1 Aufg 1

1.1 a

Define

$$\vec{r}'\frac{\vec{r}}{\sigma} \qquad E' = \frac{E}{\epsilon} \qquad m' = \frac{m}{\mu} \tag{1}$$

with $\mu = 6.69 \cdot 10^{-26}$kg. For the velocity we can calculate

$$\sqrt{\frac{\epsilon}{\mu}} =: \nu \approx 157.0\frac{\mathrm{m}}{\mathrm{s}} \qquad \Rightarrow \qquad v' = \frac{\vec{v}}{\nu} \tag{2}$$

and therefore

$$\frac{\sigma}{\nu} =: \tau \approx 2.2 \cdot 10^{-12}\mathrm{s} \qquad \Rightarrow \qquad t' = \frac{t}{\tau} \tag{3}$$

later we'll need

$$\frac{\epsilon}{k_B} =: \theta = 120\mathrm{K} \qquad \Rightarrow \qquad T' = \frac{T}{\theta} \tag{4}$$

1.2 b

We implemented the Box-Muller-Method to get a Gaussian distribution. For the velocities we multiplied the result from the gaussian distribution with the given sigma. This streches the velocity distribution, s.t. the sigma of the velocity distribution is equal to the given sigma.

1.2.1 c

We should update our neigborlist. In our Version, we put all particle as neigbours.

2 Aufg 2

2.0.1 a

2.0.2 b

$$T = \frac{1}{k_B}\langle E \rangle \qquad \Rightarrow T' = \langle E' \rangle \tag{5}$$