

**Numerical Algorithms Applied to Computational Quantum Chemistry
Homework Assignments**

January 25, 2024

1 HOMEWORK SUBMISSION GUIDELINES

Follow these steps to submit your Chem 279 homework:

1. **Code Development:** Write your own C++ code following the homework requirements
2. **Code Testing on Datahub:** Log into Datahub (<https://data.berkeley.edu/datahub>) to test your code
 - a) Select "Datahub Login", then navigate to the Terminal to upload your code for testing purpose.
 - b) Download the sample input/output files from our Github repository (<https://github.com/zhewang233/Chem-279-Spring-2024-HW.git>). Please be aware that the provided sample outputs are intended solely for reference and verification purposes. It is not mandatory for your output files to match the format of these samples.
 - c) Compile and run your code using the g++ compiler to compare your results with the provided samples. Use the command "g++ -o <execname> <filename>.cpp" for single file compilation. For projects using Armadillo for matrix operations, use "g++ -o <execname> <filename>.cpp -larmadillo". For compiling multiple C++ files, refer to <https://www.cs.fsu.edu/~lacher/lectures/Output/compiler/compiler3.html>.
3. **Code Submission:**
 - a) Create a **private** Github repository which contains all your code.

- b) Add your GSI (Github username: zhewang233) as the collaborator for your private working repository.
 - c) Upload a pdf file on Gradescope containing the link to your private Github repository before the homework submission deadline, which means you finished all the coding. Your GSI can download and grade your code then.
 - d) It would be beneficial if you could provide comments or a brief README file detailing how to execute your code with the specified input.
4. **Additional Submissions:** You can submit other homework elements, including discussions and plots, through Gradescope. Remember to submit it under the specified question.

2 GENERAL SUGGESTIONS AND GRADING RUBRICS FOR HOMEWORK

1. There are five problem sets, each worth 12 points.
2. **Grading Criteria:**
 - a) **Test Case Completion:** Full points are awarded if your code passes all the test cases and you complete the remaining non-coding assignments. If not, partial points will be assigned based on the quality of your coding and comments. Note that the test cases used for grading may differ from the sample input/output provided. However, if your code produces results similar to the sample outputs, it is likely to pass most of the test cases.
 - b) **Code Quality and Comments:** Well-written code and clear comments are crucial for understanding the functionality of your code. If your code does not pass all test cases, points can still be earned based on the relevancy and clarity of your code and comments.
 - c) **Handling Difficult Cases:** Occasionally, challenging test cases not covered in the sample input/output would be included. These are not included in the total points, but bonus points will be awarded for codes that demonstrate special consideration and successfully handle these difficult cases.
 - d) **Plagiarism:** Zero points will be awarded for plagiarized code.
3. Your GSI will provide grades and feedback for each homework assignment through Gradescope. After each homework deadline, the code solutions will be made available on GitHub (<https://github.com/zhewang233/Chem-279-Spring-2024-HW.git>).

Some suggestions for your homework:

1. The C++ standard libraries are useful. You can fully utilize the convenience offered by the C++ standard libraries.

2. If you're struggling to locate a bug, try commenting out all the suspicious code sections and then review each part gradually to identify the issue.
3. Don't worry if your test results don't align with the sample outputs. Reflect on possible causes – Could it be an algorithmic error, a typo, different parameters or initial conditions you used compared to the sample, or an oversight in the output provided by your careless GSI? There are numerous reasons why it might produce results that differ from the provided samples, even if your code is well-written.
4. If you find yourself stuck for a long time or unsure about where to start, don't hesitate to ask your classmates for help or attend our office hours.