

Molecular Dynamics Simulations of Liquid Crystals in Confined Geometries

D.Andrienko, M.P.Allen, G.Germano

H.H. Wills Physics Laboratory,
University of Bristol,
Faculty of Science,
Royal Fort, Tyndall Avenue,
Bristol BS8 1TL, UK

Abstract

The preliminary results of the molecular dynamics simulation of the system of the Gay-Berne particles in the slab geometry is presented. Each surface was modelled on a molecular level through an integrated Gay-Berne potential. The depth of the potential was taken angle dependent, favouring a molecular alignment along the surface

1 Why computer simulations?

- *Experiments* are not able to handle thin liquid crystal layers
- *Theories* have problems with convergence of the surface terms in the phenomenological free energy expansions (K_{13} problem)



Simulations of the sufficiently large systems should be able to test the lengthscales where the elastic model applies and check the validity of mean-field, density functional theories in describing the properties of the liquid crystal interface. Simulations may also give values of the macroscopic surface characteristics: anchoring energy and easy axis direction.

2 System parameters

Gay-Berne (3,5) molecules in liquid crystal phase [1].

Cell dimensions, $N_x : N_y : N_z = 8 : 8 : 13$.

Number of particles, $N = 256$.

Number density $\rho = 0.3$.

Temperature $T = 0.5 - 1.5$.

Spherical cutoff, $r_c = 4$.

Particle substrate potential - 'integrated' Gay-Berne potential [2]

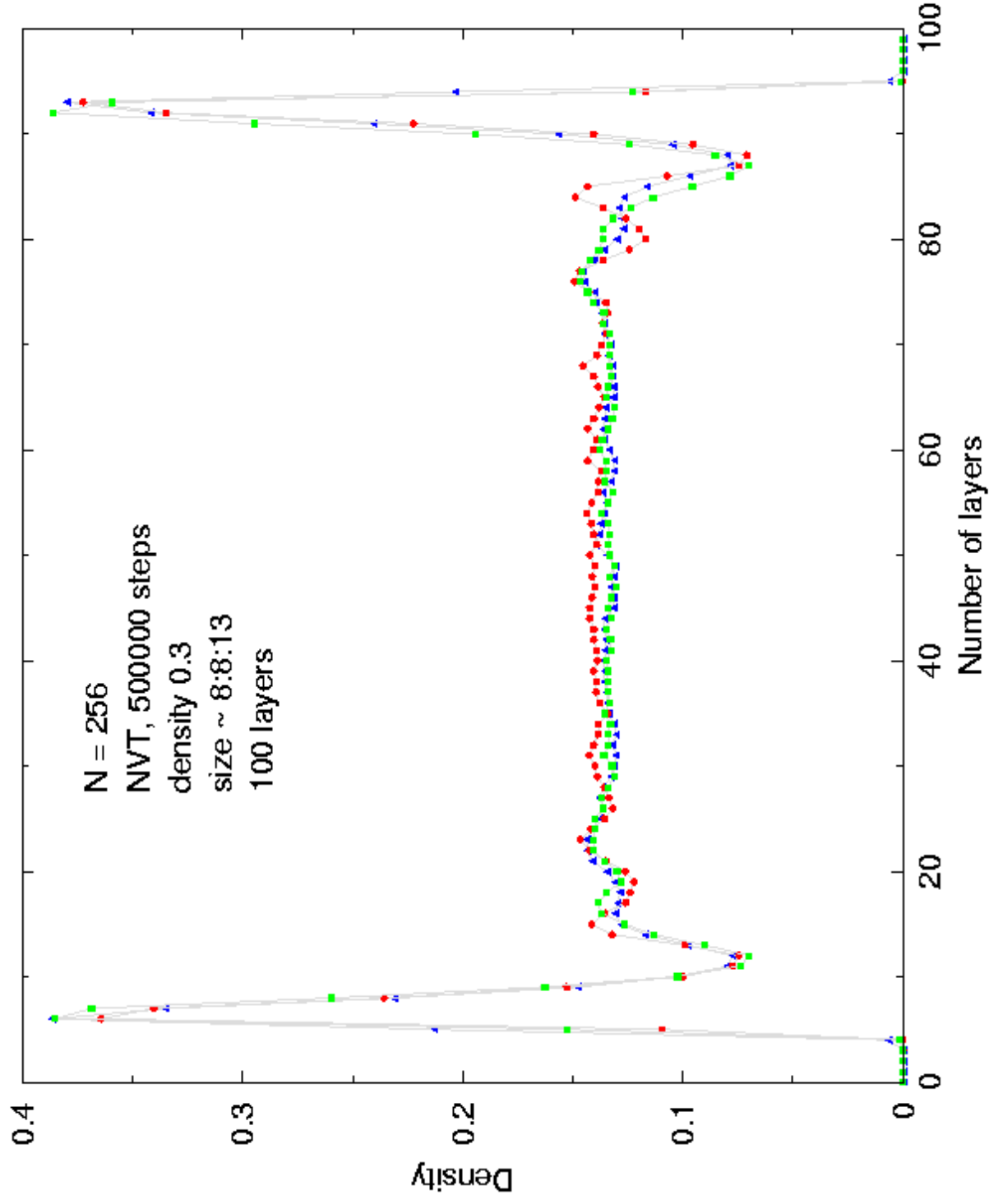
$$U_s = 4\varepsilon_s(\theta) \left\{ \begin{array}{l} \left(\frac{\sigma_s}{|z-z_0| - \sigma(\theta) + \sigma_s} \right)^9 - \\ - \left(\frac{\sigma_s}{|z-z_0| - \sigma(\theta) + \sigma_s} \right)^3 \end{array} \right\},$$

where

$$\sigma(\theta) = \sigma_s \left\{ 1 - \chi \cos^2(\theta) \right\}^{-1/2},$$

$$\varepsilon_s(\theta) = \varepsilon_0 \left[1 - \chi' \cos^2(\theta) \right]^\mu$$

GB LC with walls



3 Future work

- Influence of the wall potential on the anchoring parameters: easy orientation axis, anchoring energy [3].
- Increase of the particle number N in order to avoid cell size effects and influence of the LC bulk on the interface region.
- Different cell geometries: cylinder, sphere.
- Comparison with Onsager, DFT, Landau-de Gennes theories.

References

- [1] E. De Miguel, L.F. Rull, M.K. Challam, and K.E.Gubbins, *Mol.Phys.* 74, 405 (1991)
- [2] G. D. Wall, D. J. Cleaver, *Phys. Rev. E*, 56, 4306 (1997)
- [3] M. P. Allen, *Mol. Phys.* 96, 1391 (1999)

Acknowledgments:

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