Is TPSS an TPSSh better for TPAA calculations?

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1 Introduction

The first paragraph provides broad context and motivation for your report. It should establish a connection to your and the group's scientific long-term goals, and avoid lofty or vague statements. Popularity, recent public attention, or the observation that "our group is interested in A, B and C" etc. are insufficient motivations. You may re-use parts of this paragraph from previous reports, taking into consideration feedback you received.

The second paragraph also provides context, but much more focused on your research. For example, you may explain in the first paragraph why solvation effects are important for chemists, and then give a brief overview of work on excited state properties in the area of implicit solvent models. The purpose of this paragraph is to help the reader understand what prior work was done, and to provide the "background scenery" for the work you are reporting.

The third paragraph should explain how your work goes beyond existing methods or results, and define its specific goals and hypotheses. It is better to focus on what your work aims to do than on what you and others before you were not able to do.

While your report should efficiently communicate any recent results you have had, it also serves to help you gauge your progress, see the conclusions and broader context of your work, assess priorities, generate narratives for later use in publications, and sharpen your writing skills. Even if you spend the entire period of your report debugging code, your report can help re-state the problem, discuss strategies you employed to find the error and whether your time was well used. You might also conclude, e.g., that you need additional resources and help to tackle the problem, or that it may not be worth pursuing further.

The entire report should be written in scientific English suitable for publication, see **Strunk99** for an introduction. Try to be concise, clear, and articulate at the same time. Bullet points, unexplained abbreviations, incomplete sentences, or slang are not acceptable. References should be cited using the group's refbase cite keys. Ensure that all symbols are defined, and figures and tables are clear and have self-contained captions. For instructions on how to best display quantitative information in figures, refer to **Tufte01**. Use vector graphics (eps or pdf) when possible and appropriate, otherwise 600 dpi bitmap (png, jpeg). The report should be between 2 and 4 pages long, including references.

If you are working on more than one different projects simultaneously, you may alternate your biweekly reports over a longer period of time.

In addition to attaching an electronic version of your report to your meeting agenda, please print it (two-sided) and submit a paper copy to Filipp's office by 5:00 pm on the day before your meeting (you may slide it under the door if necessary).

2   Methods

The methods section should concisely state the methods you used to obtain your results. For a theoretical project, this section will review key assumptions and equations; for an implementation-centered project, the main working equations and implementation strategies will be stated here; for a computational project, this section will contain the computational details. Depending on the subject, parts of this section may be carried over from previous reports.

3   Results

This section states the main new results of the current reporting period. These results could be presented, e.g., in the form of equations, figures, tables, and text. Negative results are just as important as positive ones and should be carefully reported. Use a balanced tone avoiding over- and understatement.

Sometimes, it is helpful to separate statement of the results and discussion, although a strict separation of the two is often impossible. A separate discussion section may be appropriate if you are proposing a speculative rationale or if several interpretations of your results are possible. If you have no new results at all, this is the place to explain why.

4   Conclusions

This section should answer the following questions: What is the significance of your results for the question, problem, or hypothesis posed in the introduction? What, if any, are the implications in the broader context of the research area laid out in the second paragraph of the introduction?

A second paragraph should discuss any conclusions for your future work. Is there a need to change your approach or your priorities? What remains to be done to reach the goals stated in the first section?

5 Service

This section should summarize group service activities you have engaged in during the reporting period, including, e.g., related to shared governance (deputy positions), work for the high school outreach program, helping or supervising other group members to larger extent than usual.