Name: PHY401 (Fall 2006), 11/22/06

Last 4 digits of UIN: Score:

Homework Assignment #9

(*Due Date*: Friday, December 01, 12:40 pm, in class)

9.1 *Molecular Dynamics and Temperature* (cf. textbook Ex. 9.1) *(10 pts.)*
Write a FORTRAN program to perform a molecular dynamics simulation for Argon atoms (interacting via the Lennard-Jones potential with $\epsilon = 120 k_B T$) in a 2-D 20×20 box (using periodic boundary conditions). Initialize the simulation with 80 particles and initial speed of v_0=3 for each particle (pointing in a random direction). Perform about 10000 time steps (with $\Delta t = 0.01$) and extract 3 speed distributions by averaging over t=25-50, 50-75, and 75-100. Fit a Maxwell distribution to each set of points separately (finding the temperature which minimizes χ^2) and evaluate the average temperature.