Python Environments with Anaconda3 on Delta

- Recent Changes
- Batch Jobs
- Jupyter with Open OnDemand
  - For debugging purposes, try jupyter-lab from a terminal:

Recent Changes

To address a problem with `PATH` ordering when using anaconda3 modules, a warning in the module was put in place to caution loading an anaconda3 module while in a virtual environment, or if `conda init` has been used to modify one's environment.

```
(base) [arnoldg@dt-login03 ~]$ module load anaconda3_gpu
A conda environment has been detected CONDA_PREFIX=
/sw/external/python/anaconda3
anaconda3_gpu is loaded. Consider running conda deactivate and reloading it.
```

see also: https://docs.conda.io/projects/conda/en/latest/configuration.html , if you want to disable automatic conda environment activation

Batch Jobs

Batch jobs will honor the commands you execute within them. Purge/unload/load modules, or deactivate/activate environments as needed for that job.

A clean slate job might resemble:

user has a conda init clause in bashrc

```
conda deactivate
conda deactivate  # just making sure
module purge
module reset  # load the default Delta modules

conda activate base
# commands to load modules and activate environs
```

Non-python/conda HPC users would see per-job stderr from the *conda deactivate* above:

user has never ran "conda init bash"

```
[arnoldg@dt-login03 ~]$ conda deactivate
bash: conda: command not found
[arnoldg@dt-login03 ~]$

# or

[arnoldg@dt-login03 ~]$ conda deactivate

CommandNotFoundError: Your shell has not been properly configured to use 'conda deactivate'.
To initialize your shell, run

    $ conda init <SHELL_NAME>

Currently supported shells are:
  - bash
  - fish
  - tcsh
  - xonsh
  - zsh
  - powershell

See 'conda init --help' for more information and options.

IMPORTANT: You may need to close and restart your shell after running 'conda init'.
```

Jupyter with Open OnDemand

Jupyter and jupyter-lab will find the environments in your $HOME/.conda/envs -- your login shell should reflect what you want to see from Jupyter.

The list of avail. kernels for Jupyter should be the same as what you see from a login shell and python3 (https://github.com/Anaconda-Platform/nb_conda_kernels).

Jupyter needs to be installed in every virtual environment where you want to use with Jupyter-lab or Jupyter-notebook.

   $ conda install jupyter

nb_python_kernels

```
[arnoldg@dt-login03 jupyter_notebook_config.d]$ python3 -m nb_conda_kernels list
[ListKernelSpecs] WARNING | Config option `kernel_spec_manager_class` not recognized by `ListKernelSpecs`.
[ListKernelSpecs] [nb_conda_kernels] enabled, 8 kernels found
Available kernels:
  conda-env-westpa20-py          /projects/bbka/arnoldg/westpa20/share/jupyter/kernels/python3
  conda-root-py                  /sw/external/python/anaconda3/share/jupyter/kernels/python3
  conda-env-anaconda3_Rcpu-r     /sw/external/python/anaconda3_rcpu/share/jupyter/kernels/ir
  conda-env-anaconda3_Rcpu-py    /sw/external/python/anaconda3_rcpu/share/jupyter/kernels/python3
  conda-env-westpa-2022.03-py    /sw/external/python/westpa-2022.03/share/jupyter/kernels/python3
  conda-env-.conda-myclone-py    /u/arnoldg/.conda/envs/myclone/share/jupyter/kernels/python3
  conda-env-.conda-mynewenv-r    /u/arnoldg/.conda/envs/mynewenv/share/jupyter/kernels/ir
  conda-env-.conda-mynewenv-py   /u/arnoldg/.conda/envs/mynewenv/share/jupyter/kernels/python3
  python3                        /sw/external/python/anaconda3_gpu/share/jupyter/kernels/python3
```

For debugging purposes, try jupyter-lab from a terminal:

Of interest are the Searching path at the beginning, and the nb_conda_kernels outputs.

jupyter-lab --log-level=0

```
[arnoldg@dt-login03 jupyter_notebook_config.d]$ jupyter-lab --log-level=0
[D 2023-02-20 12:48:50.533 ServerApp] Searching ['/u/arnoldg/.jupyter', '/u/arnoldg/.local/etc/jupyter', '/sw
/external/python/anaconda3/etc/jupyter', '/usr/local/etc/jupyter', '/etc/jupyter'] for config files
[D 2023-02-20 12:48:50.533 ServerApp] Looking for jupyter_config in /etc/jupyter
```

```
[D 2023-02-20 12:48:50.533 ServerApp] Looking for jupyter_config in /usr/local/etc/jupyter
[D 2023-02-20 12:48:50.533 ServerApp] Looking for jupyter_config in /sw/external/python/anaconda3/etc/jupyter
[D 2023-02-20 12:48:50.534 ServerApp] Loaded config file: /sw/external/python/anaconda3/etc/jupyter
/jupyter_config.json
[D 2023-02-20 12:48:50.534 ServerApp] Looking for jupyter_config in /u/arnoldg/.local/etc/jupyter
[D 2023-02-20 12:48:50.534 ServerApp] Looking for jupyter_config in /u/arnoldg/.jupyter
[D 2023-02-20 12:48:50.537 ServerApp] Looking for jupyter_server_config in /etc/jupyter
[D 2023-02-20 12:48:50.537 ServerApp] Looking for jupyter_server_config in /usr/local/etc/jupyter
[D 2023-02-20 12:48:50.537 ServerApp] Looking for jupyter_server_config in /sw/external/python/anaconda3/etc
/jupyter
[D 2023-02-20 12:48:50.537 ServerApp] Looking for jupyter_server_config in /u/arnoldg/.local/etc/jupyter
[D 2023-02-20 12:48:50.537 ServerApp] Looking for jupyter_server_config in /u/arnoldg/.jupyter
[D 2023-02-20 12:48:50.538 ServerApp] Paths used for configuration of jupyter_server_config:
            /etc/jupyter/jupyter_server_config.json
[D 2023-02-20 12:48:50.538 ServerApp] Paths used for configuration of jupyter_server_config:
            /usr/local/etc/jupyter/jupyter_server_config.json
[D 2023-02-20 12:48:50.539 ServerApp] Paths used for configuration of jupyter_server_config:
            /sw/external/python/anaconda3/etc/jupyter/jupyter_server_config.d/jupyterlab.json
            /sw/external/python/anaconda3/etc/jupyter/jupyter_server_config.d/nbclassic.json
            /sw/external/python/anaconda3/etc/jupyter/jupyter_server_config.d/notebook_shim.json
            /sw/external/python/anaconda3/etc/jupyter/jupyter_server_config.d/panel-client-jupyter.json
            /sw/external/python/anaconda3/etc/jupyter/jupyter_server_config.json
[D 2023-02-20 12:48:50.541 ServerApp] Paths used for configuration of jupyter_server_config:
            /u/arnoldg/.local/etc/jupyter/jupyter_server_config.d/ipyparallel.json
            /u/arnoldg/.local/etc/jupyter/jupyter_server_config.json
[D 2023-02-20 12:48:50.541 ServerApp] Paths used for configuration of jupyter_server_config:
            /u/arnoldg/.jupyter/jupyter_server_config.json
Note: detected 128 virtual cores but NumExpr set to maximum of 64, check "NUMEXPR_MAX_THREADS" environment
variable.
Note: NumExpr detected 128 cores but "NUMEXPR_MAX_THREADS" not set, so enforcing safe limit of 8.
NumExpr defaulting to 8 threads.
[I 2023-02-20 12:48:51.954 ServerApp] ipyparallel | extension was successfully linked.
[W 2023-02-20 12:48:51.957 LabApp] Config option `kernel_spec_manager_class` not recognized by `LabApp`.
[W 2023-02-20 12:48:51.958 LabApp] Config option `kernel_spec_manager_class` not recognized by `LabApp`.
[W 2023-02-20 12:48:51.960 LabApp] Config option `kernel_spec_manager_class` not recognized by `LabApp`.
[I 2023-02-20 12:48:51.961 ServerApp] jupyterlab | extension was successfully linked.
[W 2023-02-20 12:48:51.962 NotebookApp] Config option `kernel_spec_manager_class` not recognized by
`NotebookApp`.
[W 2023-02-20 12:48:51.963 NotebookApp] Config option `kernel_spec_manager_class` not recognized by
`NotebookApp`.
[W 2023-02-20 12:48:51.965 NotebookApp] Config option `kernel_spec_manager_class` not recognized by
`NotebookApp`.
[I 2023-02-20 12:48:51.965 ServerApp] nbclassic | extension was successfully linked.
[D 2023-02-20 12:48:51.968 ServerApp] Paths used for configuration of jupyter_notebook_config:
            /u/arnoldg/.jupyter/jupyter_notebook_config.json
[D 2023-02-20 12:48:51.968 ServerApp] Paths used for configuration of jupyter_notebook_config:
            /etc/jupyter/jupyter_notebook_config.json
[D 2023-02-20 12:48:51.969 ServerApp] Paths used for configuration of jupyter_notebook_config:
            /usr/local/etc/jupyter/jupyter_notebook_config.json
[D 2023-02-20 12:48:51.969 ServerApp] Paths used for configuration of jupyter_notebook_config:
            /sw/external/python/anaconda3/etc/jupyter/jupyter_notebook_config.d/jupyterlab.json
            /sw/external/python/anaconda3/etc/jupyter/jupyter_notebook_config.d/panel-client-jupyter.json
            /sw/external/python/anaconda3/etc/jupyter/jupyter_notebook_config.json
[D 2023-02-20 12:48:51.971 ServerApp] Paths used for configuration of jupyter_notebook_config:
            /u/arnoldg/.local/etc/jupyter/jupyter_notebook_config.d/ipyparallel.json
            /u/arnoldg/.local/etc/jupyter/jupyter_notebook_config.json
[D 2023-02-20 12:48:51.971 ServerApp] Paths used for configuration of jupyter_notebook_config:
            /u/arnoldg/.jupyter/jupyter_notebook_config.json
[I 2023-02-20 12:48:51.971 ServerApp] notebook_shim | extension was successfully linked.
[I 2023-02-20 12:48:51.972 ServerApp] panel.io.jupyter_server_extension | extension was successfully linked.
[D 2023-02-20 12:48:51.972 ServerApp] Config changed: {'JupyterApp': {'kernel_spec_manager_class':
'nb_conda_kernels.CondaKernelSpecManager'}, 'NotebookApp': {}, 'ServerApp': {'log_level': 0,
'jpserver_extensions': <LazyConfigValue value={'jupyterlab': True, 'ipyparallel': True, 'nbclassic': True,
'notebook_shim': True, 'panel.io.jupyter_server_extension': True}>}}
[D 2023-02-20 12:48:51.972 ServerApp] Raising open file limit: soft 1024->4096; hard 262144->262144
[D 2023-02-20 12:48:51.972 ServerApp] [nb_conda_kernels] refreshing conda info
[I 2023-02-20 12:48:54.607 ServerApp] [nb_conda_kernels] enabled, 8 kernels found
[I 2023-02-20 12:48:54.645 ServerApp] notebook_shim | extension was successfully loaded.
[I 2023-02-20 12:48:54.648 ServerApp] Loading IPython parallel extension
[I 2023-02-20 12:48:54.648 ServerApp] ipyparallel | extension was successfully loaded.
[I 2023-02-20 12:48:54.649 LabApp] JupyterLab extension loaded from /sw/external/python/anaconda3/lib/python3.9
```

```
/site-packages/jupyterlab
[I 2023-02-20 12:48:54.649 LabApp] JupyterLab application directory is /sw/external/python/anaconda3/share
/jupyter/lab
[I 2023-02-20 12:48:54.652 ServerApp] jupyterlab | extension was successfully loaded.
[I 2023-02-20 12:48:54.660 ServerApp] nbclassic | extension was successfully loaded.
[I 2023-02-20 12:48:54.660 ServerApp] panel.io.jupyter_server_extension | extension was successfully loaded.
[I 2023-02-20 12:48:54.661 ServerApp] The port 8888 is already in use, trying another port.
[I 2023-02-20 12:48:54.661 ServerApp] Serving notebooks from local directory: /u/arnoldg/.local/etc/jupyter
/jupyter_notebook_config.d
[I 2023-02-20 12:48:54.661 ServerApp] Jupyter Server 1.23.4 is running at:
[I 2023-02-20 12:48:54.661 ServerApp] http://localhost:8889/lab?
token=a728f76b935d157d2eecc6a32810cf4e88ae1bc53701f4f6
[I 2023-02-20 12:48:54.661 ServerApp]  or http://127.0.0.1:8889/lab?
token=a728f76b935d157d2eecc6a32810cf4e88ae1bc53701f4f6
[I 2023-02-20 12:48:54.661 ServerApp] Use Control-C to stop this server and shut down all kernels (twice to
skip confirmation).
[C 2023-02-20 12:48:54.880 ServerApp]

    To access the server, open this file in a browser:
        file:///u/arnoldg/.local/share/jupyter/runtime/jpserver-1287615-open.html
    Or copy and paste one of these URLs:
        http://localhost:8889/lab?token=a728f76b935d157d2eecc6a32810cf4e88ae1bc53701f4f6
     or http://127.0.0.1:8889/lab?token=a728f76b935d157d2eecc6a32810cf4e88ae1bc53701f4f6
/usr/bin/xdg-open: line 862: x-www-browser: command not found
/usr/bin/xdg-open: line 862: firefox: command not found
/usr/bin/xdg-open: line 862: iceweasel: command not found
/usr/bin/xdg-open: line 862: seamonkey: command not found
/usr/bin/xdg-open: line 862: mozilla: command not found
/usr/bin/xdg-open: line 862: epiphany: command not found
/usr/bin/xdg-open: line 862: konqueror: command not found
/usr/bin/xdg-open: line 862: chromium: command not found
/usr/bin/xdg-open: line 862: chromium-browser: command not found
/usr/bin/xdg-open: line 862: google-chrome: command not found
/usr/bin/xdg-open: line 862: www-browser: command not found
/usr/bin/xdg-open: line 862: links2: command not found
/usr/bin/xdg-open: line 862: elinks: command not found
/usr/bin/xdg-open: line 862: links: command not found
/usr/bin/xdg-open: line 862: lynx: command not found
/usr/bin/xdg-open: line 862: w3m: command not found
xdg-open: no method available for opening 'file:///u/arnoldg/.local/share/jupyter/runtime/jpserver-1287615-open.
html'
```