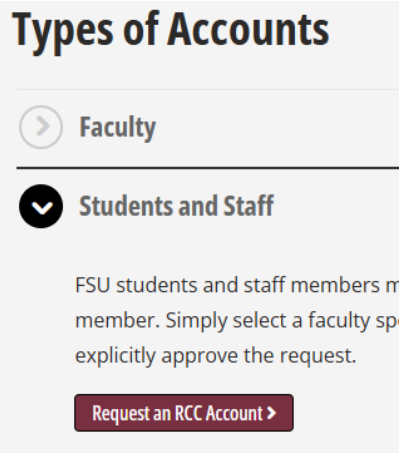
Getting set up on the HPC

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



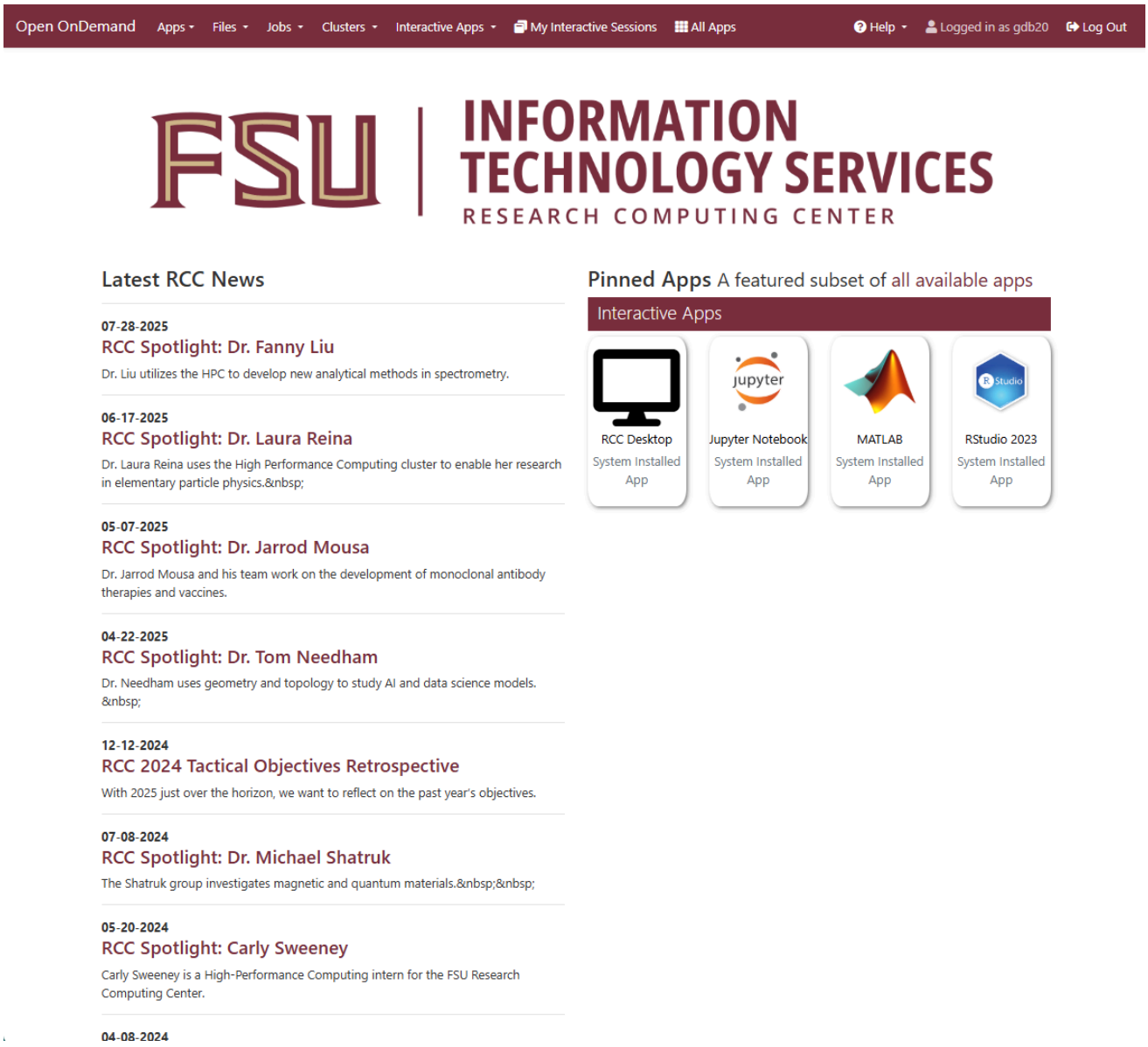
3. Log in with your normal FSU credentials
4. Fill out all the fields to request an account. As your sponsor, list the instructor in charge of your lab - in this case, Dr. Judy Clark.

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:



You may want to bookmark this page for future use.

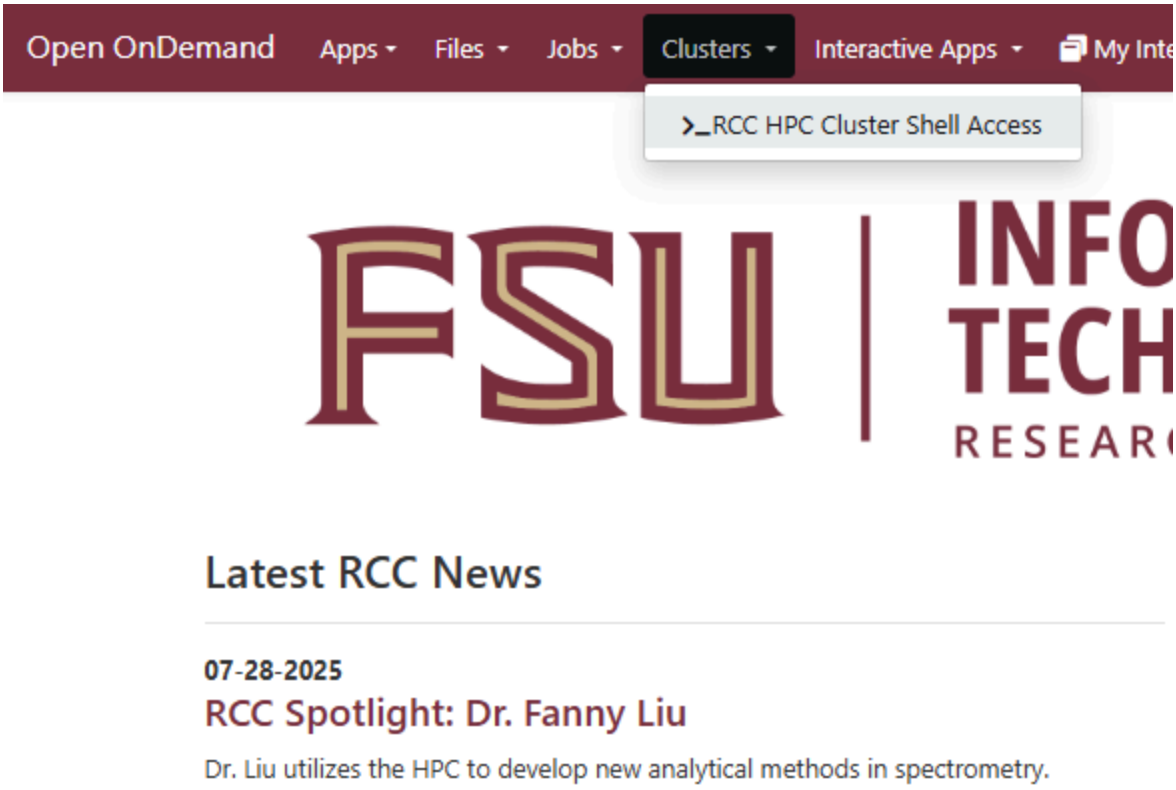
There are two primary ways we will use Open OnDemand to interface with the FSU HPC.

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`.



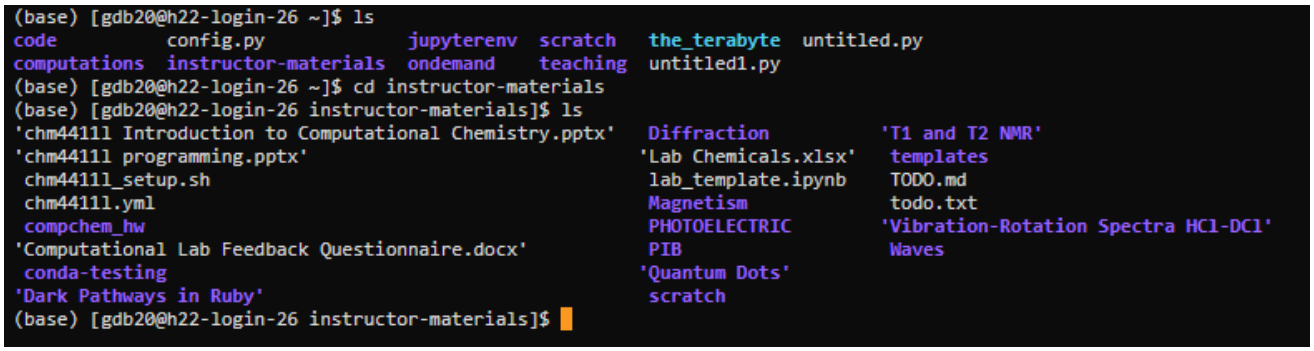
2. You should see something like this:

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/instructor-materials.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:



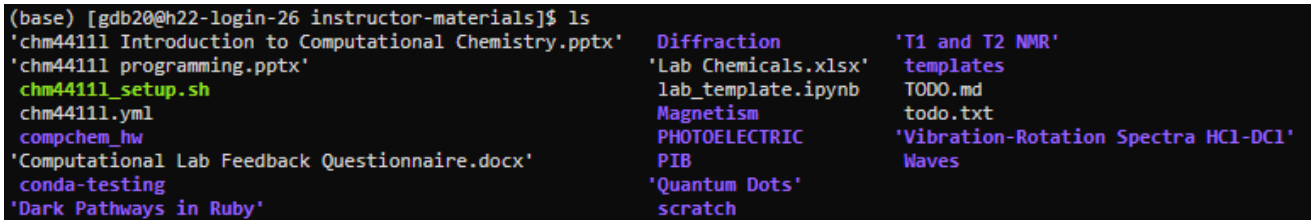
7. Check for the `chm4411l_setup.sh` file. Run the following command:

   `chmod +x chm4411l_setup.sh`

   then

   `ls`

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



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.

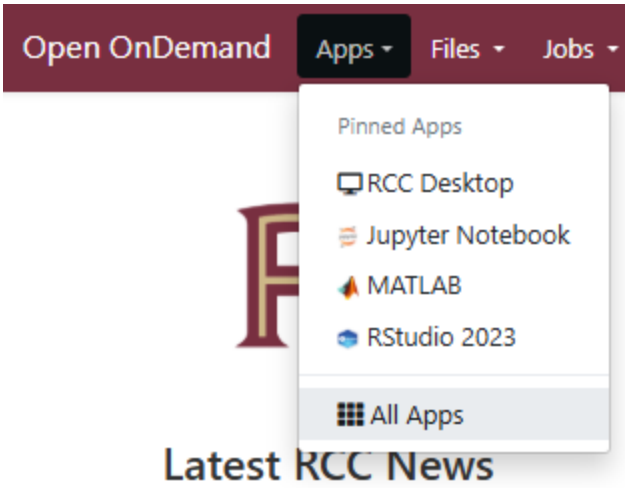
What we just did was to install all of the packages we will use for this course in a Conda virtual environment in the following directory: `~/.conda/envs/chm441l`.

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

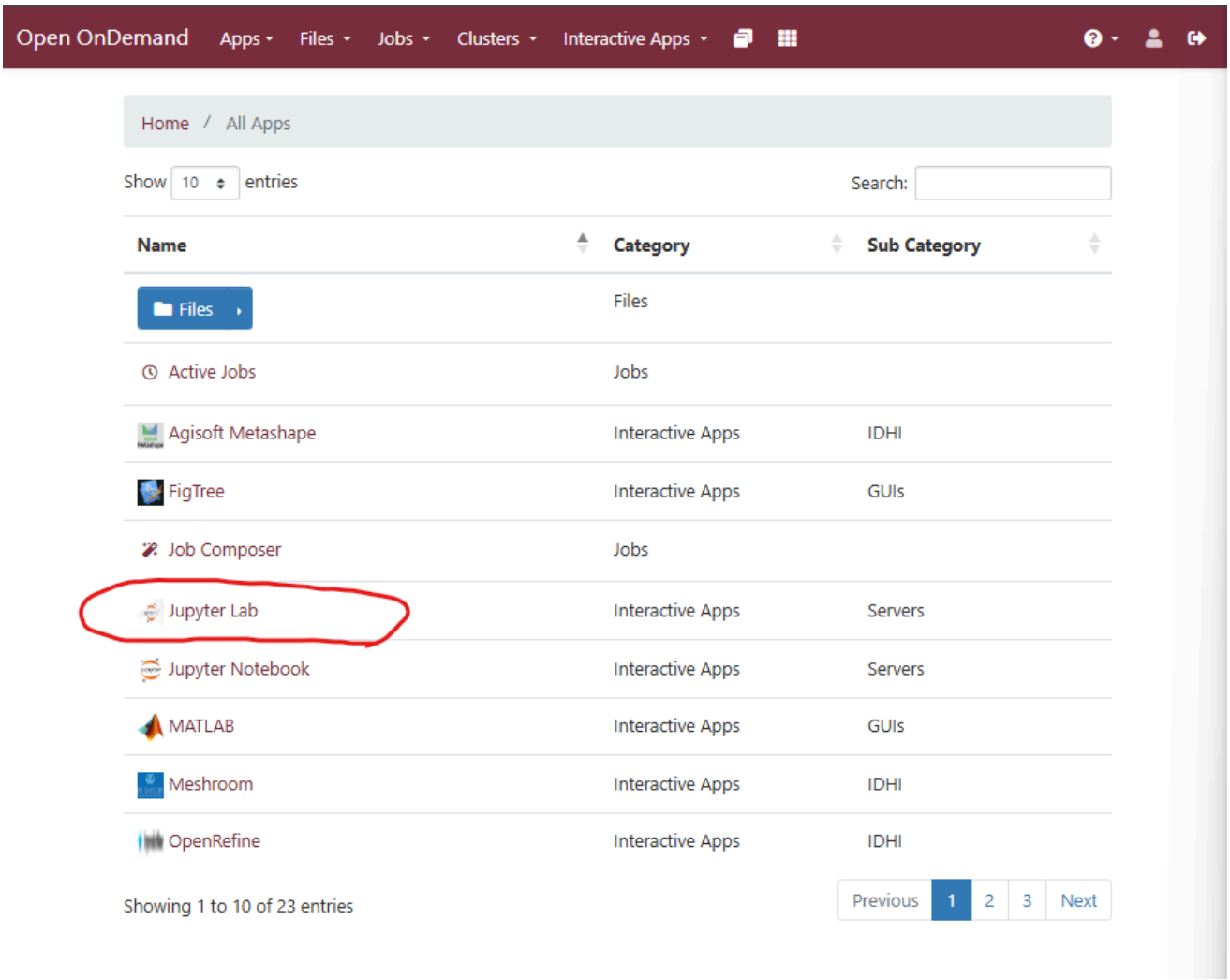
The immediate next thing we will do is open JupyterLab and use our newly created environment, where we can test if everything installed properly.

Using Jupyter Lab

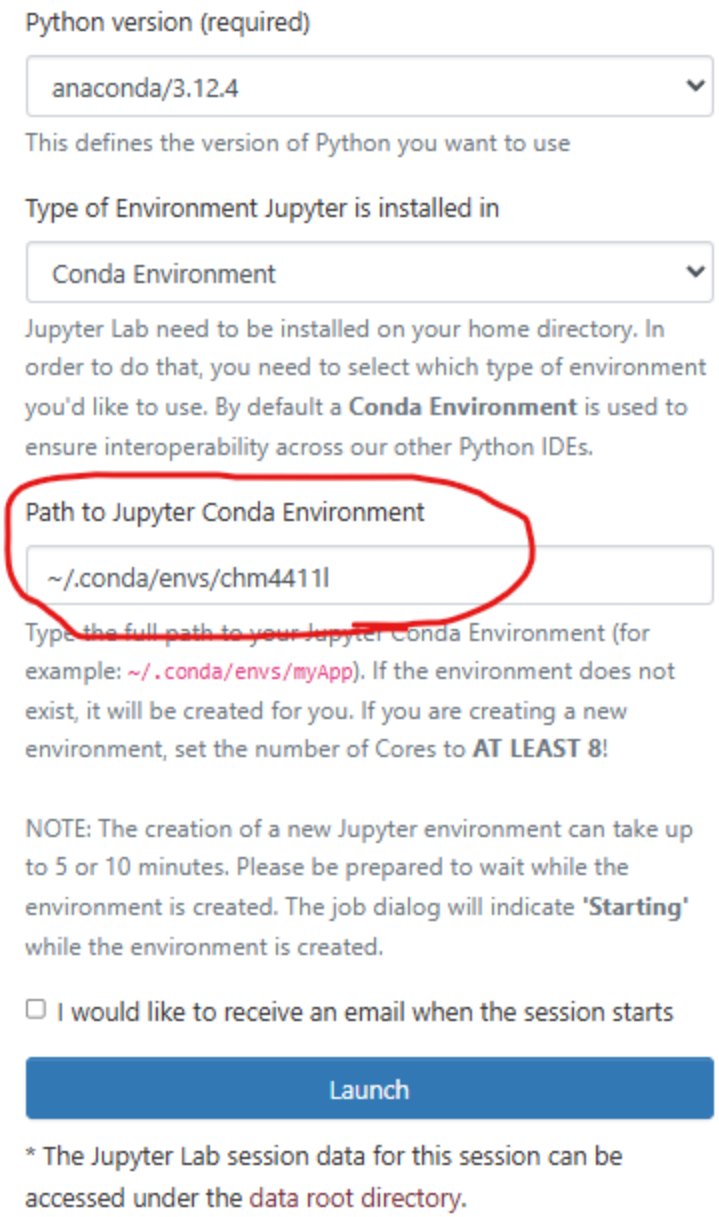
1. Navigate to `Apps > All Apps`



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`.



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.
5. You should already be acquanited with Jupyter from the first day Jupyter guide. If not, watch the video here: Jupyter video.

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.
   - [ ] todo: make key for what it should look like, maybe?
2. If all the outputs work, congratulations! You are properly set up for the rest of the course.