Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Study of liquid crystal molecular dynamics algorithm[1] JONES TSZ-KAI WAN, Department of Physics, The Chinese University of Hong Kong — Recent years have witnessed the growth in controlling liquid crystal (LC) alignment using patterned surfaces. Computer simulation of actual LC configurations that are due to different substrate surfaces is a useful tool to aid the design of practical LC cells. In liquid crystal simulations, one seeks for an optimal configuration of the LC director field n(r) that minimizes the total energy of the LC cell. For non-uniform substrate surfaces, the spatial variation of the LC is complicated and the minimization of the total energy is accomplished by advance numerical techniques like conjugate gradient (CG). In a recent work, the author proposed an efficient simulation scheme called liquid crystal molecular dynamics (LCMD), which is developed to determine liquid crystal configurations in complex physical environments. In this work, the author studies the limitation of such scheme and investigates how the simulation parameters can be tuned to achieve optimal performance.

[1]This work is supported by CUHK direct grant (project no. 2060307)

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Date submitted: 21 Nov 2008 Electronic form version 1.4