Assignments/questions TFYA90, part I: MD & MC, fall 2020
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Evaluation scale: grades (G) = 1, 2, 3, 4, 5
G=1 (points ≤ 10) ; G=2 (10 < points ≤ 25) ; G=3 (25 < points ≤ 40) ;
G=4 (40 < points ≤ 55) ; G=5 (points > 55)
Maximum = 75 points

A) What is the most crucial ingredient of molecular dynamics (MD) simulations? (**1p**)
(1) To define initial atomic positions
(2) To properly calculate atomic velocities
(3) To properly model the acceleration
(4) To choose the ensemble for the simulation

B) Briefly describe difference between “classical” MD and “ab initio (first-principles)” MD. (**2p**)

C) Briefly describe difference between a two-body and a three-body empirical model potential. (**1p**)

D) How is temperature (T) typically evaluated during MD simulations? (**1p**)

E) Write (and explain) formula to compute temperature at a given MD timestep. (**1p**)

F) What is meant with a deterministic method? (**2p**)

G) What are the advantages of using ab initio MD instead of classical MD, given that CMD is much more efficient? (**3p**)

H) Use your imagination: give examples of materials science (or chemistry, medicine etc.) problems that could not be studied (nor possibly solved) via ab initio MD in feasible time. Explain also why. (**3p**)

I) What is a statistical ensemble? Give a few examples of them and clarify what/why different ensembles are used for. (**2p**)

J) Think out of the box. Assume you start an MD simulation in the NVE ensemble by setting initial velocities which correspond to a temperature “T” (note that the system is *not* coupled to a thermostat). How do you expect (and explain why) temperature to behave after a “very long” simulation time? (Hint: consider equipartition theorem). (**4p**)

K) Why does one use a cutoff length “r_c” for neighbor lists and atomic interactions during a classical MD simulation? What is the advantage? (**2p**)

L) What are “technical problems” caused by truncation of atomic interactions beyond a distance “r_c” during MD simulations? Describe in a few words how this problem can be solved. (**2p**)

M) Still concerning interaction cutoff "r_c": would you expect that sudden truncation of the atomic interactions affects MD and Monte Carlo simulations in the same way? Why? (**4p**)

N) In the 2D Ising spin model (square lattice of n × n sites), the total magnetization M of the system (at any timestep) is defined as the sum of all spins $M=\sum_i{}^{n\wedge 2}\, s_i$, where a spin s_i can have values ±1 (arb. units).

1) The MC-Ising simulation starts with: J large and positive, B=0 and "very low" temperature (T). What is(are) the most likely expectation value(s) of the total magnetization <M> at the equilibrium? (**2p**)
2) The MC-Ising simulation starts with: J large and negative, B=0 and "very low" temperature (T). What is(are) the most likely expectation value(s) of the total magnetization <M> at the equilibrium? (**2p**)
3) Why under conditions (1) and (2) above, the system may get "trapped" into metastable states? (**2p**)
4) The MC-Ising simulation starts with: J=0, B large and positive and T "very low". What is(are) the most likely expectation value(s) of the total magnetization <M> at the equilibrium? (**2p**)
5) The MC-Ising simulation starts with: J = 0, B = 0 and T "very low". What is(are) the most likely expectation value(s) of the total magnetization <M> at the equilibrium? Do you expect that the total magnetization at the equilibrium would be different if T was "very high"? (**4p**)
6) Let's assume that J is large and positive and B=0. Under which temperature conditions you expect that the system will have total magnetization ≈0 at the equilibrium? Why? Do you remember how such magnetic state is named? (**4p**)

O) In which classes are thermostats and barostats (employed in MD simulations) divided? Briefly explain the difference between different classes (**2p**)

P) Which statistical ensemble is not well suited to be modelled in Monte Carlo sampling? Why? (**2p**)

Q) Describe your understanding of the concepts of "partition function" and "probability distribution functions" for the canonical and isothermal-isobaric ensembles (**5p**)

R) What does one mean with "importance sampling" in Monte Carlo methods? Why is that crucial to achieve statistical averages at reasonable computational efforts? (**2p**)

S) What is the difference between intensive and intensive thermodynamic variables? (**1p**)

T) Give examples of problems/phenomena that is convenient to investigate via MD simulations and others that are best solved via MC methods. Also explain why. (**3p**)

U) An adatom adsorbed in a stable surface site vibrates around the energy minimum with a frequency of 1 THz. The energy barrier that separates

adjacent adatom adsorption sites is 300 meV. Evaluate the migration rate of the adatom (using Arrhenius expression) when the temperature is 500 K and when the temperature is 2000 K. (**3p**)

V) Molecular dynamics simulations performed at different temperatures T (300, 600, 900, 1200, and 1500 K) estimate average migration rates $\Gamma(T)$ of an adatom on a surface of:
$\Gamma(300\ K) = 8 \times 10^{5}\ s^{-1}$
$\Gamma(600\ K) = 1 \times 10^{9}\ s^{-1}$
$\Gamma(900\ K) = 2 \times 10^{10}\ s^{-1}$
$\Gamma(1200\ K) = 6 \times 10^{10}\ s^{-1}$
$\Gamma(1500\ K) = 1 \times 10^{11}\ s^{-1}$
Construct an Arrhenius plot of $\log[\Gamma(T)]$ vs. 1/T. Extract the adatom migration activation energy E_a and attempt frequency ν by linear regression of $\log[\Gamma(T)]$ vs. 1/T data (**3p**)

W) You want to determine the equilibrium volume of a crystal lattice at different temperatures (the volume increases due to thermal expansion). You employ molecular dynamics simulations. Which ensembles is best to solve this problem? Why? (**2p**)

X) You intend to perform Monte Carlo (or Kinetic Monte Carlo) simulations in the NVT ensemble to model migration of adatoms on a surface at a few different temperatures. Which information you need to know beforehand in order to run your simulation? (**2p**)

Y) Describe step-by-step how the Metropolis Monte Carlo algorithm works. Describe it for the case of the Ising spin model. (**2p**)

Z) Consider the following variant of Hamiltonian for a Ising spin model on a n × n lattice and in absence of external field B:

$$U = -J_{i,j} \cdot \sum_{i,j} s_i \cdot s_j \,.$$

The products $s_i \cdot s_j$ are non-zero only if i and j are adjacent sites. The interaction constant $J_{i,j}$ is <u>large and negative</u> if site i and site j belong to the same lattice row, while $J_{i,j}$ is <u>large and positive</u> for i and j sites on a same lattice column. Assume you run MC at “very low” T. Sketch the spin configuration you expect to see at the equilibrium. What would be its total magnetization <M> ? (**4p**)