UCSB, Physics 129AL, Computational Physics: Section Worksheet, Week 10A

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Section Participation and Submission Guidelines

Section attendance is required, but you do not need to complete all the work during the section. At each section, the TA will answer any questions that you might have, and you are encouraged to work with others and look for online resources during the section and outside of sections. Unless otherwise stated, the work will be due one week from the time of assignment. The TA will give you 1 point for each task completed. You can see your grades on Canvas.

We will use GitHub for section worksheet submissions. By the due date, you should have a single public repository on GitHub containing all the work you have done for the section work. Finally, upload a screenshot or a .txt file to Canvas with your GitHub username and repository name so the TA knows who you are and which repository you are using for the section.

Remember: talk to your fellow students, work together, and use GPTs. You will find it much easier than working alone. Good luck! All work should be done in the Docker container, and don't forget to commit it to Git!

Task 1: Quantum Espresso: an Ab initio tool for electronic structure

a) Self-Consistent Field (SCF) Calculation

First, you should look at the **pw.scf.in** file I provided. Based on this information, write a bash script that updates **ecutwfc** in the **pw.scf.in** file,

- Wavefunction cutoff energy: This parameter defines the kinetic energy cutoff for the plane waves used to expand the wavefunctions in the calculation. It determines the maximum energy of the plane waves that will be included in the basis set. **ecutwfc = 10,15,20,25,30,35,40,60**

- **Charge density cutoff energy**: A large charge density energy often means faster wavefunction variations in spacial dimension. **ecutrho = 200.0**.

This bash script then run execute pw.x < *some input file* > *some output file*. You should be really careful on the naming and output directory. The pseudopotential directory should be the following, pseudo_dir = '/root/Desktop/pseudo'.

b) Energy Convergence

Write a bash script that uses **grep** to get the ground state energy (**total energy**) for each scf calculation you have done in **a)**. Plot the energy with respect to **ecutwfc** in Python.

c) Energy Minimum with various lattice constants

Write a bash script that updates the lattice constant in the lattice direction b-axis from $0.4 - 0.7$ with a uniform density 10. Similar to **b)**, grep the total energy and plot in Python. What is the optimal lattice size in this case. **This is a simple illustration of lattice relaxation in ab initio calculations.**

d) KS-orbitals (wavefunctions)

Using the **pp.in** file I provide, obtain the KS-orbitals below the highest occupied valance band and lowest unoccupied conduction band orbital at the **Gamma point**. Hint: you need to update the following, kband(1), kband(2) in the **pp.in**.

e) Band structure

Run the remaining band calculation in the provided text file, and obtain the band strcture via the gnuplot (do it in the local host). Translate it into python.