UNIVERSITY OF CALIFORNIA BERKELEY

Numerical Algorithms Applied to Computational Quantum Chemistry
Grading Rubrics for Homework 4

October 20, 2024

1 GRADING RUBRICS FOR CHEM 179/279 HW4

1. The problem set is worth 12 points. And the total points are divided into several components, as outlined below:

2. Key Points for Consideration:

   a) **Correctly build the CNDO/2 Fock matrix for some simple systems (6 points)** Read the specified format of input for some molecules composed of H, C, N, O, and F and corresponding basis sets. Correctly build and print the CNDO/2 matrix with the initial guess of density matrix ($\mathbf{P}^{\alpha} = \mathbf{P}^{\beta} = \mathbf{0}$). The accuracy of your Fock matrix will be verified using some test samples (could be different from the sample inputs provided).

   b) **Solve and print the Eigenvectors and Eigenvalues Self-Consistently (4 points):** Solve the eigenvalue problem self-consistently. Please print the final eigenvectors and eigenvalues after convergence.

   c) **Compute the total energy (2 points):** Calculate the total energy of the molecule based on the results you obtained from a converged SCF algorithm. Pay attention to units and unit conversions.

   d) **Bonus Points (2 points):**Experiment with your CNDO/2 code by applying it to molecules not included in the sample inputs, such as N_2 and O_2. Explore the chemical behaviors and properties these simulations reveal. For reference structures of common molecules, you can go to CCCBDB `https://cccbdb.nist.gov/expgeom1x.asp`. Discuss your findings and any interesting insights you gain from this exploration.

3. After completing the code, remember to submit the link to your repository to Gradescope so that your GSI is informed that you have finished your homework. Additionally, don't forget to add your GSI as a collaborator to your repository.