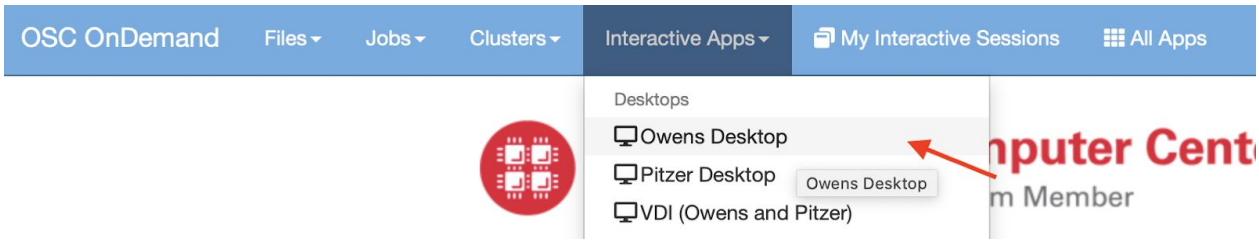
Parallel Computing

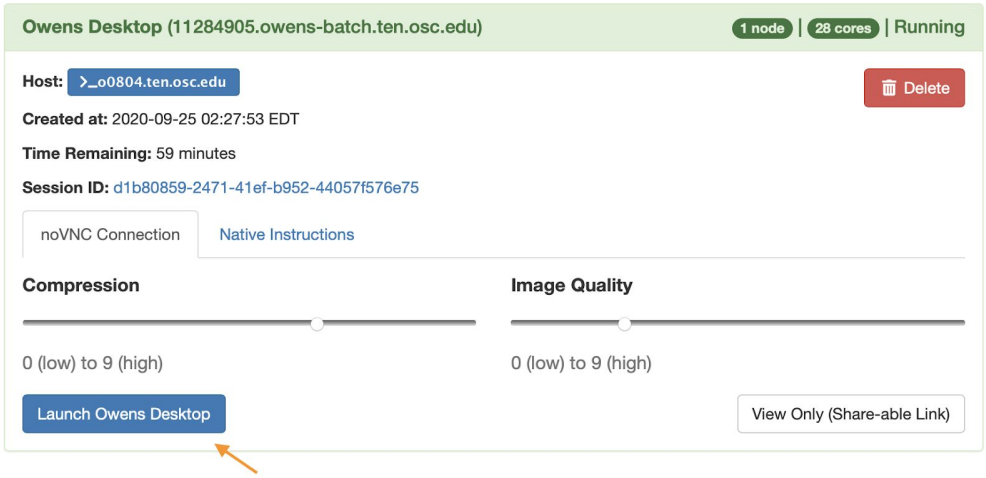
Working With Python And Numba On OSC

Getting Started

1. Go to https://ondemand.osc.edu and login into your account.
2. From the navigation menu, go to Interactive Apps -> Owens Desktop.
    a. You are able to use Pitzer as well as along you select a node type with a GPU in step 3.



3. Create an environment with the following attributes:
    a. Desktop environment: Xfce
    b. Account: PES0830 (or another account if it's different)
    c. Number of hours: 1 (provide any time you desire)
    d. Number of nodes: 1
    e. Node type: vis
4. Wait until your environment is ready.
5. When your environment is ready, you can either "Launch Owens Desktop" for a graphical interface or optionally ssh in. The rest of this guide will assume you have pressed "Launch Owens Desktop", however, you can perform the same steps through ssh.



6. In your Owens Desktop environment, open a terminal.
7. Load the latest supported version of Python and Conda module with `module load python/3.6-conda5.2`.
    a. For an updated list of supported Python and Conda modules: https://www.osc.edu/resources/available_software/software_list/python
    b. By having a Conda environment, you will be able to create multiple Python environments easily.
8. Create a Python 3.6 environment called “py36” in Conda with `conda create -n py36 python=3.6`.
9. Activate the environment: `source activate py36`.
10. Load the CUDA module: `module load cuda`.
11. Now you can install Numba and any of your other desired Python packages: `conda install numba`.
    a. Alternatively you can also use `pip3 install <package-name>` (which will be required for packages not available on Conda).

        Note: There may be issues with installing Numba with Pip so Conda will be preferred for this package.

12. At this point, as long as you’re still in your Conda environment, you can run any Python script with: `python3 <your-python-file`.

Creating Future Environments

When you create a new Owens environment in the future, most of your configuration will be saved. You will just need to load the appropriate modules again and activate your Conda environment to re-use it:

1. `module load python/3.6-conda5.2 && module load cuda && source activate py36`.

Transfer Files To And From OSC

Refer to guide this by OSC to learn how to transfer files to and from your environment:
https://www.osc.edu/resources/online_portals/ondemand/file_transfer_and_management

Numba Documentation

For information on how to work with Numba, documentation can be found here:
https://numba.readthedocs.io/en/stable/user/5minguide.html

You will also want to refer to its usage with CUDA:
https://numba.readthedocs.io/en/stable/cuda/index.html

Timing CUDA GPU Events

To time Numba CUDA GPU events, you can use either the Numba Events API or install numba_timer for a simpler interface:

1. `pip3 install numba_timer`

numba_timer documentation can be found here:
https://github.com/mihi-r/numba_timer

If you prefer to use the Numba Events API:
https://numba.pydata.org/numba-doc/latest/cuda-reference/host.html#events