CB&B752/MCDB452/MB&B752/MCDB752/CPSC752
Homework 3

Non-programming assignment

Problem 1:

Calculate the x-, y-, and z-components of the conservative forces $\vec{F} = \frac{dV}{dr_{ij}}\hat{r}_{ij}$ from the following interparticle potentials: (a) $V = \frac{\varepsilon}{2}\left(\sigma - r_{ij}\right)^2$, (b) $V = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$, and (c) $V = -\frac{\varepsilon}{2}\ln\left[1 - \left(\frac{r_{ij}}{\sigma}\right)^2\right]$. Plot $V(r_{ij})/\varepsilon$ versus r_{ij}/σ and determine which regions give repulsive forces and which give attractive forces.