Lecture 2 – questions & survey

Answer with yes/maybe/no:

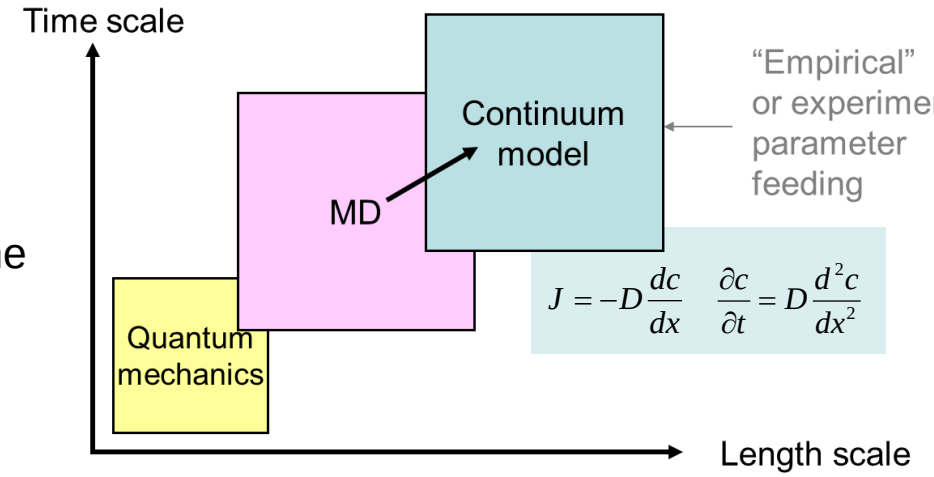
1. Explain the basic concept of molecular dynamics.
2. Do you need forces between atoms to carry out a molecular dynamics simulation?
3. What is the key physical law that goes into the formulation of molecular dynamics?
4. Explain how to calculate the diffusivity from a molecular dynamics run.
5. Explain the characteristics of a continuum model. What are its strengths, limitations? Give 2 examples of a continuum model.

On a scale from 1-7 please rate:

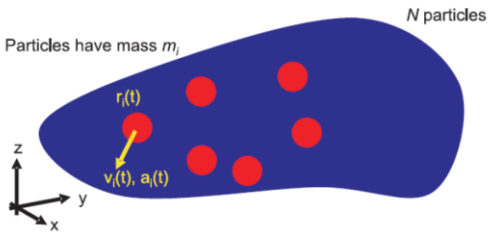
7. Were the goals of today's lecture clear?
8. Was today's lecture clear?
9. Did you feel that today's lecture contributed to your understanding of the topic?
10. What could have been improved in order to make this lecture more useful?
11. Is the level of teaching appropriate? What should we change?
12. Please give us overall feedback regarding IM/S so far how interesting are lectures, overall impression, suggestions for changes, etc.).

Lecture 2 – core concepts

MD allows to compute fundamental parameters from the atomic motions, feeds into continuum model



Conventionally, continuum models need empirical input (e.g. experiment)



Follow trajectories of atoms

$$\left\langle \Delta r^2(t) \right\rangle = \frac{1}{N}\sum_i \left(r_i(t) - r_i(t=0)\right)^2$$

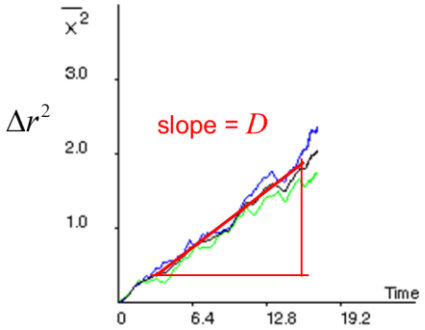
Position of atom *i* at time t — Position of atom *i* at time t=0

"Verlet central difference method"

$$r_i(t_0 + \Delta t) = 2r_i(t_0) - r_i(t_0 - \Delta t) + a_i(t_0)\Delta t^2 + \ldots$$

Positions at t_0 — Positions at t_0-Δt — Accelerations at t_0

$$a_i = f_i / m$$



$$D = \frac{1}{2d}\lim_{t\to\infty}\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \Delta r^2 \right\rangle$$

1D=1, 2D=2, 3D=3