

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 MATC-SSI 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".

The screenshot shows the MATC-SSI web interface. At the top, there is a navigation bar with 'TACC | TEXAS' and a search bar. Below the navigation bar, there is a sidebar with a menu containing 'Dashboard', 'Data Files', 'Applications', 'Allocations', 'History', and 'System Status'. The 'Applications' tab is selected. The main content area displays a tray of applications: 'Visualization [2]', 'Data Processing [5]', 'Utilities [2]', 'Paraview (Frontera)', and 'TACC Analysis Portal'. Red arrows point to the 'Applications' tab in the sidebar, the 'Visualization [2]' application in the tray, and the 'TACC Analysis Portal' application in the tray. Below the tray, there is a message: 'Select an app from the tray above to submit a job.' The URL at the bottom of the page is 'https://matcssi.tacc.utexas.edu/workbench/applications/analysis-portal?appVersion=1.0'.

► 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**".

The screenshot shows the job submission interface. On the left, the 'Submit New Job' form has dropdown menus for System, Application, Project, and Queue, and input fields for Nodes (1) and Tasks (1). Below these are 'Options' for Job Name, Time Limit, Reservation, and VNC Desktop Resolution. At the bottom, there are 'Submit' and 'Utilities' buttons. A red arrow points to the 'Utilities' button. On the right, the 'System Status' table shows three systems: Frontera (96% utilization, 338 running jobs), Lonestar6 (92% utilization, 317 running jobs), and Stampede3 (45% utilization, 182 running jobs). Below this is a 'Current Jobs' section with a 'MyJob' entry and buttons for 'Status', 'End', and 'Connect'.

► 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.

The screenshot shows the job submission interface with the form filled out. The 'Submit New Job' form has System set to 'Frontera', Application to 'Jupyter notebook', Project to 'DMR23030', and Queue to 'development'. The 'Nodes' field is set to 1 and 'Tasks' to 16. In the 'Options' section, 'Job Name' is 'MyJob' and 'Time Limit' is '2:0:0'. The 'System Status' table on the right shows the same three systems as before, but with updated job counts: Frontera (356 running), Lonestar6 (317 running), and Stampede3 (181 running).

► 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

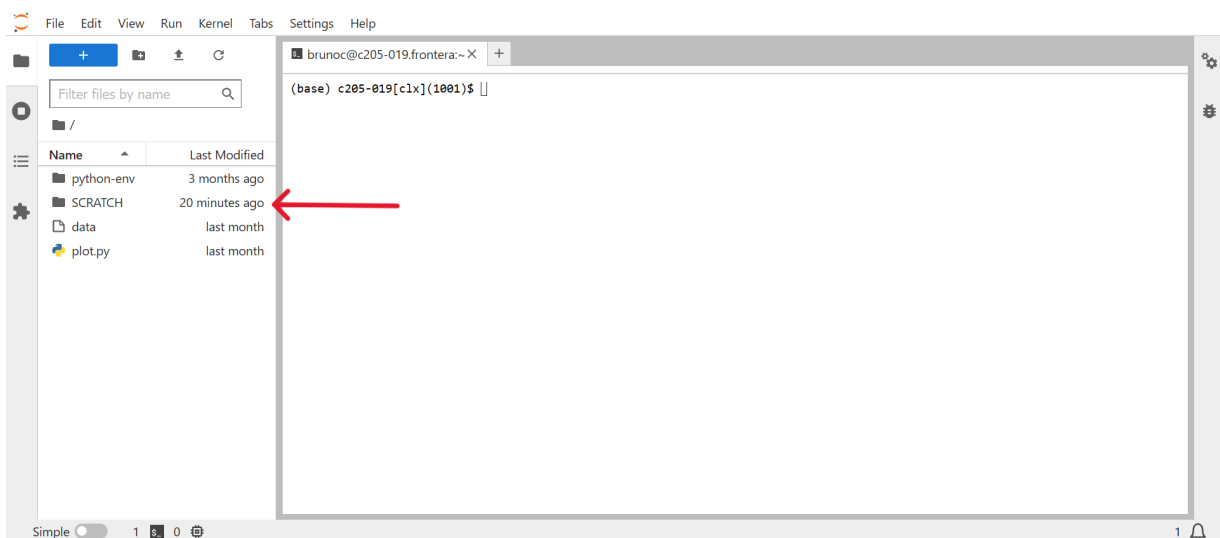
Message:

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.