BT5420: Computer Simulations of Biomolecular Systems
July – Nov 2020 Semester
Take Home Exam

Instructions:

- Submit the scanned copy of the hand written answer sheet as a pdf file on Moodle by 24th Nov 2020
- The answer sheet should include only a maximum of 6 pages
- Write your name, roll number and page number in each page of your answer sheet
- The first page should include the following oath with your name and signature: "I understand that it is a take home exam, not an assignment, and I am aware that disciplinary action would be taken if I am found to be involved in any form of malpractice."

1. Compare and contrast the explicit water models – TIP3P, TIP4P and TIP5P. Also discuss about the variants of each water model. **(8 marks)**

2. What is an *.itp file? Discuss all the possible entries in an *.itp file for a molecule, say urea. How it is related to a system *.top file? **(7 marks)**

3. Consider a two-particle system with masses m_1 and m_2, positions r_1 and r_2, and velocities $\dot{r}_1$ and $\dot{r}_2$ subject to a potential U that is a function of only the distance $|r_1 - r_2|$ between them. This is typical of a diatomic molecule. **(10 marks)**

i. Write down the Lagrangian of the system.

ii. Define new variables $R = \dfrac{m_1 r_1 + m_2 r_2}{M}$, and $r = r_1 - r_2$. R corresponds to the coordinates of the center of Mass and r is called the relative coordinate. Let's define new mass variables: total mass, $M = m_1 + m_2$, and reduced mass, $\mu = m_1 m_2 / M$. Write down the Lagrangian of the system using the new variables.

iii. Which set of variables is suitable for this problem and why?

4. Derive the ideal gas equation of state from grand canonical partition function *i.e.* prove **(5 marks)**

$$\frac{PV}{kT} = \ln \Xi = \frac{V\zeta}{\lambda^3} = \langle N \rangle$$

5. Write a brief note on **(10 marks)**

i. Site-site radial distribution function

ii. Hydrogen bond life time analysis based on autocorrelation function