Report

Serial part

Here we list the various optimization that we made in the serial program (wrt unoptimised version dubbed 0). Since we noticed using perf that the greatest part of cycles were spent in the `force` function, we tried to optimize it.

1. Apply 3rd Newton's law

Implementing this law allow us to perform the half of the calculation. In doing this one must care the potential energy that differs by a factor of 2 with the unoptimized version. With this optimization we gain a factor of ~2.

2. Avoid expensive math operation

We tried to reduce as much we could the amount of division (the inverse of the divisor were stored if we had to do repeated division by that number). The same was applied to the power function. All the constant were stored and reused. We tried also to suppress completely power function replacing it with repeated multiplication, but no benefit were found.

3. Avoid repeated computation in cycle

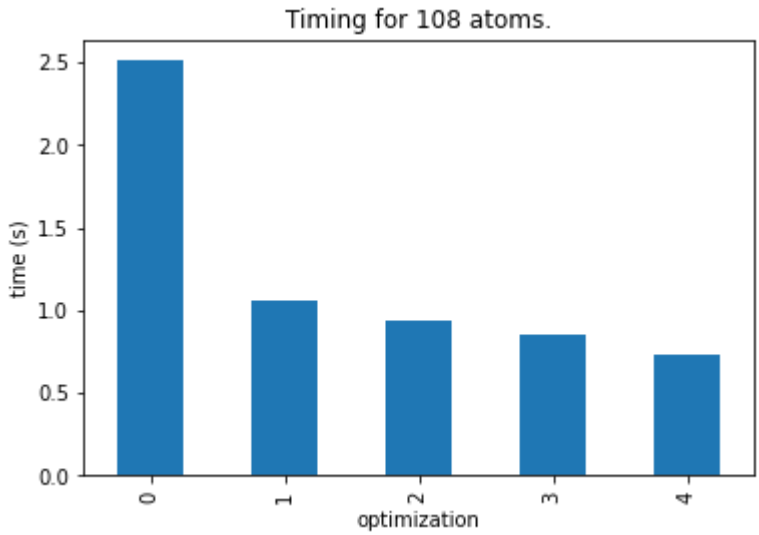
We tried to put on the outer cycle as much operation that would have been repeated in the inner cycle. Also doing this we avoided some potentially expensive cache lookup.

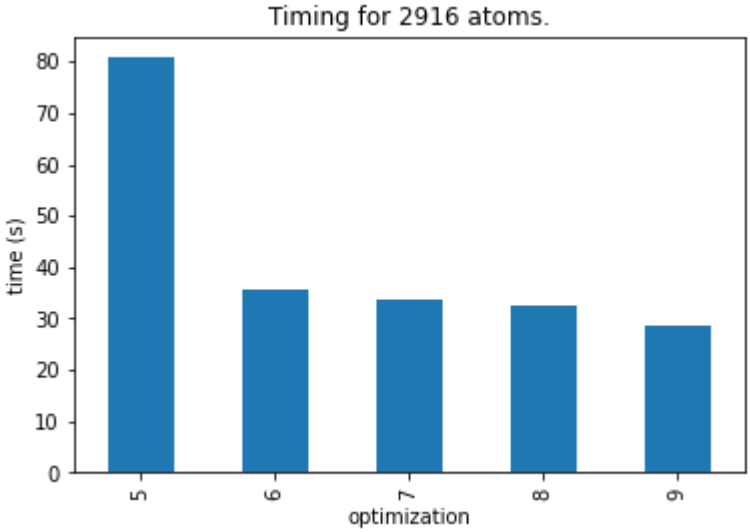
4. Repack pointer into vector struct

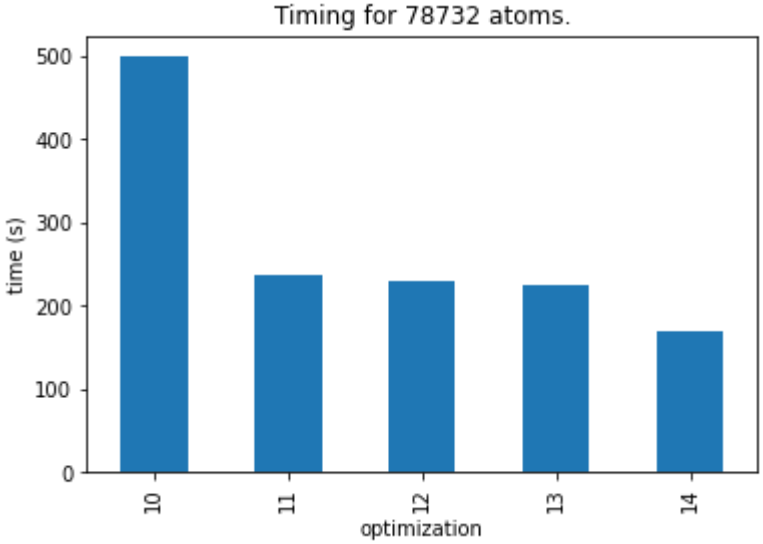
We tried to repack position, velocities and force arrays (in total 9) into 3 arrays of struct containing 3 elements.

Results

	atoms	optimisation	time (s)
0	108	0	2.51
1	108	1	1.058
2	108	2	0.944
3	108	3	0.854
4	108	4	0.734
5	2916	0	80.726
6	2916	1	35.755
7	2916	2	33.551
8	2916	3	32.522
9	2916	4	28.555
10	78732	0	498.966
11	78732	1	235.921
12	78732	2	228.585
13	78732	3	223.414
14	78732	4	168.823




Timing for 2916 atoms.
time (s)
0
10
20
30
40
50
60
70
80
5
6
7
8
9
optimization


Timing for 78732 atoms.
time (s)
0
100
200
300
400
500
10
11
12
13
14
optimization