UNIVERSITY OF CALIFORNIA BERKELEY

Numerical Algorithms Applied to Computational Quantum Chemistry
Grading Rubrics for Homework 5

November 5, 2024

1 GRADING RUBRICS FOR CHEM 179/279 HW5

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) **Calculation of Important Derivatives (9 points):** You are required to calculate and print the derivatives of overlap integrals ($S_{\mu\nu}^{\mathbf{R}_A}$), two-electron integrals ($\gamma_{AB}^{\mathbf{R}_A}$) and the nuclear repulsion energy ($V_{\text{nuc}}^{\mathbf{R}_A}$) with respect to atomic coordinates. Each derivative calculation is worth 3 points. Ensure these are printed in your output.

   b) **Compute the total gradient of CNDO/2 energy (3 points):** Construct the final gradient using the values obtained from the aforementioned steps and evaluate correct $x_{\mu\nu}$ and y_{AB}, contain them in your final output.

   c) **Bonus Points (1 point):** Derive the correct forms of $x_{\mu\nu}$ and y_{AB} for the analytical gradient of CNDO/2 energy. You can upload a PDF document that details your derivation process on Gradescope.

   d) **Bonus Points (1 point):** Experiment with your CNDO/2 gradient in conjunction with an optimization method from HW1 to optimize structures of molecules (such as N_2 and O_2). Share any interesting insights or findings from your optimization. For reference structures of common molecules, you can go to CCCBDB `https://cccbdb.nist.gov/expgeom1x.asp`.

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.