Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

A Minimal Model for the Helix-Coil Transition of Worm-like Polymers GUSTAVO A. CARRI, VIKAS VARSHNEY, TANER E. DIRAMA, The University of Akron, TANER Z. SEN, Iowa State University — We present a geometric approach to the simulation of the Helix-Coil transition in wormlike polymers. In our model, the polymer is treated as a Freely Rotating Chain with hard-core repulsion between beads. The conformational state (helix or coil) of each bead is determined by the value of its torsion. If the difference between the torsion of a bead and the one of the perfect helix is less than a cutoff value, then the bead is part of a helical domain and carries a negative energy, otherwise it is part of a random coil. We have simulated these concepts using the Wang-Landau algorithm where the density of states depends on two parameters: the number of beads in the helical state and the number of interfaces. In this talk I show that these simple ideas can account for the cooperativity of the transition explicitly and capture the known conformational, configurational and thermodynamic properties correctly. Moreover, these concepts have important theoretical implications since they lead naturally to a field-theoretic Hamiltonian of the Edwards' type that might be useful for problems of current experimental interest.

Gustavo A. Carri
The University of Akron

Date submitted: 28 Nov 2004 Electronic form version 1.4