

## Ex06-Report

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### 1. Interface for interaction function

```
int interactions(const double* pos, const box*** cellList, int idx, int idy, int idz, double cutoff2, double* distance2, int* pairs, int maxnumpairs, int* numpairs_p)
```

### 2. Description

Before the ***interactions*** function, loop through all particles and build a linked list for each bin. Then for each bin, call the ***interactions*** function in parallel. All threads read from shared ***pos*** array and 3 dimensional ***cellList***. Each thread reads the linked list in bin<idx, idy, idz> and all its 26 neighbor bins. The output is all pairs related to the particles in bin<idx, idy, idz>. The loop through the ***pairs*** array and compute forces for the particles. Finally, loop through all particles and update their locations.

Compared to the sequential version, this will double the calculation because Newton's third law is no longer applied. However, since it removed dependency between multiple threads, better performance is expected if more than 2 threads are used.