UNIVERSITY OF CALIFORNIA BERKELEY

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

March 26, 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 **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.