CSE Ex08

Cell Lists for MD are my specialty. So here is something I calculated from my Bachelor-Thesis: Let **N** be the number of particles. Furthermore, let **c** be the average number of particles in a cell, **c = N/m**, with **m** being the number of cells. For the case of brute forcing with 2-Body interaction we would have to calculate **N^2** interactions. With a cell list, we only have about **27cN** interactions. Thus, we have an improvement from **O(N^2)** to **O(cN)**.
I compared your code with mine (corrected) first version, improved version without cell list and with cell list.
CPU: R9 5950x

L = 10, rc = 2.5, N = 30

- Solution code: 124.9 it/s
- Mine basic: 327.62 it/s
- Mine fast: 590.52 it/s
- Mine fast + cell list: 833.95 it/s

L = 20, rc = 2.5, N = 128

- Solution code: 7.21 it/s
- Mine basic: 22.70 it/s
- Mine fast: 42.60 it/s
- Mine fast + cell list: 321.52 it/s

Of course the bigger the ratio L/rc the faster the cell lists method is.