Hoffman2 Happy Hour: Anaconda for HPC

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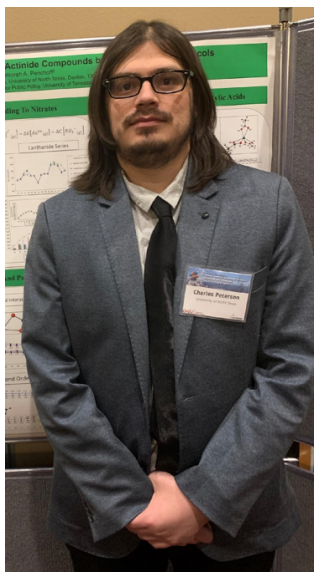
Overview

Welcome to Hoffman2 Happy Hour!

The H^{2}HH are designed to be short interactive talks that focus on a certain aspect of HPC.

- In this H^{2}HH we will go over using Anaconda on Hoffman2

- This information can be applied to other HPC resources



Any suggestions for upcoming workshops, email me at cpeterson@oarc.ucla.edu

Files for this Presentation

This presentation can be found on our UCLA OARC's github repo.

- https://github.com/ucla-oarc-hpc/H2HH_anaconda

View slides:

- PDF format: `H2HH_anaconda.pdf`
- html format:
  - The html sildes can be viewed at:
  - https://ucla-oarc-hpc.github.io/H2HH_anaconda

> **Note**
>
> This presentation was build with Quarto and RStudio.
>
> - Quarto file: `H2HH_anaconda.qmd`

What is Anaconda

- Anaconda is a very popular Python and R distribution.

- Great option for simplifying package management and pipelines.

- Easily install popular Python and R packages.

Why use Anaconda

- Easy install many python and R packages with simple `conda` commands
- Create isolated python/R environments for different projects
  - Different python/R setups and switch between them
- Checks and solve for possible version conflicts when installing packages
- Share conda env on different systems.
  - Version control!

Starting Anaconda

On Hoffman2, Anaconda is installed and can be used by loading modules

- See available anaconda versions

```
1  module av anaconda
```

- Load anaconda in your environment

```
1  module load anaconda3/2020.11
```

- Loading the anaconda module will setup anaconda in your environment and ready to be used!

> **Important**
>
> By using anaconda, you do **NOT** need to load any other python/R modules. The python/R builds will be available via anaconda.
>
> Using other python build might cause conflicts with your anaconda python (or R)

Anaconda environment

- Anaconda environments (conda env) is a virtual environment
  - install and update packages that you can control
- These conda env's will reside in your personal workspace
  - By default `$HOME/.conda`
- Conda is also a package manager
  - Many packages/software can be install via Conda's repository
  - https://anaconda.org/anaconda/repo
- Can also install python packages within your conda env outside of Conda's repo
  - PyPI's `pip` for python
  - R's CRAN software repository

Creating conda env

Creating a new conda environment

```
conda create [options]
conda create -n myconda
```

- The –n option will name your new conda env

You can install packages and software while creating the env

```
conda create -n myconda python
```

Install multiple conda packages with `conda create` command

```
conda create -n myconda python=3.9 pandas scipy r-base
```

This will install

- python version 3.9
- scipy
- R

Conda envs

See list of all your environments that you have created

```
conda env list
```

Start (activate) your conda environment

```
conda activate myconda
```

Activating the conda env gives access to the software within the env

This version of `python` and R is installed locally in your conda env and is different from the builds of python on Hoffman2.

You can see location of python in your env and check the version.

```
which python
python -V
```

Important

You do **NOT** need to load the python module if you installed python via anaconda.

Tips for running on HPC

You maybe familiar with using Anaconda on your local machine.

- Running on HPC may be different.

> ⚠ **Warning**
>
> Do not use conda's default `base` env

When conda is install, it creates an conda env named `base` that you may see when running `conda env list`

- Located in the central anaconda installation path **CANNOT** be modified by users

Tips for running on HPC

> ⚠ **Warning**
>
> Do not run `conda init` on H2.

You may see messages or online tips about running the `conda init` command.

This initializes conda but is **NOT NEEDED** to run on Hoffman2

While this does setup conda, it will change ~/.bashrc and may cause conflicts using different versions/envs.

Loading the anaconda module will already setup conda.

Installing packages

Once your conda env is activate, you can install more packages with

- `conda install`

```
conda create -n myconda
conda activate myconda
conda install python=3.9 pandas scipy tensorflow -c conda-forge
```

> **Note**
>
> The `-c` option in conda is for the "conda channel". The conda channels are different locations where packages are stored. Examples are 'conda-forge', 'bioconda', 'defaults', etc. Conda will search though the available channels for the request packages to install.

Installing packages

You can use `pip` when you are in a conda env

```
conda activate myconda
pip3 install scipy
```

> **Tip**
>
> When using pip/pip3 in a conda env, you do **NOT** need to have `--user`. Using just `pip` will install the package inside the conda env. If you use `--user`, it will install the package in outside of the conda env, inside of `~/.local` and may cause conflicts with other python builds or conda env's you have.

Tips

By default, when you install a conda env, it will install it at `~/.conda`

You can change this location, esp if you are low in space at `$HOME`

```
conda create -p $SCRATCH/mypython python=3.9
conda activate $SCRATCH/mypython
```

- Some detailed information on using Anaconda on Hoffman2 can be found on our website

- https://www.hoffman2.idre.ucla.edu/Using-H2/Software/Software.html#anaconda

Job examples

Once you create you env, you don't need to create it again.

```
qrsh -l h_data=5G
module load anaconda3/2020.11
conda activate myconda
python test.py
```

Job script example

```
#!/bin/bash
#$ -cwd
#$ -j y
#$ -l h_rt=1:00:00,h_data=5G
#$ -pe shared 1

# load the anaconda module
. /u/local/Modules/default/init/modules.sh
module load anaconda3/2020.11
# Activate the 'myconda' conda env
conda activate myconda

```

Searching for anaconda packages

Find software that is available on Anaconda's package repo

- https://anaconda.org/anaconda/repo

Here, you can search for software and other packages. It will also explain what conda commands you need to install them inside your conda env.

Using yml files

You can create a conda file from a `environment.yml` file

```yaml
name: myconda
dependencies:
  - numpy
  - pandas
  - python=3.9
```

You can create a conda env with all these packages by running:

```
conda env create -f environment.yml
```

Using yml files

An `.yml` file can be created from an existing conda env so you can create the same conda env.

```
conda activate myconda
conda env export > environment.yml
```

This file can be shared with others to reproduce any conda env.

- Keep the same versions of packages when running anaconda on different HPC resources

> **Tip**
>
> We have a collection of `.yml` files that we made to use on Hoffman2
>
> https://github.com/ucla-oarc-hpc/hpc_conda

Installing Anaconda

While Hoffman2 already has Anaconda install, you may need to install Anaconda on a separate machine or another HPC resource.

Visit https://repo.anaconda.com/archive/ for all the versions of Anaconda that are available.

In this example, anaconda is install at `$HOME/apps/anaconda/2021.11`

```
#Download anaconda script for Linux
wget https://repo.anaconda.com/archive/Anaconda3-2021.11-Linux-x86_64.sh
#Run Anaconda installer
bash Anaconda3-2021.11-Linux-x86_64.sh -p $HOME/apps/anaconda/2021.11 -b
```

Now create and activate a conda env with this new anaconda build

```
# Setup Anaconda
source $HOME/apps/anaconda/2021.11/etc/profile.d/conda.sh
# Create new conda env
conda create -n myconda python=3.9
conda activate myconda
```

Installing Anaconda

> **Tip**
>
> Don't run `conda init`
>
> Instead, `source /CONDA/PATH/etc/profile.d/conda.sh`
>
> This will setup Anaconda without changing the ~/.bashrc file

> **Tip**
>
> Miniconda is a good alternative to Anaconda.
>
> It is a Minimal installer for conda that is smaller than Anaconda.

Thank you!

Questions? Comments?

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- cpeterson@oarc.ucla.edu
- Look at for more Hoffman2 workshops at https://idre.ucla.edu/calendar
  - Search for HPC