Aliance jupyter link:

https://docs.alliancecan.ca/wiki/JupyterHub

JupyterHub is the best way to serve Jupyter Notebook for multiple users. It can be used in a class of students, a corporate data science group or scientific research group. [1]

JupyterHub provides a preconfigured version of JupyterLab and/or Jupyter Notebook; for more configuration options, please check the Jupyter page.

Click on Jupyter in selected cluster, e.g. narval

Login

Go to directory where you have files

In setup on top select show active files

Python console

The Python 3.x console launcher is available by default in a new JupyterLab session. When launched, a Python 3 interpreter is presented in a new JupyterLab tab.

Terminal

This application launcher will open a terminal in a new JupyterLab tab:

- *The terminal runs a (Bash) shell on the remote compute node without the need of an SSH connection.*
  - *Gives access to the remote filesystems (`/home`, `/project`, `/scratch`).*
  - *Allows running compute tasks.*
- *The terminal allows copy-and-paste operations of text:*
  - *Copy operation: select the text, then press Ctrl+C.*
    - *Note: Usually, Ctrl+C is used to send a SIGINT signal to a running process, or to cancel the current command. To get this behaviour in JupyterLab's terminal, click on the terminal to deselect any text before pressing Ctrl+C.*
  - *Paste operation: press Ctrl+V.*

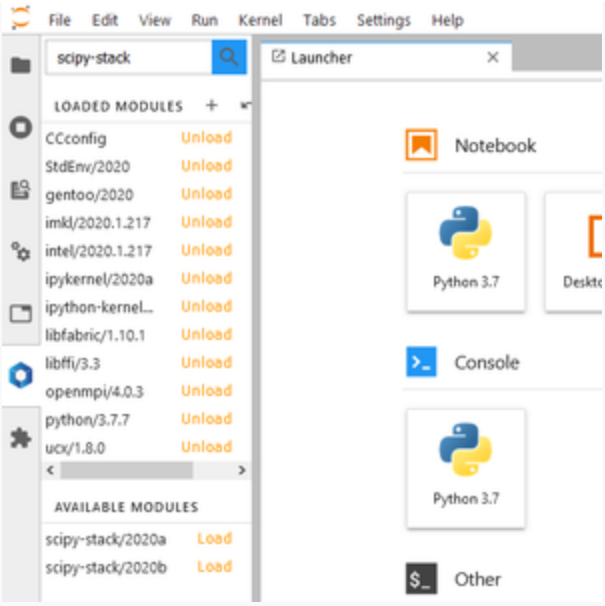
Available notebook kernels

Julia notebook

To enable the Julia 1.x notebook launcher, an `ijulia-kernel` module needs to be loaded.

When launched, a Julia notebook is presented in a new JupyterLab tab.

Python notebook



Searching for scipy-stack modules

If any of the following scientific Python packages is required by your notebook, before you open this notebook, you must load the `scipy-stack` *module from the JupyterLab Softwares tool:*

- `ipython`, `ipython_genutils`, `ipykernel`, `ipyparallel`
- `matplotlib`
- `numpy`
- `pandas`
- `scipy`

VASP

Copy to used directory toolsScriptum.tgz

Unpack it:

tar zxvf toolsScriptum.tgz

Other zip files were done using:

zip -r workshop.zip workshop

To unzip them:

unzip workshop.zip

In Jupiter type import py4vasp

To download tutorials from web: https://vasp.at/tutorials/latest/ type in terminal:

wget https://www.vasp.at/tutorials/latest/get_started.zip

unzip get_started.zip

Download also these tutorials to your PC:

https://www.vasp.at/tutorials/latest/molecules/part1/

https://www.vasp.at/tutorials/latest/md/part1/

https://www.vasp.at/tutorials/latest/md/part2/

For workshop upload them to https://hub.vasp.at/ your dir

Note unzip MD contains part1 and part2

In terminal:

Unzip zip files and run tutorials in Jupiter.

In Jupiter type import py4vasp

In Py4fVasp for exporting the data as a csv file, you need to change .plot() to .to_csv(). To create a downloadable image, change .plot() to .to_image(). You will then be able to download this. Alternatively, you could write .to_plotply() and produce a plotly graph, then download that.

To execute job in terminal in the respective directory submit it using sbatch command and respective script as listed on https://www.barbara-research.ca/nipy/CurrentlLnksBatchjobs.htm

Jupyter interface was created for convenience in VASP.

To run VASP from console you need to have the following input files: INCAR, POSCAR and POTCAR and job submission file. After your submitted job (sbatch) is completed you can analyse output files using your own software or available online as described on https://www.vasp.at/wiki/index.php/Welcome

See for example nice videos:

DOS and BANDS calculation in VASP

https://www.youtube.com/watch?app=desktop&v=RYziHtNFaPs
VASP writes the DOS after every calculation and the projected DOS if you set LORBIT in the INCAR file. You can use this class to extract this data. Typically you want to run a non self consistent calculation with a denser mesh for a smoother DOS but the class will work

independent of it. If you generated a projected DOS, you can use this class to select which subset of these orbitals to read or plot.
Extract numerical values for figures in py4vasp give answer for bands:
https://www.vasp.at/forum/viewtopic.php?p=27211