

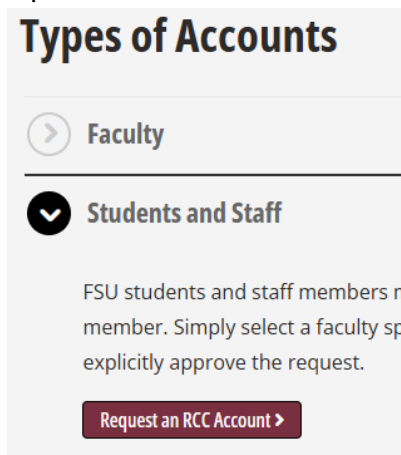
Getting set up on the HPC

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



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:



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.

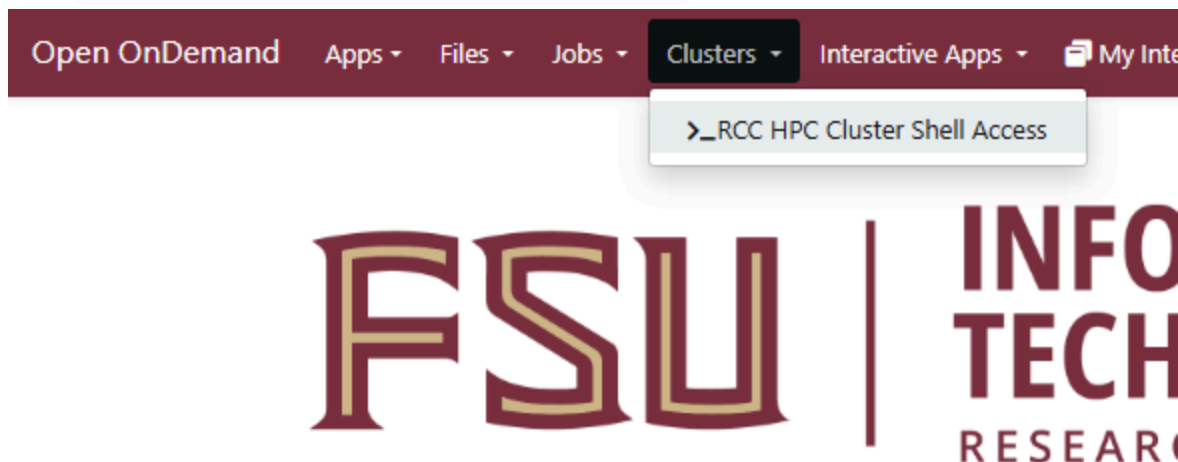
There are two primary ways we will use Open OnDemand to interface with the FSU HPC.

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.



Latest RCC News

07-28-2025

RCC Spotlight: Dr. Fanny Liu

Dr. Liu utilizes the HPC to develop new analytical methods in spectrometry.

2. You should see something like this:

```
Host: hpc-login.rcc.fsu.edu

Warning: Permanently added 'hpc-login.rcc.fsu.edu,144.174.41.24' (ECDSA) to the list of known hosts.

Welcome to the RCC

RCC/HPC Documentation can be found here:
https://rcc.fsu.edu/docs

Users of our general access scratch space, note that old data in our scratch
volume is periodically cleared. Details: https://rcc.fsu.edu/scratch

Last login: Wed Jul 30 10:18:27 2025 from 144.174.40.111

** Disk usage (GPFS) quota report: 100.26 used of 150G available
For a disk quota report, run: gpfs_quota

(base) [gdb20@h22-login-24 ~]$
```

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 instructor-materials`

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
'chm44111 Introduction to Computational Chemistry.pptx'  Diffraction          'T1 and T2 NMR'
'chm44111 programming.pptx'                            'Lab Chemicals.xlsx' templates
chm44111_setup.sh                                     lab_template.ipynb   TODO.md
chm44111.yml                                           Magnetism            todo.txt
compchem_hw                                           PHOTOELECTRIC        'Vibration-Rotation Spectra HCl-DCI'
'Computational Lab Feedback Questionnaire.docx'        PIB                  Waves
conda-testing                                          'Quantum Dots'
'Dark Pathways in Ruby'                               scratch
```

7. Check for the `chm44111_setup.sh` file. Run the following command:

```
chmod +x chm44111_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
'chm44111 Introduction to Computational Chemistry.pptx'  Diffraction          'T1 and T2 NMR'
'chm44111 programming.pptx'                            'Lab Chemicals.xlsx' templates
'chm44111_setup.sh'                                   lab_template.ipynb   TODO.md
chm44111.yml                                           Magnetism            todo.txt
compchem_hw                                           PHOTOELECTRIC        'Vibration-Rotation Spectra HCl-DCI'
'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.

```
./chm44111_setup.sh
```

Don't worry if you see error codes.

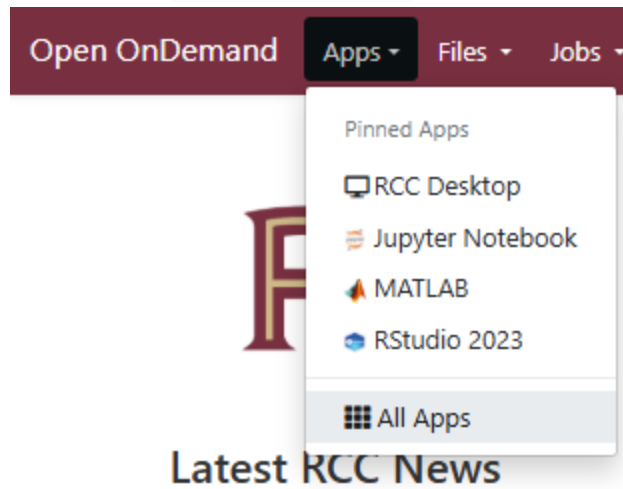
What we just did was to install all of the packages we will use for this course in a Conda virtual environment in the following directory: `~/conda/envs/chm44111`.

If we ever need to run something on the HPC in this environment, use `conda activate chm44111`

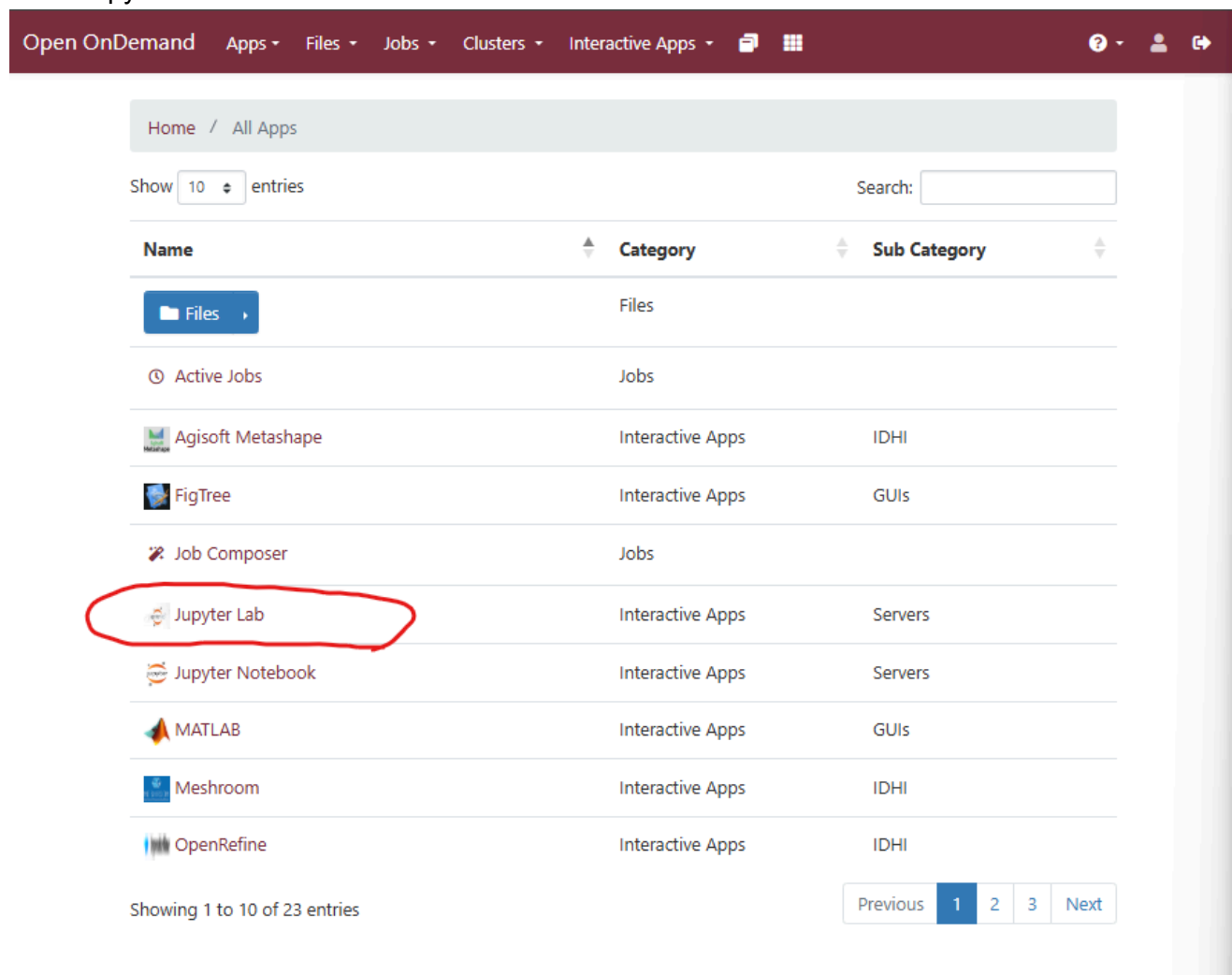
The immediate next thing we will do is open JupyterLab and use our newly created environment, where we can test if everything installed properly.

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/chm44111`.

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.