

Assignment 1 Applied Computational Science

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1. Suppose,

$$r = \sqrt{x^2 + y^2 + z^2} \quad (1)$$

then we define:

$$f_x(r) = -\frac{\partial U(r)}{\partial x} = -\frac{x}{r} \frac{\partial U(r)}{\partial r} : \text{x-component of the force.} \quad (2)$$

with

$$U(r) = 4\left(\frac{1}{r^{12}} - \frac{1}{r^6}\right) \longrightarrow f_x(r) = \frac{48x}{r^2} \left(\frac{1}{r^{12}} - \frac{1}{2} \cdot \frac{1}{r^6}\right) : \text{Lennard-Jones Potential} \quad (3)$$

Derive the f_x, f_y , and f_z component of Lennard-Jones Potential System.

From Equation (2), we know that:

$$\begin{aligned} f_x(r) &= -\frac{\partial U(r)}{\partial x} \\ &= -\frac{\partial r}{\partial x} \frac{\partial U(r)}{\partial r} \end{aligned} \quad (4)$$

then we substitute r and $U(r)$ from equation (1) and (3) \rightarrow (4)