Course project and term paper

Computational Chemistry, Spring, 2022

Each student will prepare a written paper, describing an application of computational chemistry to some problem. You should start with a research paper that has a "materials and methods" section (or equivalent) giving details of how the modeling was done. You are encouraged to choose a paper relevant to your area of research that describes a non-trivial application of computer-aided modeling. Provide a careful analysis that addresses the following points:

1. Give a brief but clear summary of what was done; it is appropriate to include figures or tables taken from the paper you chose. This should be about 4-6 paragraphs in length. The focus of this analysis should be on the modeling or methods that are used, but you should also describe the context or background involved (*e.g.* experimental results that are being interpreted.)

2. Describe (in your words this time, and in a few paragraphs) what was learned, and how the computer modeling was useful to the overall paper.

3. Provide (again, in one or two paragraphs) a careful analysis of the strengths and weaknesses of the method as used in this example. Were alternatives available? How much effort went into doing the analysis?

4. Set up and run (on Amarel) a calculation that reproduces or extends part of the work described in the paper. Your illustrative calculation will almost certainly only be a small subset of what is reported in the paper, but should represent the beginning of a serious effort to carry out or extend similar studies. Limit the size of system or basis sets (for quantum calculations), or the size and/or number of MD steps (for MD calculations), so that the total time will be limited to 1-2 hours of CPU time. In your report, discuss in some detail exactly what you did, and what the next steps would be if you had both more computer time available, and more personal time to devote to this effort. Include copies of the key input files you used as an Appendix to your report.

5. Write for an audience of your fellow students, making a real effort provide clear explanations of what was done. If the paper you choose assumes an understanding beyond that covered in the course or textbook, you may need to consult earlier papers (and add relevant information to your report).

The total length of your report should be 6-8 pages, not including citations or Appendices. The paper is due on **May 5** (the first day of the final exam period). Before you start computing or writing, send an email to me, giving information about the paper you have chosen, and about the calculations you plan to undertake. I will approve of your choice or make suggestions. **You should submit the completed paper via email, as a single PDF file**, named lastname.pdf.

Please note: both the computations and the writing of the paper are to be done by you alone, and not in concert with others.