Installing Software on Alpine with Conda and Mamba

Research Computing
UNIVERSITY OF COLORADO BOULDER

Installing software on Alpine with Conda and Mamba

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- Research Computing, User Support Team

- Website: http://www.colorado.edu/rc
- Documentation: https://curc.readthedocs.io
- Helpdesk: rc-help@colorado.edu
- Survey: http://tinyurl.com/curc-survey18

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Meet the User Support Team

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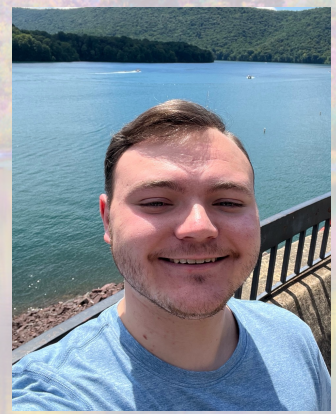

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Slides

https://github.com/ResearchComputing/alpine_conda_mamba_primer

Session Overview

- Installing software on CURC systems
- What are Conda and Mamba?
- Using Conda and Mamba on CURC systems
  - Creating environments
  - Installing packages
  - Useful commands
  - Batch jobs
- Useful strategies for complex environments

Building Software on CURC Systems

- There are numerous ways to install software on Alpine
  - Grab pre-compiled binaries
  - Compile from source
  - Using containers (Apptainer/Singularity)
  - Using a package manager for HPC systems (Spack)
  - **Within virtual environments (via Conda, Miniconda, Mamba)**

Logging into CU Research Computing

Login to CURC via your terminal:

```
ssh <username>@login.rc.colorado.edu
```

Or login to CURC via your browser:

- Navigate to https://ondemand-rmacc.rc.colorado.edu/
- Once logged in, select **Clusters → Alpine shell**

What are Conda and Mamba?

- They are a package (software) management system
  - Installs, runs, and updates packages *and their dependencies*
  - Creates, saves, loads, and switches between virtual environments
  - Created for Python programs, but can package and distribute software for any language

Why would we use Mamba?

- Mamba is a faster and more robust package manager in comparison to Conda
  - It is fully compatible with Conda packages
  - Supports **most** of Conda's commands
  - In most cases, Mamba can be used as a drop-in replacement for Conda
    - i.e. replace "conda" with "mamba" in commands

For a more detailed overview of Mamba's capabilities, please see: https://mamba.readthedocs.io

What is a .condarc file?

- The file ".condarc" is a special file that specifies configurations for Conda and Mamba
  - Specifies items such as where to store installed packages and environments
  - Located in your Home directory, **/home/$USER/.condarc**
    - We create it for you, if it doesn't exist, with the content:

```
pkgs_dirs:
  - /projects/$USER/.conda_pkgs
envs_dirs:
  - /projects/$USER/software/anaconda/envs
```

Getting access to Conda and Mamba

On CURC systems, Conda and Mamba are made available through modules

- **We highly recommend using these modules**
  - Redirects output produced by Conda and Mamba
  - Creates useful variables
  - Creates the ".condarc" file, if it doesn't exist
  - They are easier than installing it yourself!

Conda and Mamba modules

- You must be on a compute node to get access to modules!
- Conda is accessible via

```
$ module load anaconda
```

- Mamba is accessible via

```
$ module load miniforge
```

NOTE: We have retired our former "mambaforge" module, as it is deprecated; please use "miniforge".

Demo time!

Start a session and load Conda

Start a session on an Alpine compute node with **acompile**:

```
[johndoe@login11 ~]$ acompile --help
[johndoe@login11 ~]$ acompile –ntasks=4 --time=60:00
…
[johndoe@c3cpu-a5-u28-1 ~]$ module load anaconda
(base) [johndoe@c3cpu-a5-u28-1 ~]$
```

Note: when you login to CURC you'll be on a ***login*** node. You'll need to be on a ***compute*** node to use anaconda. The **acompile** command allows you to quickly start an interactive job on a compute node.

Create your first Conda environment!

- Environments are created and programs are installed in a few simple steps

```
(base) [johndoe@c3cpu-a5-u28-1 ~]$ conda create -n my_first_env python==3.10
(base) [johndoe@c3cpu-a5-u28-1 ~]$ conda activate my_first_env
(my_first_env) [johndoe@c3cpu-a5-u28-1 ~]$ python
```

Don't install packages in your base environment!

Installing packages

- Packages are installed within **activated** environments using **conda install**
- Install latest version available:

```
(my_first_env) [johndoe@c3cpu-a5-u28-1 ~]$ conda install pandas
```

- Install a specific version:

```
(my_first_env) [johndoe@c3cpu-a5-u28-1 ~]$ conda install pandas==2.2.0
```

Installing packages with “pip”

- pip installs should be done within **activated** environments

Using **pip** to install latest version:

```
(my_first_env) [johndoe@c3cpu-a5-u28-1 ~]$ pip install --no-cache-dir pandas
```

`--no-cache-dir` may be crucial on CURC systems

Useful Conda Commands

```
conda env list                              # list all environments
conda list                                  # list packages in active env
conda env remove -n <envname> --all         # remove an environment
conda config --show channels                # view configured channels
conda deactivate                            # deactivate environment
conda create --name <clonedenv> /           # clone an environment
      --clone <envtoclone>
```

Useful Conda file paths on Alpine

```
# location of python libraries
/projects/$USER/software/anaconda/<env>/lib/python3.10/site-packages

# location of package executables
/projects/$USER/software/anaconda/<env>/bin

# location of .condarc file
/home/$USER/.condarc
```

Running Alpine batch jobs with Conda

```
[johndoe@login11 ~]$ nano runconda.sh  #Step 1: open new job script in editor
```

```
#!/bin/bash
# job script name: runconda.sh

#SBATCH --partition=amilan
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --time=10:00
#SBATCH --qos=normal

module purge
module load anaconda
conda activate my_first_env
python my_python_code.py
```

```
# Step 2: Write job script
```

https://curc.readthedocs.io/en/latest/running-jobs/batch-jobs.html

```
[johndoe@login11 ~]$ sbatch runconda.sh  #Step 3: Schedule job
```

Using environments in Open OnDemand

- In Open OnDemand users can utilize their environments in Jupyter sessions. This can be done using two different methods:
  - Specifying the environment name in the "Conda environment" field
    - Allows you to launch the notebook from within your environment
    - Needed for some Jupyter extensions
  - Create a Jupyter Kernel
    - Allows you to switch between different environments while in a notebook
    - May prevent some Jupyter extensions from working
- Both methods are described at https://curc.readthedocs.io/en/latest/open_ondemand/jupyter_session.html

Strategies for complex environments

- You may have to use different channels and change channel order
- Conflicts can arise when iteratively installing packages. If this happens create a new environment and install the package that causes conflicts first.
- Use Mamba to accelerate installations

Thank you!

Survey and feedback

http://tinyurl.com/curc-survey18

Slides

https://github.com/ResearchComputing/alpine_conda_mamba_primer