Σεπτέμβριος 2022

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad r_0 = 2^{1/6}\,\sigma$$

για $\varepsilon = 1$ $\sigma = 1$ $\quad V(r) = 4\left(\frac{1}{r^{12}} - \frac{1}{r^6}\right)$

Ορίζω την συνάρτηση $u(r) = V(r) - 3$

Λύνω την $u(r) = 0$

Αλγορίθμος

$$u(r) = 4\left(\frac{1}{r^{12}} - \frac{1}{r^6}\right) - 3$$

$$u'(r) = 4\left(\frac{-12}{r^{13}} - \frac{-6}{r^7}\right) = \frac{24}{r^7} - \frac{48}{r^{12}}$$

```
x = starting_point

for i in 100:
    x = x - u(x)/u'(x)
    if ( |u(x)/u'(x)| < 10^-6 ): break
    if x<0 or x>10 : break

print x
```