Anaconda on ADAPT
(Brown Bag)

NCCS
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Anaconda is a package management system that allows users to create independent environments each with different configurations of packages within them.
Good News!

Users do NOT need to install Anaconda in personal directories!

Anaconda is already installed globally and can be imported/loaded across ADAPT VMs.
Agenda

- Anaconda location
- Anaconda Modules (Finding and loading)
- Anaconda Environments (what envs?, Activating)
- Creating a conda env (customize and configure)
Anaconda location

Which Anaconda are you pointing to?

sstrong@foyer101:~$ which conda

/att/opt/other/centos/anaconda3/bin/conda

*note-If no path is returned then an anaconda module will need to be loaded (discussed in module section)
Anaconda Modules

What is a Module
Enable “Module” commands
Finding available Modules
Loading available Modules
What is a Module

Modules are globally installed applications that ADAPT makes accessible to users across any VM on ADAPT.

Implemented by system admins, they contain commands that load specific applications into a users environment.
What is a Module

Modules

- GCC
- OpenMPI
- PGI
- Anaconda3
- ml/AIconda3

Packages
(Within each environment)

- numpy
- pandas
- matplotlib
- scipy
- netCDF4

Anaconda Environments
(Within each module)

- base
- celery
- myMongo
- mypgres
- ml
- earthml
- rapids
- tensorflow2
- tensorflow
- pytorch
- xgboost
- sk-learn
- keras
Enable "module" commands

sstrong@foyer101:~$ echo $0
-bash

sstrong@foyer101:~$ source
/att/opt/other/centos/modules/init/bash

sstrong@foyer101:~$ export
MODULEPATH=/att/opt/other/centos/modules/modulefiles
Finding Available Modules

<table>
<thead>
<tr>
<th>Module</th>
<th>Version</th>
<th>Module</th>
<th>Version</th>
</tr>
</thead>
<tbody>
<tr>
<td>anaconda3</td>
<td>jessie/R-3.6.1</td>
<td>ml/openmpi-4.0-gcc-9.1</td>
<td></td>
</tr>
<tr>
<td>anaconda3_stratus</td>
<td>lmod/lmod_8.1</td>
<td>ml/PGI-18.10-OpenMPI-CUDA</td>
<td></td>
</tr>
<tr>
<td>cmake-3.15.4</td>
<td>lmod/lua_5.1</td>
<td>module-info</td>
<td></td>
</tr>
<tr>
<td>crane/R-3.6.1</td>
<td>lmod/tcl_8.9</td>
<td>openmpi-4-gcc-9.1-foyer</td>
<td></td>
</tr>
<tr>
<td>gcc-7.4-explore</td>
<td>ml/anaconda3</td>
<td>openmpi-4.0.0-gcc-9.1</td>
<td></td>
</tr>
<tr>
<td>gcc-9.1</td>
<td>ml/bison-3.4</td>
<td>redis</td>
<td></td>
</tr>
<tr>
<td>gcc-9.1-foyer</td>
<td>ml/CUDA-10.0</td>
<td>stretch/anaconda3</td>
<td></td>
</tr>
<tr>
<td>gcc-9.1-ml4</td>
<td>ml/gcc-9.1</td>
<td>stretch/anaconda3_intern</td>
<td></td>
</tr>
<tr>
<td>git-2.23.0</td>
<td>ml/hdf5-1.10.5-openmpi-4</td>
<td>stretch/bzip2</td>
<td></td>
</tr>
<tr>
<td>hdf5-1.10.5-openmpi-gcc-9.1</td>
<td>ml/NCCL-2.3</td>
<td>stretch/jdk-13</td>
<td></td>
</tr>
<tr>
<td>intel-19.0.2.187</td>
<td>ml/openmpi-4</td>
<td>stretch/R-3.6.1</td>
<td></td>
</tr>
</tbody>
</table>

This a list of all the available system modules
(*note list is as of Dec 2019)
Loading Available Modules

strong@foyer101:~$ module list
Currently Loaded Modulefiles:
  1) anaconda3
strong@foyer101:~$ module av

------------------------- /att/opt/other/centos/modules/modulefiles -------------------------
anaconda3                jessie/R-3.6.1
anaconda3_stratus        lmod/lmod_8.1
ccmake-3.15.4            lmod/lua_5.1
cc/cmake-3.15.4          lmod/tcl_8.9
cc/gcc-7.4-explore       ml/anaconda3
cc/gcc-7.4.1             ml/bison-3.4
cc/gcc-9.1               ml/CUDA-10.0
cc/gcc-9.1.foyer         ml/gcc-9.1
cc/gcc-9.1.ml4           ml/hdf5-1.10.5-openmpi-4
cc/git-2.23.0            ml/NCCL-2.3
cc/hdf5-1.10.5-openmpi-gcc-9.1 ml/openmpi-4.0-gcc-9.1
cc/intel-19.0.2.187      ml/PGI-18.10-OpenMPI-CUDA
------------------------- /att/opt/other/centos/modules/modulefiles -------------------------

strong@foyer101:~$ module switch anaconda3 ml/anaconda3
strong@foyer101:~$ module list
Currently Loaded Modulefiles:
  1) ml/anaconda3

strong@foyer101:~$ module switch ml/anaconda3 anaconda3
strong@foyer101:~$ module list
Currently Loaded Modulefiles:
  1) anaconda3

anaconda3 module loaded
Anaconda Environments

- Conda envs
  In Anaconda3

- Find Packages
  in a conda env

- Activate and deactivate a conda env
Conda Envs within base Anaconda3

Modules

GCC
OpenMPI
PGI
Anaconda3
ml/A naconda3

base
celery
myMongo
mynsgres

base
ml
earthml
rapids
tensorflow2

Anaconda Environments
(Within each module)

13
Conda Envs within base Anaconda3

```

```

"conda env list" will list all the environments within an anaconda module as well as all of the user's personally created environments.
Pkgs within a conda env

Packages
(Within each environment)

numpy
pandas
matplotlib
scipy
netCDF4
tensorflow
pytorch
xgboost
sk-learn

Modules

base
ml
earthml
rapids
tensorflow2

* (conda envs)
Find pkgs in a conda env

```
sstrong@foyer101:~$ which conda
/att/opt/other/centos/anaconda3/bin/conda
sstrong@foyer101:~$ conda list
# packages in environment at /att/opt/other/centos/anaconda3:

<table>
<thead>
<tr>
<th>Name</th>
<th>Version</th>
<th>Build</th>
<th>Channel</th>
</tr>
</thead>
<tbody>
<tr>
<td>_ipyw_jlab_nb_ext_conf</td>
<td>0.1.0</td>
<td>py37_0</td>
<td>anacondaforge</td>
</tr>
<tr>
<td>_libgcc_mutex</td>
<td>0.1</td>
<td>main</td>
<td>anacondaforge</td>
</tr>
<tr>
<td>_r-mutex</td>
<td>1.0.0</td>
<td>anacondaforge</td>
<td></td>
</tr>
<tr>
<td>absl-py</td>
<td>0.7.1</td>
<td>py37_0</td>
<td>condaforge</td>
</tr>
<tr>
<td>affine</td>
<td>2.2.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>alabaster</td>
<td>0.7.12</td>
<td>py0</td>
<td>condaforge</td>
</tr>
<tr>
<td>anaconda-client</td>
<td>1.7.2</td>
<td>py0</td>
<td>condaforge</td>
</tr>
<tr>
<td>anaconda:navigator</td>
<td>1.9.6</td>
<td>py37_0</td>
<td>condaforge</td>
</tr>
<tr>
<td>asn1crypto</td>
<td>0.24.0</td>
<td>py37_1003</td>
<td>condaforge</td>
</tr>
<tr>
<td>astor</td>
<td>0.7.1</td>
<td>py0</td>
<td>condaforge</td>
</tr>
<tr>
<td>astroid</td>
<td>2.2.5</td>
<td>py37_0</td>
<td>condaforge</td>
</tr>
<tr>
<td>astropy</td>
<td>3.2.1</td>
<td>py37h516909a_0</td>
<td>condaforge</td>
</tr>
<tr>
<td>attrs</td>
<td>19.1.0</td>
<td>py0</td>
<td>condaforge</td>
</tr>
<tr>
<td>babel</td>
<td>2.7.0</td>
<td>py0</td>
<td>condaforge</td>
</tr>
<tr>
<td>backcall</td>
<td>0.1.0</td>
<td>py0</td>
<td>condaforge</td>
</tr>
<tr>
<td>basemap</td>
<td>1.2.0</td>
<td>py37h673bf1a_1001</td>
<td>condaforge</td>
</tr>
<tr>
<td>basemap-data-hires</td>
<td>1.2.0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>beautifulsoup4</td>
<td>4.7.1</td>
<td>py37_1001</td>
<td>condaforge</td>
</tr>
<tr>
<td>binutils_impl_linux-64</td>
<td>2.31.1</td>
<td>h6176602_1</td>
<td></td>
</tr>
</tbody>
</table>
```

Packages within the basic anaconda3 env
Conda activate

```
$ which conda
/att/opt/other/centos/anaconda3/condabin/conda

$ conda env list
# conda environments:
#
"/att/nobackup/sstrong/conda/envs/SAvEdasStratusYMLTest"
"/att/nobackup/sstrong/conda/envs/edas-stratus"

base * /att/opt/other/centos/anaconda3

celery /att/opt/other/centos/anaconda3/envs/celery
earthml /att/opt/other/centos/anaconda3/envs/earthml
myMongo /att/opt/other/centos/anaconda3/envs/myMongo
mypgres /att/opt/other/centos/anaconda3/envs/mypgres
r-environment /att/opt/other/centos/anaconda3/envs/r-environment
baseclone /home/sstrong/.conda/envs/baseclone

$ conda activate
(base) $```

"conda activate"

will activate the "base" conda env
Conda deactivate

```bash
sstrong@foyer101:~$ which conda
/att/opt/other/centos/anaconda3/condabin/conda
sstrong@foyer101:~$ conda env list
# conda environments:
#
/att/nobackup/sstrong/conda/envs/SAvEdasStratusYMLTest
/att/nobackup/sstrong/conda/envs/edas-stratus
base
* /att/opt/other/centos/anaconda3
celery
/att/opt/other/centos/anaconda3/envs/celery
earthml
/att/opt/other/centos/anaconda3/envs/earthml
myMongo
/att/opt/other/centos/anaconda3/envs/myMongo
mypgres
/att/opt/other/centos/anaconda3/envs/mypgres
r-environment
/att/opt/other/centos/anaconda3/envs/r-environment
baseclone
/home/sstrong/.conda/envs/baseclone
sstrong@foyer101:~$ conda activate
(base) sstrong@foyer101:~$ conda deactivate
sstrong@foyer101:~$
```
Conda activate another env (celery)

sstrong@foyer101:~$ which conda
/att/opt/other/centos/anaconda3/condabin/conda
sstrong@foyer101:~$ conda env list
# conda environments:
#
... (environment paths listed)

base
celery
earthml
myMongo
mypsgres
r-environment
baseclone

sstrong@foyer101:~$ conda activate (base)
sstrong@foyer101:~$ conda deactivate
sstrong@foyer101:~$ conda activate celery
(celery)
Creating new conda Envs

- Work on nobackup
- Create a new env (.../envs)
- Customize and configure
Work on ../nobackup

Due to limited storage on /home/<username>, it preferred that all new conda environments be created on /att/nobackup/<username>

To accomplish this:

sstrong@foyer101:~$ mv ~/.conda $NOBACKUP/

Make a softlink:

sstrong@foyer101:~$ ln –s $NOBACKUP/.conda ~/.conda

sstrong@foyer101:~$ ls –alt .conda

lrwxrwxrwx 1 sstrong k3000 28 Nov 8 15:58 .conda -> /att/nobackup/sstrong/.conda
Create new env

conda create -n SAvCondaEnv
Collecting package metadata (current_repodata.json): done
Solving environment: done

## Package Plan ##

   environment location: /home/sstrong/.conda/envs/SAvCondaEnv

Proceed ([y]/[n])? y

Preparing transaction: done
Verifying transaction: done
Executing transaction: done
#
# To activate this environment, use
#
#   $ conda activate SAvCondaEnv
#
# To deactivate an active environment, use
#
#   $ conda deactivate

ls -alt /att/nobackup/sstrong/.conda

SAvCondaEnv is created under
/att/nobackup/sstrong/.conda/envs
Customize and Configure

Once you have created a conda env, you can fully customize and configure your conda env by installing packages

First activate the environment..

sstrong@foyer101:~$ conda activate SAvCondaEnv
--------> (SAvCondaEnv) sstrong@foyer101:~$
Customize and Configure

In this example we will install two packages into SAvCondaEnv, dateparser and python-graphviz. First we have to locate the conda channel for the specified package.
Customize and Configure

Another option for users is to leverage a managed conda env.
If a conda env exists with most the desired packages, users can copy that managed conda env by cloning it and adding additional packages.

Here we’ll choose earthml to clone

```bash
sstrong@foyer101:~$ which conda
/att/opt/other/centos/anaconda3/condabin/conda
sstrong@foyer101:~$ conda env list
# conda environments:
#
/att/nobackup/sstrong/conda/envs/SAvEdasStratusYMLTest
/att/nobackup/sstrong/conda/envs/edas-stratus
base
* /att/opt/other/centos/anaconda3
celery
earthml
myMongo
m psycopg
r-environment
baseclone
```
Customize and Configure

earthmlPlus3 created with earthml env and ready for package installation
Summary

• No Anaconda installation neccessary
• Many available modules and can simply load the one you want.
• Can create new enviornments or leverage existing environments.
Any questions?
Assistance

“Anaconda on ADAPT”  
instructional video located at:
https://www.nccs.nasa.gov/nccs-users/instructional/instructional-videos

Email:
support@nccs.nasa.gov