# Lecture 3 – questions & survey

**Answer with yes/maybe/no:**

1. Why did computing power increase exponentially in the 2000s?
2. Can you see a difference in the Mean Square Displacement function that allows you to distinguish a crystal solid, liquid, gas? Explain details.
3. What is the ergodic hypothesis and what does it mean for MD simulations?
4. What is the difference between microscopic and macroscopic states?
5. What is the difference between MD and MC? What are identical features?
6. How do you compute a macroscopic property from microscopic variables?

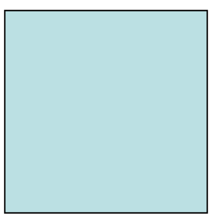
**On a scale from 1-7 please rate:**

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.).

**Ergodic hypothesis:** $< A >_{Ens} = < A >_{Time}$

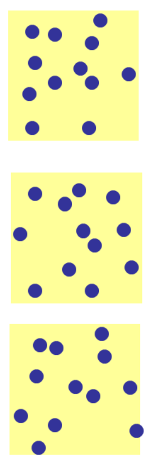
$$\underbrace{\frac{1}{N_A}\sum_{i=1..N_A} A(i)}_{\text{MC}} = < A >_{Ens} = < A >_{Time} = \underbrace{\frac{1}{N_t}\sum_{i=1..N_t} A(i)}_{\text{MD}}$$

*Canonical ensemble*



$N, V, T$

$\equiv$



$C_1 \longleftrightarrow r_1, p_1$

$C_2 \longleftrightarrow r_2, p_2$

$C_3 \longleftrightarrow r_3, p_3$

...

$C_N \longleftrightarrow r_N, p_N$

$$\boxed{< A > = \int_p \int_r A(p,r)\rho(p,r)\,dr\,dp}$$

Same macroscopic state is represented by many different microscopic configurations