

Numerical Algorithms Applied to Computational Quantum Chemistry
Grading Rubrics for Homework 1

January 25, 2024

1 GRADING RUBRICS FOR CHEM 279 HW1

1. The homework consists of three problems, with each problem valued at 4 points.
2. Key Points for Consideration:
 - a) **HW1.1:** Ensure you echo outputs and terminate the program with an error message if any atoms other than Au are present. This will be verified through a specific test case.
 - b) **HW1.2:** Produce a plot comparing the logarithm of the error in the finite difference force against the analytical force, accompanied by a discussion. You may submit both the plot and your discussion via Gradescope, or upload them to GitHub.
 - c) **HW1.3:** Implement a local optimizer that works by steepest descent with line searches. You can use golden section line search.
3. (1 Bonus Point) How would you optimize the structure when the initial distance between atoms in the gold cluster is either very large or small (so there will be extremely large/small initial force). Discuss (or implement) the strategy you use. This aspect will be evaluated through a relevant test case.