Assignment 1 Applied Computational Science

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1. Suppose,

$$r = \sqrt{x^2 + y^2 + z^2} \tag{1}$$

then we define:

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

with

$$U(r) = 4\left(\frac{1}{r^{12}} - \frac{1}{r^6}\right) \text{ : Lennard-Jones Potential System} \tag{3}$$

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

From Equation (2), we know that:

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

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

$$\begin{aligned} f_x(r) &= -\left(\frac{\partial}{\partial x}\sqrt{x^2 + y^2 + z^2}\ \frac{\partial}{\partial r}4\left(\frac{1}{r^{12}} - \frac{1}{r^6}\right)\right) \\ &= -\left(\frac{1}{2}\frac{1}{\sqrt{x^2 + y^2 + z^2}}2x\ \left(\frac{-48}{r^{13}} + \frac{24}{r^7}\right)\right) \\ &= -\left(\frac{x}{\sqrt{x^2 + y^2 + z^2}}\frac{48}{r}\left(\frac{-1}{r^{12}} + \frac{1}{2}\cdot\frac{1}{r^6}\right)\right) \\ &= \frac{x}{r}\frac{48}{r}\left(\frac{1}{r^{12}} - \frac{1}{2}\cdot\frac{1}{r^6}\right) \\ &= \frac{48x}{r^2}\left(\frac{1}{r^{12}} - \frac{1}{2}\cdot\frac{1}{r^6}\right) \end{aligned} \tag{5}$$

For the f_y component, we define:

$$\begin{aligned} f_y(r) &= -\frac{\partial U(r)}{\partial y} \\ &= -\frac{\partial r}{\partial y}\frac{\partial U(r)}{\partial r} \end{aligned} \tag{6}$$

Again we substitute r and $U(r)$ from equation (1) and (3) $\rightarrow$ (6), thus:

$$\begin{aligned} f_y(r) &= -\left(\frac{\partial}{\partial y}\sqrt{x^2+y^2+z^2}\ \frac{\partial}{\partial r}4\left(\frac{1}{r^{12}}-\frac{1}{r^6}\right)\right) \\ &= -\left(\frac{1}{2}\frac{1}{\sqrt{x^2+y^2+z^2}}2y\ \left(\frac{-48}{r^{13}}+\frac{24}{r^7}\right)\right) \\ &= -\left(\frac{x}{\sqrt{x^2+y^2+z^2}}\frac{48}{r}\left(\frac{-1}{r^{12}}+\frac{1}{2}\cdot\frac{1}{r^6}\right)\right) \\ &= \frac{y}{r}\frac{48}{r}\left(\frac{1}{r^{12}}-\frac{1}{2}\cdot\frac{1}{r^6}\right) \\ &= \frac{48y}{r^2}\left(\frac{1}{r^{12}}-\frac{1}{2}\cdot\frac{1}{r^6}\right) \end{aligned} \tag{7}$$

For the f_y component, we define:

$$\begin{aligned} f_z(r) &= -\frac{\partial U(r)}{\partial z} \\ &= -\frac{\partial r}{\partial z}\frac{\partial U(r)}{\partial r} \end{aligned} \tag{8}$$

Again we substitute r and $U(r)$ from equation (1) and (3) $\rightarrow$ (8), thus:

$$\begin{aligned} f_z(r) &= -\left(\frac{\partial}{\partial z}\sqrt{x^2+y^2+z^2}\ \frac{\partial}{\partial r}4\left(\frac{1}{r^{12}}-\frac{1}{r^6}\right)\right) \\ &= -\left(\frac{1}{2}\frac{1}{\sqrt{x^2+y^2+z^2}}2z\ \left(\frac{-48}{r^{13}}+\frac{24}{r^7}\right)\right) \\ &= -\left(\frac{x}{\sqrt{x^2+y^2+z^2}}\frac{48}{r}\left(\frac{-1}{r^{12}}+\frac{1}{2}\cdot\frac{1}{r^6}\right)\right) \\ &= \frac{z}{r}\frac{48}{r}\left(\frac{1}{r^{12}}-\frac{1}{2}\cdot\frac{1}{r^6}\right) \\ &= \frac{48z}{r^2}\left(\frac{1}{r^{12}}-\frac{1}{2}\cdot\frac{1}{r^6}\right) \end{aligned} \tag{9}$$