Molecular Dynamics Simulation Using Lennard-Jones Potential

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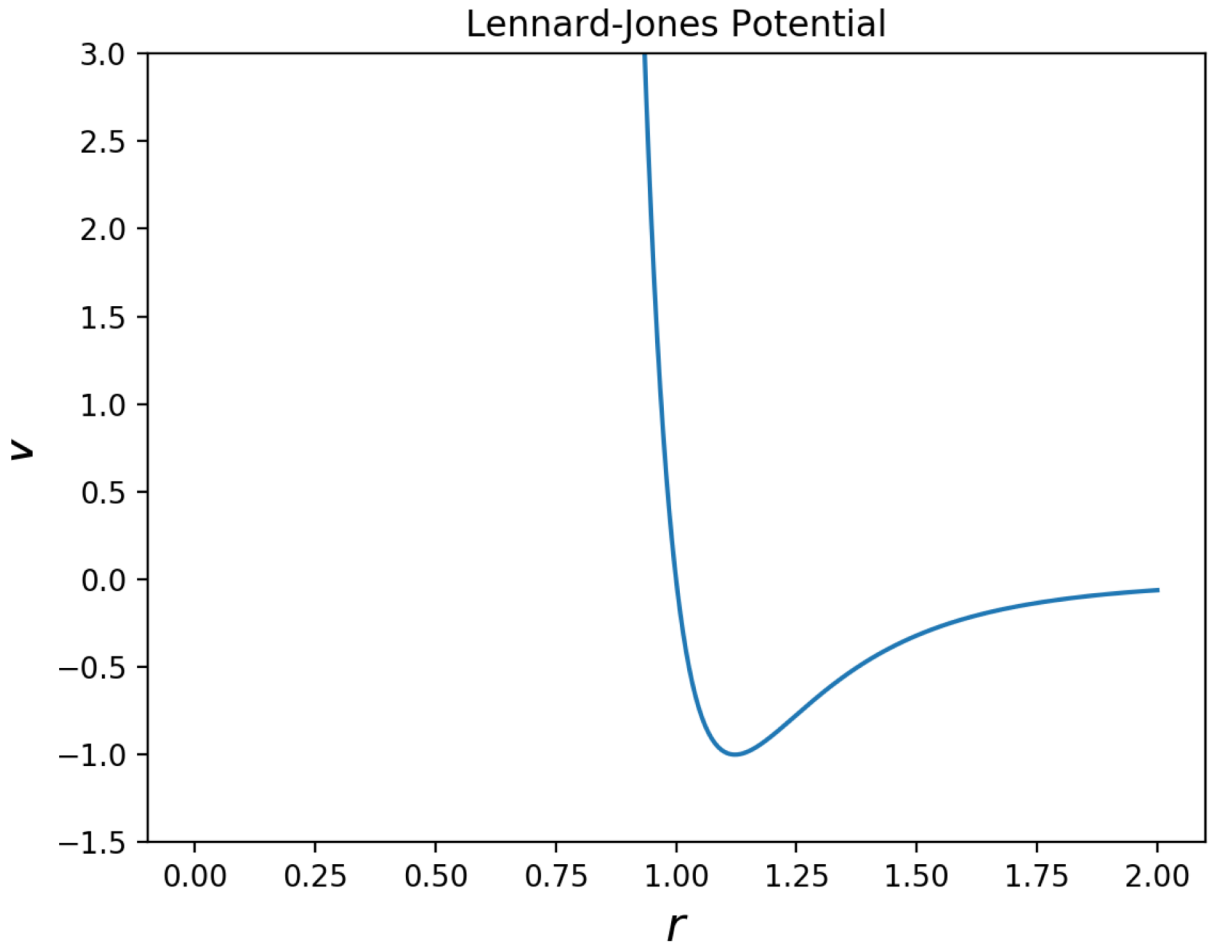
Lennard-Jones Potential

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

- Where ε is the depth of the potential well and σ is radius for zero potential.
- Approximation involving Van Der Waals Interactions (attractive) and electron orbital overlap (repulsive)

$$F_x = \sum_{i \neq j} \frac{-48\varepsilon}{r_{ij}^2}\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \frac{1}{2}\left(\frac{\sigma}{r_{ij}}\right)^{6}\right](x_i - x_j)$$

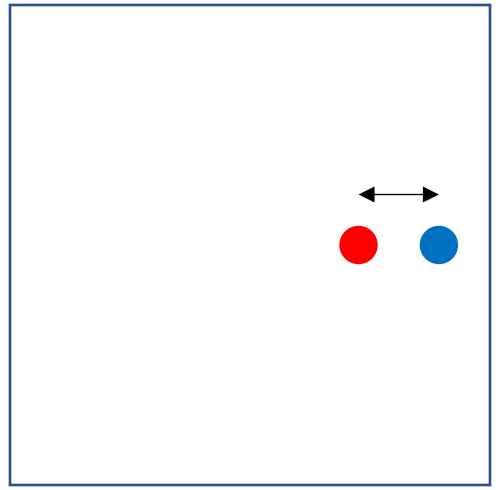
$$F_y = \sum_{i \neq j} \frac{-48\varepsilon}{r_{ij}^2}\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \frac{1}{2}\left(\frac{\sigma}{r_{ij}}\right)^{6}\right](y_i - y_j)$$

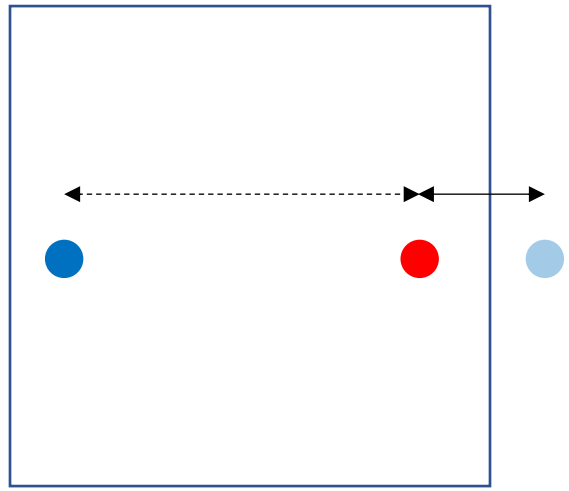


Lennard-Jones potential with $\varepsilon = \sigma = 1$

Boundary Conditions

- Periodic Boundaries
- Nearest Neighbor Force Calculations
  - When a component of the distance between two particles is greater than half the boundary size, perform force calculations using the image of the second particle outside the boundary.





Velocity Verlet

$$\vec{x}(t+\Delta t) = \vec{x}(t) + \vec{v}(t)\Delta t + \frac{1}{2}\vec{a}(t+\Delta t)\Delta t^2$$

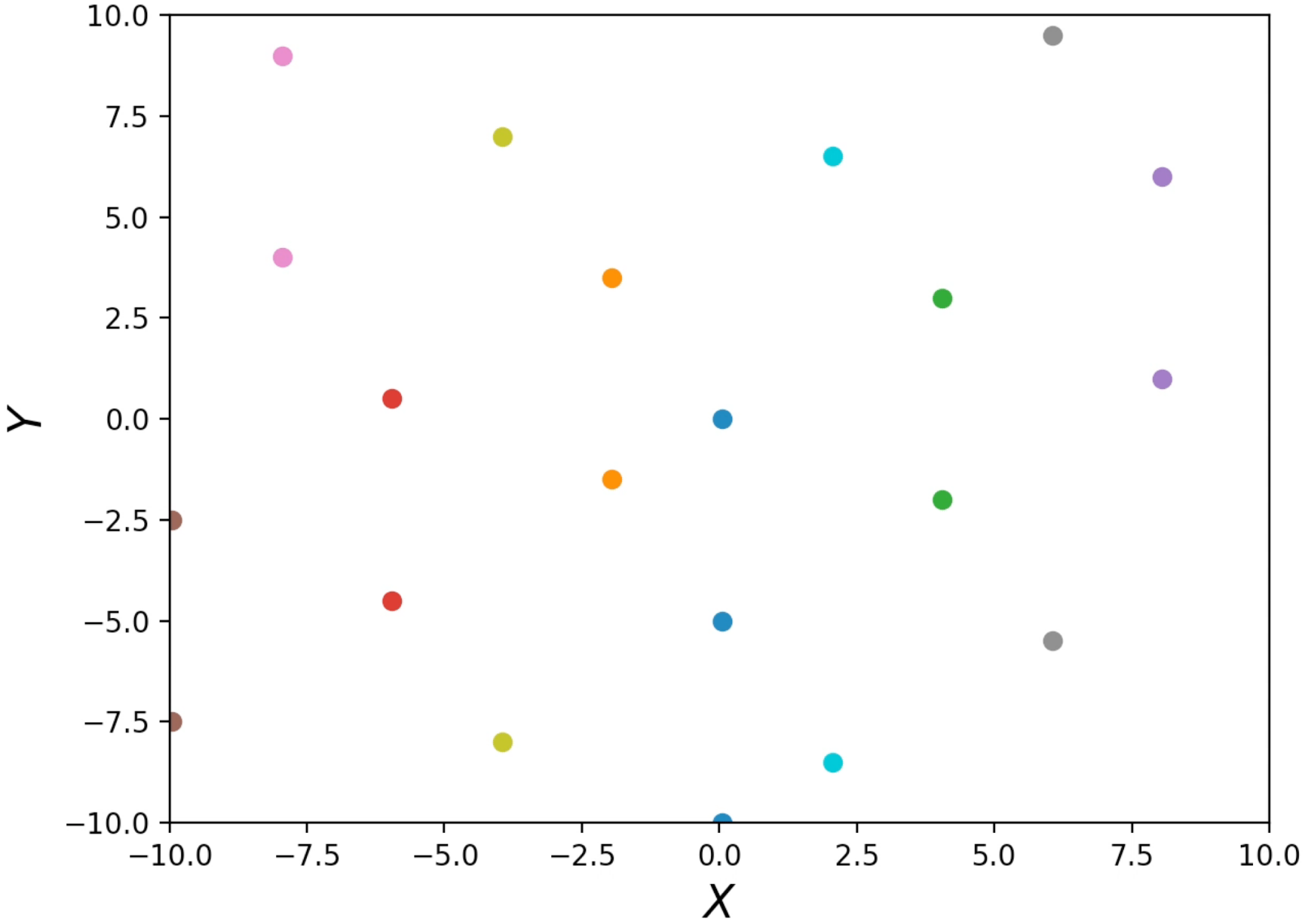
$$\vec{v}(t+\Delta t) = \vec{v}(t) + \frac{1}{2}[\vec{a}(t) + \vec{a}(t+\Delta t)]\Delta t$$

Error scales with Δt^2

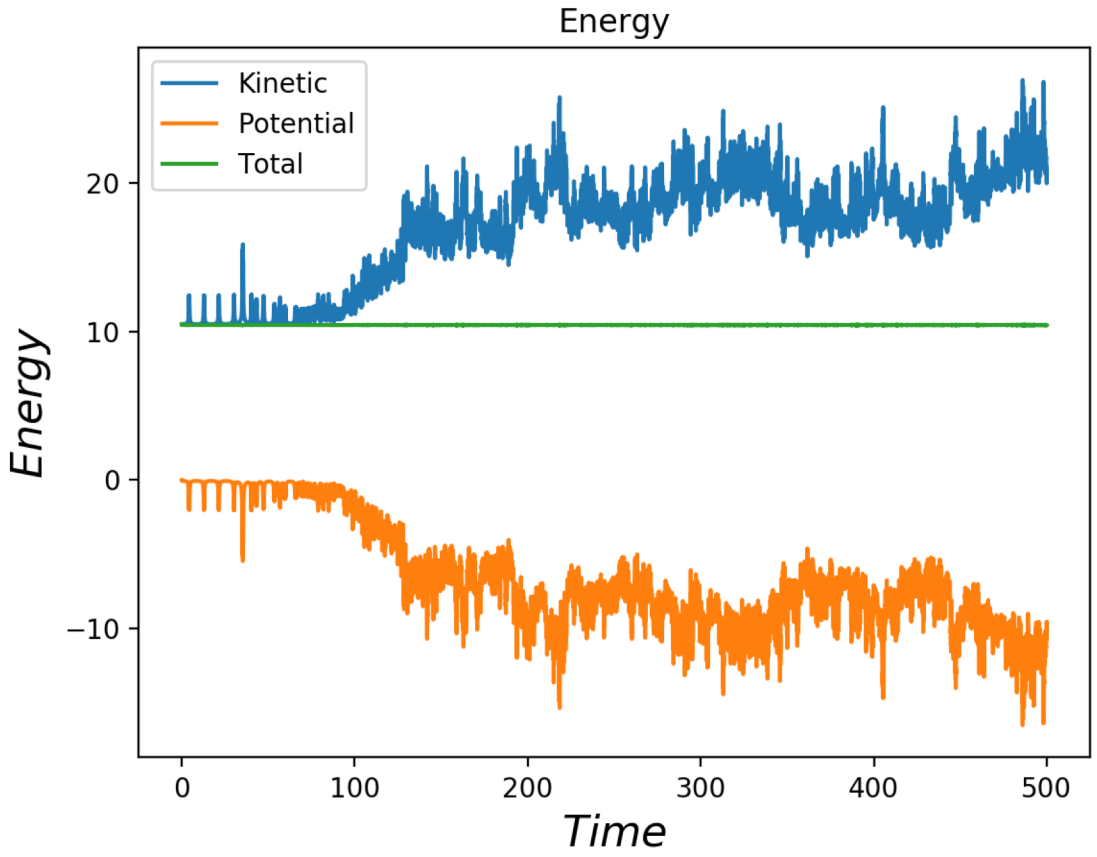
Algorithm at each time step for each particle:

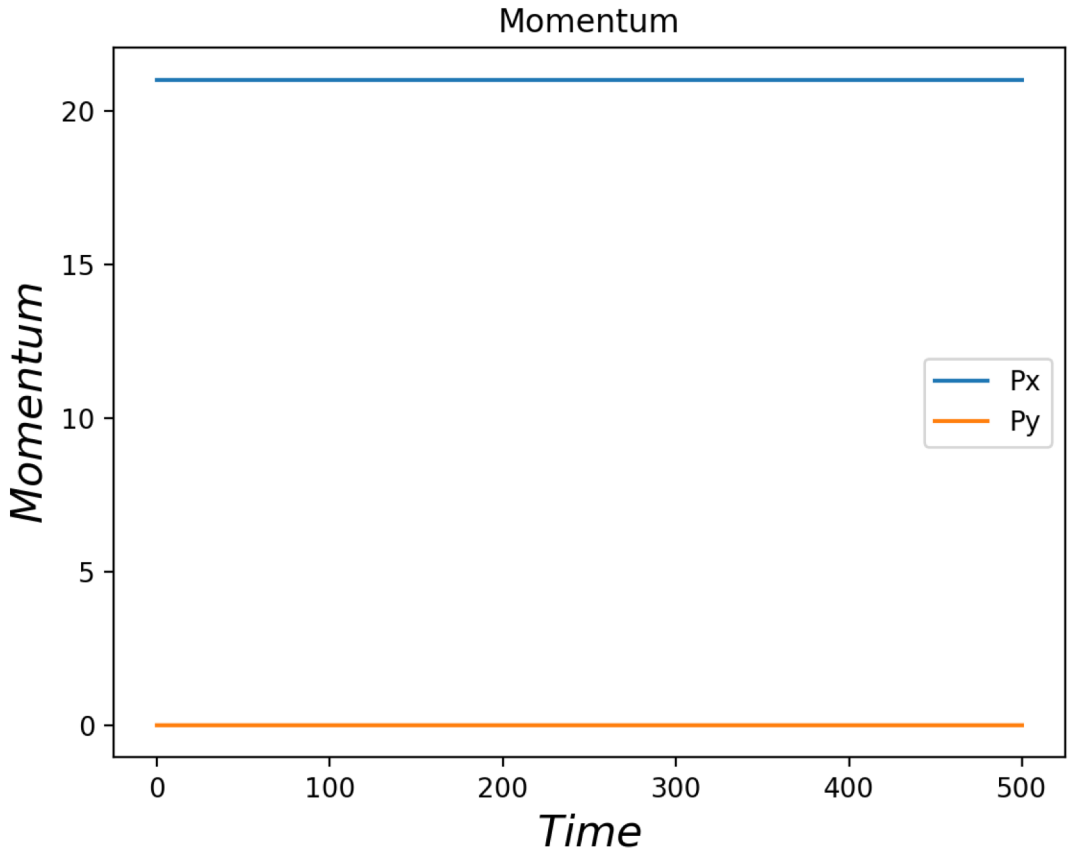
- Calculate intermediate velocity $\vec{v}_I(t) = \vec{v}(t) + \frac{1}{2}\vec{a}(t)\Delta t$
- Calculate updated position $\vec{x}(t+\Delta t) = \vec{x}(t) + \vec{v}_I(t)\Delta t$
- Calculate updated velocity $\vec{v}(t+\Delta t) = \vec{v}_I(t) + \frac{1}{2}\vec{a}(t+\Delta t)\Delta t$

Results



Results


Energy
Kinetic
Potential
Total
20
10
0
−10
Energy
0
100
200
300
400
500
Time


Momentum
20
15
10
5
0
Momentum
Px
Py
0
100
200
300
400
500
Time

Next Steps

- Flow around an object
- Polarity
- 3-Dimensions
- Introduce different molecules

Citations

[1]. Swope, W. C., Andersen, H. C., Berens, P. H., & Wilson, K. R. (1982). A computer simulation method for the calculation of equilibrium constants for the formation of physical clusters of molecules: Application to small water clusters. *The Journal of Chemical Physics*, *76*(1), 637-649.

[2]. Verlet, L. (1967). Computer "experiments" on classical fluids. I. Thermodynamical properties of Lennard-Jones molecules. *Physical review*, *159*(1), 98.