LIQUID CRYSTAL LATTICE MODELS ON QUADRICS SUPERCOMPUTER

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Abstract

The implementation on Quadrics and some tests of a Monte Carlo code for simulations of liquid crystal lattice models are described. The use of a Quadrics with 512 processors is proving essential in studying the nematic-isotropic phase transition to an unprecedented level of accuracy using over 10^6 *particles.*

1. Introduction

Liquid crystals constitute a state of aggregation of matter intermediate between solids and liquids [1]. Their main characteristic is that they possess long-range orientational molecular order while having flow properties similar to those of liquids. This orientational order can be characterized, at least for systems formed of molecules with cylindrical symmetry, by the average of the second Legendre polynomial of the angle β between molecule axis and the overall preferred orientation of the liquid crystal (the "director")

$$\langle P_2 \rangle \equiv \left\langle \frac{3}{2}\cos^2\beta - \frac{1}{2} \right\rangle . \tag{1}$$

$\langle P_2 \rangle$ is one when all molecules are perfectly aligned with the director, and decreases with increasing temperature until at a temperature T_{NI} a weak first-order transition to the isotropic liquid state is reached, where $\langle P_2 \rangle$ goes to zero. This behaviour has been fairly well studied both experimentally and theoretically, although many of the features of the phase transition, e.g. its critical exponents, are still a subject of discussion. Computer simulations have also been applied to investigate the liquid crystal physics since the pioneering work of Lebwohl and Lasher (LL) [2]. In this model attention is focused only on the orientational properties and the LL potential plays, in the field of liquid crystals, a rôle similar to that of the Heisenberg or Ising models in magnetism. The particles, represented by three dimensional spins placed at the sites of a cubic lattice, interact through the attractive nearest neighbour pair potential:

$$U_{ij} = -\epsilon_{ij}[\frac{3}{2}(\vec{S}_i \cdot \vec{S}_j)^2 - \frac{1}{2}] \quad (2)$$
$$= -\epsilon_{ij} P_2(\cos\beta_{ij}). \quad (3)$$

Here ϵ_{ij} is a positive constant, ϵ, for nearest neighbours particles i and j and zero otherwise, β_{ij} is the angle between the axis of these two molecules and P_2 is a second rank Legendre polynomial. This simple model reproduces fairly correctly the orientational phase transition and the related physical observables [2-6], while the choice of fixed positions at lattice sites, even though clearly not correct in reality, does not influence the essential orientational behaviour near the phase transition. A lot of work has been done on generalizations of the LL model [7-17] and recently, with the development of more powerful computers, potentials with traslational degrees of freedom have been introduced [18,20]. However, lattice models still present several advantages in comparison with these " more realistic" potentials. First of all on a lattice it is possible to treat a number of particles at least one or two orders of magnitude larger, so that the transition temperature can be located with a greater accuracy. This is a crucial point because the Nematic-Isotropic phase transition is not completely understood: an analytic solution of the model does not exist and while any sensible approximate theory (molecular field, Two Site Cluster, etc.) gives a phase transition, no theory has yet been able to correctly predict more subtle but fundamental features such as the pretransitional effects, taking place above the disordering transition and diverging for real systems about $1°K$ below T_{NI}. It is then essential to have reference calculations on this LL model to test if this simple potential is adequate or not. Thus the transition and its neighbourhood have to be studied with a temperature resolution as small as possible and certainly below 0.1 K equivalent and this requires very large lattices. Presently the uncertainty on the transition temperature is about .2K obtained with simulations of a $30 \times 30 \times 30$ systems [3-5]. Moreover, apart from basic research, the large number of spins permits to tackle computer simulations of certain technologically relevant systems, such as LC displays [16]. The need of powerful computers is then essential fot the aims above mentioned and here we wish to present the implementation of a MC code on a Quadrics and some tests and examples.

2. Implementation of the code on Quadrics: main features

Quadrics computers are parallel SIMD machine derived from APE100, a special purpose computer developed by INFN (National Institute for Nuclear Physics) for lattice QCD [21]. We shall see that the nearest neighbours Lebwohl-Lattice models we deal with can easily implemented on the Quadrics architecture.

Our aim is to simulate a (large) lattice of $L \times L \times L$ particles then we follow the approach of making a geometrical subdivision of the sample, following the machine architecture, placing on each processor a $l_x \times l_y \times l_z$ particles sublattice:

$$l_x = L/N_x$$

$$l_y = L/N_y$$
$$l_z = L/N_z$$

where N_x, N_y and N_z are the number of nodes for each side of the Quadrics machine.

Clearly, we have to pay attention to the interactions of the particles on the edges of the sublattice with their neighbours, because they lie on the adyacent processor and an inter-node communication is needed.

Because of the SIMD architecture of the Quadrics machines all the calculations, as well as all the communications, are globally performed at the same time on all the processors.

On the sample made of 1728000 particles we are studying, each node owns a portion made of $15 \times 15 \times 15$ particles. So there are totally $2 \times 6 \times 15^3 = 40500$ interactions to be calculated by each node. Just $2 \times 6 \times 15^2 = 2700$ of these involve a particle residing on an adjacent processor. Furthermore the number of communications is halved, because the 2 factor is needed to count both the old and the new energy calculations (to apply the Monte Carlo acception criterion), for which the neighbour particles are still the same.

Because of this it is very important to aim to the target of getting the best performance in the single processor code.

The Quadrics processors are characterized by the fast execution of the normal operation $(A \times (\pm B)) \pm C$ when the operands are still on the registers (one operation for clock cycle). So the bottle-neck in the execution is primarily due to the memory-to-register and register-to-memory data transfers; these operations can be pipelined, i.e. if we need to load into the registers a sequence of contigonous memory locations, the fetch is slow (4 clock cycles) just for the first datum, while the following ones are loaded at high rate (1 clock cycle each).

The TAO language allows the programmer to optimize the usage of the 128 hardware registers. Moreover the capabilities of the ZZ language allow the programmer to write a simplified code doing operations, such as loop-unrolling and in-line code expansion, implicitly.

The memory organization of the code has been set up *ad hoc*, to take advantage of the pipelined execution. The main idea consists in the loading of columns of particles, with their neighbours, on the registers, to allow the fast execution for more than one particle.

Using the TAO sintax, the new datatype `three` has been defined:

```
matrix real three.[3]
```

This is a generic type composed of three real number. In particular it is used for the representation of the particle orientations in terms of director cosines, i.e., using Euler angles, for the i-th particle:

$$u_{ix} = \cos\alpha_i \sin\beta_i \quad (4)$$

$$u_{iy} = \sin\alpha_i \sin\beta_i \quad (5)$$

$$u_{iz} = \cos\beta_i \quad (6)$$

To easly take advantage of the pipelined memory retrivial-storage a new type `use`, composed of `hmz` (acronimous for *How-Many-Z*) `three`, has been created:

```
three use.[hmz]
```

These are `hmz` consecutive orientations along the z direction. Finally the `u` array containing the molecular configuration has been created:

```
nz = ndz/hmz
use u[ndx,ndy,nz]
```

where `ndx`, `ndy` and `ndz` are the dimension of the portion of the whole sample owed by one node. `ndz` has to be a multiple of `hmz`.

The data needed on the registers to optimally exploit the processor performance are the following:

- $3 \times hmz$ real numbers for a block of orientations along the z direction
- $4 \times 3 \times hmz$ real numbers for the *left*, *front*, *right* and *rear* blocks of orientations with respect to the previous one.
- 2×3 real numbers for the *up* and *down* particles.
- $3 \times hmz$ real numbers for the random numbers needed for the Monte Carlo method. For each move two of them are for the Barker and Watts [22] move and the third one for the Metropolis Monte Carlo acceptance criterion. We use the Metropolis prescription [23] for the local lattice updating, which in this SIMD implementation is performed with a synchronous scanning of the different sublattices.
- $3 \times hmz$ real numbers for the trial orientations.
- 9 real numbers to accumulate the global energy (1), the ordering matrix (6) and the acception rate (2)

The optimal value without exceeding the registers at our disposal has been found to be $hmz = 3$, totally 78 physical registers (usually about 90 of the total 128 are usable).

The code is based on several libraries of Tao statments and functions, both for general Monte Carlo purposes and for Lebwohl-Lasher potential in particular. The main libraries are:

- *Algebraic library.* A general purpose library for computing operations on vectors (scalar products, normalizations, ecc.) and for diagonalizing a symmetric 3×3 matrix by means of *powers method*
- *Lebwohl Lasher library.* A library of Tao functions and statments for Lebwohl Lasher model.
- *Order library.* A library for computing ordering matrices.

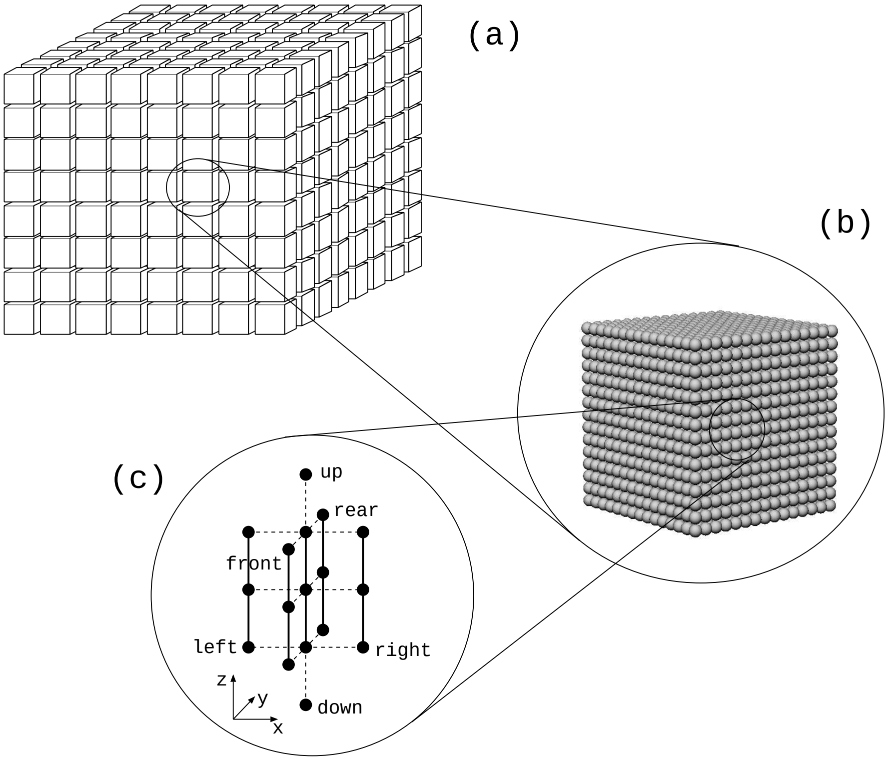

Figure 1: A schematic representation of the whole system on a QH4 machine (**a**), the spin organisation on a single processing element (**b**) and the data loaded at once on the registers for the pipelined calculation (**c**) (see text).

- *Fast memory access.* This is a library for fast memory access: i.e. we reduced the ratio of memory access time versus calculations time, using optimized *extract* and *replace* statments.

3. TESTS AND EXAMPLES

To test the code we have performed a complete simulation on a relatively small cubic lattice of $30 \times 30 \times 30$ spins. In Fig. 2. we show the second rank order parameter $< P_2 >_\lambda$ curve as obtained from the test simulation and some points of the megaparticle simulation (see next section). Results from the previous largest calculations ($N = 30 \times 30 \times 30$) [3] are also reported for comparison and provide an excellent test of the program.

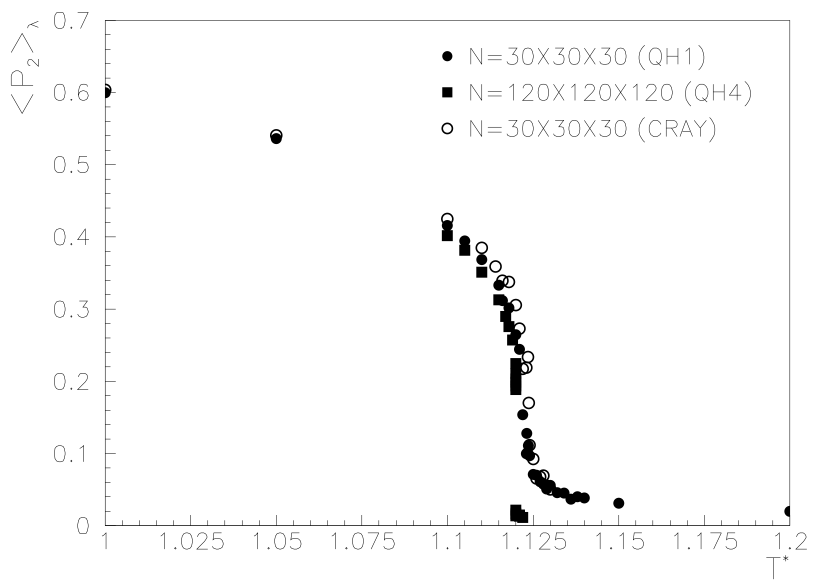

Figure 2: Second rank order parameter $\langle P_2 \rangle_\lambda$ versus reduced temperature $T^* = kT/\epsilon$ as obtained by MC simulations on Quadrics (full symbols) and on Cray [3] (empty symbols).

A number of properties are calculated. The most important are the dimensionless energy $U^* \equiv U/kT$, calculated as a sum of pair interactions (Eq. 2), the heat capacity C_V^*, obtained by differentiating the average energy with respect to temperature, and the order parameters, particularly $\langle P_2 \rangle$. The order parameter cannot be calculated directly from Eq. 2 because of director fluctuations during the simulation, and is evaluated with respect to the instantaneous preferred direction using the largest eigenvalue of a suitably defined ordering matrix [2-4]. The results are correct and reproduce well the behaviour of the thermodynamic observables versus temperature curves.

As mentioned above we are interested in two lines of work and here we summarize some preliminary results.

3.1 Phase change in very large lattice systems.

We have been using the code to simulate what is by far the largest LL system to date, i.e. $N = 120 \times 120 \times 120$ (1728000 spins). We recall that until now there are no systematic LL simulation for samples larger than 27000 spins and then the present simulations, still under way, are the largest one performed in the liquid crystal field with an improvement of nearly two orders of magnitude in the system size.

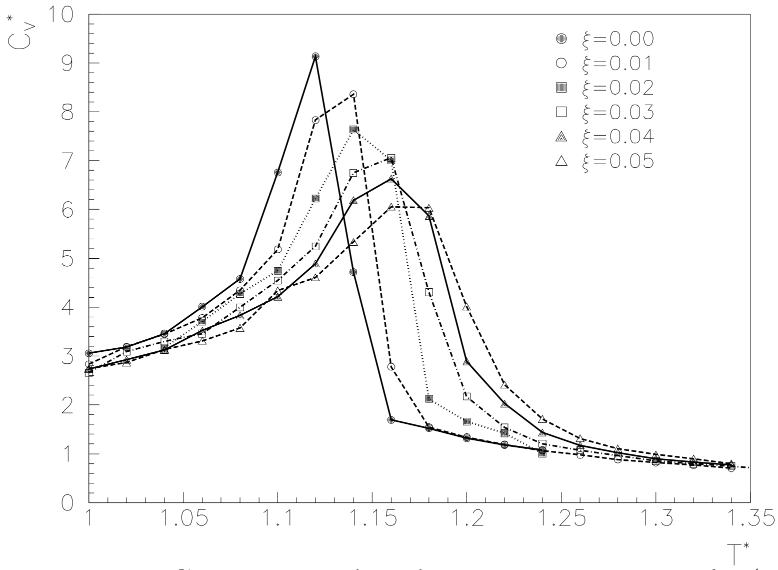

Figure 3: Heat capacity C_V^* versus reduced temperature $T^* = kT/\epsilon$ for different values of field strenght, ξ.

3.2 Simulation of the effect of an external field on a nematic system

The case we wish to tackle here is that of the effect of an applied field on the molecular organization and on the nematic isotropic phase transition. To do this, a suitable second rank term is added to the LL hamiltonian to keep into account the contribution to the orientational energy due to the interaction between the spins and the external field [15]:

$$U_N = -\sum_{\substack{i,j \\ i<j}} \epsilon_{ij} P_2(\cos\beta_{ij}) - \epsilon\xi \sum_{i=1}^{N} P_2(\cos\beta_i) \tag{7}$$

where N is the number of particles of the system, β_i is the angle between the field direction and the particle symmetry axis and ξ determines the strength of the coupling to the field. The effect of the external field is a stabilization of the ordered phase with a change in the character of the transition as the intensity of the field increases with disappearance of the transition at a critical point. We are running a set of simulations for various values of ξ to determine the critical coupling and more generally the phase diagram. In Fig. 3 we show the heat capacity plotted against the reduced temperature for some values of field strength as obtained from simulations of a $24 \times 24 \times 24$ system performed on a Quadrics Q1 machine. The shift and rounding of the transition is apparent even from this preliminary results.

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References

[1] The Molecular Physics of Liquid Crystals, eds. Luckhurst G.R. and Gray G.W., (Academic Press, New York), (1979).
[2] Lebwohl P.A. and Lasher G., *Phys Rev. A*, **6**, 426, (1972).
[3] Fabbri, U., and Zannoni, C., *Mol. Phys.*, **58**, 763, (1986).
[4] Zhang Z., Mouritsen O.G. and Zuckerman M., *Phys. Rev. Lett.* **69**, 2803 (1992).
[5] Cleaver D.G. and Allen M.P., *Phys Rev.* **A43**, 1918 (1991).
[6] Zannoni C., *J. Chem. Phys.*, **84**, 424, (1986).
[7] Chiccoli, C., Pasini, P., and Zannoni, C., *Liq. Cryst.*,**a)** **3**, 363, (1988); **b)** *Physica*, **148A**, 298, (1988); **c)** *Liq. Cryst.*, **2**, 39, (1987).
[8] Chiccoli, C., Pasini, P., Biscarini F. and Zannoni, C., **a)** *Mol. Phys.*, **65**, 1505, **b)***Mol. Phys.*, **73**, 439 (1991).
[9] Kunz H and Zumbach G., *Phys. Lett.* **B257**, 299 (1991).
[10] Caracciolo S., Edwards R.G., Pelissetto A. and Sokal A.D., *Nucl. Phys. B (Proc. Suppl.)* ***30**, 815 (1993).*
[11] Chiccoli, C., Pasini, P., Semeria F. and Zannoni, C., *Phys. Lett.* **A176**, 428 (1993).
[12] Fuller G., Luckhurst G.R. and Zannoni C., *Chem. Phys.* **92**, 105 (1985).
[13] Luckhurst G.R. and Simpson P., Chem. Phys. Lett. **95**, 149, (1983).
[14] Hashim R., Luckhurst G.R. and S. Romano, *Mol. Phys.* **53**, 1535, (1984); *Mol. Phys.* **56**, 1217, (1985); *Liq. Cryst.* **1**, 133, (1986); *Proc. R. Soc. Lond. A.*, **429**, 323, (1990).
[15] Luckhurst G.R., T.J. Sluckin and H.B. Zwedie, *Mol. Phys.* **59**, 657, (1986).
[16] Chiccoli, C., Pasini, P., Semeria F. and Zannoni, C., *Int. J. Mod. Phys. C* **6**, 135 (1995).
[17] Biscarini F. , Chiccoli, C., Pasini, P., Semeria F. and Zannoni, C., *Phys. Rev.*

Lett, ***75**, 1803 (1995).*
[18] Gay J.G and Berne B.J., *J. Chem. Phys.* **74**, 3316 (1981).
[19] De Miguel E., Rull L.F., Chalam M.K., Gubbins K.E. and Van Sivol F, *Mol. Phys.* **72**, 593 (1991).
[20] Berardi R, Emerson A.P.J. and Zannoni C., *J. Chem. Soc. Faraday Trans.* **89**, 4069 (1993).
[21] Tripiccione R. *Int. J. Mod. Phys. C* **4** 1323 (1993) *and reference therein*
[23] Barker J.A. and Watts R.O. *Chem. Phys. Lett.* **3**, 144, (1969).
[23] Metropolis N., Rosenbluth A.W., Rosenbluth M.N., Teller A.H. and Teller E., *J. Chem. Phys.* **21**, 1087, (1953).