Part 4 – First thoughts, Tomi

Applicability of current model in 3D (3D two particle harmonic oscillator and Lennard-Jones balls)

3D two particle harmonic oscillator (NON-INTERACTING MOLECULES)

At their current state the model would provide good simulations to following systems:

- **Diatomic homomolecules in a gaseous state (H_2, O_2, N_2, F_2, Cl_2, …);** non-polar
  [particles have same mass, no outward charge or polarity; issues: no induced dipolemoment)

At their current state the model would provide decent simulations to following systems:

- **Diatomic heteromolecules in a gaseous state (HCl)**; polar
  [particle masses can be changed, no outward charge; issues: no Coulombic interaction, no polarity)

At their current state the model would provide passable simulations to following systems:

- **Approximated system where a single bond is analysed ignoring other molecular structures (H_3C-CH_3)**
  [functional group masses can be changed, outwardly neutral)

Lennard-Jones balls (NEUTRAL ATOMS / MOLECULES INTERACTING)

At their current state the model would provide good simulations to following systems:

- **Noble gas atoms in a gaseous state**
  [outwardly neutral due to octet, quantum mechanics description reduces to a sphere]
- **Neutral single atoms radicals**
  [no outward charge; issues: no reaction-interaction, no reaction pathways]

At their current state the model would provide passable simulations to following systems:

- Any molecules approximated to a single ball (CH_4, polymer globules) ignoring internal state and interactions based on non-Lennard-Jones properties.

Molecular dynamic simulation - units

System energy: described as Hartree (1 Hartree = 4.359 744 650(54)×10^{-18} J)
System size: max 500 Å (1 Å = 10^{-10} m)
System timestep: picoseconds or femtoseconds (10^{-12} s, 10^{-15} s)

No results from part two