A note about reduced units in a 2D Monte Carlo simulation of hard core particles with Lennard-Jonse potantial

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The particles are interacting with a pair Lennard-Jonse potantial:

$$U = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

If we want to calculate the thrmodynamic properties of particles with differet ϵ, σ, do we realy need to run a simulation for each caes? we don't. we will run the simulation in reduced units:

$$\begin{aligned} U' &= \frac{U}{\epsilon} \\ r' &= \frac{r}{\sigma} \end{aligned}$$

so that:

$$\boxed{U' = 4 \left[\left(\frac{1}{r'}\right)^{12} - \left(\frac{1}{r'}\right)^{6} \right]}$$

if we choose:

$$T' = \frac{k_B T}{\epsilon}$$

than in the only place in the simulation where we need to use T, ϵ *and* σ are gone:

$$\boxed{e^{-\frac{dU}{k_B T}} = e^{-\frac{dU}{\epsilon T'}} = e^{-\frac{dU'}{T'}}}$$

What if we want the pressure?

$$PV = Nk_B T - \frac{1}{2} \sum_{ij} r_{ij} \frac{dU}{dr}|_{r_{ij}}$$

in the Lennard-Jonse case:

$$r_{ij} \frac{dU}{dr}|_{r_{ij}} = 4\epsilon r_{ij} \left[-12\sigma^{12} r_{ij}^{-13} + 6\sigma^{6} r_{ij}^{-7} \right] = 4\epsilon \left[-12\sigma^{12} r_{ij}^{-12} + 6\sigma^{6} r_{ij}^{-6} \right] = 4\epsilon \left[-12 \left(\frac{1}{r'_{ij}}\right)^{12} + 6 \left(\frac{1}{r'_{ij}}\right)^{6} \right]$$

so that

$$
\begin{aligned}
PV &= Nk_BT - 4\epsilon\frac{1}{2}\sum_{ij}\left[-12\left(\frac{1}{r'_{ij}}\right)^{12} + 6\left(\frac{1}{r'_{ij}}\right)^{6}\right] = N\epsilon T' - 2\epsilon\sum_{ij}\left[-12\left(\frac{1}{r'_{ij}}\right)^{12} + 6\left(\frac{1}{r'_{ij}}\right)^{6}\right] \\
\frac{PV}{\epsilon} &= NT' - 2\sum_{ij}\left[-12\left(\frac{1}{r'_{ij}}\right)^{12} + 6\left(\frac{1}{r'_{ij}}\right)^{6}\right] \\
\frac{P}{\epsilon} &= \rho T' - \frac{2}{V}\sum_{ij}\left[-12\left(\frac{1}{r'_{ij}}\right)^{12} + 6\left(\frac{1}{r'_{ij}}\right)^{6}\right] \\
\frac{P\sigma^2}{\epsilon} &= \rho T'\sigma^2 - \frac{2}{V}\sigma^2\sum_{ij}\left[-12\left(\frac{1}{r'_{ij}}\right)^{12} + 6\left(\frac{1}{r'_{ij}}\right)^{6}\right] \\
\frac{P\sigma^2}{\epsilon} &= \rho T'\sigma^2 - 2\rho\frac{\sigma^2}{N}\sum_{ij}\left[-12\left(\frac{1}{r'_{ij}}\right)^{12} + 6\left(\frac{1}{r'_{ij}}\right)^{6}\right] \\
\frac{P\sigma^2}{\epsilon} &= \rho T'\sigma^2 - 12\rho\frac{\sigma^2}{N}\sum_{ij}\left[\left(\frac{1}{r'_{ij}}\right)^{6} - 2\left(\frac{1}{r'_{ij}}\right)^{12}\right]
\end{aligned}
$$

so if we choose:

$$
\begin{aligned}
P' &= \frac{P\sigma^2}{\epsilon} \\
\rho' &= \rho\sigma^2
\end{aligned}
$$

we get:

$$
\boxed{P' = \rho' T' - 12\rho'\sum_{ij}\left[\left(\frac{1}{r'_{ij}}\right)^{6} - 2\left(\frac{1}{r'_{ij}}\right)^{12}\right]}
$$

because we use the reduced distance: $r' = \frac{r}{\sigma}$, the size of the board will be reduced. if we want a reduced density of ρ' with N particles, the reduced size of the board will be given by:

$$L' = \frac{L}{\sigma}$$

$$\rho = \frac{N}{L^2} \rightarrow \frac{\rho'}{\sigma^2} = \frac{N}{\sigma^2 L'}$$

$$\boxed{L' = \sqrt{\frac{N}{\rho'}}}$$