

Note: items marked with * you should be able to perform on a closed book exam.

Molecular Simulation Learning Objective Checklist

After studying this coursepack you should be able to:

- Explain why the total kinetic energy of the sites of a molecule is different than the kinetic energy of the center of mass.*
- Explain whether KE or PE is independent of density at a particular temperature.*
- Explain why Monte Carlo and Molecular Dynamics can both give the same results. Explain briefly how each type of simulation is performed.*
- Explain what is meant by periodic boundary conditions. Draw a sketch to illustrate how they are used.*
- Explain what is meant by the minimum image convention. Draw a sketch to illustrate how it is used.*
- List one advantage of molecular dynamics over Monte Carlo? What is one disadvantage?*
- Discuss using the terms velocity, acceleration, and position why a molecular dynamics simulation is not an exact duplication of molecular motion.*
- Explain the differences that would be expected in particle motions for the following types of simulations at the same temperature: ideal gas particles, purely repulsive particles, square-well particles.*
- Explain why the temperature fluctuates in a simulation with attractive and repulsive potential energy.*
- Given a set of purely repulsive particles in 2-D with specified velocities, and eq (10), (14) from the coursepack, decide if particles are approaching, if they will collide, and when they will collide.
- Given a set of purely repulsive particles in 2-D with specified velocities, position and collision time, and equation (23) from the coursepack, determine the coordinates when they collide, and the velocity vectors after collision.