## 2024 School on Electron-Phonon Physics, Many-body Perturbation Theory, and Computational Workflows

## Automated workflows with EPWpy

### Hands-on session (Sun.2)

## Setup for Tutorials

▶ 1st step: First, we will be installing some python libraries we will be using throughout the tutorials, including the EPWpy library. Start by logging in the Frontera supercomputer, then issue the following commands on your terminal:

```
$ cds
$ module load python3.7
$ python3.7 -m pip install alive_progress --user
$ python3.7 -m pip install request --user
$ pip install -i https://test.pypi.org/simple/ EPWpy
$ cp /work2/05193/sabyadk/stampede3/EPWSchool2024/tutorials/Sun.16.EPWpy.tar ./
$ tar xvf Sun.16.EPWpy.tar
```

▶ 2nd step: Once you set-up the libraries in your terminal session, you will want to access the MATCSSI platform website in order to be able to execute Jupyter notebooks at Frontera. The platform can be access via the following link:

https://matcssi.tacc.utexas.edu/

▶ 3rd step: Log in with your TACC username and password. You will be greet with a page just as shown below. Go to the "Applications" tab on the right, then "Visualization" and finally "TACC Analysis Portal", as indicated by the red arrows. Finally click "Launch".

► 4th step: You should see a page as shown below. Click the button "Utilities" at the bottom of the page and then "Use Python3" and "Link $SCRATCH from $HOME" in the new webpage. Finally, click "Back to Jobs".



► 5th step: Fill the information for "System", "Application", "Project", "Queue", "Tasks", "Job name", "Time Limit" and "Reservation", as shown in the figure below. Today's reservation is **DMR23030_June_2**. When you are done, start your session by clicking at "Submit" at the bottom of the page.



► 6th step: After you submit the job you will be redirected to a page as shown below. You might have to wait a couple of seconds for the job to be allocated. If it takes too long click "Check status" to refresh the page. When the status change to "Running" you can now initialize your session by clicking "Connect".

**TAP Job Status**

**Job:** MyJob
**Status:** PENDING
**Refresh:** in 53 seconds
**Message:**

TAP: Your script has been submitted to Frontera but it is not yet running.

`sinfo -p development` output is:
PARTITION        AVAIL NODES(A/I)
development*     up   175/219

[Check Status] [End Job] [Show Output] [Back to Jobs]

▶ 7th step: Once you connect you should see a page just as shown below. This is your Jupyter session. You can open multiple tabs by double clicking any file inside your folders. Navigate to your "SCRATCH" folder as shown in the figure below, and find the tutorial notebooks you have downloaded in the 1st step. Double click any of the tutorials to open it.
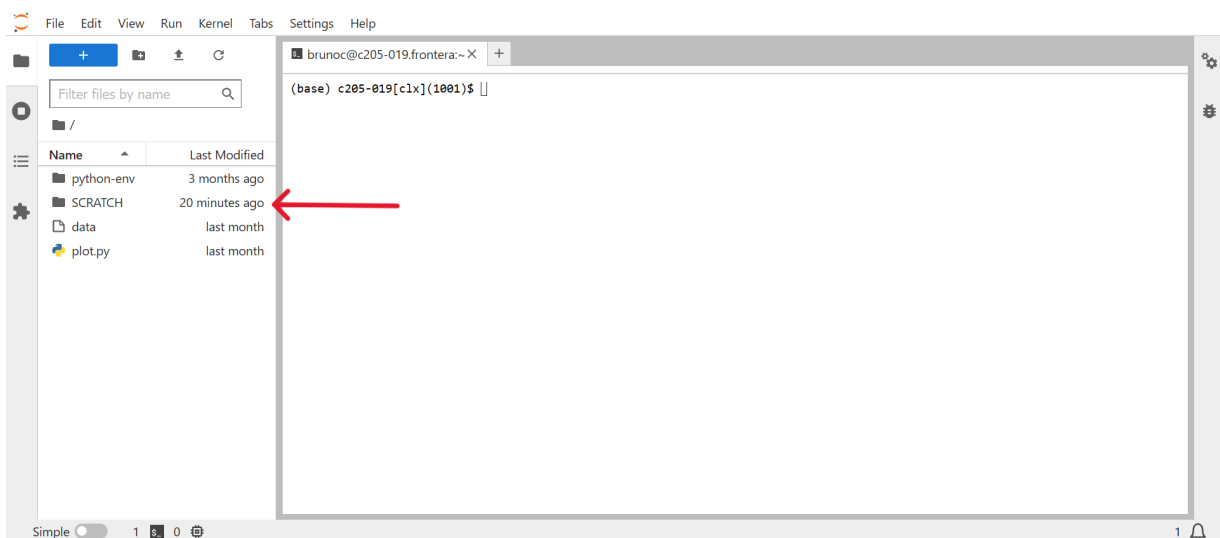


▶ 8th step: Have fun! Take your time to check the instructions throughout the notebook and also the actual python codes. These tutorials are just examples on how you can apply EPWpy to perform different types of calculation. Remember, EPWpy is a python library and you may use it as you seem fit.