UNIVERSITY OF CALIFORNIA BERKELEY

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

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) **Derivation of $x_{\mu\nu}$ and y_{AB}** Derive the correct forms of $x_{\mu\nu}$ and y_{AB} for the analytical gradient of CNDO/2 energy. You must upload a PDF document that details your derivation process on Gradescope.
      i. **Derivation of $x_{\mu\nu}$ (2 points):**
      ii. **Derivation of y_{AB} (2 points):**
   b) **Calculation of Important Derivatives:** You are required to calculate and print the the following derivatives with respect to atomic coordinates. Ensure these are printed in your output.
      i. **Overlap Integrals $S_{\mu\nu}^{\mathbf{R}_A}$ (2 points):**
      ii. **Two-Electron Integrals $\gamma_{AB}^{\mathbf{R}_A}$ (2 points):**
      iii. **Nuclear Repulsion Energy $V_{\text{nuc}}^{\mathbf{R}_A}$ (2 points):**
   c) **Compute the total gradient of CNDO/2 energy (2 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.
   d) **Bonus Points (2 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 to Gradescope.