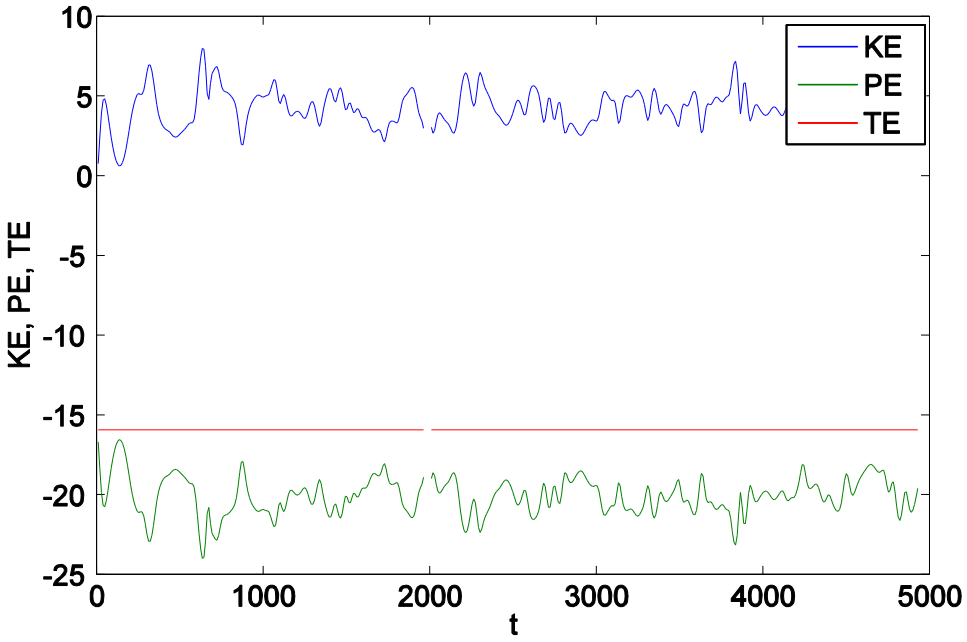
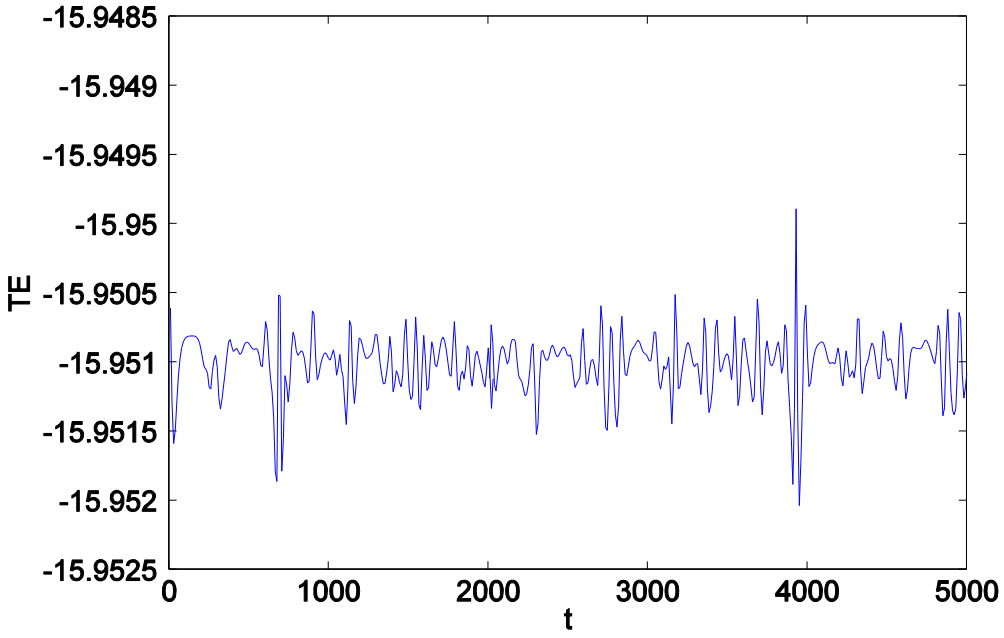
3)

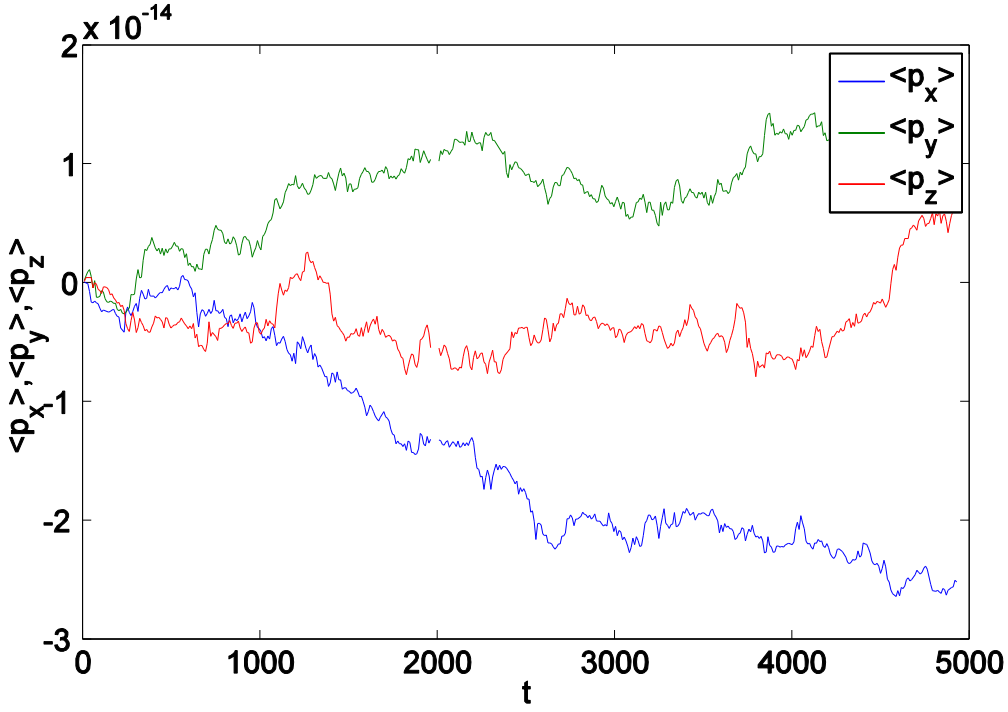
The below plot shows the Potential, Kinetic, and Total energies as functions of time. The PE and KE are (nearly) perfectly anti-correlated. That is, when the KE is decreasing, the PE is increasing and vice versa.



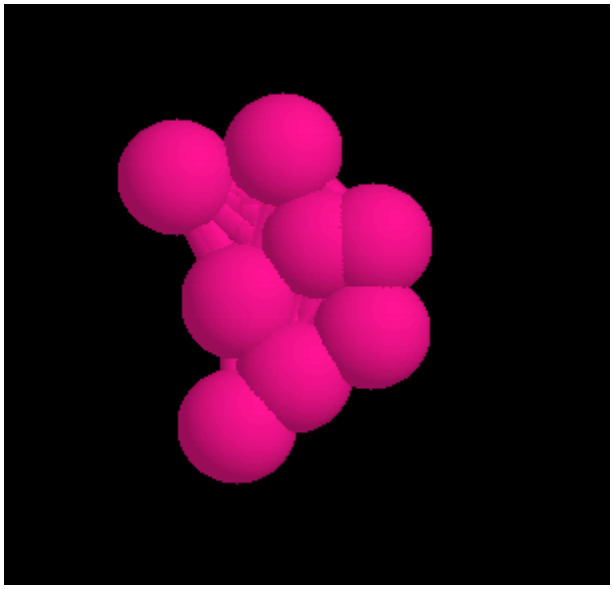
The total energy is conserved to within 10E-04 (RMS fluctuation).



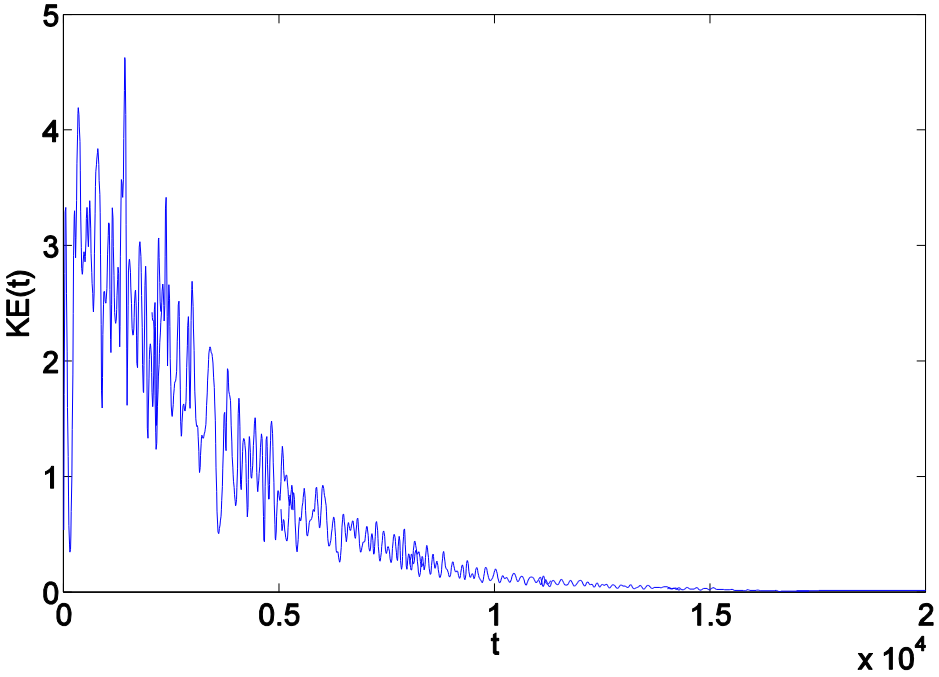
The rms fluctuations in the total energy is 2.0573e-004. Using a time step of dt=0.0005 the rms fluctuations are 1.4474e-005, which is consistent with energy conservation increasing with decreasing dt.



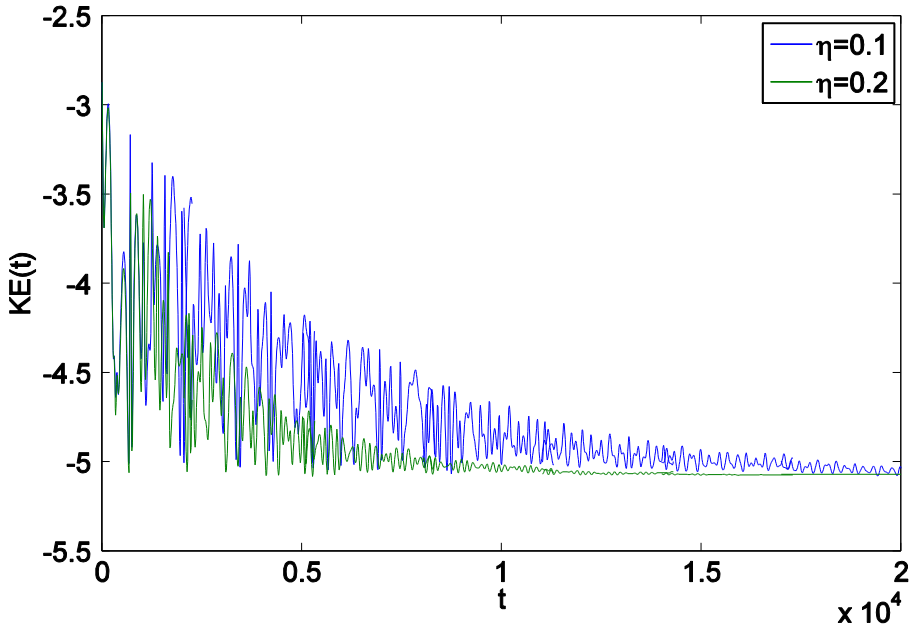
Above is a plot of the 3 components of the momentum, showing that they are conserved within 10E-14.



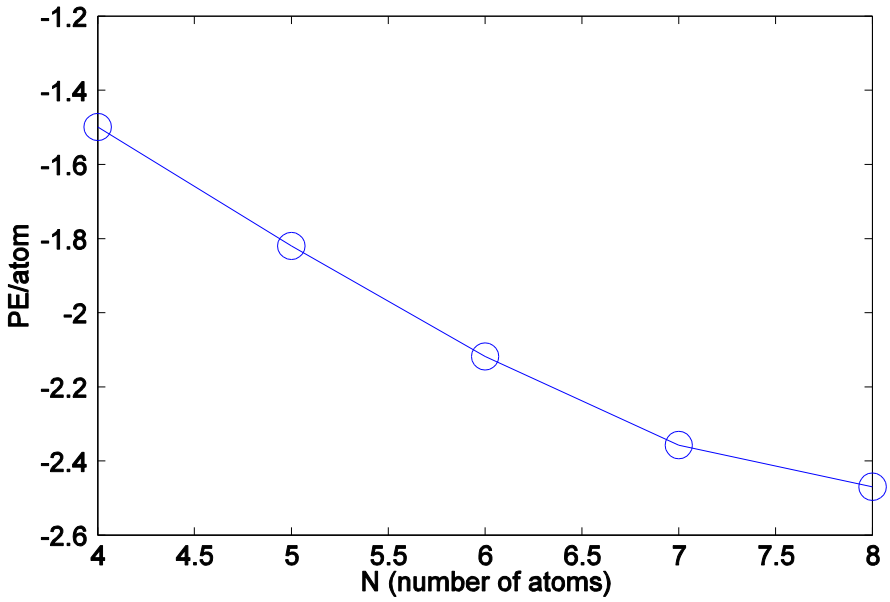
Above is a snapshot of the 10 atom nanoparticle after the time varying potential and kinetic energy have reached a steady state.



The above plot shows the kinetic energy KE(t) as the system of N=8 particles is quenched using eta=0.02. The time step dt=0.002 and the simulation was run for 20,000 time steps. The parameter eta removes KE from the system until the structure is quenched.



Above is a plot for N=10, dt=0.002, and total time 20,000. The quench parameter eta controls how fast KE is removed from the system.



Here is the Potential Energy per atom of the quenched structures. There are varying potential energy minima as the number of atoms N is varied.