# Quiz Assignment for Molecular Simulations

*In total 1.5 point,* ***1*** *point for Question 1 and 0.5 point for Question 2*

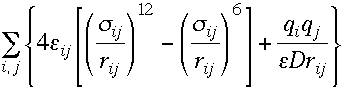
Consider following scalar ODEs for Newton’s equation of motion,

force/mass, and force = -dEpot/dr

Initial values

Given .

The equation then describes the motion of one argon atom (one particle) with mass 40 dalton (Da) respect to another argon atom kept fix. The atoms interact only with van der Waals interactions, which we model using the Lennard-Jones potential:



Epot=ELJ(rij) =

whereij=0.24 (kcal/mol) and ij=3.4Å and rij is the distance between atoms i and j.

1. Solve the position and the velocity of the moving object (i.e,  *and )* numericallywithVerlet’ algorithm for **t** *.* Use time step h=1 as a start, then use smaller time steps e.g. h = 0.3 , h=0.15 and compare the results. (Note r is simply the same as rij)
2. The total energy of the system includes kinetic energy and potential energy, i.e.

 Epot. Substitute the numerical solutions calculated above into the energy function, does the energy conserve? Discuss your findings.

Hint:

1. Acceleration *a* as a function of *r*, i.e. *a(r)* can be calculated using the provided potential function Epot according to “a= force/mass, and force = -dEpot/dr”
2. Be cautious of the unit for both questions. Following should be useful for converting unit of ij=0.24 (kcal/mol)

1 kcal/mol = 418.4 Da-Å^2/ps^2 (see following link)

<https://simtk.org/api_docs/molmodel/api_docs22/Simbody/html/group__MacroConstants.html>