23}$$

*Proposition 3.1.* We have the following relation between the sequential and parallel Curie–Weiss models

$$\psi^{\text{par}}_{\text{cw}}(\beta,h) = 2\psi^{\text{seq}}_{\text{cw}}(\beta,h). \tag{24}$$

Before giving a proof, we shall establish two lemmas. We shall use large deviation results for which the reader can refer to appendix A.

*Lemma 3.1.* Let $\{W_n,\ n\geqslant 1\}$ and $\{W'_n,\ n\geqslant 1\}$ be $\mathbb{R}$-valued random variables. For all $n\geqslant 1$, we assume $W_n$ and $W'_n$ to be independent and identically distributed. For all $a\in\mathbb{R}$, we denote

$$c_n(a) = \frac{1}{n}\ln E[\exp aW_n]. \tag{25}$$

We assume for all $a\in\mathbb{R}$ that

(i) for all $n\geqslant 1$, $c_n(a)<\infty$,

(ii) $c(a) = \lim_n c_n(a) < \infty$ and

(iii) $c_n(a)$ is differentiable.

For all $n\geqslant 1$, we denote by $Q^{(2)}_n$ the distribution of the random variable $(W_n/n, W'_n/n)$. Then, the sequence $\{Q^{(2)}_n, n\geqslant 1\}$ has a large deviations property with reference sequence $a_n = n$ and entropy function

$$\forall (a,b)\in\mathbb{R}^2 \qquad I^{(2)}(a,b) = c^*(a)+c^*(b) \tag{26}$$

where $c^*$ denotes the Legendre–Frenchel transform of $c$.

*Proof.* For all $a,b\in\mathbb{R}$, we have

$$\begin{aligned} c_n(a,b) &= \frac{1}{n}\ln E[\exp(aW_n+bW'_n)] \\ &= \frac{1}{n}\ln(E[\exp aW_n]E[\exp bW'_n]) \\ &= c_n(a)+c_n(b). \end{aligned} \tag{27}$$

Hence, we have $c^*(a,b) = c^*(a)+c^*(b)$ for all $a,b\in\mathbb{R}$. The proof is concluded by a straightforward application of theorem II.6.1 of Ellis (1985). □

Now, we have a remark about convex functions.

*Lemma 3.2.* Let $f$ be a real convex function. If $(a, b) \in \mathbb{R}^2$ is a solution of the system

$$\begin{cases} f'(a) = b \\ f'(b) = a \end{cases} \tag{28}$$

then, we have $a = b$.

*Proof.* Let $a \leqslant b$. Then, $f'(b) \leqslant f'(a)$ and $b \leqslant a$ by convexity. □

*Proof of proposition 3.1.* For all $n \geqslant 1$, we denote by $Q_n$ the distribution of

$$S_n(\eta) = \frac{1}{|\Lambda_n|} \sum_{x \in \Lambda_n} \eta(x). \tag{29}$$

By lemma 3.1, the sequence $\{Q_n \otimes Q_n, n \geqslant 1\}$ has a large deviations property with reference sequence $a_n = |\Lambda_n|$ and entropy function

$$\forall (a, b) \in \mathbb{R}^2 \qquad I(a, b) = I(a) + I(b). \tag{30}$$

According to theorem II.7.1 of Ellis (1985), the long-range behaviour of $\frac{1}{|\Lambda_n|} \ln Z(\Lambda_n, \beta, h)$ is determined by the minimum points of

$$i_{\beta,h}(a, b) = I(a, b) - \beta(\mathcal{J}ab + h(a + b)). \tag{31}$$

These points are the solutions to the system

$$\begin{cases} I'(a) = \beta(\mathcal{J}b + h) \\ I'(b) = \beta(\mathcal{J}a + h). \end{cases} \tag{32}$$

Since $I$ is convex, we have

$$\begin{aligned} -\beta\psi_{\mathrm{cw}}^{\mathrm{par}}(\beta, h) &= \sup_{(a,b)\in\mathbb{R}^2} \{\beta(\mathcal{J}ab + h(a + b)) - I(a, b)\} \\ &= \sup_{a\in\mathbb{R}} \{\beta(\mathcal{J}a^2 + 2ha) - 2I(a)\} \\ &= -2\beta\psi_{\mathrm{cw}}^{\mathrm{seq}}(\beta, h). \end{aligned} \tag{33}$$

□

*Comments.* Proposition 3.1 states that the parallel Curie–Weiss and mean-field models have the same features in the long-range limit. The magnetization can be explicitly computed from the variational expression. Thus, we have

$$m_{\mathrm{cw}}^{\mathrm{par}} = \tanh \beta(\mathcal{J} m_{\mathrm{cw}}^{\mathrm{par}} + h) \tag{34}$$

and

$$m_{\mathrm{cw}}^{\mathrm{par}} = m_{mf}^{\mathrm{par}} = m_{\mathrm{cw}}^{\mathrm{seq}}. \tag{35}$$

## 4. Thermodynamical limits

In this section, we shall focus on the existence of the specific free energy and the magnetization function for the Gibbs states that result from a parallel updating of ferromagnetic spins. For a finite subset $\Lambda \subset \mathbb{Z}^d$, lemma 2.1 showed that $M^{\text{par}}(\Lambda, \beta, h)$ and $\Psi^{\text{par}}(\Lambda, \beta, h)$ could be computed as the thermodynamical quantities of a 'bigger' model. This model was obtained by dedoubling the set of spins and the set of interactions. A short calculation shows the connection between both quantities

$$-\frac{\partial \Psi^{\text{par}}}{\partial h}(\Lambda, \beta, h) = -\frac{1}{\beta Z^{\text{par}}(\Lambda, \beta, h)} \frac{\partial Z^{\text{par}}}{\partial h}(\Lambda, \beta, h) = 2M^{\text{par}}(\Lambda, \beta, h). \tag{36}$$

This easy statement has a deep consequence. The existence of the thermodynamical quantities that we defined in section 2 can be formally established by using convexity arguments. These arguments are close to those developed in Georgii (1988) or Ellis (1985). We shall give the existence result and defer the proof to appendix B.

*Proposition 4.1.*

(a) For all $\beta > 0$, the limit

$$\psi^{\text{par}}(\beta, h) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \Psi^{\text{par}}(\Lambda, \beta, h) \tag{37}$$

exists, it is a concave and pair function of $h \in \mathbb{R}$. It is differentiable for $h \neq 0$.

(b) For all $\beta > 0$, $h \in \mathbb{R}$,

$$m^{\text{par}}(\beta, h) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} M^{\text{par}}(\Lambda, \beta, h) \tag{38}$$

exists and for $h \neq 0$

$$m^{\text{par}}(\beta, h) = -\frac{1}{2} \frac{\partial \psi^{\text{par}}}{\partial h}(\beta, h). \tag{39}$$

*Proof.* See appendix B. □

*Comments.* The coefficient $\frac{1}{2}$ in equation (39) can be explained in the following manner. If no interaction exists between the spins, the parallel partition function would be the square of the sequential one. Then the parallel free energy would be twice the sequential one. However, according to the law of large numbers the magnetization would be the same.

We now focus on the relationships between parallel and sequential models. We shall see that in some cases the relation can be written explicitly, i.e. the parallel quantities will express from the sequential ones. First, we concentrate on ferromagnetic models with the property that

$$\text{for all even } k \in \mathbb{Z}^d, \quad J(k) = 0. \tag{40}$$

Even $k$ means that the sum of the coordinates of $k$ is an even integer.

As a relevant situation, we have used the Ising model on the $d$-dimensional lattice. Let $J$ be a positive number. The parallel Ising model can be defined through the doubled Hamiltonian

$$\forall (\eta, \zeta) \in X_\Lambda \times X_\Lambda \qquad H^{(2)}_{\Lambda,h}(\eta, \zeta) = -\sum_{|x-y|=1} J\eta(x)\zeta(y) - h\sum_{x\in\Lambda}(\eta(x) + \zeta(x)). \tag{41}$$

The following statement holds.

*Proposition 4.2.* For any ferromagnetic model satisfying condition (40)

$$\psi^{\mathrm{par}}(\beta, h) = 2\psi^{\mathrm{seq}}(\beta, h). \tag{42}$$

*Proof.* Let $\Lambda$ be a symmetric hypercube of $\mathbb{Z}^d$. The key argument is the following. For the interaction graph induced on $\mathbb{Z}^d$ by the potential $J$, the chromatic number is 2. Hence, a partition of $\Lambda$ in two independent subsets $\Lambda_1$ and $\Lambda_2$ exists. The importance of such a property has been noticed for a long time in order to optimize the sequential updating procedure. This time, we use it to change variables in the parallel partition function. Define a new configuration, $\eta_{\Lambda_1}\zeta_{\Lambda_2}$, from $\eta$ and $\zeta$ by

$$\forall x \in \Lambda \qquad \eta_{\Lambda_1}\zeta_{\Lambda_2}(x) = \begin{cases} \eta(x) & \text{if } x \in \Lambda_1 \\ \zeta(x) & \text{if } x \in \Lambda_2. \end{cases} \tag{43}$$

We have

$$H^{(2)}_{\Lambda,h}(\eta, \zeta) = H^{\mathrm{seq}}_{\Lambda,h}(\eta_{\Lambda_1}\zeta_{\Lambda_2}) + H^{\mathrm{seq}}_{\Lambda,h}(\eta_{\Lambda_2}\zeta_{\Lambda_1}). \tag{44}$$

We can compute the parallel partition function in the following way

$$\begin{aligned} Z^{\mathrm{par}}(\Lambda, \beta, h) &= \sum_{\eta,\zeta\in X_\Lambda} \exp -\beta H^{(2)}_{\Lambda,h}(\eta, \zeta) \\ &= \sum_{\eta\in X_\Lambda}\sum_{\zeta\in X_\Lambda} \exp -\beta (H^{\mathrm{seq}}_{\Lambda,h}(\eta_{\Lambda_1}\zeta_{\Lambda_2}) + H^{\mathrm{seq}}_{\Lambda,h}(\eta_{\Lambda_2}\zeta_{\Lambda_1})) \\ &= \sum_{\sigma\in X_\Lambda}\sum_{\sigma'\in X_\Lambda} \exp -\beta H^{\mathrm{seq}}_{\Lambda,h}(\sigma) \exp -\beta H^{\mathrm{seq}}_{\Lambda,h}(\sigma') \\ &= \{Z^{\mathrm{seq}}(\Lambda, \beta, h)\}^2 \end{aligned} \tag{45}$$

since $\sigma$ and $\sigma'$ are independent. The result is obtained by letting $\Lambda$ grow to $\mathbb{Z}^d$. □

*Comments*. By the previous proposition, the magnetization is the same for both sequential and parallel Ising models. As stressed in the proof, this result is true whenever $\mathbb{Z}^d$ can be separated in two independent sublattices. In such a case, the doubled model contains two independent versions of the original one. This property fails to hold when the chromatic number of the interaction graph is greater than 3.

We now study some more complicated situations. The parallel updating will be performed in models for which the chromatic number is greater than or equal to three. We emphasize in an indirect manner the need to use parallel simulation. Parallel simulation allows us to simulate models for which the chromatic number of the interaction graph is equal to 2 by using a reduced system. The models that we wish to simulate are Ising models on product graphs with chromatic number 2 (we shall assume the existence of the thermodynamical functions by the techniques used in appendix B). From proposition 4.2, it would be sufficient to apply parallel updating of spins without changing anything.

Our technique consists of considering the original graph as the doubled graph (which is always bipartite) of a parallel model. Thus, parallel updating can be performed on the corresponding reduced graph. Of course, this procedure is not systematic. It works in some particular cases. For instance, we consider the Ising model on the graphs

$$G_1 = \mathbb{Z}/6\mathbb{Z} \times \mathbb{Z} \qquad \text{and} \qquad G_2 = \mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}. \tag{46}$$

It can be easily checked that the reduced graph of $\mathbb{Z}/6\mathbb{Z}$ is the clique $C_3$ of the order of 3 (i.e. the graph $\mathbb{Z}/3\mathbb{Z}$). Then the reduced graph of $G_1$ is $\mathbb{Z}/3\mathbb{Z} \times \mathbb{Z}$. The reduced graph of the hypercube (with eight vertices) is the clique $C_4$ of the order of 4. Then the reduced graph of $G_2$ is $D_4 \times \mathbb{Z}^+$ where $D_4 = C_4$ for $i = 0$ and $D_4 = \mathbb{Z}/4\mathbb{Z}$ for $i \geqslant 1$. By the dedoubling argument, we have

$$m^{\text{par}}_{\text{reduced}}(\beta, h) = m^{\text{seq}}_G(\beta, h) \tag{47}$$

where $m^{\text{par}}_{\text{reduced}}(\beta, h)$ is the magnetization function of the parallel model on the reduced graph and $m^{\text{seq}}_G(\beta, h)$ is the magnetization function of the sequential model on the original graph. The chromatic number of the reduced graph is equal to 3 for $G_1$ and equal to 4 for $G_2$.

Numerical simulations performed on lattice graphs $G_1$ and $G_2$ for different values of the parameter $\beta$ confirm the later results (figures 1 and 2). We deliberately chose small graphs as the efficiency of the method is proved by proposition 4.1 in the limit of large sizes. Furthermore, we did not observe a phase transition for these models.

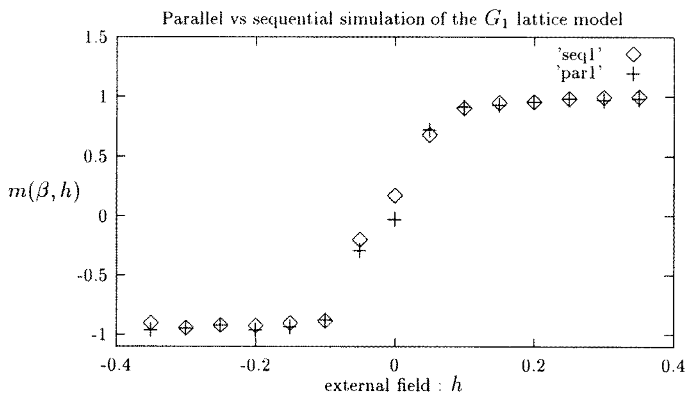


**Figure 1.** Magnetization as a function of the external field. 500 spins. $\beta = 0.6$.

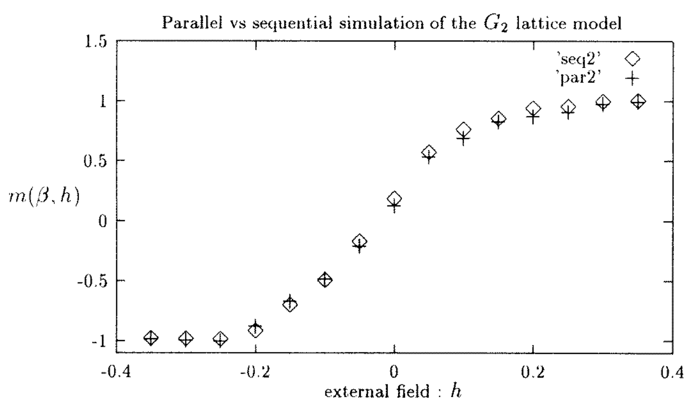


**Figure 2.** Magnetization as a function of the external field. 1000 spins. $\beta = 0.8$.

## 5. Conclusion

The results given in this article constitute a step towards a better understanding of the use of parallelism in spin systems simulation. We obtained ‘rigorous’ results which concern the use of parallel updating in ferromagnetic spin systems simulation. We proved the existence of parallel free energy and magnetization functions. In addition, we gave some relationships between both the quantities. The study of the Curie temperature of the parallel models by these quantities is thus relevant. We tried to establish formal links between the parallel and the sequential quantities. We identified two classes of models for which the relationships are clear: the mean-field models and the two-coloured lattice models. For such models parallelism introduces no bias when one is interested in the study of the sequential Curie temperature. Before concluding, we suggested through examples a different manner of using parallelism to simulate a two-coloured lattice model. It is often possible to perform a parallel simulation on a reduced lattice. Doing so we gain by using parallelism and by dividing the simulation size by two.

Finally, we conclude with the emphasis that the simulation procedure itself was not studied. To analyse the simulation results, the size-fluctuations of the order parameters must be taken into account. Moreover, a thorough study would also require the control of the relaxation time of the parallel Markov chain. Such an analysis is difficult in general due to the existence of a critical region for the parameters (see Frigessi *et al* 1993) and will be given in a forthcoming paper.

## Appendix A.

We recall some results concerning large deviations. These results can be found in Ellis (1985).

Let $\mathcal{X}$ be a complete metric space endowed with its Borel algebra $\mathcal{B}(\mathcal{X})$ and $\{Q_n,\ n \geqslant 1\}$ be a sequence of probability distributions on $(\mathcal{X},\ \mathcal{B}(\mathcal{X}))$.

*Definition A.1.* The sequence $\{Q_n, n \geqslant 1\}$ has a large deviations property if there exists a sequence $\{a_n\ \ n \geqslant 1\}$ of positive numbers $a_n \to \infty$ and a function $I : \mathcal{X} \to \mathbb{R}^+$ satisfying

(a) $I$ is lower semi-continuous,

(b) $I$ has compact level sets,

(c) for all closed subset $K$

$$\overline{\lim}\, a_n^{-1} \ln Q_n\{K\} \leqslant - \inf_{x\in K} I(x). \tag{A1}$$

(d) for all open subset, $O$,

$$\underline{\lim}\, a_n^{-1} \ln Q_n\{O\} \geqslant - \inf_{x\in G} I(x). \tag{A2}$$

The sequence $\{a_n\}$ is called the reference sequence and $I$ the entropy function.

Let $\{W_n,\ n \geqslant 1\}$ be $\mathbb{R}^d$-valued random variables ($d \geqslant 1$) and $\{a_n,\ n \geqslant 1\}$ be a sequence of positive numbers such that $a_n \to \infty$. We denote

$$\forall t \in \mathbb{R}^d \qquad c_n(t) = \frac{1}{a_n} \ln E_n[\exp\langle t, W_n\rangle] \tag{A3}$$

and assume that for all $n \geqslant 1$, $c_n(t) < \infty$ and $c(t) = \lim_n c_n(t)$ exists. Let $c^*$ be the Legendre–Frenchel transform of $c$

$$\forall z \in \mathbb{R}^d \qquad c^*(z) = \sup_{t\in\mathbb{R}^d}\{\langle t, z\rangle - c(t)\}. \tag{A4}$$

Let $Q_n$ be the probability distribution of $W_n/a_n$. Then, the sequence $\{Q_n, n \geqslant 1\}$ has a large deviations property with reference sequence $\{a_n\}$ and entropy function $I = c^*$. Moreover, for all continuous functions, $F$,

(a) $\sup_{\mathcal{X}} F(x) < \infty$ implies $\sup_{\mathcal{X}}\{F(x) - I(x)\} < \infty$

(b) $\lim_n \frac{1}{a_n} \ln \int \exp a_n F(x) Q_n(\mathrm{d}x) = \sup_{\mathcal{X}}\{F(x) - I(x)\}$.

## Appendix B.

In this section, we will give a proof of proposition 4.1. We will need the following results. For all $R \subset \Lambda$, we shall denote

$$\chi_R(\eta) = \prod_{x \in R} \eta(x). \tag{B1}$$

We recall the classical correlation inequalities which hold for ferromagnetic models

*GKS1 inequality*. For all $R \subset \Lambda$,

$$\langle \chi_R(\eta) \rangle \geqslant 0. \tag{B2}$$

*GKS2 inequality*. For all $R, T \subset \Lambda$,

$$\langle \chi_R(\eta)\chi_T(\eta) \rangle \geqslant \langle \chi_R(\eta) \rangle \langle \chi_T(\eta) \rangle. \tag{B3}$$

*GHS inequality*. For all $x, y, z \in \Lambda$,

$$\langle (\eta(x) - \langle \eta(x) \rangle)(\eta(y) - \langle \eta(y) \rangle)(\eta(z) - \langle \eta(z) \rangle) \rangle \leqslant 0. \tag{B4}$$

*Proposition B.1.* For all $\beta > 0$

(a) $M^{\mathrm{par}}(\Lambda, \beta, 0) = 0$;

(b) $M^{\mathrm{par}}(\Lambda, \beta, -h) = -M^{\mathrm{par}}(\Lambda, \beta, h)$ for all $h \in \mathbb{R}$;

(c) $M^{\mathrm{par}}(\Lambda, \beta, h) \geqslant 0$ if $h \geqslant 0$ and $|M^{\mathrm{par}}(\Lambda, \beta, h)| \leqslant |\Lambda|$;

(d) $M^{\mathrm{par}}(\Lambda, \beta, h)$ is a concave function of $h \geqslant 0$;

(e) $M^{\mathrm{par}}(\Lambda, \beta, h)$ is an increasing function of $h \geqslant 0$.

*Proof.* Let $h \geqslant 0$. According to the $GKS$ 1 inequality, we have

$$\langle \chi_R \rangle_\Lambda^{\mathrm{par}} = \langle \chi_R \rangle_\Lambda^{(2)} \geqslant 0. \tag{B5}$$

According to $GKS$ 2, we have, for all $R, R', T, T' \subset \Lambda$,

$$\langle \chi_R(\eta)\chi_T(\zeta)\chi_{R'}(\eta)\chi_{T'}(\zeta) \rangle_\Lambda^{(2)} \leqslant \langle \chi_R(\eta)\chi_T(\zeta) \rangle_\Lambda^{(2)} \langle \chi_{R'}(\eta)\chi_{T'}(\zeta) \rangle_\Lambda^{(2)}. \tag{B6}$$

Let $h \in \mathbb{R}$ and $x, y, z \in \Lambda$. According to $GHS$, for any choice

$$\alpha(x) = \eta(x) \text{ or } \zeta(x) \qquad \alpha(y) = \eta(y) \text{ or } \zeta(y) \qquad \alpha(z) = \eta(z) \text{ or } \zeta(z) \tag{B7}$$

we have

$$\langle (\alpha(x) - \langle \alpha(x) \rangle_\Lambda)(\alpha(y) - \langle \alpha(y) \rangle_\Lambda)(\alpha(z) - \langle \alpha(z) \rangle_\Lambda) \rangle_\Lambda^{(2)} \geqslant 0. \tag{B8}$$

Then, it is easily checked that

$$\frac{\partial}{\partial h} \langle \eta(x) \rangle_\Lambda^{\mathrm{par}} \geqslant 0 \tag{B9}$$

and

$$\frac{\partial^2}{\partial h} \langle \omega(x) \rangle_\Lambda^{\mathrm{par}} \leqslant 0 \tag{B10}$$

which proves (d) and (e).

By checking the other statements, in particular, we have

$$\pi^{\mathrm{par}}_{\Lambda,\beta,-h}(\eta) = \sum_{\zeta\in X_\Lambda} \frac{1}{Z^{\mathrm{par}}(\Lambda,\beta,h)} \exp\left\{\beta\sum_{x,y\in\Lambda} J(x-y)\eta(x)\zeta(y) - h\sum_{x\in\Lambda}(\eta(x)+\zeta(x))\right\}$$

$$= \sum_{(-\eta)\in X_\Lambda} \frac{1}{Z^{\mathrm{par}}(\Lambda,\beta,h)} \exp\beta\Bigg[\sum_{x,y\in\Lambda} J(x-y)(-\eta(x))(-\zeta(y))$$

$$+h\sum(-\eta(x)-\zeta(x))\Bigg]$$

$$= \pi^{\mathrm{par}}_{\Lambda,\beta,h}(-\eta). \tag{B11}$$

This proves (a) and (b). □

*Proof of proposition 4.1.* (a) The existence of $\psi^{\mathrm{par}}(\beta,h)$ is a consequence of a general result that can be found for instance in Ellis (1985) appendix D 1. Concavity follows from the Hölder inequality. Let $h_1, h_2 \in \mathbb{R}$ and $\lambda \in [0,1]$, we have

$$Z^{\mathrm{par}}(\Lambda,\beta,\lambda h_1+(1-\lambda)h_2) = \sum_{(\eta,\zeta)\in X_\Lambda\times X_\Lambda} \exp\left(\beta\lambda h_1\left\{\sum_{x\in\Lambda}\eta(x)+\zeta(x)\right\}\right)$$

$$\times \exp\left(\beta(1-\lambda)h_2\left\{\sum_{x\in\Lambda}\eta(x)+\zeta(x)\right\}\right)\exp(-\beta H^{(2)}_{\Lambda,0}(\eta,\zeta)) \tag{B12}$$

and thus

$$Z^{\mathrm{par}}(\Lambda,\beta,\lambda h_1+(1-\lambda)h_2) \leqslant \left\{\sum_{(\eta,\zeta)\in X_\Lambda\times X_\Lambda}\exp-\beta H_{\Lambda,h_1}(\eta,\zeta)\right\}^{\lambda}$$

$$\times\left\{\sum_{(\eta,\zeta)\in X_\Lambda\times X_\Lambda}\exp-\beta H_{\Lambda,h_2}(\eta,\zeta)\right\}^{1-\lambda}. \tag{B13}$$

Then, we obtain

$$\Psi^{\mathrm{par}}(\Lambda,\beta,\lambda h_1+(1-\lambda)h_2) \geqslant \lambda\Psi^{\mathrm{par}}(\Lambda,\beta,h_1)+(1-\lambda)\Psi^{\mathrm{par}}(\Lambda,\beta,h_2). \tag{B14}$$

Taking the thermodynamical limit, $\psi^{\mathrm{par}}(\beta,h)$ is a concave function of $h$.

Parity is a consequence of the relation

$$H^{\mathrm{par}}_{\Lambda,\beta,h}(-\eta) = H^{\mathrm{par}}_{\Lambda,\beta,-h}(\eta). \tag{B15}$$

To prove the second statement of proposition 4.1, fix $h \geqslant 0$. Then, we have, according to relation (36)

$$\frac{1}{|\Lambda|}(\Psi^{\mathrm{par}}(\Lambda,\beta,h)-\Psi^{\mathrm{par}}(\Lambda,\beta,0)) = -2\int_0^h \frac{1}{|\Lambda|}M^{\mathrm{par}}(\Lambda,\beta,s)\,\mathrm{d}s. \tag{B16}$$

Since $\frac{1}{|\Lambda|}M^{\mathrm{par}}(\Lambda,\beta,h)$ is a concave and bounded function of $h \geqslant 0$, the limit $m^{\mathrm{par}}(\beta,h)$ exists and is continuous. By Lebesgue's convergence theorem, we have

$$\psi^{\mathrm{par}}(\beta,h)-\psi^{\mathrm{par}}(\beta,0) = -2\int_0^h m^{\mathrm{par}}(\beta,s)\,\mathrm{d}s. \tag{B17}$$

This proves (b) when $h \geqslant 0$ and a similar argument holds when $h < 0$. □

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