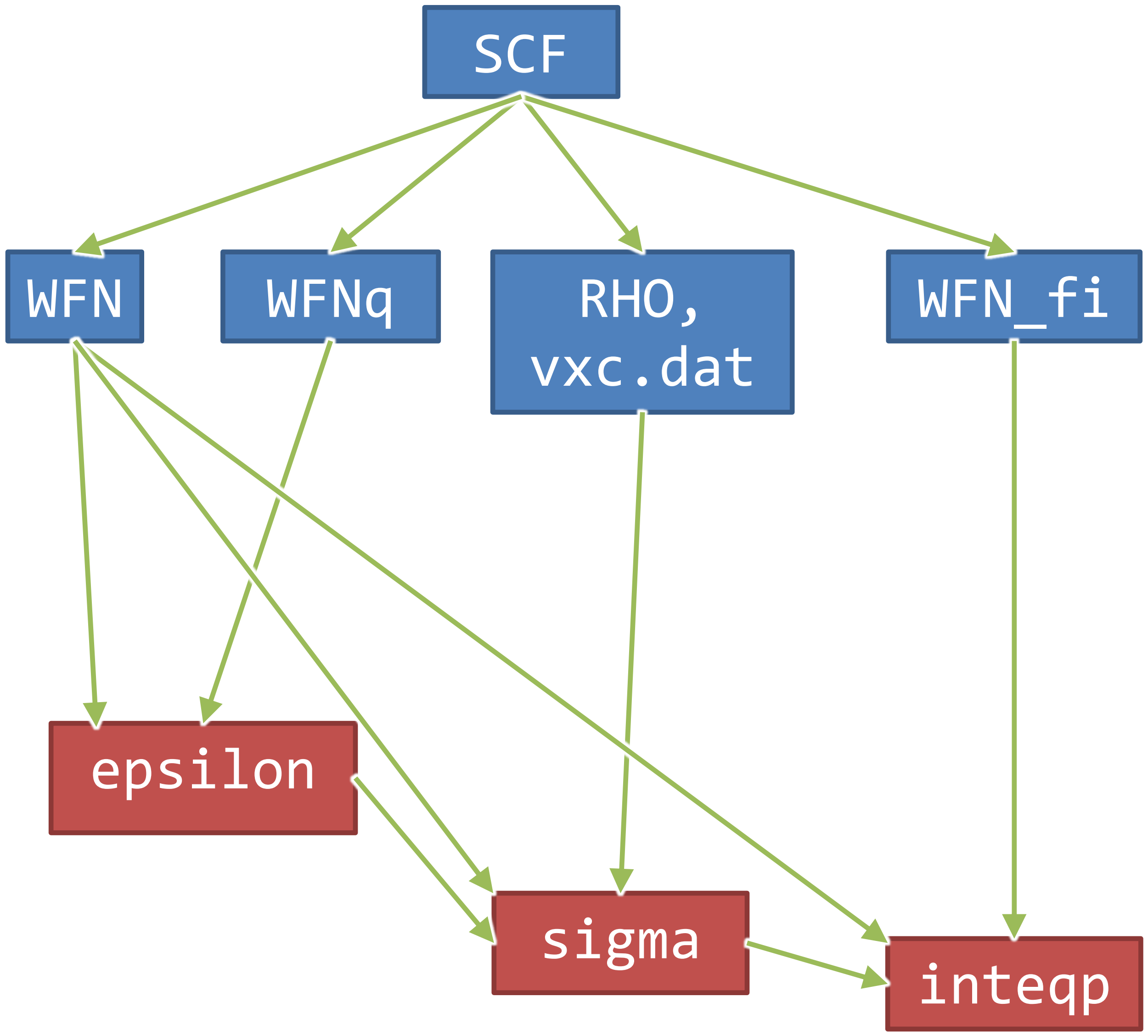
TUTORIAL 1: BASIC GW CALCULATIONS – SILICON

Felipe H. da Jornada (Stanford), David A. Strubbe (UC Merced), Bradford Barker (UC Merced), Zhenglu Li (UC Berkeley), Meng Wu (UC Berkeley)

vES BerkeleyGW Mini-Workshop – June 5th, 2020

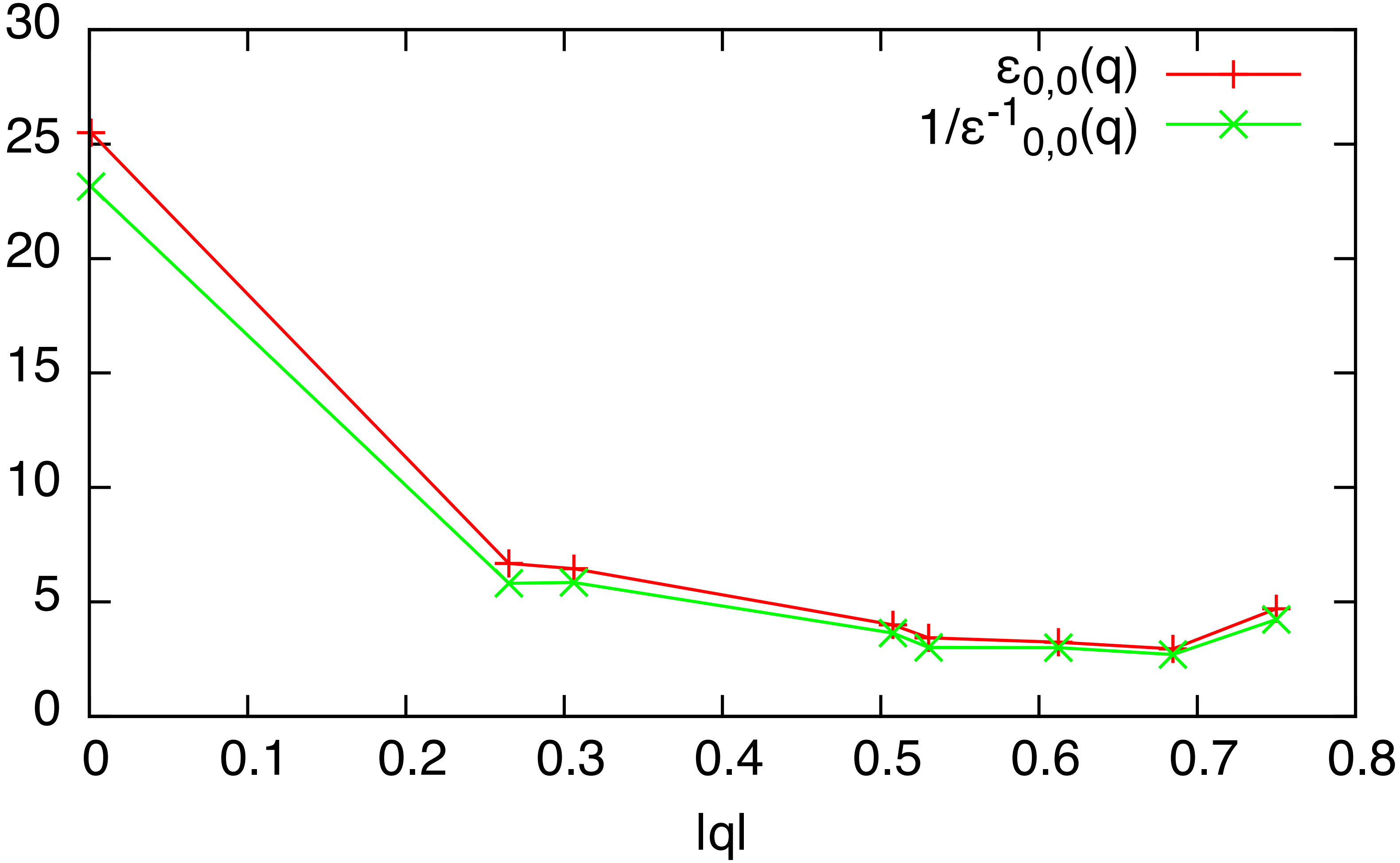
1-silicon_GW: Workflow

```
kgrid.x
wfn_rho_vxc_info.x
```

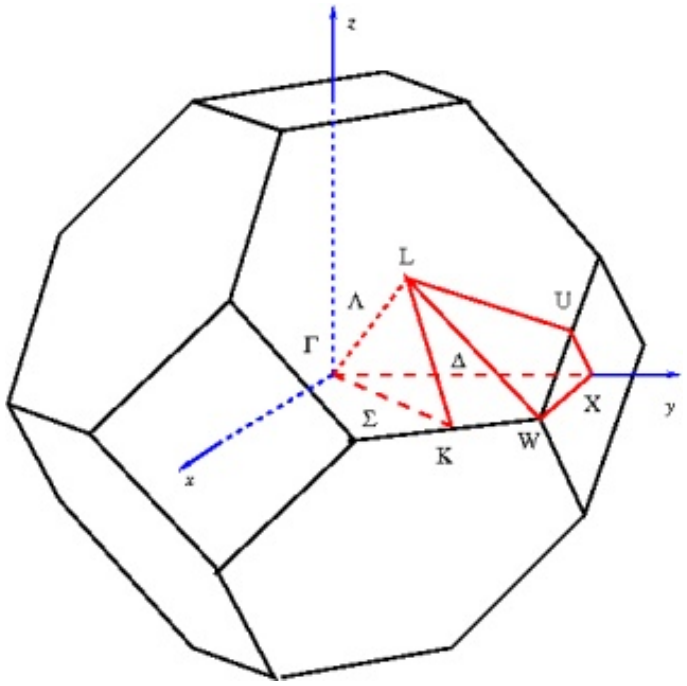


BerkeleyGW

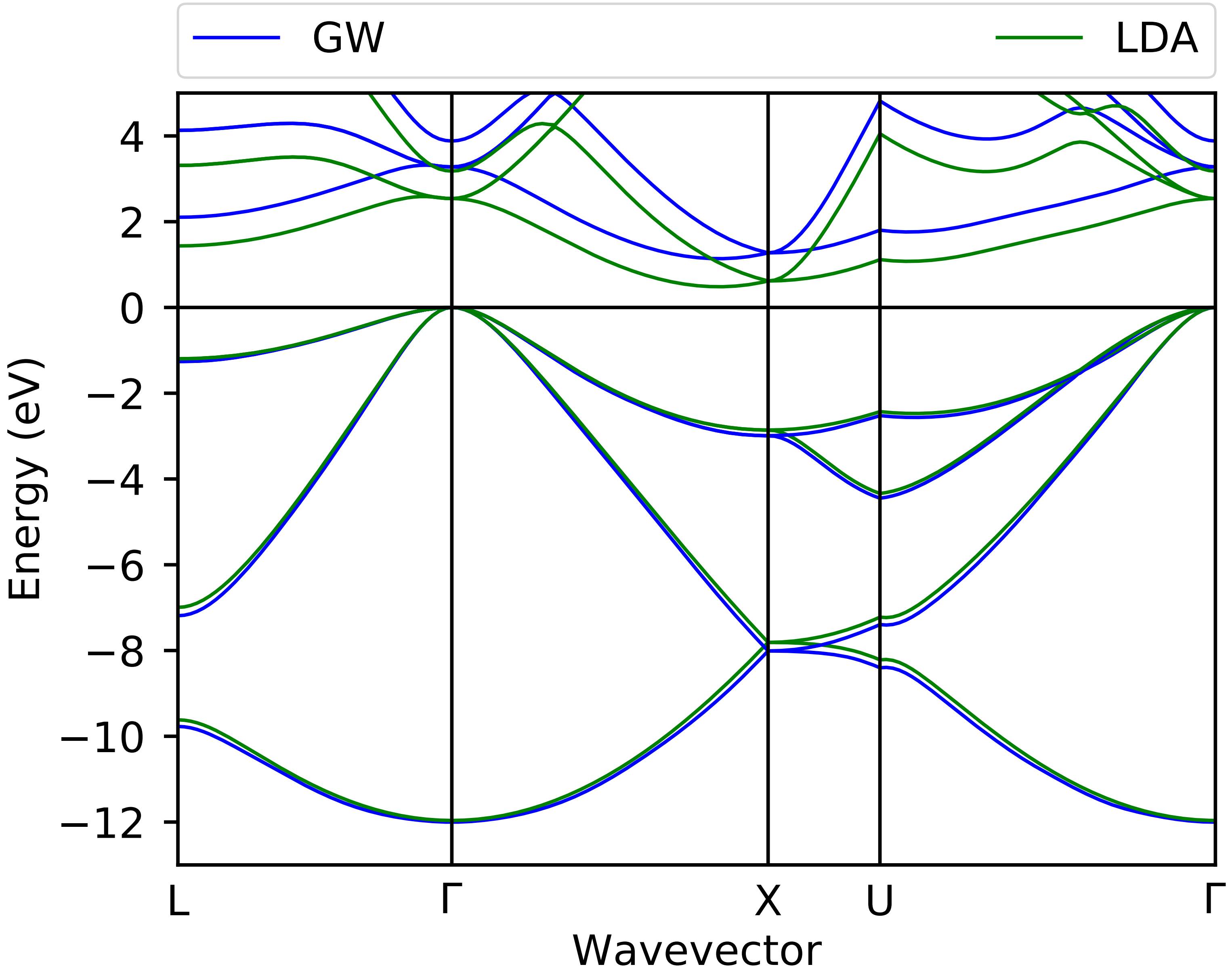
1a-silicon_GW: Epsilon: screening as a function of |q|



1-silicon_GW: inteqp – interpolated bandstructure



LDA gap: 0.483 eV
GW gap: 1.137 eV



`1-silicon_GW`: Goals

Basic goals:

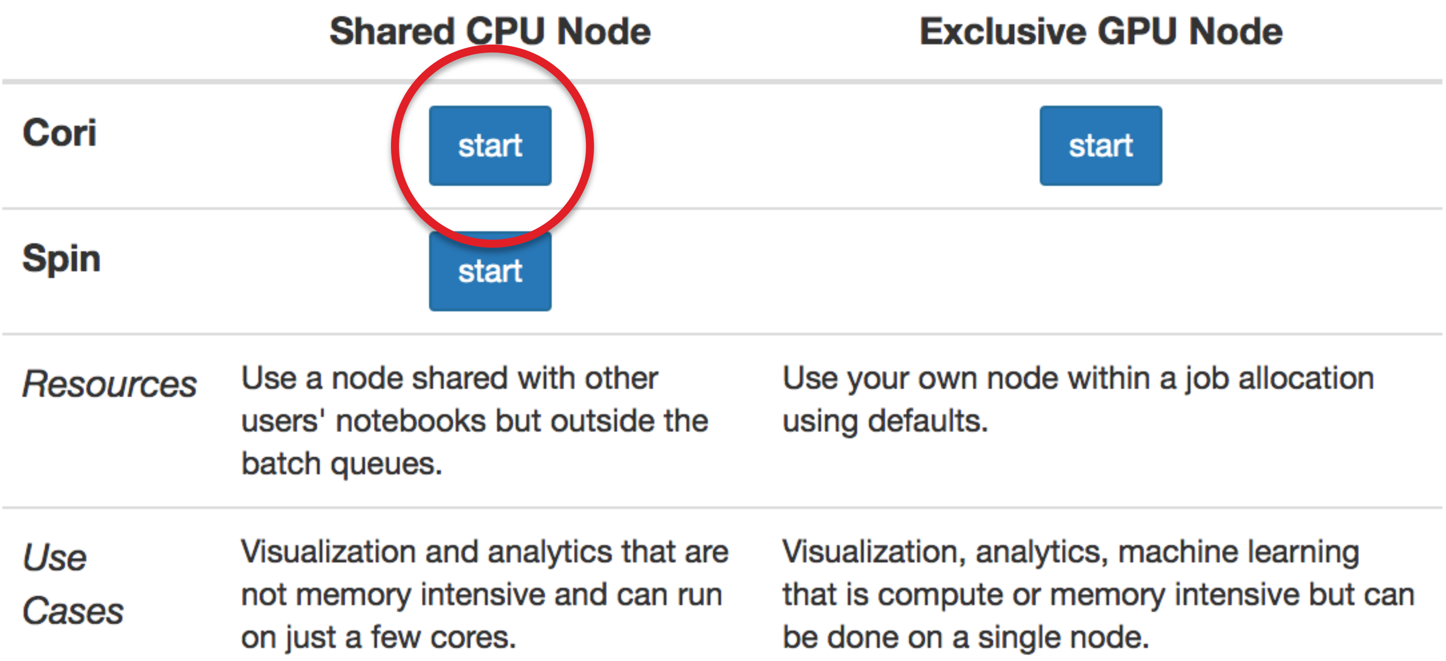
1. Understand the basic workflow of BerkeleyGW, and the relation between the **k**-grids, wavefunctions, `epsilon`, `sigma`, and `inteqp`.
2. Run a basic GW calculation on silicon.
3. Construct an interpolated bandstructure using the `inteqp` code.

Stretch goals:

1. Compare your Sigma GW results with Hartree-Fock and/or static COHSEX.
   What inputs are no longer necessary? How do the results compare?
2. Modify the example for GaAs and repeat each step of the calculation.
3. Adapt calculation to use half-shifted **k**-grids.

Logging in with Jupyter

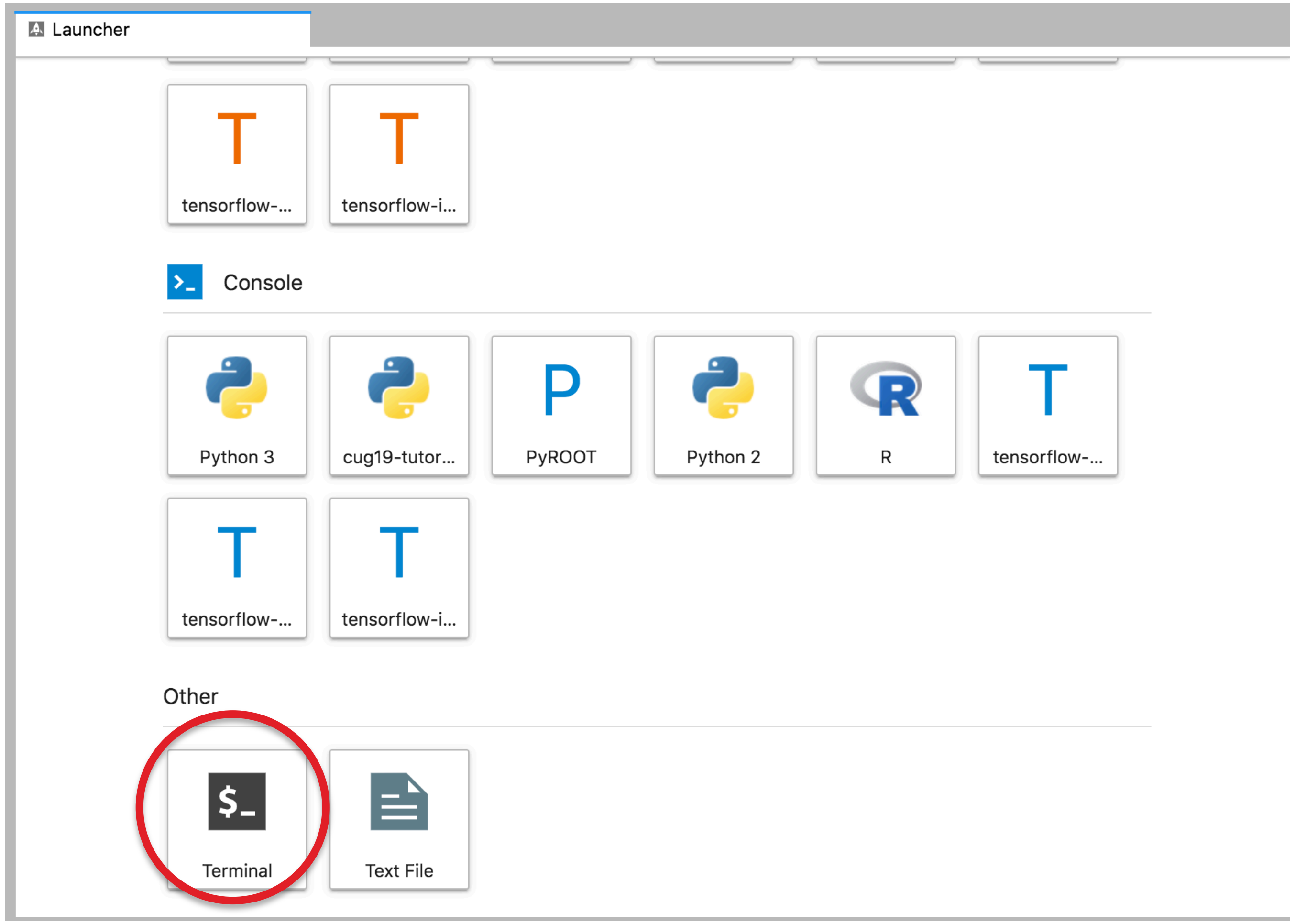
1. Go to https://jupyter.nersc.gov
2. Log in
3. Click on on the button for "Cori" / "Shared CPU Node"



	Shared CPU Node	Exclusive GPU Node
Cori	start	start
Spin	start	
Resources	Use a node shared with other users' notebooks but outside the batch queues.	Use your own node within a job allocation using defaults.
Use Cases	Visualization and analytics that are not memory intensive and can run on just a few cores.	Visualization, analytics, machine learning that is compute or memory intensive but can be done on a single node.

Logging in with Jupyter

4. Click on "Terminal"



Logging in with Jupyter

5. Copy the workshop examples to your $SCRATCH folder. Type the following commands into the new Jupyter console:

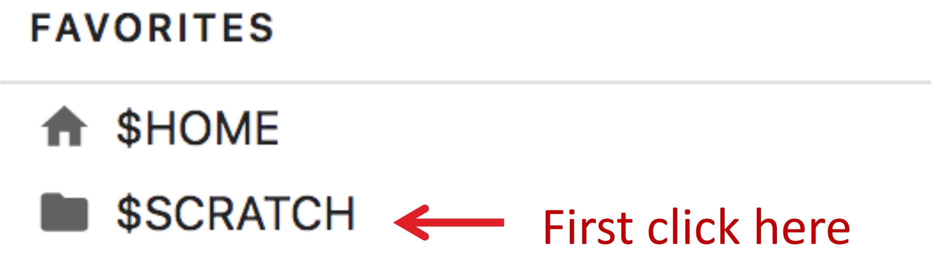
```
# Go to scratch space to run jobs
cd $SCRATCH

# Copy tutorial directory to your directory
cp -rP /project/projectdirs/m3034/vESW_2020/BerkeleyGW/1-silicon_GW .

# Enter your local folder
cd 1-silicon_GW
```

Logging in with Jupyter

6. Navigate to the corresponding tutorial folder

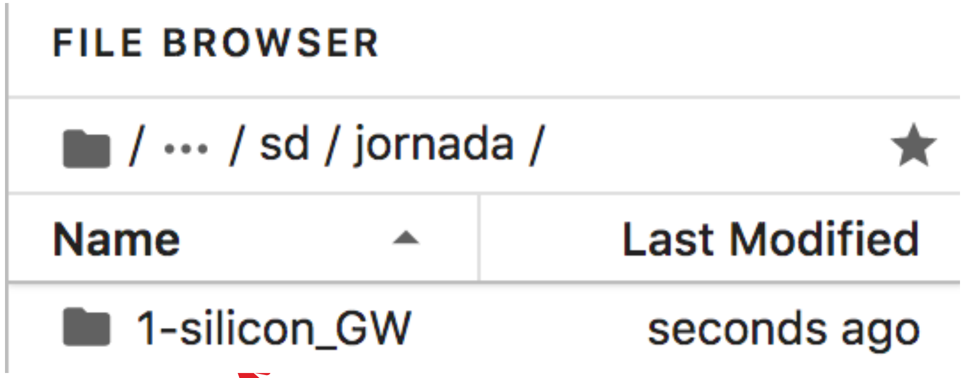


FAVORITES

$HOME

$SCRATCH

First click here



FILE BROWSER

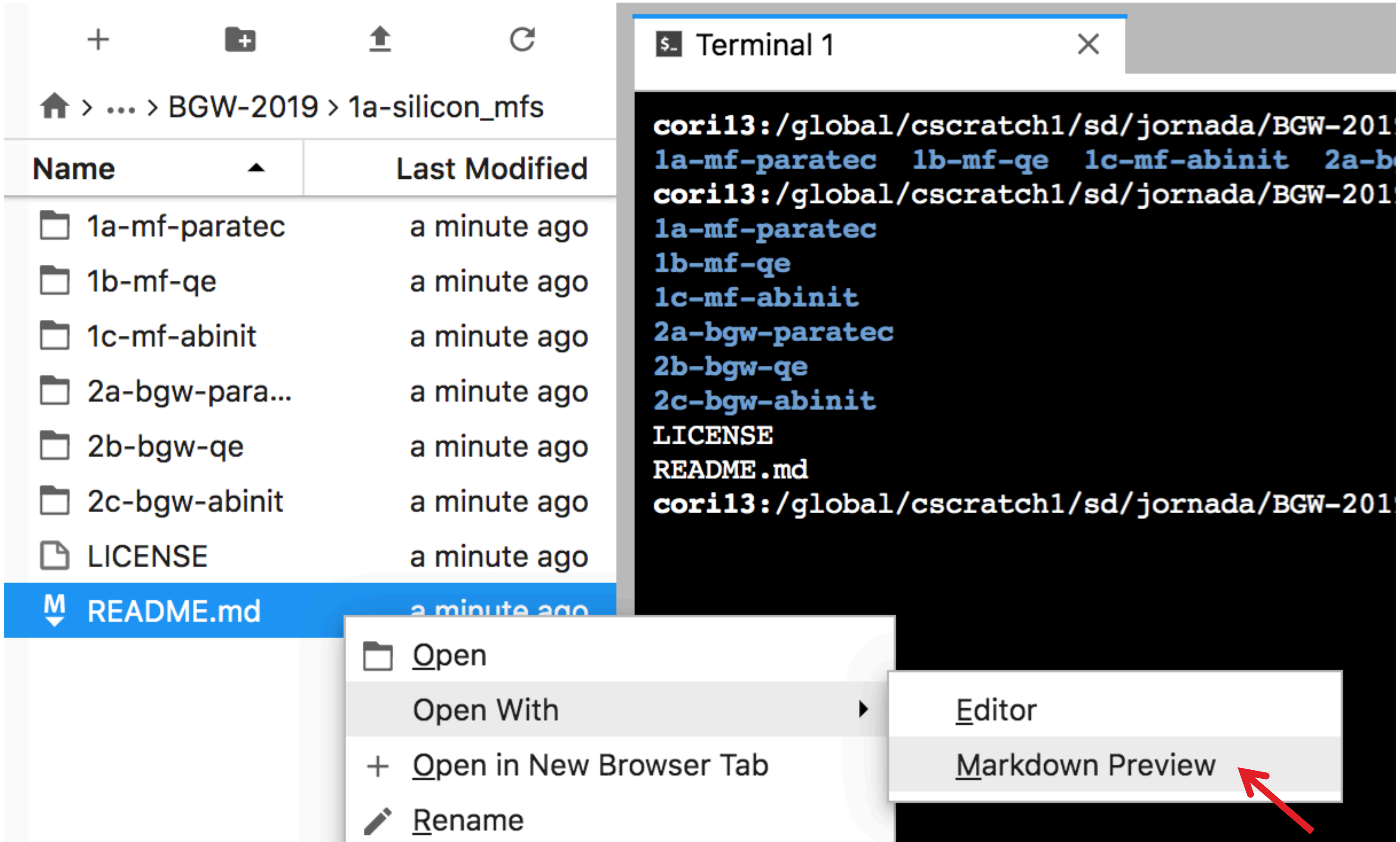
/ ··· / sd / jornada /

Name	Last Modified
1-silicon_GW	seconds ago

Then here

Logging in with Jupyter

7. Once you find the correct folder, right click on the "README.md" file, select "Open With" -> "Markdown Preview"

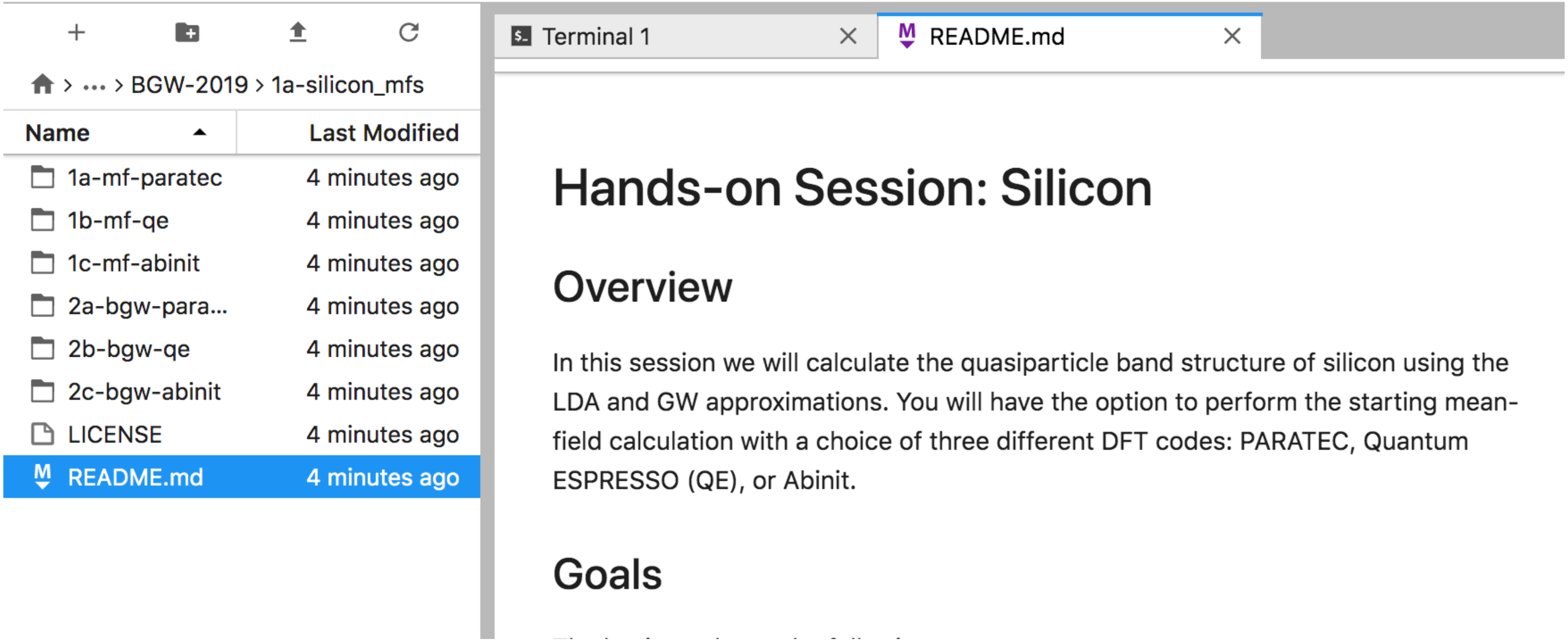


Name	Last Modified
1a-mf-paratec	a minute ago
1b-mf-qe	a minute ago
1c-mf-abinit	a minute ago
2a-bgw-para...	a minute ago
2b-bgw-qe	a minute ago
2c-bgw-abinit	a minute ago
LICENSE	a minute ago
README.md	a minute ago

```
cori13:/global/cscratch1/sd/jornada/BGW-201
1a-mf-paratec  1b-mf-qe  1c-mf-abinit  2a-b
cori13:/global/cscratch1/sd/jornada/BGW-201
1a-mf-paratec
1b-mf-qe
1c-mf-abinit
2a-bgw-paratec
2b-bgw-qe
2c-bgw-abinit
LICENSE
README.md
cori13:/global/cscratch1/sd/jornada/BGW-201
```

Logging in with Jupyter

8. Now, you can work on the terminal, read the instructions (`README.md` files) and see files all from the same interface



Name	Last Modified
1a-mf-paratec	4 minutes ago
1b-mf-qe	4 minutes ago
1c-mf-abinit	4 minutes ago
2a-bgw-para...	4 minutes ago
2b-bgw-qe	4 minutes ago
2c-bgw-abinit	4 minutes ago
LICENSE	4 minutes ago
README.md	4 minutes ago

Hands-on Session: Silicon

Overview

In this session we will calculate the quasiparticle band structure of silicon using the LDA and GW approximations. You will have the option to perform the starting mean-field calculation with a choice of three different DFT codes: PARATEC, Quantum ESPRESSO (QE), or Abinit.

Goals

Final instructions

Always load the `berkeleygw/2.1–beta` module before running any command!

```
module load berkeleygw/2.1-beta
```

Additional resources:

- BerkeleyGW manual: http://manual.berkeleygw.org/2.2/
- 2019 workshop examples: http://workshop.berkeleygw.org