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Monte Carlo Simulations of a Biaxial Liquid Crystal Model using the Condor processing System

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Abstract. We study a lattice system of biaxial particles interacting with a second rank anisotropic potential by means of Monte Carlo simulations over a wide distributed network. We use the Condor processing system installed on the Italian Nuclear Physics Institute computer network. We have done calculations for a large number of different values of molecular biaxiality and we have determined a phase diagram for the system that we compare with previous simulations. The results of this work seems to be very promising and will allow us to use the Condor system for our large scale simulation studies.

1 Introduction

Computer simulations are a useful tool for investigating many fields of physics and are currently widely used in condensed matter research. We are interested in studying states of condensed matter intermediate between solids and liquids. These states are indicated by the somewhat contradictory name of liquid crystals (LC) and consist of various phases with different molecular organizations [1]. The main characteristic of liquid crystals at molecular level is that they possess orientational order, together with a translational mobility similar to that of liquids in nematic phases and reduced in other, so called smectic, types. A theoretical investigation of LC can be undertaken, as for any other complex fluids, by means of approximate theories or by performing numerical experiments on models. The Monte Carlo method, one of the foremost simulation techniques [2], commonly used in studying phase transitions and critical phenomena, plays an important role also in the investigation of liquid crystals [3]. One of the most important approaches deals with lattice models [3] where the molecules, or tightly ordered cluster of molecules, represented by three dimensional unit vectors ("spins") are considered to have a fixed position at the lattice sites. The spins possess full rotational freedom, subject to a certain intermolecular potential, so that this restriction does not affect their long range orientational ordering. The main advantage in using lattice models is the great number of particles which can be treated in comparison with off-lattice systems. A detailed investigation of these models requires, however, a very significant amount of

computing power which can imply using parallel computing, typically when studying large lattices, or employing distributed resources for smaller lattices but with many different values of parameters corresponding to different physical conditions.

Here we wish to present a distributed approach for studying a biaxial liquid crystal model by means of the software CONDOR [4] developed at the Computer Science Department at the University of Wisconsin-Madison and implemented on the network of the Italian National Institute for Nuclear Physics. The paper is organized as follows: first we briefly summarize the main features of the Monte Carlo simulation model; then we describe the CONDOR software and finally we discuss how we have performed the simulations of the biaxial liquid crystal system.

2 The Biaxial Liquid Crystal Lattice Model

The prototype lattice model for modelling nematic liquid crystals formed of uniaxial molecules was devised many years ago by Lebwohl and Lasher (LL) [5] and is the simplest one with the correct symmetry for nematics (in particular the potential is invariant for an head-tail flip of the molecules). The LL interaction tends to bring molecules parallel to one another and effectively models whatever underlying intermolecular interaction either attractive or repulsive that does that. While in this model, as in the large majority of theoretical calculations of liquid crystals, the mesogenic molecules are assumed to be cylindrically symmetric, it is important to recall that nematogenic molecules are invariably non cylindrically symmetric and that a much more realistic approximation is to treat them at least as biaxial objects. A simple lattice model of a biaxial system is defined by the second rank attractive pair potential [6]:

$$U(\omega_{ij}) = - \varepsilon_{ij} \{ P_2 (\cos \beta_{ij}) + 2 \lambda [R_{02}^{2}(\omega_{ij}) + R_{20}^{2}(\omega_{ij})] + 4 \lambda^2 R_{22}^{2}(\omega_{ij}) \} \qquad (1)$$

where ε_{ij} is a positive constant, ε, for nearest neighbour molecules i and j and zero otherwise, P_2 is the second Legendre polynomial. $\omega \equiv (\alpha , \beta, \gamma)$ is the set of Euler angles specifying the orientation of a molecule and R_{mn}^{L} are symmetrized combinations of Wigner functions [7]. The parameter λ takes into account the deviation from cylindrical molecular symmetry: when λ is zero, the biaxial potential reduces to the Lebwohl - Lasher P_2 one , while for λ different from zero the particles tend to align not only their major axis, but also their short axis. In this latter case and varying the temperature then there is the presence of different orientational phases (see Fig. 1), as shown by Luckhurst and Romano for λ=0.2 [8] and by us on a L x L x L cubic lattice for a fairly large set of biaxialities [9].

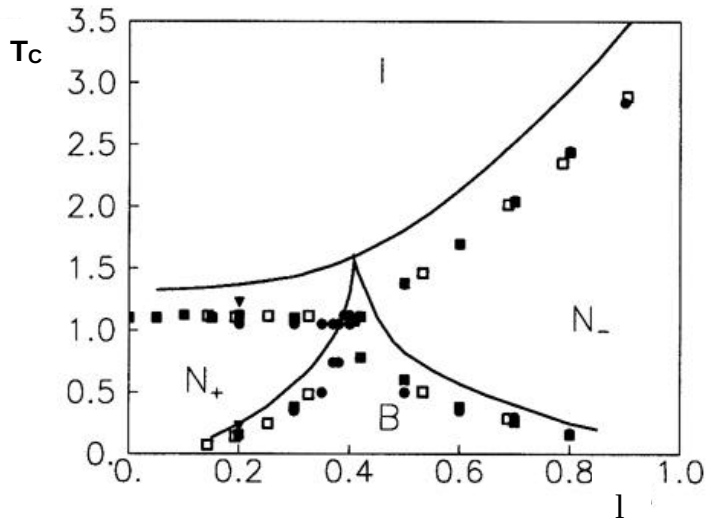

Fig. 1 Phase diagram showing the transition temperature T_C (in reduced units $T^* = kT/\varepsilon$) vs. λ as obtained by MC simulations (symbols) and Mean Field Theory (lines) from Ref. [9]. N_+, N_-,B represent regions of uniaxial and biaxial nematic phases.

The Monte Carlo simulation are performed using a standard Metropolis algorithm [10] with periodic boundary conditions for the lattice updates. The configuration of the system is given by a set of N trebles of unitary vectors $\mathbf{u}_{ij}$, i=1,2,3, where N is the number of particles. A new configuration is generated by moving a particle at random and we call a set of N attempted moves a cycle. To change the particle orientation we firstly choose at random an integer number $k \in [0,1,2]$ to identify the rotation axis. Then the orientation of the chosen particles is changed by generating a new uniformly distributed random value of the rotation angle. The maximum angular jump is chosen so as to maintain a rejection ratio not too far from 0.5. In this preliminary work we have used at least 30000 equilibration cycles far from the transition and 40000 in the pseudo critical regions. Apart from equilibration, production runs were also of varying length, according to the distance from the transition. Close to a phase change typical sequences of 20 kcycles have been used to produce the averages. We routinely determine a number of observables. In particular we calculate the heat capacity by differentiating the energy against temperature and the full set of second rank order parameters which are essential to define the different type of ordering in the different phases [9].

3 The CONDOR Processing System

CONDOR [4] is a processing system that allows the use of very large collections of available non-dedicated, pre-existing computing resources, such as (but not only) personal workstations or other distributed ownership machines. CONDOR provides an environment (a CONDOR Pool) for High Throughput Computing (HTC). The key idea of HTC is to use large amounts of computing power for very lengthy periods, with no concern in the instantaneous performance of the system typical of the traditional High Performance Computing (HPC). CONDOR creates a HTC environment by assigning idle CPUs (CPUs not used by their owners) belonging to the Pool, to jobs submitted by other machines in the Pool. When the owner starts using the workstation which a CONDOR job is running on, the job is suspended, and eventually a checkpoint of the job (a snapshot of the current state of a program) is done and the job migrates over the network to another idle machine in the Pool, on which the job is restarted from precisely where it left off. If no machine in the Pool is available, then the checkpoint is stored on disk until a machine becomes available. CONDOR also makes periodic checkpointing, providing fault tolerance. In this way two results are fulfilled: 1) the owner of the workstation should not notice any impact on the use of the workstation itself, 2) the job, migrating from one machine to another, restarting from the last checkpoint, will eventually come to the end of its execution. The Italian National Institute for Nuclear Physics (INFN) has developed a wide academic computer network linking its 24 sites since 1982. In 1998 the INFN project of building a CONDOR Pool over the INFN network was started, using already existing machines in many INFN sites. The Pool has been used by many INFN groups. In 1999 the equivalent of 38 years of CPU have been deployed. The Pool has presently more than 200 Unix machines, mainly Compaq Alpha and Linux PC.

4 LC Simulations Using the INFN CONDOR Pool

We have started to use the INFN CONDOR Pool for Monte Carlo simulation of the Liquid Crystal model formed by biaxial molecules to test if this processing system can be used for further studies in our research field. As can be seen from equation 1) the intermolecular potential depends on the biaxiality parameter λ, which has to be varied to study in detail the model. Of course for each value of λ an independent simulation has to be performed over a wide range of temperatures. This problem is then in principle well suited for the use of CONDOR because each simulation can be submitted on different computers. In this way we can send a CONDOR job for each value of the parameter, performing many simulations in parallel. For each value of the parameter λ we start the simulation with a low temperature from a totally aligned configuration of the molecules. For each of the subsequent temperatures the starting configuration was the last one of the previous temperature. We thus need a system for

taking into account these jobs' dependencies (the job for a temperature must only start when the run of the previous job is completed). This mechanism is provided by CONDOR with a tool called DAGMan (Directed Acyclic Graph Manager). In this way we can submit a job for each temperature and for each value of the parameter λ, but only one job for each value of the parameter λ (corresponding to a particular temperature) is executing at any time. We have made the simulation for 15 values of the parameter λ and about 20 values of the temperature for each of them. So the total number of jobs submitted was about 300. CONDOR took care of the sequencing and the management (checkpointing, migration etc.) of all these jobs. We have performed the simulations of a 40 x 40 x 40 lattice system and we have been able to reproduce the complete study performed some years ago [9] in just two weeks. In Fig.2 we report as an example a plot of the orientational order $\langle P_2 \rangle = \langle 3 \cos^2\beta - 1 \rangle / 2$, where β is the angle between long molecular axis and preferred ordering direction, as a function of reduced temperature obtained from our CONDOR runs at various λ.

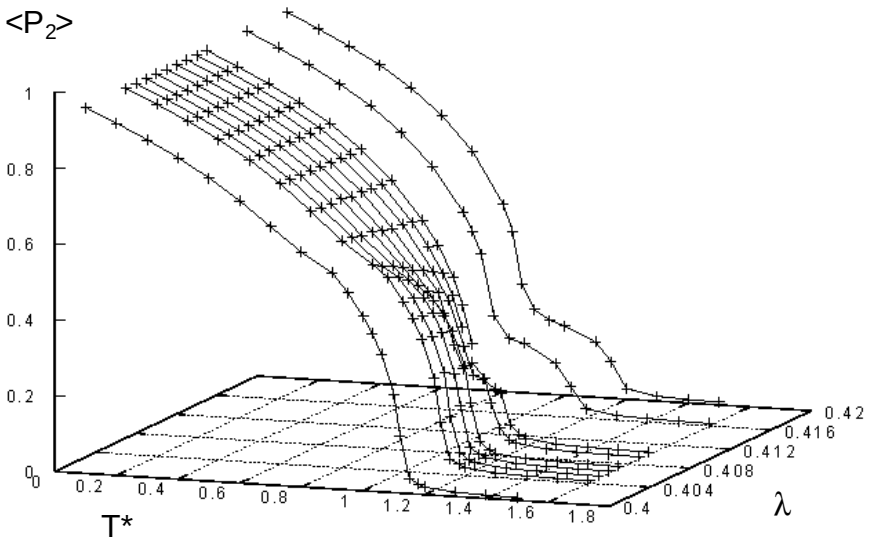

Fig. 2 A summary plot of the orientational order $\langle P_2 \rangle$ for models of various biaxiality λ as a function of the reduced transition temperature $T^* = kT/\varepsilon$.

In practice we have submitted our jobs to a CONDOR Pool of 70 Linux PCs but imposing the condition that the processor speed should be at least 200 MIPS. We report in Table 1 an excerpt of the log file for the simulation of the case $\lambda = 0.3$ where the machines used can be identified, together with the values of some performance parameters, such as the CPU Usage.

Host/Job	Wall Time (hours)	Good Time (hours)	CPU Usage (hours)	Avg Alloc (minutes)	Avg Lost (minutes)	Goodput	Util.
p3d450.bo.infn.it	44	44	43	872	0	100.0%	97
chandra.bo.infn.it	47	47	47	565	0	100.0%	99
Pcmzz.bo.infn.it	19	19	19	564	0	100.0%	99
Pceng2.bo.infn.it	50	50	50	745	0	100.0%	99
linux1.ba.infn.it	0	0	0	0	0	0.0 %	0
to414xl.to.infn.it	27	27	26	536	0	100.0%	99
to44xl.to.infn.it	13	13	13	763	0	100.0%	99
pcl3c.bo.infn.it	12	12	12	705	0	100.0%	99
pcglob.bo.infn.it	22	22	22	658	0	100.0%	99
Pceng4.bo.infn.it	13	13	13	756	0	100.0%	99
Pceng3.bo.infn.it	13	13	13	751	0	100.0%	99
to40xl.to.infn.it	2	0	0	133	133	0.0%	0

Table 1

From the log file we can check that we have used 16 PCs for a total of about 1700 hours CPU time. Since we estimated that a full study of the phase diagram, should take at least ten times as much, particularly because of the need of very long runs near the transition and of refining the grid on the biaxiality parameter λ, we see that the use of distributed resources afforded by CONDOR is particularly useful and could make possible detailed and systematic studies of this type of models in a way not easily possible until now.

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