Distance of closest approach of two hard ellipses[1] XIAOYU ZHENG,
*Department of Mathematical Sciences, KSU, PETER PALFFY-MUHORAY, Liquid Crystal Institute, KSU, *DEPARTMENT OF MATHEMATICAL SCIENCES TEAM, LIQUID CRYSTAL INSTITUTE TEAM — The distance of closest approach of hard particles is a key parameter in their interaction and plays an important role in the resulting phase behavior. The distance of closest approach of the centers of hard spheres in 3-D or of hard circles in 2-D is the diameter. For non-spherical particles, the distance depends on orientation, and its calculation is surprisingly difficult. Although overlap criteria have been developed(1,2) for use in computer simulations, no analytic solutions have been obtained for ellipsoids in 3-D, or, until now, for ellipses in 2-D. We have succeeded in deriving an analytic expression for the distance of closest approach of the centers of two arbitrary hard ellipses as function of their orientation relative to the line joining their centers. We describe our method for solving this problem, illustrate our result, and discuss its usefulness in modeling and for simulating systems of anisometric particles such as liquid crystals.

Michele Moreira
Liquid Crystal Institute

Date submitted: 03 Dec 2006

Electronic form version 1.4