

Numerical Algorithms Applied to Computational Quantum Chemistry
Grading Rubrics for Homework 2

1 GRADING RUBRICS FOR CHEM 279 HW2

1. The homework consists of two problems, with each problem valued at 6 points.
2. Key Points for Consideration:
 - a) **HW2.1:** Select a numerical method to compute the 1-D overlap integral. Choose the integration interval and the number of segments judiciously to ensure convergence of the integral within certain limits. Pay special attention to more diffused Gaussian functions. You will be graded based on the accuracy of your results against a predefined test set.
 - b) **HW2.2:** Ensure you calculate the correct number of integrals when performing overlap integration between two pairs of shells. You will be graded based on your results against a predefined test set.
3. After completing the code, remember to submit your repo in addition to submitting the write up on Gradescope