

MiniMD Performance

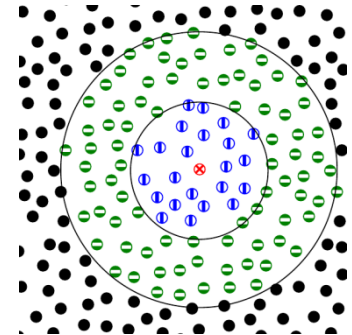
Lennard Jones force model using atom neighbor list

- Solve Newton's equations for N particles

- Simple Lennard Jones force model:
$$F_i = \sum_{j, r_{ij} < r_{cut}} 6\epsilon \left[\left(\frac{s}{r_{ij}} \right)^7 - 2 \left(\frac{s}{r_{ij}} \right)^{13} \right]$$

- Use atom neighbor list to avoid N^2 computations

```
pos_i = pos(i);  
for( jj = 0; jj < num_neighbors(i); jj++) {  
    j = neighbors(i, jj);  
    r_ij = pos_i - pos(j); //random read 3 floats  
    if ( |r_ij| < r_cut )  
        f_i += 6*e*( (s/r_ij)^7 - 2*(s/r_ij)^13 )  
}  
f(i) = f_i;
```



- Moderately compute bound computational kernel
- On average 77 neighbors with 55 inside of the cutoff radius