

Molecular Dynamics Simulation Applets

A nice overview of MD by Dr. Charles Brooks III from a workshop at Pittsburgh Supercomputing Center:

<http://www.psc.edu/general/software/packages/charmm/tutorial/brooks/mmd.pdf>

Arjan's introduction to MD can be found here: https://wiki.asu.edu/biophysics-outreach/index.php/Molecular_dynamics

http://galileo.phys.virginia.edu/classes/109N/more_stuff/Applets/newt/newtmtn.html - Newtonian Mountain

<http://www.phy.ntnu.edu.tw/ntnujava/index.php?topic=25> - MD simulation of an ideal gas. Allows for determining the gas law relationships.

<http://michele.usc.edu/java/HSgas/Hsgas.html> - simulates a gas and draws a distribution of speeds.

http://Galileo.phys.Virginia.EDU/classes/109N/more_stuff/Applets/brownian/brownian.html - Brownian motion (macroscopic and microscopic) applet.

<http://www.physics.orst.edu/~rubin/CPUG/CPlab/MoleDynam/md.html> - molecular dynamics applet that allows velocity scaling (yes/no), temperature control, and will plot energy, temperature, LJ potential (allows for setting parameters), or radial distribution function versus timestep.

http://comp.uark.edu/~jgeabana/mol_dyn/KinThI.html - stat mech applet that looks at the kinetic theory, approach to equilibrium, Maxwell-Boltzmann speed distribution, and reversibility.

<http://physics.weber.edu/schroeder/software/MDApplet.html> - an MD applet that runs the Verlet integrator. Allows manipulation of timestep, mass, number of particles. Writes t, V, N, T, P, and E which can be copied into MS Excel for analysis.

<http://atoms.alife.co.uk/links/index.html> - an index of physics links and applets