

# Assignment 1 Applied Computational Science

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1. Suppose,

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

then we define:

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

with

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

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), therefore:

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

For the  $f_y$  component, we define:

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

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  $f_z$  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:

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