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Algorithms of Scientific Computing II

Exercise 3 - Discretization, Short-Range Potentials

1) Time Discretization

The movement of the molecules is being described by the following ordinary differential equation: $F_i = m_i \ddot{r}_i$.

In the lecture different methods for the discretization of that ODE have been introduced. In this exercise we will deal with those methods in more detail.

a) Use the Taylor-Series to derive the position equation of the *Explicit- Euler*-method

ANSWER:

Taylor-Series:

$$\vec{r}(t+\Delta t) = \vec{r}(t) + \Delta t \cdot \dot{\vec{r}}(t) + \frac{1}{2}\Delta t^2 \cdot \ddot{\vec{r}}(t) + \frac{\Delta t^i}{i!} \cdot \vec{r}^{(i)}(t) + \dots$$

truncate after first derivative:

$$\begin{aligned} \vec{r}(t+\Delta t) &= \vec{r}(t) + \Delta t \cdot \dot{\vec{r}}(t) = \vec{r}(t) + \Delta t \cdot \vec{v}(t) \\ \vec{v}(t+\Delta t) &= \vec{v}(t) + \Delta t \cdot \vec{a}(t) \end{aligned}$$

b) The "Störmer Verlet"-method is given by the following formulas:

$$\vec{r}(t+\Delta t) = 2 \cdot \vec{r}(t) - \vec{r}(t-\Delta t) + \Delta t^2 \cdot \vec{a}(t) \quad (1)$$

$$\vec{v}(t) = \frac{\vec{r}(t+\Delta t) - \vec{r}(t-\Delta t)}{2\Delta t} \quad (2)$$

Use the Taylor-Series to derive the position equation of the *Störmer-Verlet*-method

ANSWER:

Develop the Taylor-Series for $t + \Delta t$ and $t - \Delta t$:

$$\vec{r}(t + \Delta t) = \vec{r}(t) + \Delta t \cdot \dot{\vec{r}}(t) + \frac{\Delta t^2}{2} \cdot \ddot{\vec{r}}(t) + \frac{\Delta t^3}{6} \cdot \dddot{\vec{r}}(t) + O(\Delta t^4)$$
$$\vec{r}(t - \Delta t) = \vec{r}(t) - \Delta t \cdot \dot{\vec{r}}(t) + \frac{\Delta t^2}{2} \cdot \ddot{\vec{r}}(t) - \frac{\Delta t^3}{6} \cdot \dddot{\vec{r}}(t) + O(\Delta t^4)$$

Only the signs in front of terms with odd derivatives are different. Adding the two formulas yields:

$$\vec{r}(t + \Delta t) + \vec{r}(t - \Delta t) = 2 \cdot \vec{r}(t) + \Delta t^2 \cdot \ddot{\vec{r}}(t) + O(\Delta t^4)$$

This gives us the formula for the position:

$$\vec{r}(t + \Delta t) = 2 \cdot \vec{r}(t) - \vec{r}(t - \Delta t) + \Delta t^2 \cdot \ddot{\vec{r}}(t) + O(\Delta t^4)$$

c) What are the drawbacks of the *Störmer-Verlet*-method?

ANSWER:

- At the beginning of the simulation, the position of the particles is known. But the *Störmer-Verlet*-method requires the position to be known at two different timesteps.
- You always have to store the position for the two latest timesteps.
- The velocity is not being calculated.

d) In exact arithmetics, the *Störmer Verlet-* and the *Velocity-Störmer-Verlet-*method are equivalent. Prove the equivalence of the two schemes by starting from the *Störmer Verlet*-method and derive the *Velocity-Störmer-Verlet-*method:

$$r(t + \Delta t) = r(t) + \Delta t \cdot v(t) + \frac{\Delta t^2}{2} \cdot a(t) \tag{3}$$
$$v(t + \Delta t) = v(t) + \frac{\Delta t}{2} \cdot (a(t) + a(t + \Delta t)) \tag{4}$$

ANSWER:

From (2) we get:

$$\vec{r}(t - \Delta t) = \vec{r}(t + \Delta t) - 2\Delta t \cdot v(t) \tag{5}$$

substituting (5) into (1) and further transformations lead to the formula for the position:

$$\vec{r}(t + \Delta t) = 2 \cdot \vec{r}(t) - \vec{r}(t + \Delta t) + 2\Delta t \cdot v + \Delta t^2 \cdot \vec{a}(t)$$
$$2 \cdot \vec{r}(t + \Delta t) = 2 \cdot \vec{r}(t) + 2\Delta t \cdot v + \Delta t^2 \cdot \vec{a}(t)$$

$$\vec{r}(t+\Delta t) \;=\; \vec{r}(t) + \Delta t \cdot v + \frac{\Delta t^2}{2} \cdot \vec{a}(t) \tag{6}$$

To get a formula for the velocity, we substitute (1) into (2):

$$v(t) \;=\; \frac{\vec{r}(t)}{\Delta t} - \frac{\vec{r}(t-\Delta t)}{\Delta t} + \frac{\Delta t}{2} \cdot \vec{a}(t) \tag{7}$$

construct the same formula for the next time step:

$$\vec{v}(t+\Delta t) \;=\; \frac{\vec{r}(t+\Delta t)}{\Delta t} - \frac{\vec{r}(t)}{\Delta t} + \frac{\Delta t}{2} \cdot \vec{a}(t+\Delta t) \tag{8}$$

add (7) and (8)

$$\vec{v}(t) + \vec{v}(t+\Delta t) \;=\; \frac{\vec{r}(t+\Delta t) - \vec{r}(t-\Delta t)}{\Delta t} + \frac{(\vec{a}(t+\Delta t) + \vec{a}(t))\Delta t}{2}$$

$$\vec{v}(t+\Delta t) \;=\; \vec{v}(t) + \frac{(\vec{a}(t+\Delta t) + \vec{a}(t))\Delta t}{2} \tag{9}$$

Eq. 6 and eq. 9 are the desired Velocity Störmer Verlet method.

e) The Euler discretisation scheme is not time reversible. Analyse the *Velocity-Störmer-Verlet*-method to find out whether it is time reversible.

To find out wheter the method is time reversible, one calculates backwards, so starting from the calculated positions and velocites at time $(t+\Delta t)$, one calculates those at time t by using $\tilde{\Delta} t = -\Delta t$ from the previous formula as a time step. We call the resulting values at time $(t + \Delta t + \tilde{\Delta} t) = t$ $\tilde{r}$ and $\tilde{v}$, as we don't know yet wheter they are really equal to r and v. So be replacing Δt by $\tilde{\Delta} t$ and t by $t + \Delta t$ in eq. (3) and (4) we get:

$$\tilde{r}(t+\Delta t+\tilde{\Delta} t) \;=\; r(t+\Delta t) + \tilde{\Delta} t \cdot v(t+\Delta t) + \frac{\tilde{\Delta} t^{\,2}}{2} \cdot a(t+\Delta t) \tag{10}$$

$$\tilde{v}(t+\Delta t+\tilde{\Delta} t) \;=\; v(t+\Delta t) + \frac{\tilde{\Delta} t}{2} \cdot (a(t+\Delta t) + \tilde{a}(t+\Delta t+\tilde{\Delta} t)) \tag{11}$$

Replacing $\tilde{\Delta} t$ by $-\Delta t$ in 10:

$$\tilde{r}(t) \;=\; r(t+\Delta t) - \Delta t \cdot v(t+\Delta t) + \frac{\Delta t^2}{2} \cdot a(t+\Delta t) \tag{12}$$

Substituting (3) and (4) into (12):

$$\begin{aligned}
\tilde{r}(t) &= (r(t) + \Delta t \cdot v(t) + \frac{\Delta t^2}{2} \cdot a(t)) && (13)\\
&\quad -\Delta t \cdot (v(t) + \frac{\Delta t}{2} \cdot (a(t) + a(t + \Delta t))) + \frac{\Delta t^2}{2} \cdot a(t + \Delta t) && (14)\\
&= r(t) && (15)
\end{aligned}$$

Concerning the calculation of the positions, the Velocity Störmer Verlet method is time reversible. This also means that $\tilde{a}(t)$ equals $a(t)$ Now we will have a look at the velocities. Replacing $\tilde{\Delta t}$ by $-\Delta t$ in 11:

$$\begin{aligned}
\tilde{v}(t) &= v(t + \Delta t) - \frac{\Delta t}{2} \cdot (a(t + \Delta t) + \tilde{a}(t)) && (16)\\
&= v(t + \Delta t) - \frac{\Delta t}{2} \cdot (a(t + \Delta t) + a(t)) && (17)
\end{aligned}$$

Substituting (4) into (17):

$$\begin{aligned}
\tilde{v}(t) &= v(t) + \frac{\Delta t}{2} \cdot (a(t) + a(t + \Delta t)) - \frac{\Delta t}{2} \cdot (a(t + \Delta t) + a(t)) && (18)\\
&= v(t) && (19)
\end{aligned}$$

So also the velocity calculation and therefore the whole Velocity Störmer Verlet method is time reversible.

f) For the derivation of the Euler method, which is a first order method, all terms of second or higher order were neglected. In the derivetion of the Störmer Verlet method, all terms of fourth or higher order were neglected. Yet, the Störmer Verlet method is not a third order, but only a second order method. Show why this is the case.

ANSWER:

The Störmer-Verlet method is given by

$$\vec{r}(t + \Delta t) = 2 \cdot \vec{r}(t) - \vec{r}(t - \Delta t) + \Delta t^2 \cdot \vec{a}(t) + O(\Delta t^4).$$

Assume, that $\vec{r}(t)$ and $\vec{r}(t-\Delta t)$ are known exactly. Then the error for $\vec{r}(t+\Delta t)$ is

$$\text{Error}(\vec{r}(t + \Delta t)) = O(\Delta t^4).$$

Neglecting errors in $\vec{a}(t + \Delta t)$, we apply the scheme several times and determine the errror:

– At time $t + 2 \cdot \Delta t$:

$$\vec{r}(t + 2 \cdot \Delta t) = 2 \cdot \vec{r}(t + \Delta t) - \vec{r}(t) + \Delta t^2 \cdot \vec{a}(t + \Delta t) + O(\Delta t^4)$$

$$\Rightarrow \text{Error}(\vec{r}(t + 2 \cdot \Delta t)) = 2 \cdot \text{Error}(\vec{r}(t + \Delta t)) + ? + O(\Delta t^4) = 3 \cdot O(\Delta t^4)$$

– At time $t + 3 \cdot \Delta t$:

$$\vec{r}(t + 3 \cdot \Delta t) = 2 \cdot \vec{r}(t + 2 \cdot \Delta t) - \vec{r}(t + \Delta t) + \Delta t^2 \cdot \vec{a}(t + 2 \cdot \Delta t) + O(\Delta t^4)$$

$$\begin{aligned} \Rightarrow \text{Error}(\vec{r}(t + 3 \cdot \Delta t)) &= 2 \cdot \text{Error}(\vec{r}(t + 2 \cdot \Delta t)) - \text{Error}(\vec{r}(t + \cdot \Delta t)) + ? + O(\Delta t^4) = 3 \cdot \\ &= 6 \cdot O(\Delta t^4) - O(\Delta t^4) + ? + O(\Delta t^4) = 6 \cdot O(\Delta t^4) \end{aligned}$$

– At time $t + n \cdot \Delta t$: By induction, one can show:

$$\text{Error}(\vec{r}(t + n \cdot \Delta t)) = \frac{n \cdot (n-1)}{2} \cdot O(\Delta t^4)$$

So at time $T = n \cdot \Delta t$ we get

$$\begin{aligned} \text{Error}(\vec{r}(t + n \cdot \Delta t)) &= (\frac{n^2}{2} + \frac{n}{2}) \cdot O(\Delta t^4) \\ &\overset{n=\frac{T}{\Delta t}}{=} (\frac{T^2}{2 \cdot \Delta t^2} + \frac{T}{2 \cdot \Delta t}) \cdot O(\Delta t^4) \\ &= O(\Delta t^2) \end{aligned}$$

2) Short-range Potentials

a) Assume we simulate a molecular dynamics scenario with N molecules. If we explicitely compute the forces between all pairs of molecules, O(N^2) operations are necessary. For short-range potentials, we neglect interactions between particles that have a mutual distance bigger than a certain cut-off radius. This reduces the number of required operations to O(N).

Someone tries to convince you that this is not true: *A*ssume that a simulation with N molecules requires C operations for the force calculations. Double the number of molecules in the domain. Then we of course have to compute forces for twice as many molecules. But, in addition, the number of molecules within the cut-off radius of a certain molecule doubles, too. Such,

we need 4C operations, which means that the number of operations behaves like $O(N^2)$.

Why is that argumentation faulty?

ANSWER: The fault is that with doubling the number of molecules in a domain the scenario changes completely, as we now deal with matter of double the density. Thus doubling the problem size doesn't correspond to simply doubling the number of molecules, but rather to doubling the size of the domain, with constant density. In that case the algorithm really needs only twice the number of calculations.

b) For short-range potentials it is sufficient to consider only neighbouring particles for the force calculation. That means that all particles which are farther away as the cutoff-radius are neglected. But this is only allowed when the integral over the cut-away potential (from r_c to inf is finite. In the lecture you have seen for 2D potentials of the form $U(r) = c \cdot r^{-p}$ this is the case for $p > 2$

Now consider a 3D potential of the same form ($U(r) = c \cdot r^{-p}$). For which values of p is this potential short-range in 3D?

ANSWER: In order to be a short-range potential, the integral over the cut-off area has to be finite.

In the following we consider the integrals in 1d, 2d and 3d

1D:

$$\int_{\|\vec{r}\|>rc} U(\vec{r})d\vec{r}$$

As we only want to analyze if the integral is finite, it is sufficient to consider positive distances:

$$\int_{r>rc} U(r)dr \quad = \quad \int_{r>rc} c \cdot r^{-p} = c\left[\frac{r^{1-p}}{1-p}\right]_{rc}^{\infty} = c\left(\frac{\infty^{1-p}}{1-p} - \frac{rc^{1-p}}{1-p}\right)$$

Thus, for $p \leq 1$ the integral approaches infinity. For $p > 1$ the 1d-potential is short-range.

2D: The calculation of the two-dimensional integral over the cutoff-area is simpler to perform in polar coordinates. Therefore we perform a transformation of the coordinates before. The transformation function $\Psi(r, \alpha)$ reads:

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \Psi(r, \alpha) = \begin{pmatrix} r\cos\alpha \\ r\sin\alpha \end{pmatrix}$$

With that function the integral can be written as

$$\int_{\|\vec{r}\|>rc} U(\vec{r})d\vec{r} = \int_0^{2\pi}\int_{rc}^{\infty} U(r)det(J(\Psi(r,\alpha)))drd\alpha \qquad (20)$$

First we determine the determinant of the Jacobian matrix:

$$\begin{aligned} det(J(\Psi(r,\alpha))) &= \begin{vmatrix} \frac{\partial}{\partial r}\Psi_1(r,\alpha) & \frac{\partial}{\partial r}\Psi_2(r,\alpha) \\ \frac{\partial}{\partial \alpha}\Psi_1(r,\alpha) & \frac{\partial}{\partial \alpha}\Psi_2(r,\alpha) \end{vmatrix} = \begin{vmatrix} \cos\alpha & \sin\alpha \\ -r\sin\alpha & r\cos\alpha \end{vmatrix} \\ &= r\cos^2\alpha + r\sin^2\alpha = r \end{aligned}$$

That result put into (20) gives us:

$$\int_{\|\vec{r}\|>rc} U(\vec{r})d\vec{r} = \int_0^{2\pi}\int_{rc}^{\infty} U(r)\cdot r\ drd\alpha$$

Now we replace the potential with the one given:

$$\begin{aligned} \int_{\|\vec{r}\|>rc} U(\vec{r})d\vec{r} &= \int_0^{2\pi}\int_{rc}^{\infty} c\cdot r^{-p}\cdot r\ drd\alpha = \int_0^{2\pi}\int_{rc}^{\infty} c\cdot r^{1-p}drd\alpha \\ &= 2\pi\int_{rc}^{\infty} c\cdot r^{1-p}dr = 2\pi c\left[\frac{r^{2-p}}{2-p}\right]_0^{\infty} \\ &= 2\pi c\left(\frac{\infty^{2-p}}{2-p} - \frac{0^{2-p}}{2-p}\right) \end{aligned}$$

As we can see, the integral is finite for $p > 2$, thus the potential is short-range in that case.

3D: We want fo find out for wich potentials $U(r)$ the integral $\int_{\|\vec{r}\|>r_c} U(\|\vec{r}\|)d\vec{r}$ is finite.

First, we have to do a coordinate transformation to polar coordinates:

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \Psi(r,\alpha,\beta) = \begin{pmatrix} r\cdot\cos\alpha\cdot\cos\beta \\ r\cdot\sin\alpha\cdot\cos\beta \\ r\cdot\sin\beta \end{pmatrix}$$

$$\int_{\|\vec{r}\|>r_c} U(\|\vec{r}\|)d\vec{r} = \int_{-\frac{pi}{2}}^{\frac{pi}{2}}\int_0^{2\pi}\int_{r_c}^{\infty} U(\|\vec{r}\|)\cdot det(J(\Psi(r,\alpha,\beta)))drd\alpha d\beta \qquad (21)$$

Calcuate the determinant of the Jacobi-matrix

$$\begin{aligned}
det(J(\Psi(r,\alpha,\beta))) &= \begin{vmatrix} \frac{\partial}{\partial r}\Psi_1(r,\alpha,\beta) & \frac{\partial}{\partial r}\Psi_2(r,\alpha,\beta) & \frac{\partial}{\partial r}\Psi_3(r,\alpha,\beta) \\ \frac{\partial}{\partial \alpha}\Psi_1(r,\alpha,\beta) & \frac{\partial}{\partial \alpha}\Psi_2(r,\alpha,\beta) & \frac{\partial}{\partial \alpha}\Psi_3(r,\alpha,\beta) \\ \frac{\partial}{\partial \beta}\Psi_1(r,\alpha,\beta) & \frac{\partial}{\partial \beta}\Psi_2(r,\alpha,\beta) & \frac{\partial}{\partial \beta}\Psi_3(r,\alpha,\beta) \end{vmatrix} \\
&= \begin{vmatrix} \cos\alpha\cdot\cos\beta & \sin\alpha\cdot\cos\beta & \sin\beta \\ -r\cdot\sin\alpha\cdot\cos\beta & -r\cdot\cos\alpha\cdot\cos\beta & 0 \\ -r\cdot\cos\alpha\cdot\sin\beta & -r\cdot\sin\alpha\cdot\sin\beta & r\cdot\cos\beta \end{vmatrix} \\
&= r^2\cos^2\alpha\cos^3\beta r^2\sin^2\alpha\sin^2\beta\cos\beta + r^2\cos^2\alpha\sin^2\beta\cos\beta r^2\sin^2\alpha\c \\
&= r^2(\cos^3\beta(\cos^2\alpha+\sin^2\alpha)+\sin^2\beta\cdot\cos\beta(\sin^2\alpha+\cos^2\alpha)) \\
&= r^2(\cos^3\beta+\sin^2\beta\cdot\cos\beta) \\
&= r^2\cdot\cos\beta
\end{aligned}$$

and the norm of $\vec{r}$:

$$\begin{aligned}
\|\vec{r}\| &= \sqrt{r^2(\cos^2\alpha\cos^2\beta+\sin^2\alpha\cos^2\beta+\sin^2\beta)} \\
&= \sqrt{r^2(\cos^2\beta(\cos^2\alpha+\sin^2\alpha)+\sin^2\beta)} \\
&= r
\end{aligned}$$

Using this with (21):

$$\begin{aligned}
\int_{\|\vec{r}\|>r_c} U(\|\vec{r}\|)d\vec{r} &= \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\int_0^{2\pi}\int_{r_c}^{\infty} U(\|\vec{r}\|)\cdot det(J(\Psi(r,\alpha,\beta)))drd\alpha d\beta \\
&= \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\int_0^{2\pi}\int_{r_c}^{\infty} c\cdot r^{-p}r^2\cos\beta drd\alpha d\beta \\
&= 2\pi\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\int_{r_c}^{\infty} c\cdot r^{2-p}\cos\beta drd\beta \\
&= 2\pi c\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\left[\frac{r^{3-p}}{3-p}\right]_{r_c}^{\infty}\cos\beta d\beta \\
&= 2\pi c\left[\frac{r^{3-p}}{3-p}\right]_{rc}^{\infty}[\sin\beta]_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \\
&= 2\pi c\left(\frac{\infty^{3-p}}{3-p}-\frac{r_c^{3-p}}{3-p}\right)\left(\sin(\frac{\pi}{2})-\sin(-\frac{\pi}{2})\right) \\
&= \begin{cases} -4\pi c\frac{r_c^{3-p}}{3-p} & \text{if} \quad p>3 \\ \infty & \text{if} \quad p\leq 3 \end{cases}
\end{aligned}$$

3) Linked Cells

a) The linked cell datastructure is used to access neighbouring molecules. In the most simple case, the cells are cubic and the side length of a cell equals the cutoff radius. In 3D, apart from the cell itself, 26 additional cells have to be examined (8 cells in 2D). By reducing the size of the cells, more cells have to be used, but the volume covered by these cells is smaller. As the covered volume corresponds to the number of distance calculations, smaller cell sizes can increase the performance. Calculate the covered volume for $l = rc$, $l = \frac{rc}{2}$, $l = \frac{rc}{4}$ and $l \to 0$ in 2D and 3D.

	$l = rc$	$l = \frac{rc}{2}$	$l = \frac{rc}{4}$	...	$L \to 0$
$2D$					
(% unnecessary)					
$3D$					
(% unnecessary)					

ANSWER:

i) $l = rc$: In this case, we have to consider only the directly neighbouring cells:

	2D: 9 cells	3D: 27 cells
A_{cells}	$9rc^2$	$27rc^3$
$A_{\text{in cutoff}}$	πrc^2	$\frac{4}{3}\pi rc^3$
$A_{\text{in cutoff}}$ / A_{cells}	$\frac{\pi}{9} \approx 35\%$	$\frac{4\pi}{81} \approx 16\%$
$\Rightarrow$ unneccessary:	$\approx 65\%$	$\approx 84\%$

ii) $l = \frac{rc}{2}$: In this case, we have to consider two neighbouring cells in each direction, thus five cells per dimension:

	2D: 25 cells	3D: 125 cells
A_{cells}	$25(\frac{rc}{2})^2 = \frac{25}{4}rc^2$	$\frac{125}{8}rc^3$
$A_{\text{in cutoff}}$	πrc^2	$\frac{4}{3}\pi rc^3$
$A_{\text{in cutoff}}$ / A_{cells}	$\frac{4\pi}{25} \approx 50\%$	$\frac{32\pi}{375} \approx 27\%$
$\Rightarrow$ unneccessary:	$\approx 50\%$	$\approx 73\%$

iii) $l = \frac{rc}{4}$: Here we have to take 9 cells in each dimension into consideration. But now we can get rid of some cells. In 2d, e.g. the smallest distance possible between a particle in the middle cell to a particle in a corner cell is $\sqrt{2(\frac{3}{4}rc)^2} = 1.06rc$. Thus we don't have to search the corner cells for particles within the cutoff-radius.

In 3d, searching all cells along the edges is unneccessary. Moreover we can save 4 more cells per surface of the cube.

	2D: 77 cells	3D: 613 cells
A_{cells}	$77(\frac{rc}{4})^2 = \frac{77}{16}rc^2$	$\frac{613}{64}rc^3$
$A_{in\ cutoff}$	πrc^2	$\frac{4}{3}\pi rc^3$
$A_{in\ cutoff}$ / A_{cells}	$\frac{16\pi}{77} \approx 65\%$	$\frac{256\pi}{3 \cdot 613} \approx 44\%$
$\Rightarrow$ unneccessary:	$\approx 35\%$	$\approx 56\%$

Here is an overview of all the results:

	$l = rc$	$l = \frac{rc}{2}$	$l = \frac{rc}{4}$	...	$L \to 0$
$2D$	9	6.25	4.81		3.14
(% unneccessary)	65%	50%	35%		0%
$3D$	27	15.63	9.58		4.19
(% unneccessary)	84%	73%	56%		0%

b) As investigated in part a), the computational time to evaluate the force on one particle depends on the size of the cells of the linked-cells datastructure. Try to determine further factors which influence the computational time and construct a formula!

ANSWER:

The time for dealing with one cell consists of the time to access the cell plus the time to access the cell's particle and calculating the distances of the particles. If the particles are equally distributed, the number of molecules in a cell is proportional to the density ρ:

$$t_{Cell} = c_{Cell} + c_{distance} \cdot \rho \cdot V_{Cell}$$

The number of force calculations is independent of the size of the cells, as only the forces between those molecules are calculated which ly within the cutoff radius, but it depends on the density:

$$t_{force} = (c_{force} \cdot \rho \cdot \frac{4}{3}\pi \cdot rc^3) \cdot \rho \cdot V_{domain}$$

Thus, the total time is $t_{total} = N_{cells} \cdot t_{cell} + t_{force}$