Lab 2
Multiscale Computational Mechanics

1. Familiarizing yourself with Quantum Espresso (QE)

Units in QE:
1 bohr = 0.529177249 Å
1 Rydberg (R) = 13.6056981 eV
1 eV = 1.60217733 x 10^{-19} Joules

We will use QE to perform DFT simulations and review concepts from Weeks 1 and 2.

Open terminal and do
```
conda activate qe
```

Create a directory anywhere you prefer and name it mae6260_lab2. Within this directory, create another directory named `simple_scf`. From Canvas, download `simple_scf.in` into this directory.

In this first exercise, we will determine the energy of a primitive Si system of two atoms in a face-centered cubic lattice (this will be explained subsequently). We will execute a self-consistent field (scf) calculation without geometry optimization, i.e., all atoms are fixed in their initial positions.

a. Let's analyze the input script, `simple_scf.in`, what do you observe?

b. Where do we obtain the pseudopotential in the `&control` name list? (https://www.quantum-espresso.org/pseudopotentials)

c. What is going on in the `&system` name list? We can look at this in Ubuntu using the software XCrySDen:
```
xcrysden --pwi simple_scf.in
Display > Primitive cell mode
```

d. Run QE:
```
cd wherever_your_directory_is/mae6260_lab2/simple_scf/
pw.x -in simple_scf.in > simple_scf.out
```

e. Let's analyze the output, `simple_scf.out`:
```
awk '/total energy/' simple_scf.out
```

What do you observe?

Can you extract the values into a text file? I tried the following:
```
cat simple_scf.out | grep -oP '(?<=total energy).*?(?=Ry)' | awk '{print $2}'
```

Can you write a Python script to plot these values?

2. Energy convergence test

In this second exercise, we run convergence tests to determine the ground-state energy of our system of interest. Ideally, convergence tests must be performed prior to starting any studies of new systems due to the variational nature of DFT calculations.

Create a directory in `mae6260_lab2` named `energy_convergence`. From Canvas, download `batch.sh` into this directory.

a. To execute the script, do:

```
cd /content/mae6260_lab2/energy_convergence/
chmod +x batch.sh
./batch.sh
```

Did you run into any errors?

b. While that is running, let's analyze the script, `batch.sh`, what can you infer?

c. Can you create scripts for extracting all final energies and plot this data?

3. Vacancy formation energy

In the third exercise, we will synthesize everything that we have touched on so far to calculate the vacancy formation energy in silicon.

a. So far, we have been using the minimal number of atoms required to minimize computational costs, using two Si atoms in a primitive cell. To introduce a single vacancy defect in a bigger cell (supercell), we need to use a conventional, cubic simulation box.

Create a directory in `mae6260_lab2` named `vacancy`. Copy the `simple_scf.in` script into this directory, rename it as `perfect_crystal.in` and open it using `xcrysden`. Go to `Display > Unit of Repetition > Translational asymmetric unit`. Then, save it using `File > Save XSF Structure`.

Open the saved .xsf file, what can you observe?

Copy and paste the conventional cell coordinates into `perfect_crystal.in` and change the atomic number `14` to `Si`. Change the `ATOMIC_POSITIONS` card to `angstroms`.

As we are now using conventional coordinates, we need to include a card called `CELL_PARAMETERS`. Where can we get this information and what units should we specify?

What other parameters do we need to modify?

Run the simulation and extract the total energy for this system.

b. Now that we have the total energy of a perfect Si crystal, let's introduce single vacancy defect. Copy `perfect_crystal.in` and rename it as `single_vacancy.in`.

   How can we introduce a single vacancy? What parameters need to be changed?

   Visualize your new input file, does everything make sense?

   Run the simulation and extract the total energy for this system.

c. To get an accurate ground-state energy, we will need to "relax" the system. Copy `single_vacancy.in` and rename it as `single_vacancy_relax.in`. Change the following name lists:

```
&control
 calculation = 'relax'.
 …

&electrons
 conv_thr = 1.0d-8
 …

&ions
 ion_dynamics = 'bfgs'
```

   Run the simulation and extract the total energy for this system.
   Visualize the output. What can you observe?

d. Let's calculate the vacancy formation energy using a simple approximation:

$$E_f = E_v - \frac{7}{8}E_p$$

   Compare your values with literature values (https://doi.org/10.1103/PhysRevLett.108.066404). What can you observe and how do you explain these observations?

REMEMBER TO BACKUP EVERYTHING YOU NEED!