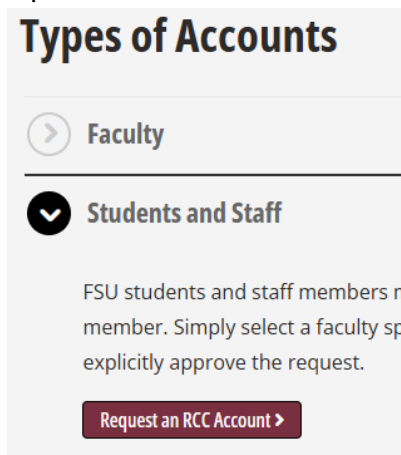# Getting set up on the HPC

The HPC is FSU's own supercomputer. You'll have the keys to it this semester. To learn more: https://its.fsu.edu/services/high-performance-compute-cluster

Getting user credentials (THIS PART MIGHT CHANGE - CONTACT HPC STAFF ABOUT CLASSROOM ACCOUNTS)

1. Navigate to https://its.fsu.edu/research/rcc-user-accounts
2. Open "Students and Staff" and click to request an RCC Account

Types of Accounts

> Faculty

⊙ Students and Staff

FSU students and staff members m
member. Simply select a faculty sp
explicitly approve the request.

Request an RCC Account >

3. Log in with your normal FSU credentials
4. Fill out all the fields to request an account. As your sponsor, list the instructor in charge of your lab - in this case, Dr. Judy Clark.

Connecting to the HPC

More information: https://docs.rcc.fsu.edu/hpc/connecting-and-using/#connecting
We will be using Open OnDemand, which allows us to access the HPC and run applications on it through our web browser. For further information, see the documentation:
https://docs.rcc.fsu.edu/hpc/ood/

The first thing we must do is to get user credentials.

1. Navigate to https://ood.rcc.fsu.edu/
2. Enter the username and password you obtained earlier
   You should see a page like this:

FSU | INFORMATION TECHNOLOGY SERVICES
RESEARCH COMPUTING CENTER

Latest RCC News

07-28-2025
RCC Spotlight: Dr. Fanny Liu
Dr. Liu utilizes the HPC to develop new analytical methods in spectrometry.

06-17-2025
RCC Spotlight: Dr. Laura Reina
Dr. Laura Reina uses the High Performance Computing cluster to enable her research in elementary particle physics.

05-07-2025
RCC Spotlight: Dr. Jarrod Mousa
Dr. Jarrod Mousa and his team work on the development of monoclonal antibody therapies and vaccines.

04-22-2025
RCC Spotlight: Dr. Tom Needham
Dr. Needham uses geometry and topology to study AI and data science models.

12-12-2024
RCC 2024 Tactical Objectives Retrospective
With 2025 just over the horizon, we want to reflect on the past year's objectives.

07-08-2024
RCC Spotlight: Dr. Michael Shatruk
The Shatruk group investigates magnetic and quantum materials.

05-20-2024
RCC Spotlight: Carly Sweeney
Carly Sweeney is a High-Performance Computing intern for the FSU Research Computing Center.

04-08-2024

Pinned Apps A featured subset of all available apps

Interactive Apps

RCC Desktop — System Installed App

Jupyter Notebook — System Installed App

MATLAB — System Installed App

RStudio 2023 — System Installed App

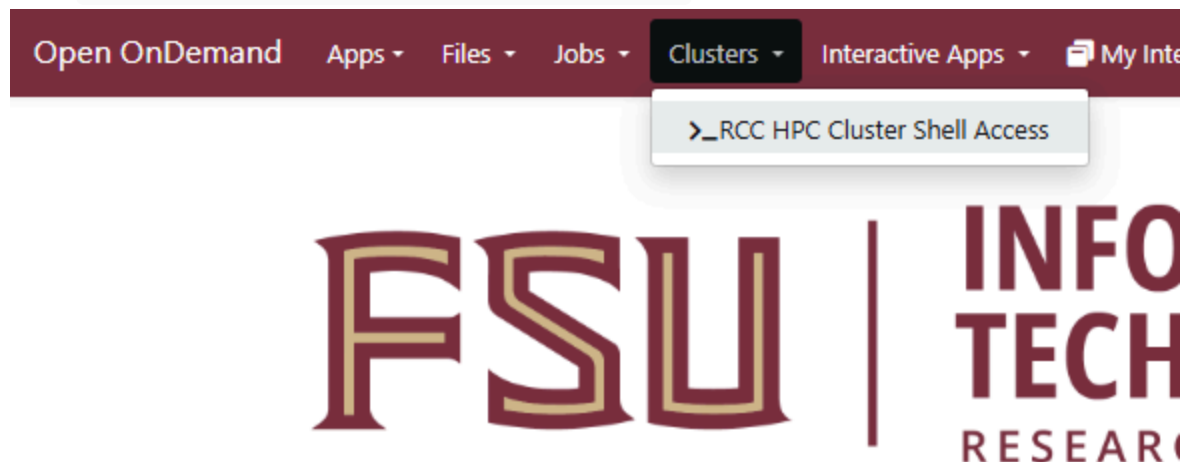You may want to bookmark this page for future use.

There are two primary ways we will use Open OnDemand to interface with the FSU HPC.

1. Using the Terminal
2. Using the Jupyter Lab app

We will not need to use the Terminal very much, except to install the software we are going to use at the beginning of the course, and to get all the labs we will use.

Obtaining the notebooks and setup script

1. click `Clusters > RCC HPC Cluster Shell Access`.

2. You should see something like this:

3. First, follow the instructions for setting up Conda on the HPC, which can be found here: https://docs.rcc.fsu.edu/software/conda/#conda-vs-pip

4. Enter the following command:
   ```
   git clone git@github.com:/zedo-heptulose/pchem-lab-II-materials-worked.git
   ```

5. If this worked, you should have a new directory with all of the course materials. Run the following command to show this:
   ```
   ls
   ```
   then
   ```
   cd pchem-lab-II-materials-worked
   ```

then

```
ls
```

6. You should see something like this:

```
(base) [gdb20@h22-login-26 ~]$ ls
code           config.py            jupyterenv  scratch   the_terabyte  untitled.py
computations   instructor-materials ondemand    teaching  untitled1.py
(base) [gdb20@h22-login-26 ~]$ cd instructor-materials
(base) [gdb20@h22-login-26 instructor-materials]$ ls
'chm4411l Introduction to Computational Chemistry.pptx'  Diffraction          'T1 and T2 NMR'
'chm4411l programming.pptx'                              'Lab Chemicals.xlsx'  templates
 chm4411l_setup.sh                                        lab_template.ipynb   TODO.md
 chm4411l.yml                                             Magnetism            todo.txt
 compchem_hw                                              PHOTOELECTRIC        'Vibration-Rotation Spectra HCl-DCl'
'Computational Lab Feedback Questionnaire.docx'           PIB                  Waves
 conda-testing                                           'Quantum Dots'
'Dark Pathways in Ruby'                                   scratch
(base) [gdb20@h22-login-26 instructor-materials]$
```

7. Check for the `chm4411l_setup.sh` file. Run the following command:

```
chmod +x chm4411l_setup.sh
```

then

```
ls
```

You should see that the color of this file has changed to green.

```
(base) [gdb20@h22-login-26 instructor-materials]$ ls
'chm4411l Introduction to Computational Chemistry.pptx'  Diffraction          'T1 and T2 NMR'
'chm4411l programming.pptx'                              'Lab Chemicals.xlsx'  templates
 chm4411l_setup.sh                                        lab_template.ipynb   TODO.md
 chm4411l.yml                                             Magnetism            todo.txt
 compchem_hw                                              PHOTOELECTRIC        'Vibration-Rotation Spectra HCl-DCl'
'Computational Lab Feedback Questionnaire.docx'           PIB                  Waves
 conda-testing                                           'Quantum Dots'
'Dark Pathways in Ruby'                                   scratch
```

8. Run the script. This will install all of the programs we will use in this course.

```
./chm4411l_setup.sh
```

Don't worry if you see error codes.

What we just did was to install all of the packages we will use for this course in a Conda virtual environment in the following directory: `~/.conda/envs/chm441l` .

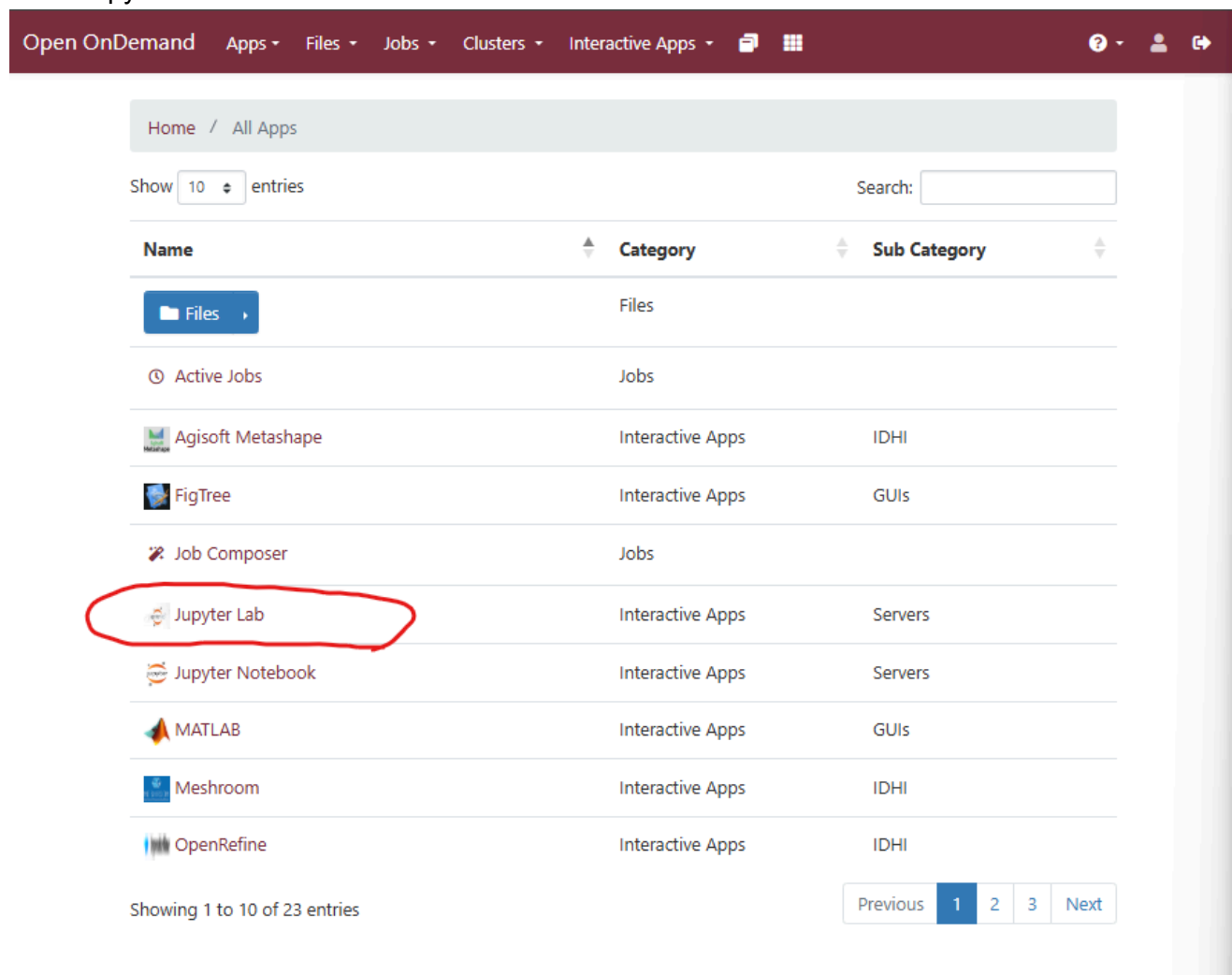> If we ever need to run something on the HPC in this enviornment, use `conda activate chm4411l`

The immediate next thing we will do is open JupyterLab and use our newly created environment, where we can test if everything installed properly.

Using Jupyter Lab

1. Navigate to `Apps > All Apps`
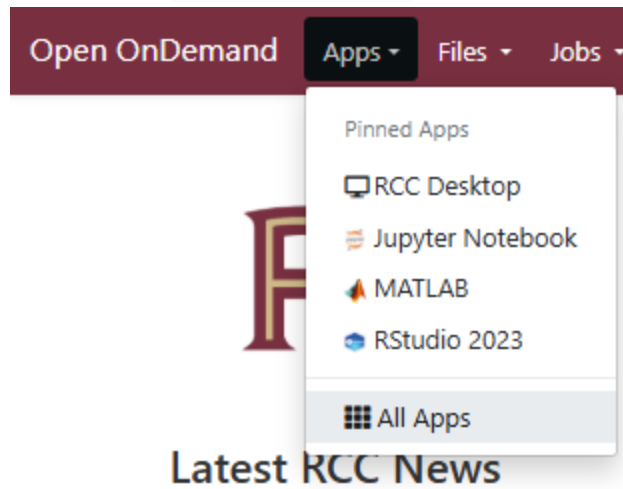
2. Click Jupyter Lab

3. Ensure that "Type of Environment Jupyter is installed in" is set to "Conda Environment", then in the "Path to Jupyter Conda Environment" field, enter `~/.conda/envs/chm4411l` .

Python version (required)

anaconda/3.12.4 ▾

This defines the version of Python you want to use

Type of Environment Jupyter is installed in

Conda Environment ▾

Jupyter Lab need to be installed on your home directory. In order to do that, you need to select which type of environment you'd like to use. By default a **Conda Environment** is used to ensure interoperability across our other Python IDEs.

Path to Jupyter Conda Environment

~/.conda/envs/chm4411l

Type the full path to your Jupyter Conda Environment (for example: `~/.conda/envs/myApp`). If the environment does not exist, it will be created for you. If you are creating a new environment, set the number of Cores to **AT LEAST 8!**

NOTE: The creation of a new Jupyter environment can take up to 5 or 10 minutes. Please be prepared to wait while the environment is created. The job dialog will indicate **'Starting'** while the environment is created.

☐ I would like to receive an email when the session starts

[Launch]

* The Jupyter Lab session data for this session can be accessed under the data root directory.

4. Click "Launch" and wait for your Jupyter Lab session to start up. This may take a few minutes; when it is finished, click the "Connect to Jupyter" button.

Checking that installation worked

1. Using the directory tree (on the left), navigate to the `pchem-II-lab-materials-worked` directory. Open the `chm4411l_installation_test.ipynb` file, and execute every cell. See if everything works.
2. If all the outputs work, congratulations! You are properly set up for the rest of the course.