UNIVERSITY OF CALIFORNIA BERKELEY

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

March 5, 2024

1 GRADING RUBRICS FOR CHEM 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 **private** 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.