Short Course on Molecular Dynamics Simulation

Lecture 6:
Neighbor Lists

Professor A. Martini
Purdue University

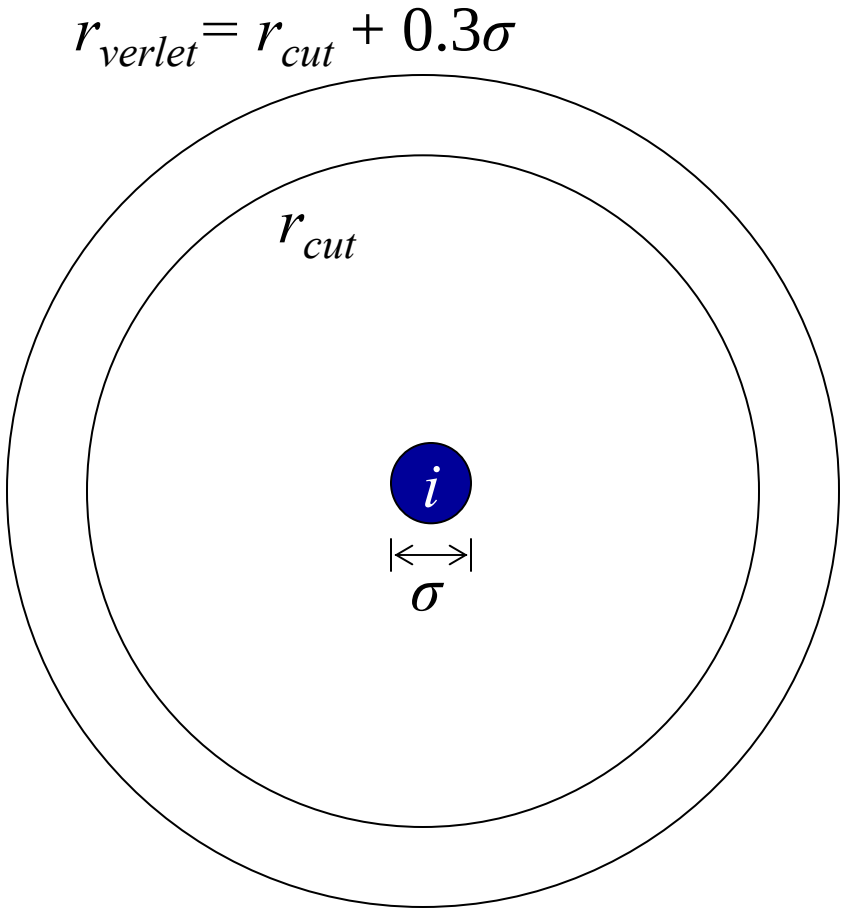
High Level Course Outline

1. MD Basics
2. Potential Energy Functions
3. Integration Algorithms
4. Temperature Control
5. Boundary Conditions
6. Neighbor Lists
7. Initialization and Equilibrium
8. Extracting Static Properties
9. Extracting Dynamic Properties
10. Non-Equilibrium MD

Saving CPU Time

- Most time-consuming part of the simulation is calculating interaction forces
- With a truncated potential, zero force at $r_{ij} > r_{cut}$
- Calculating force at $r_{ij} > r_{cut}$ just wastes time
- Solutions
  - Neighbor lists
  - Cell lists
  - Combination of the above

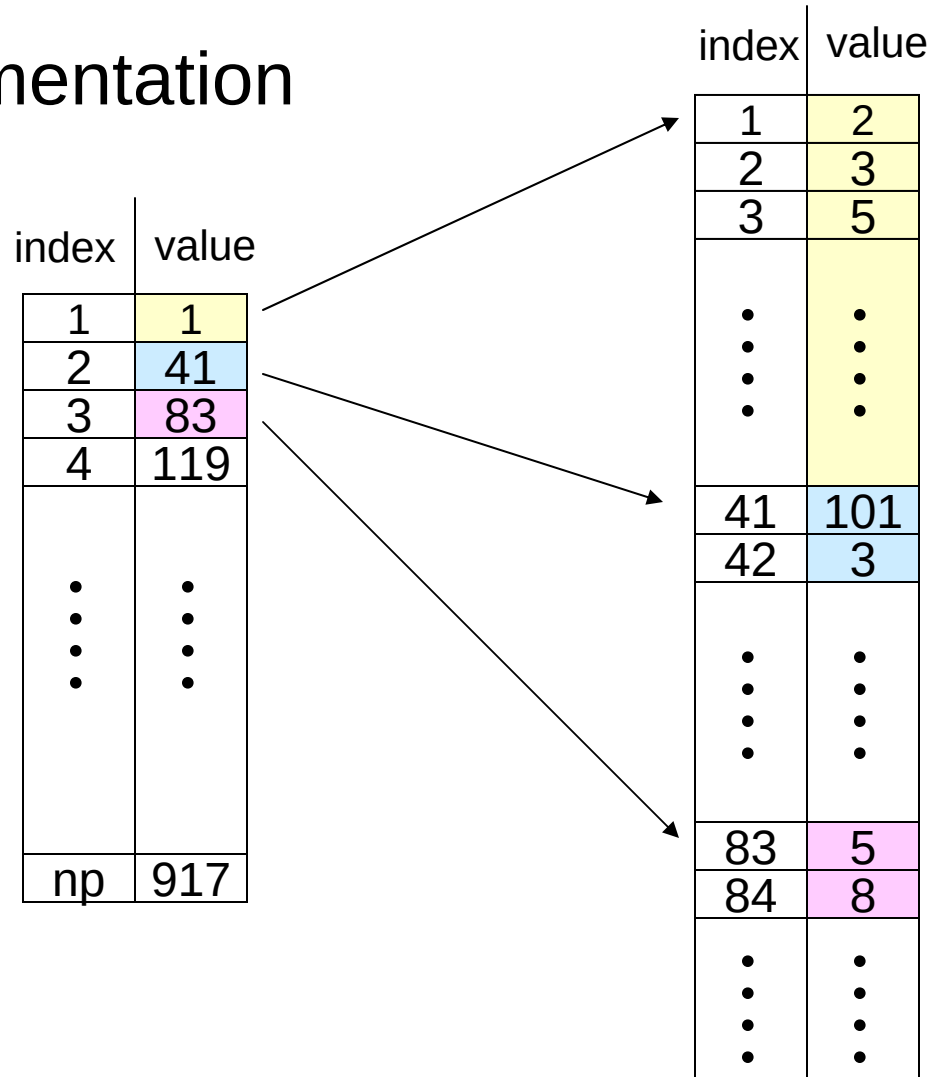
Neighbor Lists



- LJ fluid with $\rho\sigma^3 = 0.8$
- Typically ~75 atoms with $r_{ij} < r_{verlet}$
- Need only track $j > i$
- So on average the neighbor list of atom i contains ~40 atoms

Neighbor Lists

- Simple implementation



Neighbor Lists

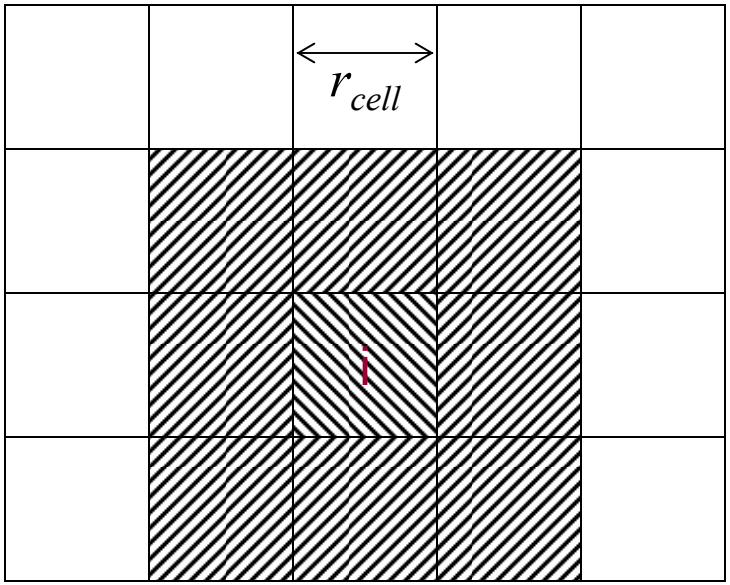
- Updating neighbor lists
  - Typical update frequency ~ 10-20 timesteps
    - Too high → method inefficient
    - Too low → forces calculated incorrectly
- Correcting for inherent error
  - Some fraction of the potential energy is always ignored → add at simulation end

$$E_{correction} = 2\pi\rho N \int_{r_{verlet}}^{\infty} r^2 U(r) dr$$

$$E_{correction,LJ} = 8\pi\rho N\varepsilon\left[\frac{\sigma^{12}}{9r_{verlet}^{9}} - \frac{\sigma^{6}}{3r_{verlet}^{3}}\right]$$

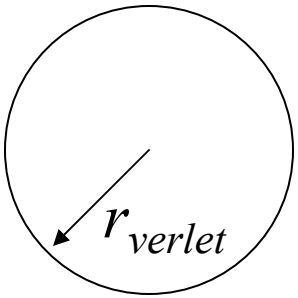
Cell Lists

- Simulation box divided into cells with size equal to or slightly larger than r_{cell}
- Each particle only interacts with others in its own cell or adjacent cells



Comparison of Methods

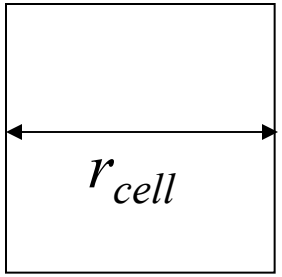
- Verlet List



$$n_{verlet} = \frac{4}{3}\pi\rho r_{verlet}^3$$

$$r_{verlet} = 2.7\sigma$$

- Cell List



$$n_{cell} = 27\rho r_{cell}^3$$

$$r_{cell} = 2.5\sigma$$

$$n_{cell} = 5n_{verlet}$$

Comparison of Methods

- Verlet List – scales with N^2
  - Loop over i and j
  - Calculate distance between i and j
  - If less than r_{verlet} add to neighbor list

- Cell List – scales with N
  - Identify cell boundaries
  - Loop over i and the number of cells
  - If i is in a given cell add to cell list