

Assignment 1

- All questions are of equal value.
- **Important: Use the template for assignments provided at OWL and follow the instructions in it for returning the assignment**

Due: Friday January 22, 2021 at midnight.

Read through the material of the first week at the web site and answer the following questions:

1. List the different *simulation software packages* mentioned in the text and classify them to a) classical MD b) quantum mechanical and c) others.
2. List all the *water models* mentioned in the sections. Separate them to a) classical MD level, b) quantum mechanical and c) coarse-grained.
3. List the different simulation *methods* mentioned in the sections.
4. Assume that you have a nanoscopic box of size 15 x 15 x 15 nm. How many water molecules can you put in there (assume normal water density)? Show all the details and assumptions of your calculation.
5. Computing can be done at single or double precision. Discuss the pros and cons of them. Which one should be used for MD simulations and why?
6. When performing computation, the CPU cores can use data and instructions in various manners depending on their design. List the different approaches and discuss which one(s) is (are) relevant in the case of GPUs.