

Pressure (LJ unit) (Here d note dimensionless, instead of asteria, so sorry)

Formula:

$$P = N k_b T / V + \sum_{i=1}^N (\mathbf{f}_i \cdot \mathbf{r}_i) / 3V$$

Dimensionless form derivation:

Temperature:

$$T^d = \frac{T k_b}{\epsilon}$$

Then,

$$T = \frac{T^d \epsilon}{k_b}$$

Volume:

$$V^d = V \sigma^{-3}$$

Then,

$$V = V^d \sigma^3$$

coordinates,

$$r_i^d = r_i / \sigma$$

Then,

$$r_i = r_i^d \sigma$$

force,

$$f_i^d = f_i \sigma / \epsilon$$

Then,

$$f_i = f_i^d \epsilon / \sigma$$

Pressure,

$$P^d = P \sigma^3 / \epsilon$$

Then,

$$P = P^d \sigma^{-3} \epsilon$$

substitute into pressure computation formula, I obtain dimensionless form which is,

$$P^d = N T^d / V^d + \sum_{i=1}^N (f_i^d \cdot r_i^d) / 3 V^d$$

=====start calculating pressure=====

from the first file, **argon.1.lj**,

Printed pressure for 1st timestep is -4.3008571 while the one calculate from formula is 0.738729.
so I was so confused by this result for several days? What's wrong with my calculation? Pressure
at other timestep are also quite different. I get same value both from excel and my own program,
so the only reason lead to the huge difference must comes from the data.

Thanks for your attention.