Units

We will measure distance in units of σ, so

$$\bar{r} = \frac{r}{\sigma}.$$

We measure energy in units of ϵ, so we have

$$\bar{U} = \frac{U}{\epsilon}.$$

The force is given as the derivative of the potential

$$F = -\frac{\mathrm{d}U}{\mathrm{d}r},$$

substituting $\bar{U}$ and $\bar{r}$ gives

$$F = \left(\frac{\epsilon}{\sigma}\right)\left(-\frac{\mathrm{d}\bar{U}}{\mathrm{d}\bar{r}}\right) = \left(\frac{\epsilon}{\sigma}\right)\bar{F},$$

so we see that

$$\bar{F} = \left(\frac{\sigma}{\epsilon}\right)F.$$

We want Newton's 2. law to simplify to

$$\bar{a} = \bar{F},$$

let us see what this means. From the definition of acceleration we get

$$a = \frac{\mathrm{d}^2 r}{\mathrm{d}t^2} = \frac{\sigma}{t_0^2}\frac{\mathrm{d}^2\bar{r}}{d\bar{t}^2} = \frac{\sigma}{t_0^2}\bar{a}.$$

So we have

$$a = \frac{F}{m} \qquad \Rightarrow \qquad \frac{\sigma}{t_0^2}\bar{a} = \left(\frac{\epsilon}{\sigma}\right)\frac{\bar{F}}{m} \qquad \Rightarrow \qquad \frac{\sigma}{t_0^2} = \left(\frac{\epsilon}{m\sigma}\right).$$

Solving for t gives

$$t_0 = \sigma\sqrt{\frac{m}{\epsilon}}.$$

Which will be our unit of time.

This means we find the kinetic energy from

$$K = \frac{1}{2}mv^2 = \frac{1}{2}\frac{\sigma}{mt_0^2}\bar{v}^2 = \frac{1}{2}\epsilon\bar{v}^2 \quad \Rightarrow \quad \bar{K} = \frac{1}{2}\bar{V}^2.$$