

## **Computer simulation of liquid crystals on the T3D**

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Over the last few years, CCP5 has supported a collaboration of U.K. simulation groups interested in the modelling of liquid crystals (M. P. Allen, Physics, Bristol University; C. M. Care, Physics, Sheffield Hallam University; D. J. Cleaver, Physics, Sheffield Hallam University; G. Jackson, Chemistry, Sheffield University; G. R. Luckhurst, Chemistry, Southampton University; A. J. Masters, Chemistry, Manchester University; M. Neal, Mathematics, Derby University; M. R. Wilson, Physics and Materials, Lancaster University). This has now evolved into a so-called ‘Consortium’ using the new Cray T3D parallel supercomputer at Edinburgh, within the EPSRC’s High-Performance Computing Initiative.

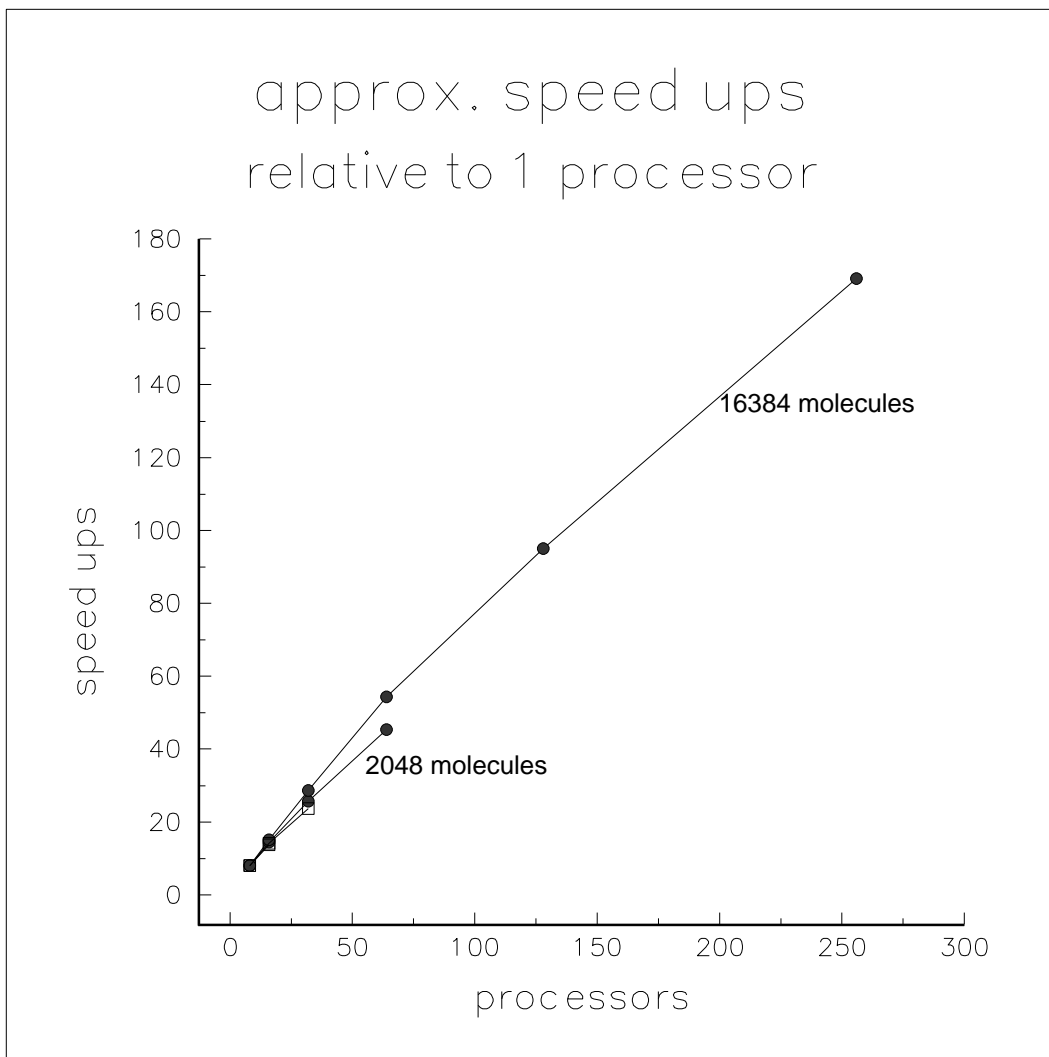
Liquid crystals are important because of their technological properties; they also provide fascinating challenges in statistical mechanics. To understand them from the theoretical perspective, we frequently adopt very simple models of the constituent molecules. Representing the molecule as a hard, elongated, rigid body is a good starting point, as it includes the fundamental physics associated with packing effects in the liquid. Softening the repulsive potential, and adding simple attractive forces between the molecules, are the obvious next steps.

One of the standard models of this kind, the ‘Gay-Berne’ model has been extensively studied in recent years. As well as the isotropic, or disordered liquid, it exhibits several liquid crystal phases, the simplest of which is the nematic: here the molecular orientations are preferentially aligned in space, but all other kinds of order are short-ranged. Various layered, smectic, phases are also seen. By applying suitable periodic boundary conditions, it is possible to twist the preferred direction (the ‘director’) into a helical structure, of the kind used in display devices. When such a twist is applied to a smectic phase, the director almost always finds it impossible to vary in a uniform fashion, because this would entail a substantial distortion energy for the layers; instead it forms domains of more-or-less uniform alignment, separated by grain boundaries at which a sudden jump in alignment occurs. These ‘twist grain boundary phases’ have become hot topics in theory and experiment over the last few years. To simulate them requires very large system sizes, both along the axis of twist (so that the twist period is not too short) and in the transverse directions (to allow the layers as much freedom as possible to choose an orientation subject to periodic boundary conditions).

We have recently developed an efficient code for running molecular dynamics of the Gay-Berne system on parallel computers. It is based on the CCP5 code for atomic fluids, MDMEGA. It uses a domain decomposition technique with linked lists, and message-passing via PVM. This program has been benchmarked on a range of parallel computers including the new T3D at Edinburgh. It shows excellent speedup characteristics with increasing numbers of processors (see the figure) for

system sizes of interest to us.

## GBMEGA PROGRAM - DOMAIN DECOMPOSITION APPROACH



We have completed our preliminary simulations in which a twisted nematic liquid crystal system is cooled into the smectic region of the phase diagram, and the grain boundary formation is observed directly. We used 27000 Gay-Berne molecules, equilibrated for several tens of thousands of steps, and observed three smectic domains within the modified periodic boundaries. This is encouraging, but to increase our confidence that the domain orientation and thickness are not strongly influenced by the boundary conditions, we shall have to repeat the exercise with larger samples. As a separate exercise, we have quenched a 64000-particle isotropic system into the nematic phase, with the intention of examining the large-scale processes of defect annealing that accompany orientational ordering. There is the prospect of extending this work to look at long-ranged director correlations in the equilibrated nematic sample, something that again requires large system sizes and reasonably long runs. Some colour pictures of configurations produced on the Edinburgh T3D may be seen on our WWW pages, starting at <http://www.phy.bris.ac.uk/research/theory/simulation.html>.

Other members of the consortium are now actively looking at various extensions of the Gay-Berne potential which may produce liquid crystal phases with large-scale structural features of the kind that can only be investigated with powerful parallel computing facilities. At the same time, the Consortium has a code development programme, supported via the HPCI Centre at Southampton University, which should increase the range of models and simulation techniques that we can use on the T3D. We hope to produce reports on these activities in due course.