HW 6 Environment Set-up

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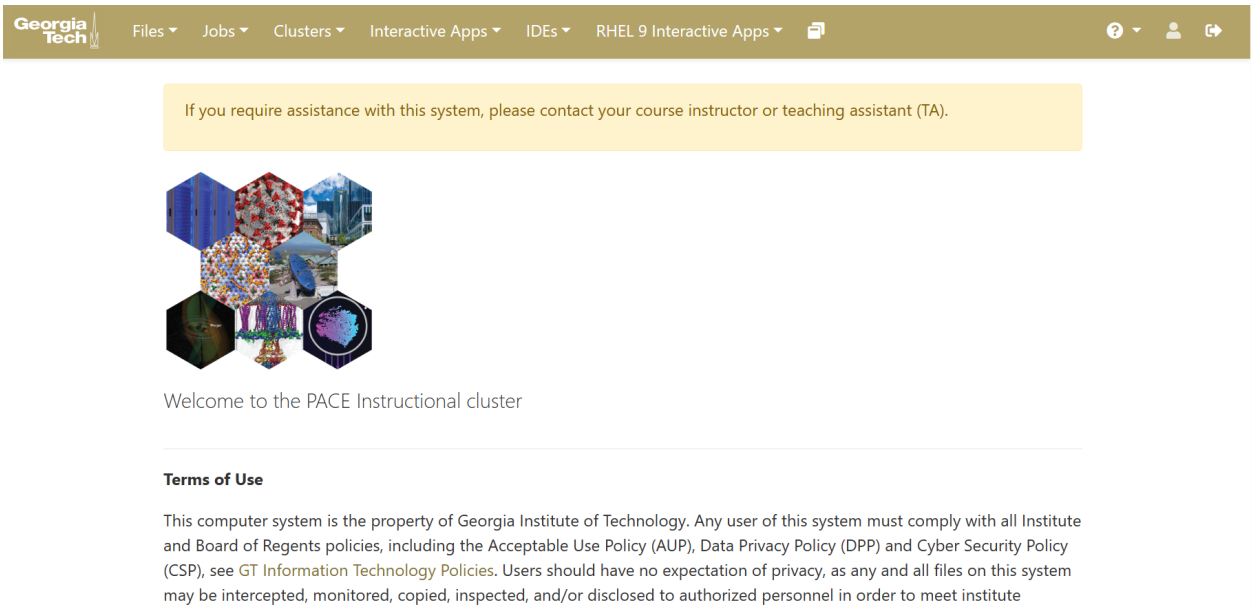
1. Prerequisites

Get familiar with step 1&2 and do step 3&4.

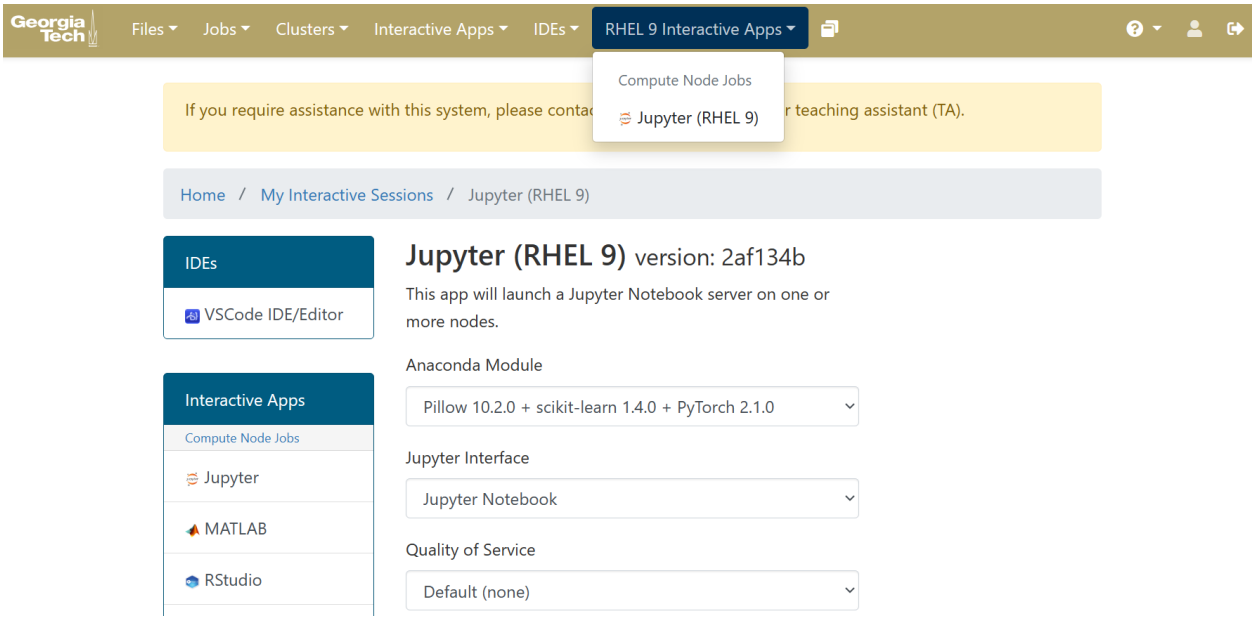
1. PACE Instructional Cluster Environment COC-ICE: https://docs.pace.gatech.edu/ice_cluster/ice/
2. Storage on ICE: https://gatech.service-now.com/technology?id=kb_article_view&sysparm_article=KB0042094
3. Download VPN client for your OS: https://gatech.service-now.com/home?id=kb_article_view&sysparm_article=KB0042139 (first to enter vpn.gatech.edu, then use your GT username and password to login.)
4. Login to the ICE cluster
    a. (ICE On Demand): https://gatech.service-now.com/home?id=kb_article_view&sysparm_article=KB0042133 (click the "ICE OnDemand", a new Dashboard window will pop out.). "Files→ Home Directory", it will show all your folders/files in your home directory. Click "Clusters→_ICE Shell Access" to open the shell, before opening HW6, we need to do environment set-up and install necessary ML libraries. (Prefer this option in your HW6.)
    b. Alternatively, via ssh, use `ssh someuser3@login-ice.pace.gatech.edu` , replace `someuser3` with your GT username.

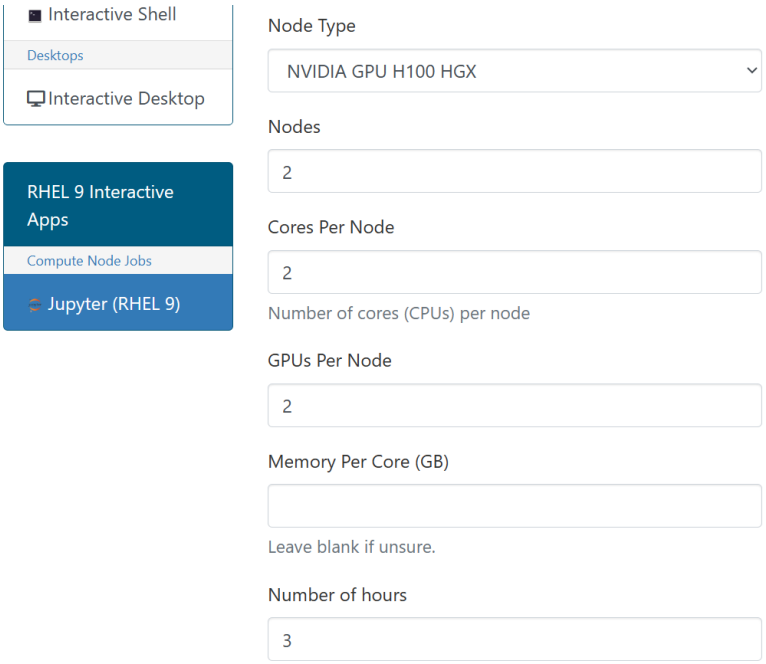
2. Open Jupyter Notebook and Run Your HW6

1. If you log in to ICE OnDemand successfully, then you should be able to see this interface: Dashboard - PACE ICE OnDemand (gatech.edu)

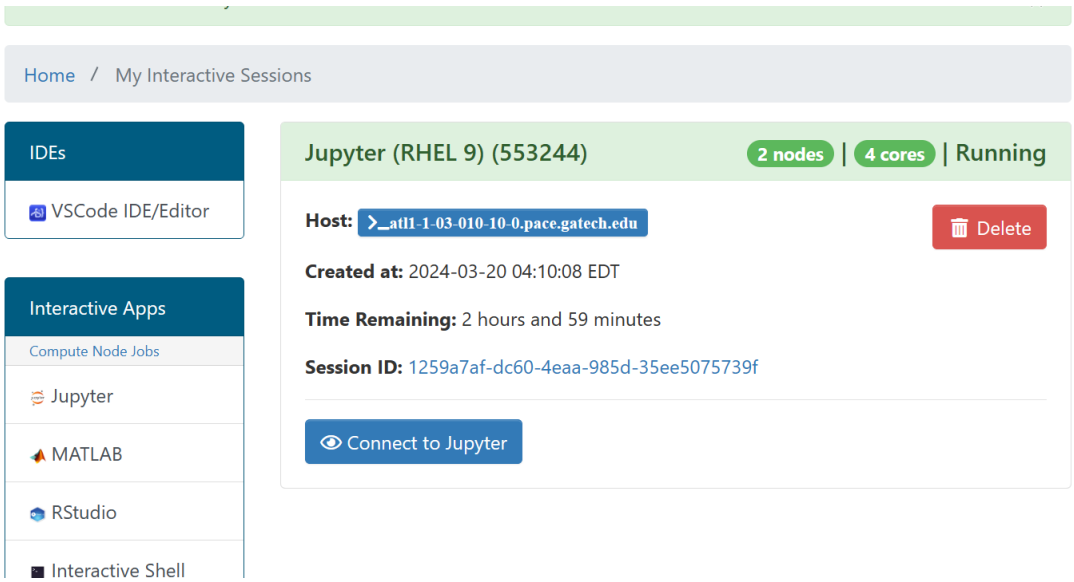


2. Click RHEL 9 Interactive Apps → Jupyter (RHEL 9), this is exclusively for the interactive App job creation on H100 nodes and you should be able to see this interface (~visualization to submit a slurm job). Under Anaconda Module, just choose “Pillow 10.2.0 + scikit-learn 1.4.0 + PyTorch 2.1.0” and thanks to Yongnuo Yang(yyang879@gatech.edu), it is all you need to implement your HW6 for this course! Choose Node Type as NVIDIA GPU H100 HGX, then launch.





3. You will see your job is whether queued, starting and running. If it is running, then you can click “Connect to Jupyter” to redirect to the jupyter notebook. Put your hw6 file under the “scratch” folder.



For HW6, you are all set! If you want to dive deeper about PACE-ICE, Anaconda, conda environment, you can refer below for some commands you may need to

build your own environment.

3. Module Load Anaconda

1. First, you can check on the current python version:

   ```
   [xchen920@login-ice-1 ~]$ python -V
   Python 2.7.5  # right
   ```

   If your python version is already python3.8 or python3.9, you are good. If not, follow step 2-3 below to upgrade your python.

2. You CANNOT directly install conda in your home directory which has a relatively small storage quota, rather you should place everything involving HW6 in your scratch directory, which has more storage quota.

3. Fortunately, PACE has several anaconda installations available, you do not have to install anaconda from the source by yourself and you can simply use module load instead. Remember every time you log in to PACE, you should re-load module load procedure.

   a. Check available anaconda installations by this command `module spider anaconda`

   ```
   [xchen920@login-ice-1 ~]$ module spider anaconda
   ----------------------------------------------------------
     anaconda3:
   ----------------------------------------------------------
        Versions:
           anaconda3/2021.05
           anaconda3/2022.05
           anaconda3/2022.05.0.1
   ----------------------------------------------------------
     For detailed information about a specific "anaconda3" pa
     Note that names that have a trailing (E) are extensions
     For example:
        $ module spider anaconda3/2022.05.0.1
   ```

b. Download the conda by using the command: `module load anaconda3/2022.05.0.1`

```
[xchen920@login-ice-1 ~]$ module load anaconda3/2022.05.0
(base) [xchen920@login-ice-1 ~]$
```

if you see the base environment, then you are all set. Remember, you need to reload the module everytime you re-log into shell.

c. Last, check your python version again, it should be python3. Mine is python3.9.12.

```
(base) [xchen920@login-ice-1 ~]$ python -V
Python 3.9.12
```

4. Conda Virtual Environment and Conda Install Packages

1. Before we install packages like `pytorch` , we need to create conda virtual environment.

   a. Use command line `conda env list` to check what environments you have. You should have a base environment and see an output like this:

```
(base) [xchen920@login-ice-1 ~]$ conda env list

# conda environments:
#
base                  *  /usr/local/pace-apps/manual/packages
```

   b. Use `conda create --name funml` to create the virtual environment. (You can replace funml with your own ENV-NAME). Then use `conda env list` again, you should see an output like this:

```
(base) [xchen920@login-ice-1 ~]$ conda env list
# conda environments:
#
funml                    /home/hice1/xchen920/.conda/envs/fu
base                  *  /usr/local/pace-apps/manual/package
```

c. If you want to delete the virtual environment, then use commands below. It might take some time.

```
(funml) [xchen920@login-ice-1 ~]$ conda deactivate
(base) [xchen920@login-ice-1 ~]$ conda remove -n funml --all

...
#[y/n]? simply enter y as yes to delete
...
```

2. Install packages:

   a. `conda install pytorch::pytorch` to install pytorch

```
(funml) [xchen920@login-ice-1 ~]$ conda install pytorch::pyt

...
[y/n]? -y
...
```

b. `conda install pytorch::torchvision` to install torchvision, similarly.

c. How to check if your packages are installed correctly? In terminal, you can do this:

```
(funml) [xchen920@login-ice-1 ~]$ python
Python 3.12.2 | packaged by Anaconda, Inc. | (main, Feb 27 2
Type "help", "copyright", "credits" or "license" for more in
>>> import torch
>>> from torchvision.datasets import ImageFolder
```

```
>>> from torchvision import transforms
>>> exit()
(funml) [xchen920@login-ice-1 ~]$
```

5. Conda install Jupyter Notebook

1. Conda install Jupyter Notebook:

```
conda install -c conda-forge jupyterlab # or alternatively, c
```

2. Conda install the `ipykernel` package to support Jupyter:

```
conda install ipykernel
```

See **Open OnDemand section** to open your file in Jupyter Notebook: https://gatech.service-now.com/home?id=kb_article_view&sysparm_article=KB0043479

Appendix

1. Intro to H100 nodes (the ones for AI-Makerspace):

   https://gatech.service-now.com/home?id=kb_article_view&sysparm_article=KB0043479

2. Anaconda:

   https://gatech.service-now.com/home?id=kb_article_view&sysparm_article=KB0041621

3. Pytorch:

   https://gatech.service-now.com/home?id=kb_article_view&sysparm_article=KB0041546