Quantum Espresso on HPC

What is Quantum Espresso?

Quantum ESPRESSO is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.

It has evolved to a distribution independent and inter-operable codes in the spirit of an open-source project. Moreover, it implements several MPI parallelization levels, in which both calculations and data structures are distributed across processors.

More info on Quantum Espresso:

User Guide

Official Website

HPC Guide

Versions Available:

The following versions are available on the cluster:

- Espresso –v6.1
- Espresso –v6.7
- Espresso –V6.8

How to load Quantum Espresso?

To load Quantum Espresso on the HPC, use the following commands:

```
module avail physical/espresso
#This will show all the available versions of espresso
```

Use the following command to load the desired version.

```
module load physical/espresso/6.8
```

To verify if the module and dependencies are loaded correctly, use the following command.

```
module list
```

This should list all the software and dependencies that are loaded.

How to use Quantum Espresso?

There are two ways to use most of the software on the cluster.

The Interactive Way:

To run the espresso in an interactive session, jump into a bash terminal of a compute node using the following command:

```
srun -p main --qos main -n 1 -c 12  --mem 16G --pty bash
```

Now, load the quantum espresso module and start your operation on the terminal.

Note: This is preferred usage in case of short runtime jobs and debugging. After you exit the terminal session, your job will be terminated unlike batch method.

The Script method:

To use this method, the user will need to write a batch script and submit it to a slrum.

To copy the example script, use the following command,

```
mkdir ~/qe-test && cd ~/qe-test
cp /share/apps/espresso/example/* ~/qe-test
```

The run_example_diamond script will be copied over. Edit the directory path and link the pseudopotential files to the script. Then the use the below script to run quantum espresso.

```
#!/bin/bash
#SBATCH --job-name=qe-test        # create a short name for your job
#SBATCH --nodes=2                 # node count
#SBATCH --ntasks-per-node=12       # number of tasks per node
#SBATCH --cpus-per-task=1         # cpu-cores per task
#SBATCH --mem=16G                 # total memory per node
#SBATCH --time=00:15:00           # total run time limit (HH:MM:SS)
#SBATCH -p main
#SBATCH --qos main
#SBATCH -e err.err
#SBATCH -o out.out

module load physical/espresso/

cd $SLURM_SUBMIT_DIR
#Use Quantum Expresso commands here
srun sh run_example_diamond -npool 2
```

All the output will be saved in the directory you specified on the script.

Where to find help?

If you are stuck on some part or need help at any point, please contact OIT at the following address.

OIT Help