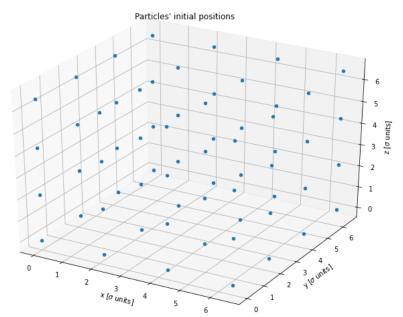
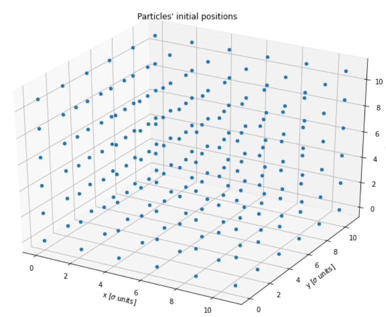
Computational physics sheet2,
Eleonora Foschino

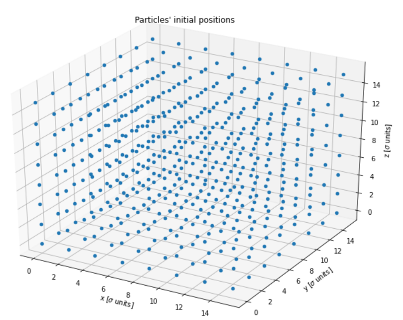
- a) The initial positions of the atoms are distributed along a cubic lattice, within a cubic simulation box (figure 1). Since density ρ and the number of particle N are fixed to $\rho = \frac{N}{V} = 0.1\sigma^{-3}$ and $N = n^3$: $L = n\sigma\sqrt[3]{10}$; also, from $L = p\sigma$ and $L = na_{lat} \rightarrow p\sigma = na_{lat}$ (in code, lengths are expressed in units of σ, so p is just the length of L).



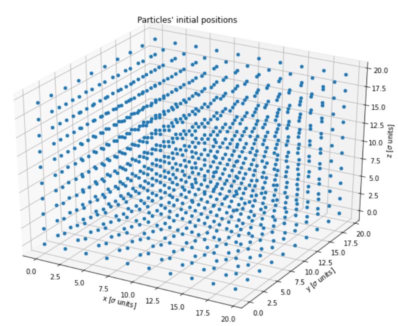
(a) n=4



(b) n=6



(c) n=8



(d) n=10

Figure 1: Snapshot of the initial conditions with n=4,6,8,10.

- e) Kinetic, potential and total energy $(K + U)$ during the production run are plotted in the following pictures. As it is possible to notice from figure 4, variations in the total energy are negligible.

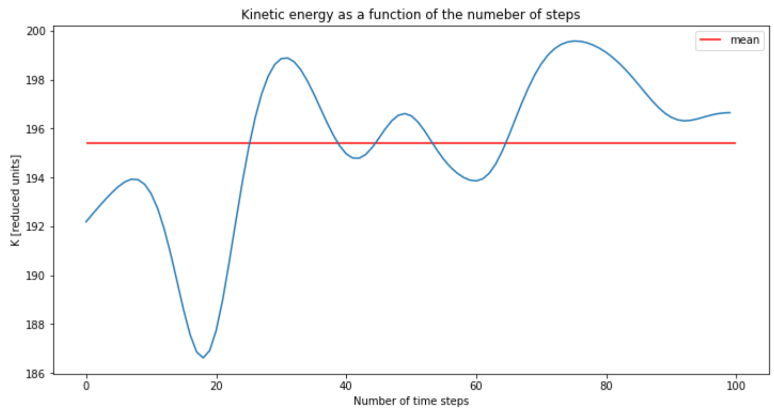


Figure 2: Kinetic energy in production with step $dt = 0.0002$.

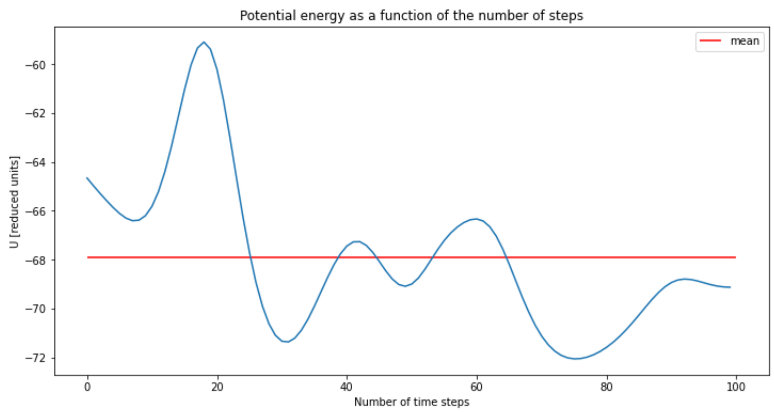


Figure 3: Potential energy in production run with step $dt = 0.0002$.

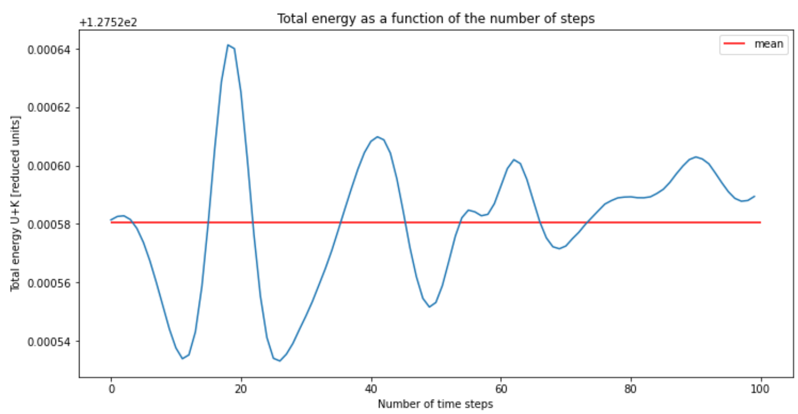


Figure 4: Total energy in production run with step $dt = 0.0002$.

Energy (dt = 0.0002)	mean	variance	standard deviation
Kinetic energy	200.2	34.2	5.8
Potential energy	-71.5	34.2	5.8
Total energy	128.77712	$1. \cdot 10^{-10}$	$4 \cdot 10^{-5}$

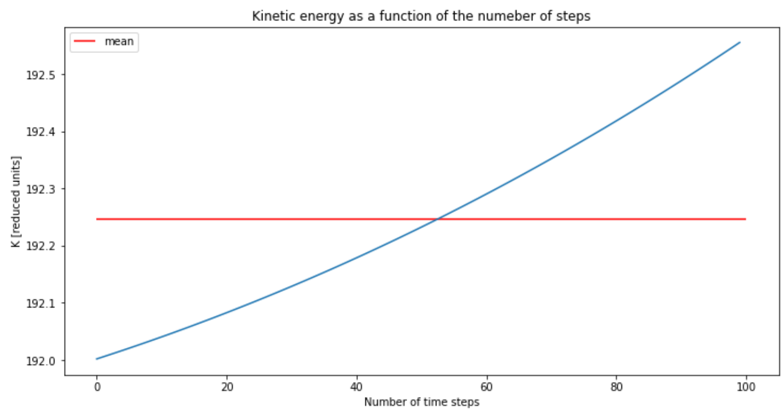


Figure 5: Kinetic energy in production with step $dt = 0.00002$.

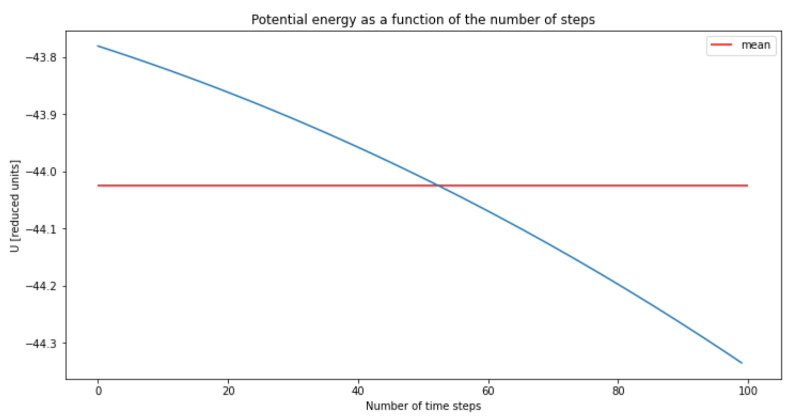


Figure 6: Potential energy in production run with step $dt = 0.00002$.

Energy (dt = 0.00002)	mean	variance	standard deviation
Kinetic energy	192.25	0.02	0.16
Potential energy	-44.02	0.02	0.16
Total energy	148.22102	$2. \cdot 10^{-19}$	$5 \cdot 10^{-10}$

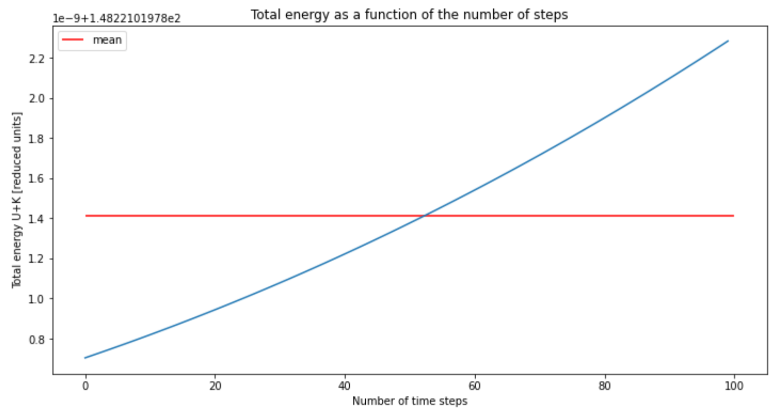


Figure 7: Total energy in production run with step $dt = 0.00002$.

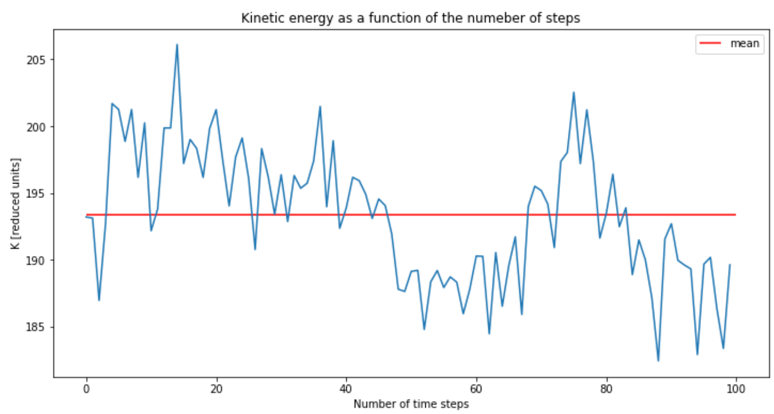


Figure 8: Kinetic energy in production with step $dt = 0.002$.

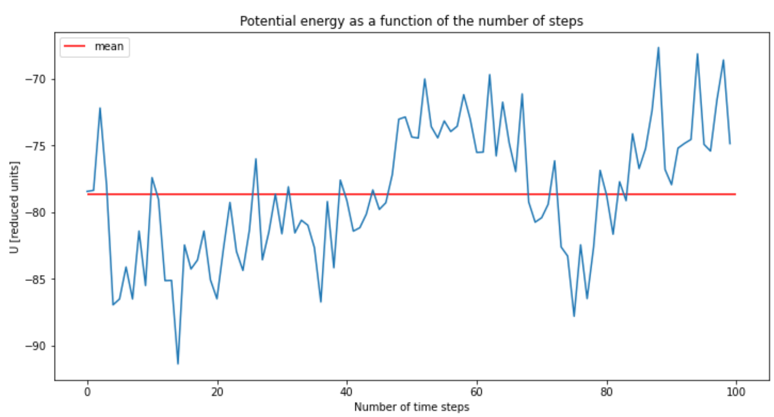


Figure 9: Potential energy in production run with step $dt = 0.002$.

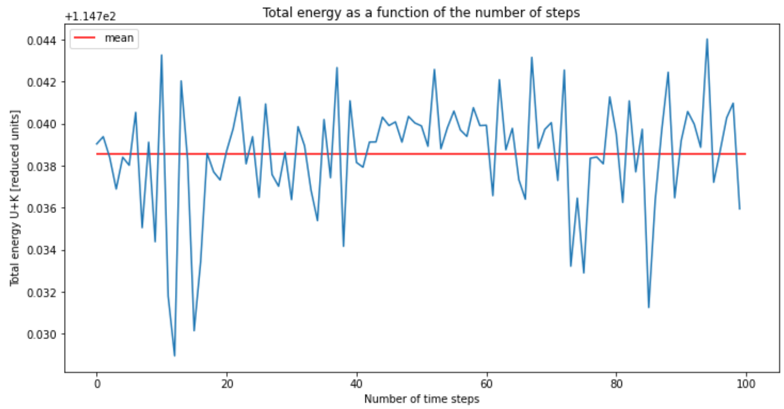


Figure 10: Total energy in production run with step $dt = 0.002$.

Energy (dt = 0.002)	mean	variance	standard deviation
Kinetic energy	193	24	5
Potential energy	-78	24	5
Total energy	114.739	$7. \cdot 10^{-6}$	0.002

With smaller integration step, the energy (and thus the algorithm?) becomes more stable.

The following graph shows the values of v_i^2 during the production run.

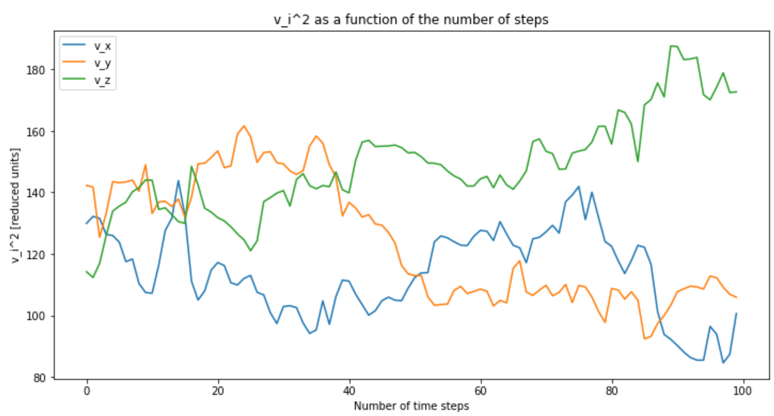


Figure 11: Velocities squared during production run.

- f) Figure 12 reports the computing time as a function of the number of steps. Estimated α is ≈ 1.6. Therefore $n = 50 \rightarrow N = 2500 \rightarrow \approx 273341s \approx 3days$.

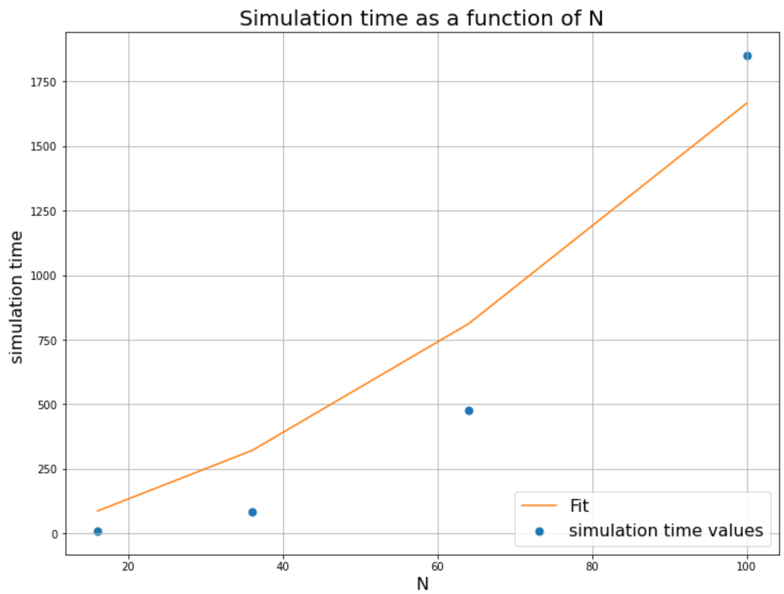


Figure 12: Computational time as a function of the number of particles.

- g) Figure 13 reports the velocities distribution (similar to the analytical Maxwell-Boltzmann distribution shape).
- h) The energy during doesn't seem to vary significantly with different r_{cuts} (figure 14 reports kinetic energy as an example).
- i) In the code, ϵ, m and σ were chosen as system units and set to 1 (calculations in 15).

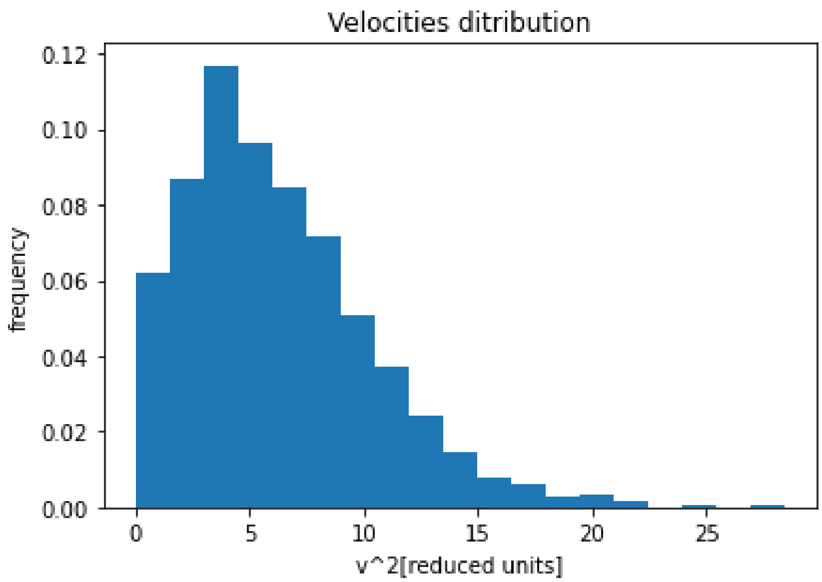
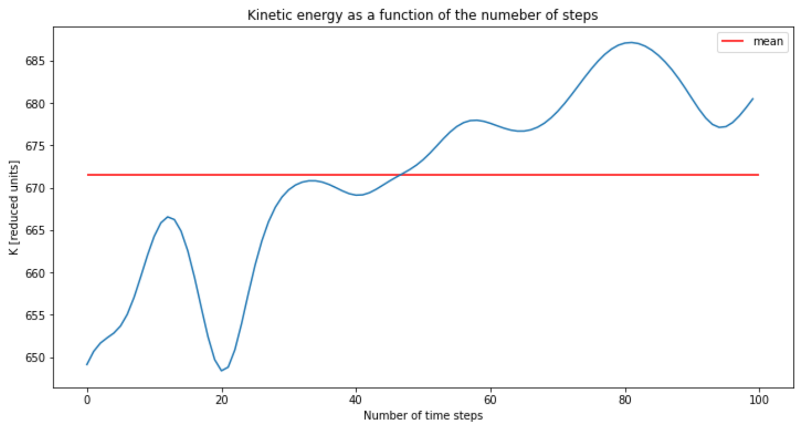
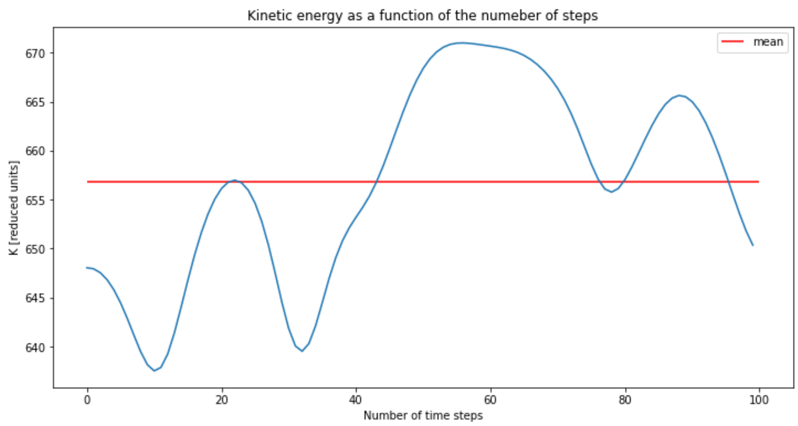


Figure 13: Velocity distribution with n=10.



(a)



(b)

Figure 14: Kinetic energy during the production run with $n = 6$ and $r_cut = 3.25\sigma$ (above) and $r_cut = 4.00\sigma$(below).

$\varepsilon = 1$ $\quad$ mass $= 1$ $\quad$ $\sigma = 1$

- 1 mass $= 105{,}52 \cdot 10^{-27}$ kg $\rightarrow$ 1 kg $= \frac{1}{105{,}52} \cdot 10^{27}$ mass
- $1\sigma = 2{,}55 \cdot 10^{-10}$ m $\rightarrow$ 1 m $= \frac{1}{2{,}55} \cdot 10^{10}\,\sigma$
- $k_B T = 2\,\varepsilon$

$$k_B T = 1{,}38 \cdot 10^{-23} \cdot 300 \ \frac{m^2\,kg}{s^2}$$

$$\Downarrow$$

$$\varepsilon = \frac{1{,}38 \cdot 10^{-23} \cdot 300}{2} \ \frac{m^2\,kg}{s^2}$$

$$\Downarrow$$

$$s^2 = \frac{1{,}38 \cdot 10^{-23} \cdot 300}{2\,\varepsilon} \ m^2\,kg =$$

$$= \frac{1{,}38 \cdot 10^{-23} \cdot 300}{2} \left(\frac{1}{2{,}55}\right)^2 \cdot 10^{20} \ \frac{1}{105{,}52} \cdot 10^{27} \ \frac{\sigma^2\,mass}{\varepsilon}$$

$$1\,s = \sqrt{\frac{1{,}38 \cdot 300}{2\,(2{,}55)^2 (105{,}52)}} \cdot 10^{14} \ \sigma \sqrt{\frac{m}{\varepsilon}}$$

- $\Delta t = 10^{-15}\,s \Rightarrow \approx 0{,}0001736 \cdot \sigma \sqrt{\frac{m}{\varepsilon}} \sim 0{,}0002$ in natural units

unit of length: σ

unit of time: $\sigma \sqrt{\frac{m}{\varepsilon}}$

unit of energy: ε

unit of temperature: $\frac{k_B}{\varepsilon}$

unit of pressure: $\frac{\sigma^3}{\varepsilon}$

- $\varepsilon = m = \sigma = k_B = 1$ in natural units
- since $\varepsilon = 0{,}5\,k_B T \Rightarrow T^* = 2$ in natural units

Figure 15