

Task

Consider a simulation box of size $10 \times 10 \times 10$ without periodic boundary conditions. Place N uniformly distributed particles into the box. Now implement:

- A naive neighbor list with cutoff radius $r_c = 1.2$,
- a Verlet list with cutoff radius $r_c = 1.2$ and skin $r_s = 0.2$,
- a cell linked-list with a cell-edge length of at least 1.2.

Measure the time how long it takes to create each kind of neighbor list depending on the number of particles N .

Also, simulate a energy/force calculation by looping over all particle's i neighbors j with $i < j$ and increase a counter, essentially counting the number of particle-neighbor tuples. Again, measure the time how long it takes to execute this depending on N .

Tips

- Generating N uniformly distributed particle positions with numpy:

```
import numpy as np

def generate(N):
    particles = np.random.rand(N, 3)
    particles *= 10
    return particles
```

- Note that this way of generating particle positions assumes a simulation box that is not centered around the origin but shifted by $(5, 5, 5)$, which should be considered when calculating cell indices in cell-linked lists.
- Measure execution time of code:

```
import time

start = time.time()
perform()
elapsed = time.time() - start

print("Elapsed: %s seconds" % elapsed)
```
