International Journal of Modern Physics C, Vol. 8, No. 3 (1997) 0–0

S. Boschi, M. P. Brunelli, C. Zannoni, C. Chiccoli, P. Pasini,
Liquid Crystal Lattice Models on Quadrics Supercomputers,
Int. J. Mod. Phys. C , 8, 547-554 (1997)

LIQUID CRYSTAL LATTICE MODELS ON QUADRICS SUPERCOMPUTERS*

SIGISMONDO BOSCHI, MARCO P. BRUNELLI, CLAUDIO ZANNONI
Dipartimento di Chimica Fisica ed Inorganica dell' Università
Viale Risorgimento 4, 40136 Bologna, Italy

and

CESARE CHICCOLI, PAOLO PASINI†
Istituto Nazionale di Fisica Nucleare, Sezione di Bologna
Via Irnerio 46, 40126 Bologna, Italy
†*E-mail: Paolo.Pasini@.bo.infn.it*

Received 5 March 1997

The implementation of a Monte Carlo code for simulations of liquid crystal lattice models on the Quadrics massively parallel SIMD supercomputer is 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 more than 10^6 particles. Here some tests on the Lebwohl–Lasher model with and without an applied field are presented.

Keywords: Computer Simulations; Supercomputers; Liquid Crystals.

1. Introduction

Liquid crystals constitute a state of aggregation of matter intermediate between solids and liquids.[1] Their main characteristic is the presence of long-range orientational molecular order together with 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 behavior has

*A preliminary version of this work was presented at the Workshop "From APE100 to APEmille: Results and Perspectives", Frascati, Italy, 17-19 February 1997.

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 physics of liquid crystals 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 LL model is mathematically equivalent also to the ferromagnetic RP^2 system of interest in lattice field theory.[3,4] The particles, represented by three-dimensional spins placed at the sites of a cubic lattice, interact through the attractive nearest-neighbor pair potential:

$$U_{ij} = -\epsilon_{ij}[\frac{3}{2}(\mathbf{u}_i \cdot \mathbf{u}_j)^2 - \frac{1}{2}] \tag{2}$$

$$= -\epsilon_{ij} P_2(\cos\beta_{ij}). \tag{3}$$

Here ϵ_{ij} is a positive constant, ϵ, for nearest-neighboring particles i and j, and zero otherwise; and β_{ij}, is the angle between the axis of these two molecules $\mathbf{u}_i$, $\mathbf{u}_j$. This simple model reproduces fairly well the orientational phase transition and the related physical observables,[2,5–8] thus the choice of fixed positions at lattice sites, even though clearly not correct in reality, does not influence the essential orientational behavior near the phase transition. A large amount of work has been done on generalizations of the LL model[9–17] and recently, with the development of more powerful computers, potentials with translational 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 1K below T_{NI}. It is then essential to have reference calculations on the LL model to test if this simple potential is adequate or not. Thus the transition and its neighborhood 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 0.2K obtained with simulations of a $30 \times 30 \times 30$ system.[5–7] 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] In this case investigating the model in the presence of external fields of different type and intensity is important. The availability of powerful computers is then essential for the aims mentioned above 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 machines derived from APE100, a special purpose computer originally developed by INFN (National Institute for Nuclear Physics, Italy) for lattice QCD.[21] In particular we have used Q1 and QH4 Quadrics machines with 8 and 512 processors respectively. We shall see that the nearest-neighboring Lebwohl-lattice models we deal with can be easily implemented on the Quadrics architecture.

Since our aim is to simulate a (large) lattice of $L \times L \times L$ particles we follow a domain decomposition approach, making a geometrical subdivision of the sample and following the machine architecture by 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 shall have to pay attention to the interactions of the particles on the edges of the sublattice with their neighbors, because they reside on the adjacent processor and an inter-node communication is needed. We also recall that, 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 a sample made of 1728000 particles, each node owns a domain made of $15 \times 15 \times 15$ particles. So there are a total of $2 \times 6 \times 15^3 = 40500$ 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 factor 2 is needed to count both the old and the new energy calculations (to apply the Monte Carlo acceptance criterion), for which the neighboring particles are still the same. Because of this it is very important to aim at 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 bottleneck 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 contiguous memory locations, the fetch is slow (four clock cycles) just for the first data item, while the following ones are loaded at high rate (one clock cycle each).

The TAO language[22] allows an optimization of the usage of the 128 hardware registers. Moreover the features of the Quadrics 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 neighbors, on the registers, to allow the fast execution for more than one particle.

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

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

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

$$u_{ix} = \cos\alpha_i \sin\beta_i \tag{4}$$

$$u_{iy} = \sin\alpha_i \sin\beta_i \tag{5}$$

$$u_{iz} = \cos\beta_i. \tag{6}$$

To easily take advantage of the pipelined memory retrieval-storage a new type `use`, composed of `hmz` (acronym 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 dimensions of the portion of the whole sample owned 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[23] move and the third one for the Metropolis Monte Carlo acceptance criterion. We use the Metropolis prescription[24] 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.
- nine real numbers to accumulate the global energy (1), the ordering matrix (6) and the acceptance rate (2).

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

The code is based on several libraries of TAO statements and functions, both for general Monte Carlo purposes and for the Lebwohl–Lasher potential in particular. The main libraries are:

- *Algebraic library.* A general purpose library for computing operations on vectors (scalar products, normalizations, etc.) and for diagonalizing a symmetric 3×3 matrix.
- *Lebwohl–Lasher library.* A library of TAO functions and statements for Lebwohl–Lasher model.
- *Order library.* A library for computing ordering matrices.[5]
- *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* statements.

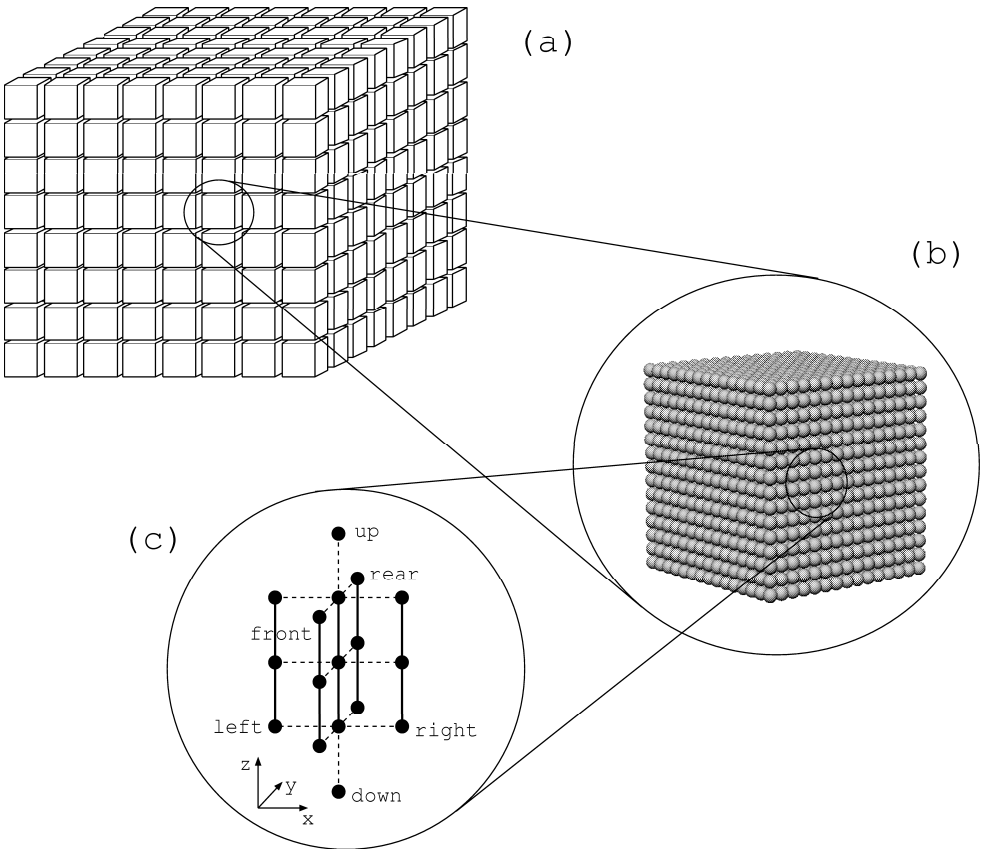

Fig. 1. A schematic representation of the whole system on a QH4 machine (a), the spin organisation on a single processing element (b) and the data loaded on the registers for the pipelined calculation (c) (see text).

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.

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 potential 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.[2,5,6] In Fig. 2 we show this second-rank order parameter $< P_2 >_\lambda$ as obtained from the test simulation and some points of the megaparticle simulation (see next section). Results from the 30^3 previous calculations[5] are also reported for comparison and provide an excellent test of the program. The results are correct and reproduce well the behavior of the thermodynamic observables versus temperature curves.

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

3.1. *Very large scale 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. Here we report in Fig. 2 some preliminary results (squares) that are already sufficient to indicate the large improvement in the sharpness of the transition.

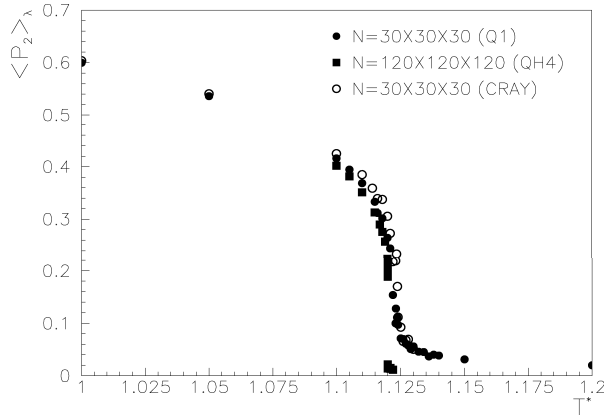

Fig. 2. Second-rank order parameter $\langle P_2 \rangle_\lambda$ versus reduced temperature $T^* = kT/\epsilon$ as obtained by MC simulations on Quadrics (full symbols) and on Cray-XMP[5] (empty symbols).

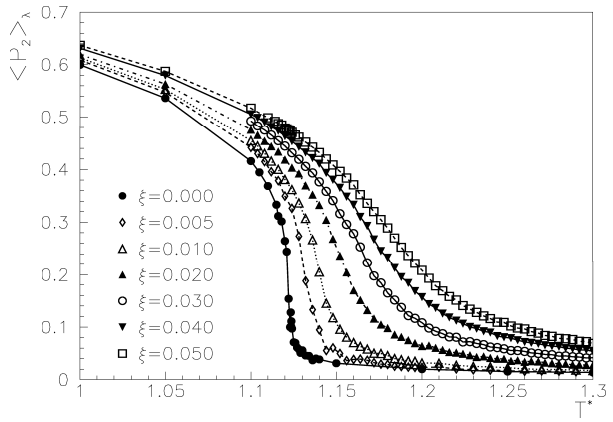

Fig. 3. Second-rank order parameter $\langle P_2 \rangle_\lambda$ versus reduced temperature $T^* = kT/\epsilon$ for different values of field strength, ξ.

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 "field" 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[13]:

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

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 from first to second order as the intensity of the field increases with disappearance of the transition at a critical point. In Fig. 3 we show the second-rank order parameter, $\langle P_2 \rangle_\lambda$, plotted against the reduced temperature for some values of field strength as obtained from simulations of a $30 \times 30 \times 30$ system performed on a Quadrics Q1 machine. The shift and rounding of the transition is apparent even from this preliminary results.

4. Conclusions

The Monte Carlo simulation of models of the Lebwohl–Lasher type, widely used in the study of liquid crystals and their phase transitions can be effectively implemented on Quadrics supercomputers. Our results show that systems up to $120 \times 120 \times 120$ can be studied, opening the way to significant improvement in the determination of transition properties.

Acknowledgments

We wish to thank G. Marchesini (Milan) and C. Catelli (Enea Bologna) for the use of their APE computers at an early stage of this work. We are particularly grateful also to A. Mathis and V. Rosato (Enea Rome) for the use of the Casaccia QH4 Quadrics. M.B. thanks INDAM for a fellowship. We are grateful to MURST and CNR for support.

References

1. G. R. Luckhurst and G. W. Gray (eds.) *The Molecular Physics of Liquid Crystals* (Academic Press, New York, 1979).
2. P. A. Lebwohl and G. Lasher, *Phys Rev. A* **6**, 426 (1972).
3. H. Kunz and G. Zumbach, *Phys. Lett. B.* **257**, 299 (1991).
4. S. Caracciolo, R. G. Edwards, A. Pelissetto, and A. D. Sokal, *Nucl. Phys. B (Proc. Suppl.)* **30**, 815 (1993).
5. U. Fabbri and C. Zannoni, *Mol. Phys* **58**, 763 (1986).
6. Z. Zhang, O. G. Mouritsen, and M. Zuckerman, *Phys. Rev. Lett.* **69**, 2803 (1992).
7. D. G. Cleaver and M. P. Allen, *Phys Rev. A* **43**, 1918 (1991).
8. C. Zannoni, *J. Chem. Phys.*, **84**, 424 (1986).
9. C. Chiccoli, P. Pasini, and C. Zannoni, *Liq. Cryst.*, **3**, 363 (1988); *Physica*, **148A**, 298 (1988); *Liq. Cryst.* **2**, 39 (1987).
10. C. Chiccoli, P. Pasini, F. Biscarini, and C. Zannoni, *Mol. Phys.* **65**, 1505 (1988); *Mol. Phys.*, **73**, 439 (1991).
11. C. Chiccoli, P. Pasini, F. Semeria, and C. Zannoni, *Phys. Lett.* **A176**, 428 (1993).
12. G. Fuller, G. R. Luckhurst, and C. Zannoni, *Chem. Phys.* **92**, 105 (1985).
13. G. R. Luckhurst, P. Simpson, and C. Zannoni, *Chem. Phys. Lett.* **78**, 429 (1981); G. R. Luckhurst and P. Simpson, *Chem. Phys. Lett.* **95**, 149 (1983).
14. E. Berggren, C. Zannoni, C. Chiccoli, P. Pasini, and F. Semeria, *Phys. Rev. E* **49**, 614 (1994).
15. R. Hashim, G. R. Luckhurst, 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).
16. C. Chiccoli, P. Pasini, F. Semeria, and C. Zannoni, *Int. J. Mod. Phys. C* **6**, 135 (1995).
17. F. Biscarini, C. Chiccoli, P. Pasini, F. Semeria, and C. Zannoni, *Phys. Rev. Lett* **75**, 1803 (1995).
18. J. G Gay and B. J. Berne, *J. Chem. Phys.* **74**, 3316 (1981).
19. E. De Miguel, L. F. Rull, M. K. Chalam, K. E. Gubbins and F. Van Sivol, *Mol. Phys.* **72**, 593 (1991).
20. R. Berardi, A. P. J. Emerson, and C. Zannoni, *J. Chem. Soc. Faraday Trans.* **89**, 4069 (1993).
21. R. Tripiccione, *Int. J. Mod. Phys. C* **4**, 1323 (1993) *and references therein.*
22. A. Bartoloni *et al.*, *Int. J. Mod. Phys. C* **4**, 955 (1993).
23. J. A. Barker and R. O. Watts, *Chem. Phys. Lett.* **3**, 144 (1969).
24. N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, *J. Chem. Phys.* **21**, 1087 (1953).