Molecular Dynamics Simulation of Noble Gases

CSE 6010 Final Project, Fall 2018

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Project Overview

The goal of this project is to create code that can perform simple Molecular Dynamics simulations on noble gases and report results, to assess the complexity of the simulation by comparing the runtime with different random number generators, to find the relative accuracy of different methods in calculating the velocity/ location, and to utilize parallel computing to decrease the total runtime.

I/O Module

Input File

Two types of input files:

1. Actual Raw Input for each atom
2. Randomly Generated Data Configuration

Raw Data

Number of lines in the file

6

x y vx vy

4.0,2.0,3.0,2.0
2.0,1.0,1.0,3.0
1.0,1.0,3.0,1.0
1.0,1.0,3.0,1.0
2.0,1.0,1.0,3.0
4.0,2.0,3.0,2.0

Randomly Generated Data Configuration

Number of lines in the file: 15

4,1,1

x y vx vy

1,3,1,2,1,1,3,1,1,4,1,1,5
3,4,6,1,1,1,1,1,1,1,1,1,5
1,3,1,2,1,1,3,1,1,4,1,1,5
3,4,6,1,1,1,1,1,1,1,1,1,5
1,3,1,2,1,1,3,1,1,4,1,1,5
...
1,3,1,2,1,1,3,1,1,4,1,1,5

4 is indicator of which Random Variable to use. (1: Exponential, 2: Normal, 3: Gamma, 4: Pareto)
1 is first parameter for respective Random Variable
1 is second parameter for respective Random Variable

Number of atoms with this configuration

Output File

Two output files for visualization:

1. Configuration file indicating the type of atoms that are simulated
2. Timestamped positions of the simulated atoms

Configuration Output

Type of atom (mono-atomic)
Radius in (angstrom)
He, 4.003, 0.31, 100
Atomic weight
Number of Atoms

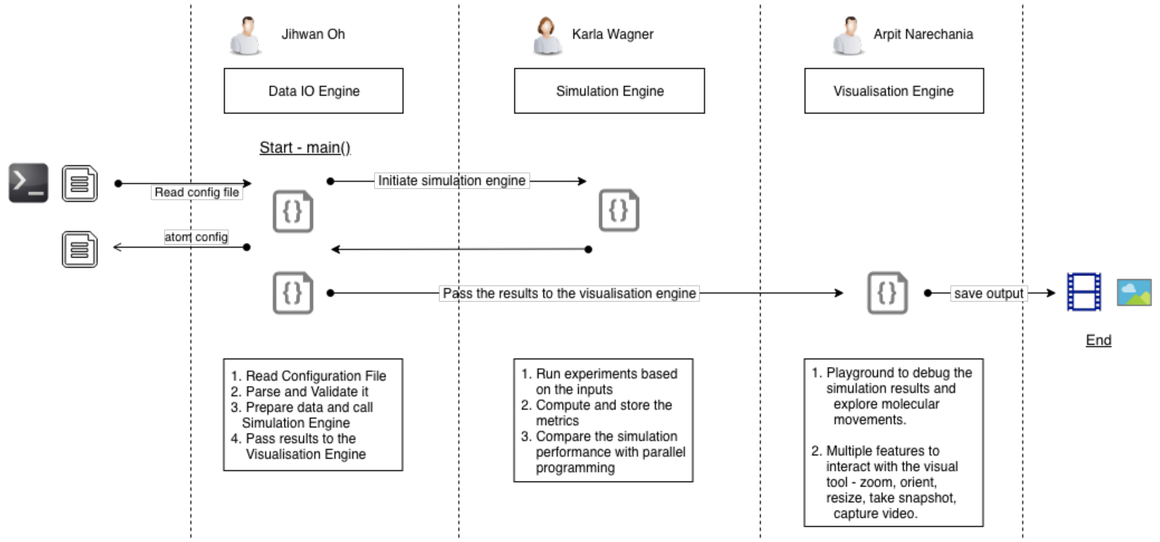
Output for Visualization

Time Stamp
Position for atom 1 at time t

t,x1,y1,x2,y2,x3,y3,...,x100,y100
0,3.0,1.0,2.0,1.0,1.0,3.0,...,1.0,1.0
1,4.0,6.0,1.0,1.0,1.0,1.0,...,1.0,1.0
2,3.0,1.0,2.0,1.0,1.0,3.0,...,1.0,1.0
3,4.0,6.0,1.0,1.0,1.0,1.0,...,1.0,1.0
4,3.0,1.0,2.0,1.0,1.0,3.0,...,1.0,1.0
...
1000,3.0,1.0,2.0,1.0,1.0,3.0,...,1.0,1.0

Position for atom 100 at time 4

Project Architecture



Simulation Module

Random Number Generator

Two types of Uniform[0,1] Generator

1. C innate rand() function
2. MRG32k3a, from L'Ecuyer

That generates:

1. Exponential – Inverse Transform
2. Normal – Box-Muller Transform
3. Gamma – Accept-Reject Method
4. Pareto – Inverse Transform

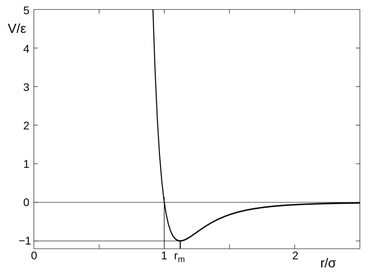
Simulation

Simulation Steps:

1. Initial atom states received from IO module
2. Interatomic forces are calculated by the Lennard-Jones potential energy (right)
3. Atom accelerations, then velocities, then positions (with periodic boundaries) are updated
4. Total energy (potential + kinetic) is confirmed to be conserved
5. Time is advanced by a step of 1.0 femtosecond

Atom Representation

- Atomic information: element, mass, and radius
- Initial conditions: atom position and atom velocity are fed into the simulation per the RNG described on the left.
- Atoms held in a linked list data structure
- Atom interactions calculated per the Lennard-Jones 6-12 potential, seen below -this is a simplification that nonetheless holds well for monoatomic systems such as a noble gas



$$V_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12}\right] - \left[\left(\frac{\sigma}{r}\right)^{6}\right]$$

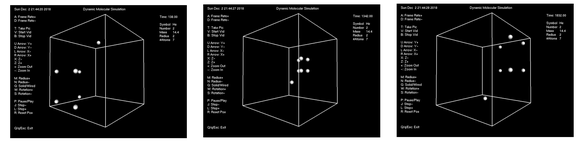
Visualization Module

Built using OpenGL, this visualization software accepts timeseries data for atoms and renders them in order.

t	x1	y1	z1	x2	y2	z2
0	-10.90186	-7.035725	-10.90186	2.993904	-5.792433	-5.792433
1	-20.396914	-10.227119	-20.396914	3.64778	-7.886058	-7.886058
2	-29.891341	-13.418429	-29.891341	4.301631	-9.979687	-9.979687
3	-39.385709	-16.609731	-39.385709	4.955478	-12.073316	-12.073316
4	-48.880066	-19.801032	-48.880066	5.609323	-14.166945	-14.166945

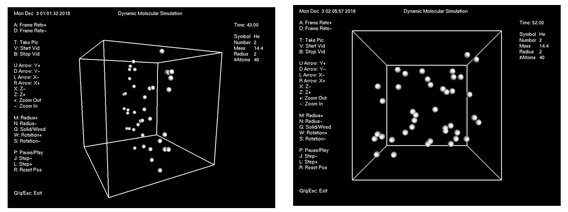
- Orientation
- Zoom Level
- Size
- Rotation
- Texture
- Frame Rate
- Pause/ Play
- Reset
- Save Screenshot
- Save Screencast
- Resize
- Metrics
- Manual Step Up Down

Simulation of 7 atoms across opposite faces of a cube at different time intervals



t=0 t=T/2 t=T

By visualizing the position and movement of atoms over time, it enables finding anomalies (eg. behaviour near edges v/s centre), understand the system and debug the code. Below are two views of a 40 atoms system for 100 timesteps.



Future Work

- Model non-noble gases or multi-element systems
- Model liquid and solid atomic systems
- Simulate system reacting to some event
- 3D simulation and visualization
- Dynamically adding atoms to the viz. software