Parallel Computing

Molecular Dynamics Simulations: A short overview

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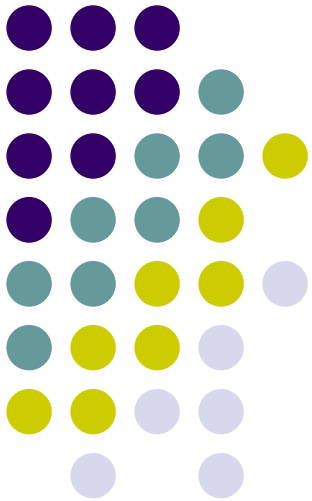
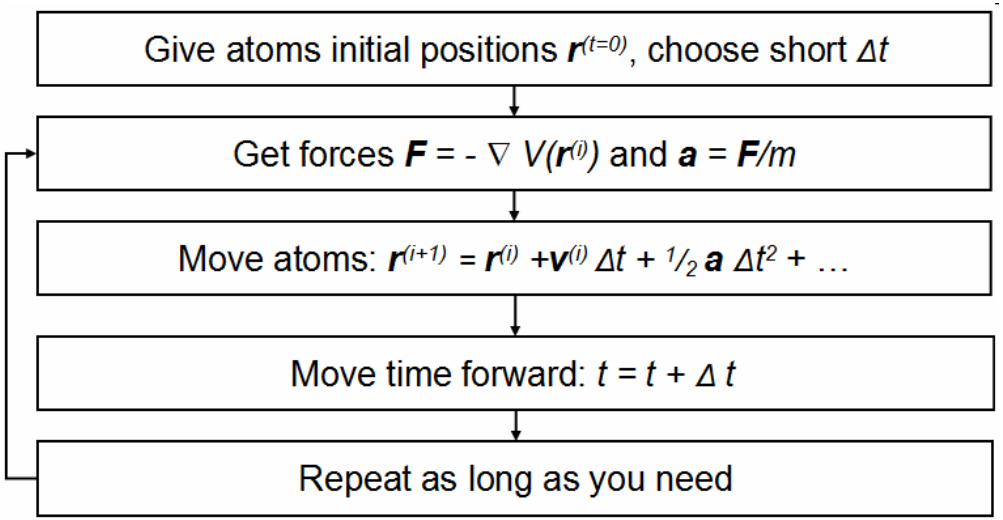


Molecular Dynamics (MD) Simulations

- A molecular dynamics simulation aims to compute thermodynamic properties of a material (such as pressure)
- The dynamics can be approximated by classical mechanics: N particles are moving according to the laws of Newton's mechanics, with each particle feeling a force generated by the N−1 other particles

Simplified code skeleton of a simulation

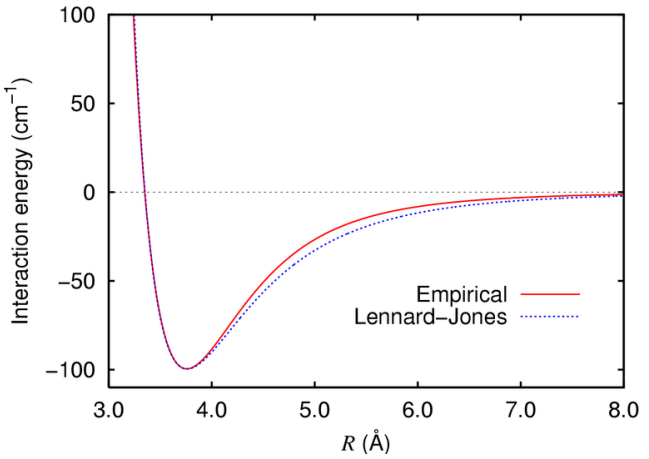


MD Simulations

Lennard-Jones potential

- Simplified model to describe interactions among particles:

$$\phi(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$



- r – distance between particles
- ε = field depth
- σ = distance where the field is null
- ε and σ are specific for each material (commonly set to 1 in simulations)

MD Simulations

Simulation Model (simplified)

- The system energy is the sum of Potential and Kinetic energy
  - The potential energy (V) is the sum the interactions between all pairs of particles

$$V(r_1,...,r_N) = \sum_i \sum_{j>i} \phi(|r_i - r_j|)$$

  - Kinetic energy is computed using the particles velocity

$$K(t) = \frac{1}{2}\sum_i m_i[v_i(t)]^2$$

- Forces between particles are given by the gradient of the potential (e.g., Lennard-Jones potential)

$$\mathbf{F}(r) = -\nabla V(r) = -\frac{d}{dr}V(r)\hat{\mathbf{r}} = 4\epsilon\left(12\frac{\sigma^{12}}{r^{13}} - 6\frac{\sigma^6}{r^7}\right)\hat{\mathbf{r}}$$

- These equations cannot be solved exactly, but need to be numerically solved. One commonly used method is the Verlet Integration algorithm:

$$\mathbf{r}(t+\Delta t) = \mathbf{r}(t) + \mathbf{v}(t)\Delta t + (1/2)\mathbf{a}(t)\Delta t^2$$

$$\mathbf{v}(t+\Delta t) = \mathbf{v}(t+\Delta t/2) + (1/2)\mathbf{a}(t+\Delta t)\Delta t$$

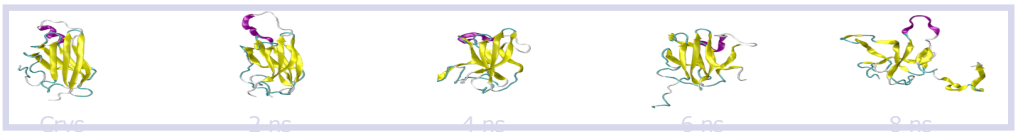
- How to deal with the simulations borders?
  - Replicate the simulation (*periodic boundary conditions)*
  - Other approaches

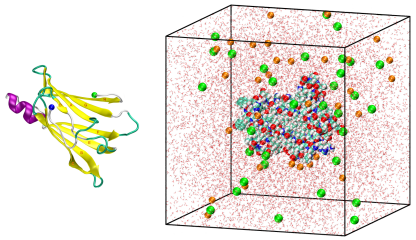
MD Simulations

Simulation examples

- **Satellite Tobacco Mosaic Virus – one of the smallest reproducing units in nature**
  - 2006, 1 million atoms for over 50 ns
  - NAMD software (would require 35 years of simulation on a desktop computer at the time)

- P-Found – L55P-TTR - Transtirretina, “Doença dos Pezinhos” (1:1000 in Portugal)
  - **2004, 44k** atoms **(**Protein: 1912 atoms; Water: 3*14137 atoms; Na^+ Cl^-: 71 ions**)**
  - **Computation run time: 4-6 weeks** using 8-12 Pentium-4 CPUs
  - **Binary file capturing the coordinates of all atoms: ≈ 4 GB**
  - **Binary file capturing the coordinates of protein’s atoms: ≈ 180 MB**

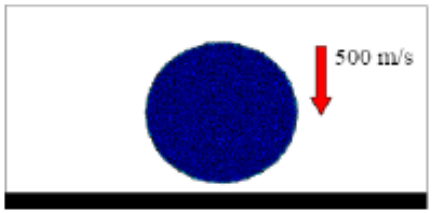




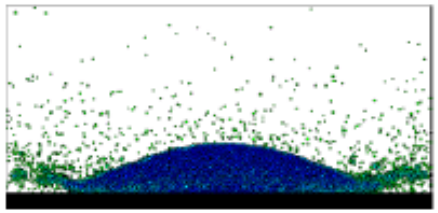
Molecular Dynamics

Example: collision of a droplet with a substrate

(by Yasushi Katsumi)



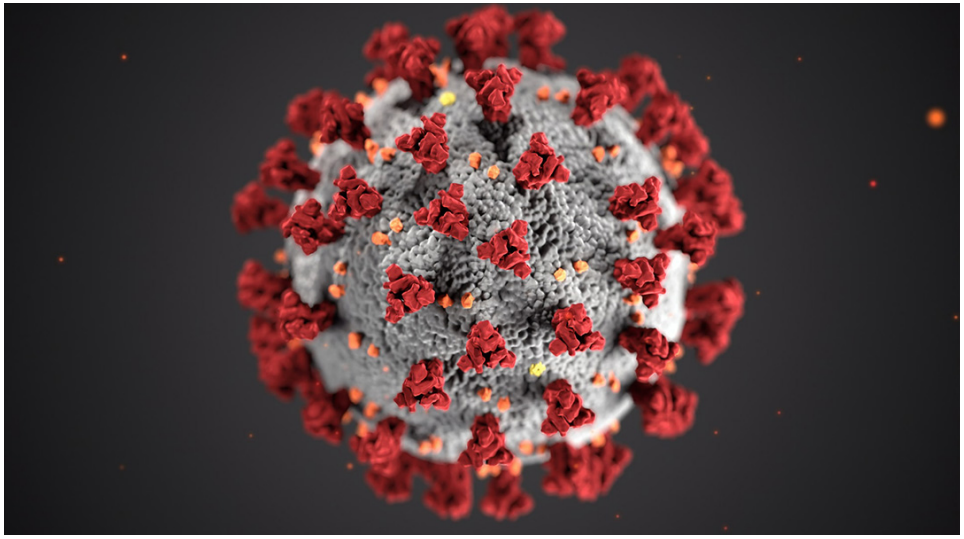
Initial conditions are specified, $r_i(t_0)$ and $v_i(t_0)$



Snapshot from MD simulation at time t_n = 100 ps

MD Simulations

Supercomputer simulates molecular model of SARS-CoV-2



- Rommie Amaro is leading efforts to build the first complete **all-atom model** of the SARS-COV-2 coronavirus envelope
- The coronavirus model is anticipated contain roughly **200 million atoms**
- The Frontera supercomputer aided efforts of the Amaro Lab on March 12-13, 2020, by running NAMD molecular dynamics simulations on up to 4,000 nodes, or about **250,000** cores.