

I. Molecular Dynamics — Neighbor

Molecular Dynamics **Improving Neighbor Table**

https://en.wikipedia.org/wiki/Lennard-Jones_potential

Sahan Bandara



Problem Statement

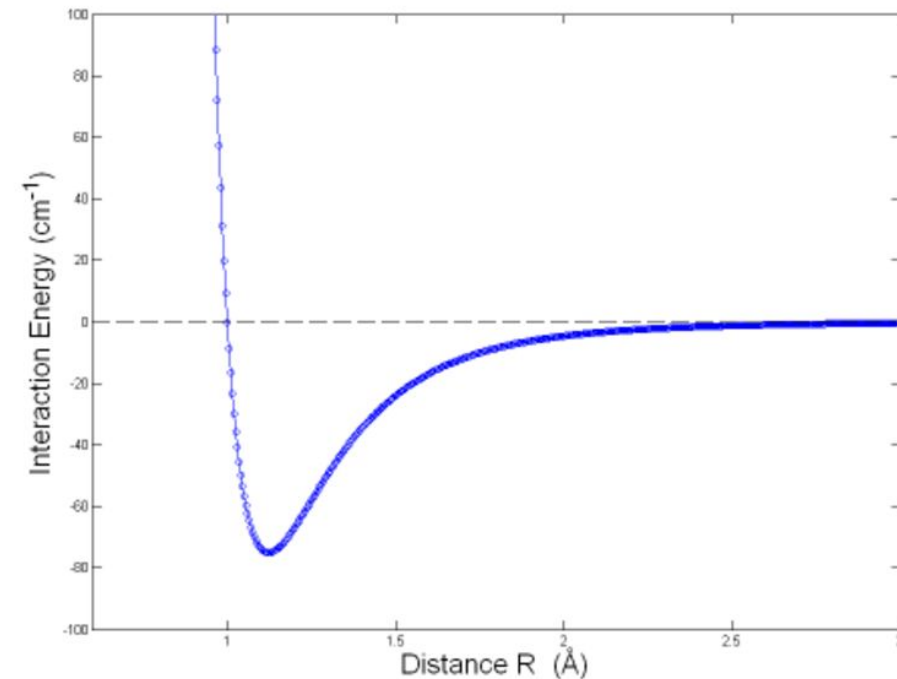
- Molecular dynamics systems = very common model
 - Two-body interatomic interactions (Lennard-Jones potential function)
 - Periodic boundaries to represent “infinite” space
- Brute Force -> $O(N^2)$ performance when comparing atom pairs
- Improvement: Verlet Table Algorithm / Cell Linked List Algorithm
- Further improvement: <https://arxiv.org/pdf/physics/0311055.pdf>
 - Combines above techniques
 - Uses additional techniques to improve table update frequency/memory organization
- How does parallelization of system work?



Molecular Dynamics Basics

- Interaction between particles in a “infinite” space
 - Utilize periodic boundaries
- Conservation of total energy
 - $E = E_{kin} + E_{pot}$
 - $E_{pot} = \sum_{i=1..N} \sum_{j>i} e_{pot}(r_{ij})$ where r_{ij} = distance between particles “i” and “j” (Equation 2.2)¹
- Lennard-Jones Potential
 - Neutral particles
 - Repulsion Forces (no collisions)

Simulation of Lennard-Jones potential ²



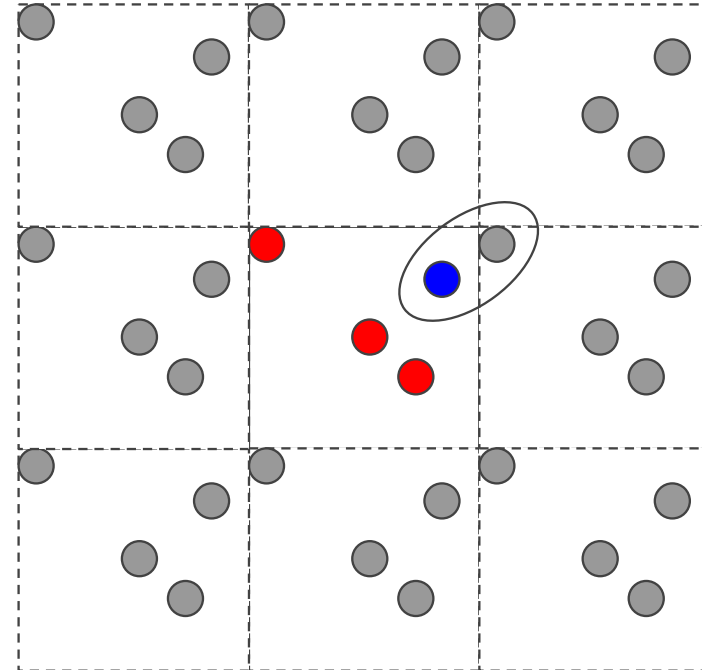
¹ Basics of Molecular Dynamics. Available from: C2_for.pdf

² Six Degree-of-Freedom Haptic Rendering for Biomolecular Docking - Scientific Figure on ResearchGate. Available from: https://www.researchgate.net/The-simulation-of-Lennard-Jones-potential_fig1_220110295 [accessed 1 May, 2018]



Periodic Boundaries

- Avoid surface effects
- Simulation particles see “images”
 - Image particles follow movement of simulation particle
- Pair interaction with closest particle
 - Minimum Image Criterion
- Constant number of particles
 - Simulation exit -> Image enter



Neighbor Table

- R_{Cut} -> Potential Cutoff
- R_{Skin} -> Considered Particle
- Circular boundaries
 - Used Square boundaries
- Data Structure for N particles:
 - Array (size N) of...
 - Pointers
 - Linked-Lists
 - Vectors
- Vector chosen for simplicity
 - Not efficiency
- Table reconstructed a set number of iterations

