Creating a Custom Python Environment on Nova

Caleb Leedy

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There are several methods to use Python modules on the Jupyter Lab server on Nova. This document discusses two different techniques.

Method 1: Nova Modules

Method 2: Custom Virtual Environments

When you open Jupyter Lab, there are two icons that initally appear. One that says "Python (ipykernel)" and another that says "default-env". These are the default virtual environments. This guide explains how to create custom ones.

1. Connect to the Nova terminal. This can be done via `ssh`, Nova OnDemand Desktop terminal, Nova OnDemand Shell, or a terminal with the Jupyter or RStudio Server environment.
2. On the command line load the Python module

```
module load python/3.11.9-i2aasxp
```

3. Create if needed (using `mkdir`) and then go to project directory

```
cd /work/LAS/zhuz-lab/<USERNAME>/<DIRNAME>
```

4. Create a virtual environment

```
python -m venv venv
```

5. Source the virtual environment

```
source venv/bin/activate
```

6. Install all needed packages AND ipykernel

```
python -m pip install torch torchvision \
  torchaudio --index-url https://download.pytorch.org/whl/cu118
python -m pip install matplotlib
python -m pip install ipykernel
```

7. Create the kernel

```
python -m ipykernel install --user --name "<KERNELNAME>"
```

8. Deactivate the virtual environment

```
deactivate
```

9. (Optional) Add soft link to home

```
cd
ln -s /work/LAS/zhuz-lab/<USERNAME>/<DIRNAME> <DIRNAME>
```

To check that this worked do the following:

1. Go back to Nova OnDemand and start a Jupyter Lab session. (Under the Interactive Apps tab.)
2. Wait until the Connect to Jupyter button appears. Then click it.
3. When the Jupyter Lab launcher appears click the KERNELNAME notebook.

To add additional modules, we do not need to create our environment. This means that we only need to run the following shell commands:

```
module load python/3.11.9-i2aasxp
cd /work/LAS/zhuz-lab/<USERNAME>/<DIRNAME>
source venv/bin/activate
python3 -m pip install <PACKAGENAME>
deactivate
```