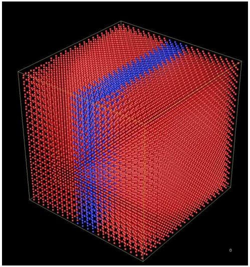
1. Molecular Dynamics: Introduction

June 25, 2012

1.1. Orders of Magnitude (Homework Exercise)



Length / distance measures in Angstrom: $1Å = 10^{-10}m = 0.1nm$

- Typical size of simulation domain: 10 - 1000 Å.
- Typical size of a time step: 1 fs (10^{-15}s).
- Number of timesteps 10^6 – 10^9.

Simulation of 1l of Beer

The molar mass of water is $18\frac{g}{mol}$, so 1 l of water contains

$$\frac{1000g}{18\frac{g}{mol}} = 55.5mol \approx 50mol.$$

Avogadro constant ($6 \cdot 10^{23}\frac{1}{mol}$): $\Rightarrow$ 1l of water contains

$$6 \cdot 10^{23}\frac{1}{mol} \cdot 50mol = 3 \cdot 10^{25}\mathrm{Molecules}.$$

As we have a great algorithm, that's also the number of calculations per time step. Our supercomputer can perform 10^{15} operations per second, so the time needed to calculate one time step is

$$\frac{10^{25}}{10^{15}} = 10^{10}.$$

As one year has 10^7 seconds, we need **1000 years** to calculate **one time step**.

This means, we need

$$1000\,\text{years} \cdot 10^{15} = 10^{18}\text{years}.$$

For comparison: the age of the universe is approximately 10^{10} years, so we had to wait only 100 Million times as long!

According to Moore's Law computational power doubles every 18 months, so in 3 years the calculation will take only $2.5 \cdot 10^{17}$ years...:

$$0.5^n \cdot 10^{18}\text{years} \leq 1\text{year}.$$

$$0.5^n \leq 10^{-18}$$

$$n \cdot \ln 0.5 \leq \ln 10^{-18}$$

$$\Rightarrow n \geq \frac{\ln 10^{-18}}{\ln 0.5} \approx 59.8$$

Thus, it would make sense to start the simulation in 90 years.

Dense Packing in 3D

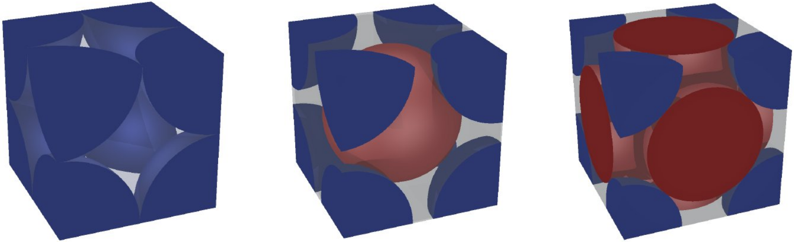


Figure: From left to right: corner-centered, cell-centered, surface-centered

What is the relative density of the different configurations?

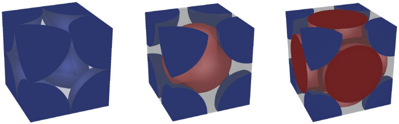


Figure: From left to right: corner-centered, cell-centered, surface-centered

- corner-centered:
  - Volume of a cube: $V_{cube} = (2r)^3$
  - Volume covered by molecules: $V_{molecules} = \frac{4}{3}\pi r^3$
  - Relative density. $\rho = \frac{V_{molecules}}{V_{cube}} = \frac{\frac{4}{3}\pi r^3}{(2r)^3} = \frac{1}{6}\pi \approx 52\%$
- cell-centered:
  - Volume of a cube: $V_{cube} = \frac{64r^3}{3\sqrt{3}}$
  - Volume covered by molecules: $V_{molecules} = 2 \cdot \frac{4}{3}\pi r^3$
  - Relative density. $\rho = \frac{V_{molecules}}{V_{cube}} = \frac{2 \cdot \frac{4}{3}\pi r^3}{\frac{64r^3}{3\sqrt{3}}} \approx 68\%$

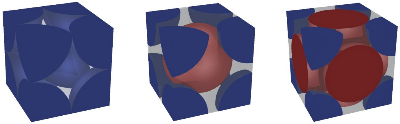


Figure: From left to right: corner-centered, cell-centered, surface-centered

- surface-centered:
  - Volume of a cube: $V_{cube} = \left(2\sqrt{2}r\right)^3$
  - Volume covered by molecules: $V_m = \frac{4}{3}\pi r^3 \cdot 4$
  - Relative density. $\rho = \frac{V_{molecules}}{V_{cube}} = \frac{\frac{4}{3}\pi r^3 \cdot 4}{(2\sqrt{2}r)^3} = \frac{\frac{16}{3}\pi r^3}{16\sqrt{2}} \approx 74\%$

Example: Gold

- Molar Volume = $10.2 \frac{\text{cm}^3}{\text{mol}}$
- $\Rightarrow 1cm^3$ contains $5.9 \cdot 10^{20}$ molecules
- Atom radius $r = 135 \cdot 10^{-12}$ m
- $\Rightarrow$ Volume covered by one molecule $V_m = 1.03 \cdot 10^{-23}\text{cm}^3$
- $\Rightarrow$ Volume covered by $5.9 \cdot 10^{2}0$ molecules $\approx 0.61\text{cm}^3$
- $\Rightarrow$ Relative density $\approx 0.61\%$

Only lower bound, as molecules don't really touch each other!