Abstract Submitted for the NWS09 Meeting of The American Physical Society

Coarse-grained molecular dynamics simulations of DNA using ellipsoids ALEX MORRISS-ANDREWS, UBC — We are developing a coarse-grained computational model of DNA using ellipsoids, and simulating the DNA using molecular dynamics simulations. We represent the bases using the RE2 potential, as these molecules are better represented by ellipsoids than spheres. Our model gives greater resolution than traditional coarse-grained models but requires less computational power than all-atom simulations.

Alex Morriss-Andrews UBC

Date submitted: 16 Apr 2009 Electronic form version 1.4