

Intro to Using Conda: Creating Python/R and other Application Environments

Introduction: This workshop will introduce what Conda is and how it can be used to create a variety of environments, such as Python/R and contained applications.

Course Goals:

1. Introduce Conda and what it is good for, and how to use on ARCC's clusters.
2. How to use Conda to create a variety of environments - based on Python, R and standalone applications.
3. Detail some of the core Conda configurations that affect your environment.

Notes:

1. This workshop focuses purely on using Conda. We have a more advanced workshop that details the interplay between Python, Conda and Pip.
 2. If you have existing conda environments, or have installed your own version of Anaconda, then the examples within this workshop might provide different results.
 3. You will need to *modify* user and project names to apply to yourself.
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Sections

1. [What is Conda? Using Miniconda3 on the Cluster](#): Introduce conda, define some terminology, how to use on the cluster and finding help.
2. [Example 01: Python, Numpy and Pandas Environment](#): Demonstrate a basic conda environment creation workflow by creating a Python environment that contains the numpy and pandas packages.
3. [Conda Configuration and Environments](#): Understand some of the basic conda configurations and where environments are stored.
4. [Example 02: R and TidyVerse](#): Create an environment using the R language that includes the TidyVerse library.
5. [Conda Channels](#): What are channels and how can they be used and configured.
6. [Example 03: Applications: SLiM](#): Demonstrate using conda to install a command-line application.
7. [Reproducibility and Sharing](#): Introduce how conda environments can be reproduced and shared.
8. [Example 04: Application: Qiime Ecosystem](#): Demonstrate importing the large qiime application ecosystem.
9. [Conda with salloc and sbatch](#): Demonstrate best practices using Conda environments with `salloc` and `sbatch`.

10. [Conda Workshop: Summary](#): Summarize the concepts covered across the workshop.
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What is Conda? Using Miniconda3 on the Cluster

Goal: Introduce conda, define some terminology, how to use on the cluster and finding help.

- [What is Conda?](#)
 - [Getting Conda: Miniconda vs Anaconda vs Miniforge](#)
 - [Terminology](#)
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What is Conda?

- [Getting Started with Conda](#): A powerful **command line tool** for **package and environment management** that runs on Windows, macOS, and Linux.
 - [Conda Documentation](#): Provides package, dependency, and environment management for any language.
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Getting Conda: Miniconda vs Anaconda vs Miniforge

[Miniconda](#): (<0.5G) A **free minimal installer for conda**. It is a small bootstrap version of Anaconda that includes only conda, Python, the packages (<70) they both depend on, and a small number of other useful packages (like pip, zlib, and a few others).

- This is what ARCC provides.

[Anaconda](#): (4.4G) (The Company) Anaconda® Distribution is a free Python/R data science distribution that contains:

- Conda and Anaconda Navigator (a desktop GUI application built on conda, with options to launch other development applications from your managed environments).
- 250 automatically-[installed packages](#) and access to the Anaconda Public Repository (>8K open-source data science and ML packages).

[Miniforge](#): This **community driven** repository holds the minimal installers for Conda and [Mamba](#) (a reimplementation of the conda package manager in C++) specific to [conda-forge](#) (Community-led recipes, infrastructure and distributions for conda - the default and only channel).

[Should I use Anaconda Distribution or Miniconda?](#)

Terminology

[Glossary](#):

Term	Definition
package manager	A collection of software tools that automates the process of installing, updating, configuring, and removing computer programs for a computer's operating system.
conda	Conda is a package manager. The package and environment manager program ... that installs and updates conda packages and their dependencies .
conda package	A compressed file that contains everything that a software program needs in order to be installed and run , so that you do not have to manually find and install each dependency separately.
conda environment	A folder or directory that contains a specific collection of conda packages and their dependencies , so they can be maintained and run separately without interference from each other.
conda repository	A cloud-based repository that contains packages that are easily installed.
channels	The locations of the repositories where conda looks for packages .

Using Miniconda3/Conda on the Cluster

You do NOT need to install `miniconda3` yourself. It is provided as pre-installed module.

```
[salexan5@mblog1 ~]$ module spider miniconda3
```

```
-----  
miniconda3: miniconda3/24.3.0  
-----
```

You will need to load all module(s) on any one of the lines below before the "miniconda3/24.3.0" module is available to load.

```
arcc/1.0
```

Help:

The minimalist bootstrap toolset for conda and Python3.

We update miniconda3 on a semi-frequent basis.

You *can* install miniconda and anaconda yourself - but this will modify your cluster environment.

Make sure you understand what you're doing.

Conda Version and Help

```
[salexan5@mblog1 ~]$ module load miniconda3/24.3.0
```

```
[salexan5@mblog1 ~]$ conda --version
```

```
conda 24.3.0
```

```
[salexan5@mblog1 ~]$ conda --help
```

```
usage: conda [-h] [-v] [--no-plugins] [-V] COMMAND ...
```

```
conda is a tool for managing and deploying applications, environments and packages.
```

```
...
```

```
[salexan5@mblog1 ~]$ conda install --help
```

```
usage: conda install [-h] [--revision REVISION] [-n ENVIRONMENT | -p PATH] [-c CHANNEL] [--use-local] [--override-channels] [--repopdata-fn REPODATA_FNS] [--experimental {jlap,lock}] [--no-lock] [--repopdata-use-zst | --no-repopdata-use-zst] [--strict-channel-priority] [--no-channel-priority]
```

```
                [--no-deps | --only-deps] [--no-pin] [--copy] [--no-shortcuts] [--shortcuts-only SHORTCUTS_ONLY] [-C] [-k] [--offline] [--json] [-v] [-q] [-d]
```

```
                [-y] [--download-only] [--show-channel-urls] [--file FILE] [--solver {classic,libmamba}] [--force-reinstall]
```

```
                [--freeze-installed | --update-deps | -S | --update-all | --update-specs] [-m] [--clobber] [--dev] [package_spec ...]
```

```
...
```

conda --help : list of all commands

```
[salexan5@mblog1 ~]$ conda --help
```

```
usage: conda [-h] [-v] [--no-plugins] [-V] COMMAND ...
```

```
conda is a tool for managing and deploying applications, environments and packages.
```

options:

-h, --help Show this help message and exit.
-v, --verbose Can be used multiple times. Once for detailed output, twice for INFO logging, thrice for DEBUG logging, four times for TRACE logging.
--no-plugins Disable all plugins that are not built into conda.
-V, --version Show the conda version number and exit.

commands:

The following built-in and plugins subcommands are available.

COMMAND	
activate	Activate a conda environment.
clean	Remove unused packages and caches.
compare	Compare packages between conda environments.
config	Modify configuration values in .condarc.
content-trust	Signing and verification tools for Conda
create	Create a new conda environment from a list of specified packages.
deactivate	Deactivate the current active conda environment.
doctor	Display a health report for your environment.
export	Export a given environment
info	Display information about current conda install.
init	Initialize conda for shell interaction.
install	Install a list of packages into a specified conda environment.
list	List installed packages in a conda environment.
notices	Retrieve latest channel notifications.
package	Create low-level conda packages. (EXPERIMENTAL)
remove (uninstall)	Remove a list of packages from a specified conda environment.
rename	Rename an existing environment.
repoquery	Advanced search for repodata.
run	Run an executable in a conda environment.
search	Search for packages and display associated information using the MatchSpec format.
update (upgrade)	Update conda packages to the latest compatible version.

conda install --help : list of install options

```
[salexan5@mblog1 ~]$ conda install --help
usage: conda install [-h] [--revision REVISION] [-n ENVIRONMENT | -p PATH] [-c CHANNEL] [--use-local] [--override-channels] [--repodata-fn REPODATA_FNS] [--experimental {jlap,lock}] [--no-lock] [--repodata-use-zst | --no-repodata-use-zst] [--strict-channel-priority] [--no-channel-priority] [--no-deps | --only-deps] [--no-pin] [--copy] [--no-shortcuts] [--shortcuts-only SHORTCUTS_ONLY] [-C] [-k] [--offline] [--json] [-v] [-q] [-d] [-y] [--download-only] [--show-channel-urls] [--file FILE] [--solver {classic,libmamba}] [--force-reinstall] [--freeze-installed | --update-deps | -S | --update-all | --update-specs] [-m] [--clobber] [--dev] [package_spec ...]
```

Install a list of packages into a specified conda environment.

This command accepts a list of package specifications (e.g, bitarray=0.8) and installs a set of packages consistent with those specifications and compatible with the underlying environment. If full compatibility cannot be assured, an error is reported and the environment is not changed.

Conda attempts to install the newest versions of the requested packages. To accomplish this, it may update some packages that are already installed, or install additional packages. To prevent existing packages from updating, use the `--freeze-installed` option. This may force conda to install older versions of the requested packages, and it does not prevent additional dependency packages from being installed.

If you wish to skip dependency checking altogether, use the `'--no-deps'` option. This may result in an environment with incompatible packages, so this option must be used with great caution.

conda can also be called with a list of explicit conda package filenames (e.g. `./lxml-3.2.0-py27_0.tar.bz2`). Using conda in this mode implies the `--no-deps` option, and should likewise be used with great caution. Explicit filenames and package specifications cannot be mixed in a single command.

positional arguments:

package_spec List of packages to install or update in the conda environment.

options:

-h, --help Show this help message and exit.
--revision REVISION Revert to the specified REVISION.
--file FILE Read package versions from the given file. Repeated file specifications can be passed (e.g. `--file=file1 --file=file2`).
--dev Use ``sys.executable -m conda`` in wrapper scripts instead of `CONDA_EXE`. This is mainly for use during tests where we test new conda sources against old Python versions.

Target Environment Specification:

-n ENVIRONMENT, --name ENVIRONMENT Name of environment.
-p PATH, --prefix PATH Full path to environment location (i.e. prefix).

Channel Customization:

-c CHANNEL, --channel CHANNEL Additional channel to search for packages. These are URLs searched in the order they are given (including local directories using the `'file://'` syntax or simply a path like `'/home/conda/mychan'` or `'../mychan'`). Then, the defaults or channels from `.condarc` are searched (unless `--override-channels` is given). You can use `'defaults'` to get the default packages for conda. You can also use any name and the `.condarc` channel_alias value will be prepended. The default channel_alias is `https://conda.anaconda.org/`.
--use-local Use locally built packages. Identical to `'-c local'`.
--override-channels Do not search default or `.condarc` channels. Requires `--channel`.

`--repopdata-fn REPODATA_FNS`
Specify file name of repodata on the remote server where your channels are configured or within local backups. Conda will try whatever you specify, but will ultimately fall back to `repodata.json` if your specs are not satisfiable with what you specify here. This is used to employ repodata that is smaller and reduced in time scope. You may pass this flag more than once. Leftmost entries are tried first, and the fallback to `repodata.json` is added for you automatically. For more information, see `conda config --describe repodata_fns`.

`--experimental {jlap,lock}`
jlap: Download incremental package index data from `repodata.jlap`; implies 'lock'. **lock**: use locking when reading, updating index (`repodata.json`) cache. Now enabled.

`--no-lock`
Disable locking when reading, updating index (`repodata.json`) cache.

`--repopdata-use-zst, --no-repopdata-use-zst`
Check for/do not check for `repodata.json.zst`. Enabled by default.

Solver Mode Modifiers:

`--strict-channel-priority`
Packages in lower priority channels are not considered if a package with the same name appears in a higher priority channel.

`--no-channel-priority`
Package version takes precedence over channel priority. Overrides the value given by ``conda config --show channel_priority``.

`--no-deps`
Do not install, update, remove, or change dependencies. This WILL lead to broken environments and inconsistent behavior. Use at your own risk.

`--only-deps`
Only install dependencies.

`--no-pin`
Ignore pinned file.

`--solver {classic,libmamba}`
Choose which solver backend to use.

`--force-reinstall`
Ensure that any user-requested package for the current operation is uninstalled and reinstalled, even if that package already exists in the environment.

`--freeze-installed, --no-update-deps`
Do not update or change already-installed dependencies.

`--update-deps`
Update dependencies that have available updates.

`-S, --satisfied-skip-solve`
Exit early and do not run the solver if the requested specs are satisfied. Also skips aggressive updates as configured by the 'aggressive_update_packages' config setting. Use `'conda info --describe aggressive_update_packages'` to view your setting. `--satisfied-skip-solve` is similar to the default behavior of `'pip install'`.

`--update-all, --all`
Update all installed packages in the environment.

`--update-specs`
Update based on provided specifications.

Package Linking and Install-time Options:

`--copy` Install all packages using copies instead of hard- or soft-linking.
`--no-shortcuts` Don't install start menu shortcuts
`--shortcuts-only SHORTCUTS_ONLY` Install shortcuts only for this package name. Can be used several times.
`-m, --mkdir` Create the environment directory, if necessary.
`--clobber` Allow clobbering (i.e. overwriting) of overlapping file paths within packages and suppress related warnings.

Networking Options:

`-C, --use-index-cache` Use cache of channel index files, even if it has expired. This is useful if you don't want conda to check whether a new version of the repodata file exists, which will save bandwidth.
`-k, --insecure` Allow conda to perform "insecure" SSL connections and transfers. Equivalent to setting 'ssl_verify' to 'false'.
`--offline` Offline mode. Don't connect to the Internet.

Output, Prompt, and Flow Control Options:

`--json` Report all output as json. Suitable for using conda programmatically.
`-v, --verbose` Can be used multiple times. Once for detailed output, twice for INFO logging, thrice for DEBUG logging, four times for TRACE logging.
`-q, --quiet` Do not display progress bar.
`-d, --dry-run` Only display what would have been done.
`-y, --yes` Sets any confirmation values to 'yes' automatically. Users will not be asked to confirm any adding, deleting, backups, etc.
`--download-only` Solve an environment and ensure package caches are populated, but exit prior to unlinking and linking packages into the prefix.
`--show-channel-urls` Show channel urls. Overrides the value given by ``conda config --show show_channel_urls``.

Examples:

Install the package 'scipy' into the currently-active environment::

```
conda install scipy
```

Install a list of packages into an environment, myenv::

```
conda install -n myenv scipy curl wheel
```

Install a specific version of 'python' into an environment, myenv::

```
conda install -p path/to/myenv python=3.11
```

Example 01: Python, Numpy and Pandas Environment

Goal: Demonstrate a basic conda environment creation workflow by creating a Python environment that contains the numpy and pandas packages.

- [General Process](#)
 - [Search for Packages](#)
 - [Create an Environment](#)
 - [Create an Environment: Proceed](#)
 - [Activate an Environment](#)
 - [Conda Install a Version of Python](#)
 - [Conda Install the numpy Package](#)
 - [Conda Deactivate your Environment](#)
 - [Using the Environment](#)
 - [Adding to an Existing Environment](#)
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General Process

```
[salexan5@mblog1 ~]$ module load miniconda3/24.3.0
[salexan5@mblog1 ~]$ conda search python
[salexan5@mblog1 ~]$ conda create -n py_env
[salexan5@mblog1 ~]$ conda activate py_env
(py_env) [salexan5@mblog1 ~]$ conda install python=3.12.4
(py_env) [salexan5@mblog1 ~]$ python --version
Python 3.12.4
(py_env) [salexan5@mblog1 ~]$ conda search numpy
(py_env) [salexan5@mblog1 ~]$ conda install numpy
(py_env) [salexan5@mblog1 ~]$ python -c "import numpy;
print(numpy.__version__)"
1.26.4
(py_env) [salexan5@mblog1 ~]$ conda deactivate
[salexan5@mblog1 ~]$
```

Search for Packages

```
[salexan5@mblog1 ~]$ conda search python
Loading channels: done
# Name                               Version           Build           Channel
python                               2.7.13           hac47a24_15    pkgs/main
...
python                               3.12.3           h996f2a0_1     pkgs/main
python                               3.12.4           h5148396_1     pkgs/main
```

Notice: Although Python version 2 has been deprecated, it is still used for old packages/modules/scripts. You can create a conda environment that provides this old, no longer supported version.

This is how ARCC provides this version on the cluster.

```
(py_env) [salexan5@mblog1 ~]$ conda search numpy
Loading channels: done
# Name                               Version                Build Channel
numpy                                1.9.3 py27_nomklhbee5d10_3 pkgs/main
...
numpy                                1.26.4 py39heeff2f4_0 pkgs/main
```

Create an Environment

```
[salexan5@mblog1 ~]$ conda create -n py_env
Channels:
- defaults
Platform: linux-64
Collecting package metadata (repodata.json): done
Solving environment: done

## Package Plan ##
  environment location: /home/salexan5/.conda/envs/py_env

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

Note the location that the environment will be saved to: environment location:
/home/salexan5/.conda/envs/py_env

Create an Environment: Proceed

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

Note the command required to activate your environment: `conda activate py_env`

This will be required every time you wish to use it.

Activate an Environment

```
[salexan5@mblog1 ~]$ conda activate py_env
(py_env) [salexan5@mblog1 ~]$
```

Note how the command line prompt has changed once the environment has been activated:
(py_env) [...]

This indicates the name of the conda environment that is currently active.

Conda Install a Version of Python

```
(py_env) [salexan5@mblog1 ~]$ conda install python=3.12.4
```

▼ Output of what is happening:

```
(py_env) [salexan5@mblog1 ~]$ conda install python=3.12.4
```

Channels:

- defaults

Platform: linux-64

Collecting package metadata (repodata.json): done

Solving environment: done

Package Plan

environment location: /home/salexan5/.conda/envs/py_env

added / updated specs:

- python=3.12.4

The following packages will be downloaded:

package	build	
-----	-----	
pip-24.0	py312h06a4308_0	3.3 MB
setuptools-69.5.1	py312h06a4308_0	1.3 MB
wheel-0.43.0	py312h06a4308_0	142 KB
-----	-----	
	Total:	4.7 MB

The following NEW packages will be INSTALLED:

_libgcc_mutex	pkgs/main/linux-64::_libgcc_mutex-0.1-main
_openmp_mutex	pkgs/main/linux-64::_openmp_mutex-5.1-1_gnu
bzip2	pkgs/main/linux-64::bzip2-1.0.8-h5eee18b_6
ca-certificates	pkgs/main/linux-64::ca-certificates-2024.3.11-h06a4308_0
expat	pkgs/main/linux-64::expat-2.6.2-h6a678d5_0
ld_impl_linux-64	pkgs/main/linux-64::ld_impl_linux-64-2.38-h1181459_1
libffi	pkgs/main/linux-64::libffi-3.4.4-h6a678d5_1
libgcc-ng	pkgs/main/linux-64::libgcc-ng-11.2.0-h1234567_1
libgomp	pkgs/main/linux-64::libgomp-11.2.0-h1234567_1

```
libstdcxx-ng      pkgs/main/linux-64::libstdcxx-ng-11.2.0-h1234567_1
libuuid           pkgs/main/linux-64::libuuid-1.41.5-h5eee18b_0
ncurses           pkgs/main/linux-64::ncurses-6.4-h6a678d5_0
openssl           pkgs/main/linux-64::openssl-3.0.14-h5eee18b_0
pip               pkgs/main/linux-64::pip-24.0-py312h06a4308_0
python            pkgs/main/linux-64::python-3.12.4-h5148396_1
readline          pkgs/main/linux-64::readline-8.2-h5eee18b_0
setuptools        pkgs/main/linux-64::setuptools-69.5.1-py312h06a4308_0
sqlite            pkgs/main/linux-64::sqlite-3.45.3-h5eee18b_0
tk                pkgs/main/linux-64::tk-8.6.14-h39e8969_0
tzdata            pkgs/main/noarch::tzdata-2024a-h04d1e81_0
wheel             pkgs/main/linux-64::wheel-0.43.0-py312h06a4308_0
xz                pkgs/main/linux-64::xz-5.4.6-h5eee18b_1
zlib              pkgs/main/linux-64::zlib-1.2.13-h5eee18b_1
```

Proceed ([y]/n)? y

Downloading and Extracting Packages:

```
Preparing transaction: done
Verifying transaction: done
Executing transaction: done
```

Note all the addition dependencies/libraries that are being installed into the environment

Lets check the version installed, within are *active environment*.

```
(py_env) [salexan5@mblog1 ~]$ python --version
Python 3.12.4
```

Conda Install the numpy Package

```
(py_env) [salexan5@mblog1 ~]$ conda install numpy
```

▼ Output of what is happening:

```
(py_env) [salexan5@mblog1 ~]$ conda install numpy
```

Channels:

- defaults

Platform: linux-64

Collecting package metadata (repodata.json): done

Solving environment: done

Package Plan

environment location: /home/salexan5/.conda/envs/py_env

added / updated specs:

- numpy

The following packages will be downloaded:

package	build
-----	-----

mkl-service-2.4.0		py312h5eee18b_1	66 KB
mkl_fft-1.3.8		py312h5eee18b_0	204 KB
mkl_random-1.2.4		py312hdb19cb5_0	284 KB
numpy-1.26.4		py312hc5e2394_0	11 KB
numpy-base-1.26.4		py312h0da6c21_0	7.7 MB

Total:			8.2 MB

The following NEW packages will be INSTALLED:

blas	pkgs/main/linux-64::blas-1.0-mkl
intel-openmp	pkgs/main/linux-64::intel-openmp-2023.1.0-hdb19cb5_46306
mkl	pkgs/main/linux-64::mkl-2023.1.0-h213fc3f_46344
mkl-service	pkgs/main/linux-64::mkl-service-2.4.0-py312h5eee18b_1
mkl_fft	pkgs/main/linux-64::mkl_fft-1.3.8-py312h5eee18b_0
mkl_random	pkgs/main/linux-64::mkl_random-1.2.4-py312hdb19cb5_0
numpy	pkgs/main/linux-64::numpy-1.26.4-py312hc5e2394_0
numpy-base	pkgs/main/linux-64::numpy-base-1.26.4-py312h0da6c21_0
tbb	pkgs/main/linux-64::tbb-2021.8.0-hdb19cb5_0

Proceed ([y]/n)? y

Downloading and Extracting Packages:

```
Preparing transaction: done
Verifying transaction: done
Executing transaction: done
```

Again, note all the addition dependencies/libraries that are being installed into the environment

If no package version is defined, typically it'll install the latest version.

Lets check the version installed, within are *active environment*.

```
(py_env) [salexan5@mblog1 ~]$ python -c "import numpy;
print(numpy.__version__)"
1.26.4
```

Conda Deactivate your Environment

```
(py_env) [salexan5@mblog1 ~]$ conda deactivate
[salexan5@mblog1 ~]$
```

Note how the command line prompt has changed, reverting back to before being activated:

```
[...]
```

The conda environment is no longer activate and can not be used.

```
[salexan5@mblog1 ~]$ python --version
Python 3.12.2
```

```
[salexan5@mblog1 ~]$ python -c "import numpy; print(numpy.__version__)"
Traceback (most recent call last):
  File "<string>", line 1, in <module>
ModuleNotFoundError: No module named 'numpy'
```

Using the Environment

```
[salexan5@mblog1 ~]$ module load miniconda3/24.3.0
[salexan5@mblog1 ~]$ conda activate py_env
(py_env) [salexan5@mblog1 ~]$ python --version
Python 3.12.4
(py_env) [salexan5@mblog1 ~]$ python -c "import numpy;
print(numpy.__version__)"
1.26.4
(py_env) [salexan5@mblog1 ~]$ conda deactivate
[salexan5@mblog1 ~]$
```

Note how the conda environment must be *activated* to use it.

Adding to an Existing Environment

```
[salexan5@mblog1 ~]$ module load miniconda3/24.3.0
[salexan5@mblog1 ~]$ conda activate py_env
(py_env) [salexan5@mblog1 ~]$ conda install pandas
(py_env) [salexan5@mblog1 ~]$ python py_test.py
Python: 3.12.4 | packaged by Anaconda, Inc. | (main, Jun 18 2024, 15:12:24)
[GCC 11.2.0]
Numpy: 1.26.4
Pandas: 2.2.2
(py_env) [salexan5@mblog1 ~]$ conda deactivate
  ~ py_test.py
import sys
import numpy
import pandas

print("Python: " + str(sys.version))
print("Numpy: " + str(numpy.__version__))
print("Pandas: " + str(pandas.__version__))
  ~ Installation Output:
(py_env) [salexan5@mblog1 ~]$ conda install pandas
Channels:
  - defaults
Platform: linux-64
Collecting package metadata (repodata.json): done
Solving environment: done

## Package Plan ##
```

environment location: /home/salexan5/.conda/envs/py_env

added / updated specs:

- pandas

The following packages will be downloaded:

package	build	
bottleneck-1.3.7	py312ha883a20_0	140 KB
numexpr-2.8.7	py312hf827012_0	149 KB
pandas-2.2.2	py312h526ad5a_0	15.4 MB
python-dateutil-2.9.0post0	py312h06a4308_2	318 KB
pytz-2024.1	py312h06a4308_0	220 KB
Total:		16.2 MB

The following NEW packages will be INSTALLED:

bottleneck	pkgs/main/linux-64::bottleneck-1.3.7-py312ha883a20_0
numexpr	pkgs/main/linux-64::numexpr-2.8.7-py312hf827012_0
pandas	pkgs/main/linux-64::pandas-2.2.2-py312h526ad5a_0
python-dateutil	pkgs/main/linux-64::python-dateutil-2.9.0post0-
py312h06a4308_2	
python-tzdata	pkgs/main/noarch::python-tzdata-2023.3-pyhd3eb1b0_0
pytz	pkgs/main/linux-64::pytz-2024.1-py312h06a4308_0
six	pkgs/main/noarch::six-1.16.0-pyhd3eb1b0_1

Proceed ([y]/n)? y

Downloading and Extracting Packages:

Preparing transaction: done

Verifying transaction: done

Executing transaction: done

Example 02: R and TidyVerse

Goal: Create an environment using the R language that includes the TidyVerse library.

- [General Process](#)
- [Create R Environment](#)
- [How to Activate](#)
- [Did Search Work?](#)
- [Conda Install TidyVerse](#)
- [How Large is this Environment?](#)
- [Using R Environment](#)

General Process

```
[salexan5@mblog1 ~]$ conda create -n r_env r=4.3.1
salexan5@mblog1 ~]$ conda activate r_env
(r_env) [salexan5@mblog1 ~]$ R --version
R version 4.3.1 (2023-06-16) -- "Beagle Scouts"
...
(r_env) [salexan5@mblog1 ~]$ conda search tidyverse
...
(r_env) [salexan5@mblog1 ~]$ conda install r-tidyverse=2.0.0
(r_env) [salexan5@mblog1 ~]$ R
> library(tidyverse)
— Attaching core tidyverse packages

----- tidyverse 2.0.0 -----
...
> quit()
Save workspace image? [y/n/c]: n
(r_env) [salexan5@mblog1 ~]$ conda deactivate
[salexan5@mblog1 ~]$
```

Create R Environment

```
[salexan5@mblog1 ~]$ conda create -n r_env r=4.3.1
Channels:
 - defaults
Platform: linux-64
Collecting package metadata (repodata.json): done
Solving environment: done

## Package Plan ##
  environment location: /project/arcc/salexan5/conda/envs/r_env
  added / updated specs:
    - r=4.3.1
...
```

Notice we can include the R language package (previously defined in a separate `conda install` ... in the creation line.

The environment install location has been updated to: `environment location: /project/arcc/salexan5/conda/envs/r_env` as configured.

How to Activate

...

Downloading and Extracting Packages:

Preparing transaction: done

Verifying transaction: done

Executing transaction: done

#

To activate this environment, use

#

\$ conda activate r_env

#

To deactivate an active environment, use

#

\$ conda deactivate

▼ Full Details: 10s of R library dependencies

[salexan5@mblog1 ~]\$ conda create -n r_env r=4.3.1

Channels:

- defaults

Platform: linux-64

Collecting package metadata (repodata.json): done

Solving environment: done

Package Plan

environment location: /project/arcc/salexan5/conda/envs/r_env

added / updated specs:

- r=4.3.1

The following packages will be downloaded:

package	build	
----- -----		
_libgcc_mutex-0.1	main	3 KB
_openmp_mutex-5.1	1_gnu	21 KB
_r-mutex-1.0.0	anacondar_1	2 KB
_sysroot_linux-64_curr_repodata_hack-3	haa98f57_10	12 KB
binutils_impl_linux-64-2.38	h2a08ee3_1	5.2 MB
binutils_linux-64-2.38.0	hc2dff05_0	24 KB
blas-1.0	openblas	46 KB
bwidget-1.9.16	h9eba36c_0	219 KB
bzip2-1.0.8	h5eee18b_6	262 KB
c-ares-1.19.1	h5eee18b_0	118 KB
ca-certificates-2024.3.11	h06a4308_0	127 KB
cairo-1.16.0	hb05425b_5	1.2 MB
curl-8.7.1	hdbd6064_0	86 KB
expat-2.6.2	h6a678d5_0	177 KB
fontconfig-2.14.1	h4c34cd2_2	281 KB
freetype-2.12.1	h4a9f257_0	626 KB
fribidi-1.0.10	h7b6447c_0	103 KB
gcc_impl_linux-64-11.2.0	h1234567_1	22.2 MB
gcc_linux-64-11.2.0	h5c386dc_0	25 KB
gfortran_impl_linux-64-11.2.0	h1234567_1	10.2 MB
gfortran_linux-64-11.2.0	hc2dff05_0	24 KB
glib-2.78.4	h6a678d5_0	508 KB

glib-tools-2.78.4		h6a678d5_0	115 KB
graphite2-1.3.14		h295c915_1	97 KB
gxx_impl_linux-64-11.2.0		h1234567_1	10.6 MB
gxx_linux-64-11.2.0		hc2dff05_0	24 KB
harfbuzz-4.3.0		hf52aaf7_2	1.3 MB
icu-73.1		h6a678d5_0	25.9 MB
jpeg-9e		h5eee18b_1	262 KB
kernel-headers_linux-64-3.10.0		h57e8cba_10	952 KB
krb5-1.20.1		h143b758_1	1.3 MB
ld_impl_linux-64-2.38		h1181459_1	654 KB
lerc-3.0		h295c915_0	196 KB
libcurl-8.7.1		h251f7ec_0	424 KB
libdeflate-1.17		h5eee18b_1	64 KB
libedit-3.1.20230828		h5eee18b_0	179 KB
libev-4.33		h7f8727e_1	111 KB
libffi-3.4.4		h6a678d5_1	141 KB
libgcc-devel_linux-64-11.2.0		h1234567_1	2.5 MB
libgcc-ng-11.2.0		h1234567_1	5.3 MB
libgfortran-ng-11.2.0		h00389a5_1	20 KB
libgfortran5-11.2.0		h1234567_1	2.0 MB
libglib-2.78.4		hdc74915_0	1.5 MB
libgomp-11.2.0		h1234567_1	474 KB
libiconv-1.16		h5eee18b_3	759 KB
libnghttp2-1.57.0		h2d74bed_0	674 KB
libopenblas-0.3.21		h043d6bf_0	5.4 MB
libpng-1.6.39		h5eee18b_0	304 KB
libssh2-1.11.0		h251f7ec_0	282 KB
libstdcxx-devel_linux-64-11.2.0		h1234567_1	14.6 MB
libstdcxx-ng-11.2.0		h1234567_1	4.7 MB
libtiff-4.5.1		h6a678d5_0	533 KB
libuuid-1.41.5		h5eee18b_0	27 KB
libwebp-base-1.3.2		h5eee18b_0	387 KB
libxcb-1.15		h7f8727e_0	505 KB
libxml2-2.10.4		hfdd30dd_2	754 KB
lz4-c-1.9.4		h6a678d5_1	156 KB
make-4.2.1		h1bed415_1	415 KB
ncurses-6.4		h6a678d5_0	914 KB
openssl-3.0.14		h5eee18b_0	5.2 MB
pango-1.50.7		h05da053_0	427 KB
pcre2-10.42		hebb0a14_1	1.3 MB
pip-24.0		py312h06a4308_0	3.3 MB
pixman-0.40.0		h7f8727e_1	373 KB
python-3.12.4		h5148396_1	34.8 MB
r-4.3.1		r43_0	4 KB
r-base-4.3.1		h1ae530e_0	23.9 MB
r-boot-1.3_28.1		r43h6115d3f_0	609 KB
r-class-7.3_22		r43h76d94ec_0	105 KB
r-cluster-2.1.4		r43h640688f_0	551 KB
r-codetools-0.2_19		r43h6115d3f_0	103 KB
r-foreign-0.8_85		r43h76d94ec_0	249 KB
r-kernsmooth-2.23_22		r43h640688f_0	94 KB
r-lattice-0.22_5		r43h76d94ec_0	1.3 MB
r-mass-7.3_60		r43h76d94ec_0	1.1 MB
r-matrix-1.6_1.1		r43h76d94ec_0	3.7 MB
r-mgcv-1.9_0		r43h76d94ec_0	3.1 MB
r-nlme-3.1_163		r43h640688f_0	2.2 MB
r-nnet-7.3_19		r43h76d94ec_0	129 KB

r-recommended-4.3.1		r43_0	4 KB
r-rpart-4.1.21		r43h76d94ec_0	683 KB
r-spatial-7.3_17		r43h76d94ec_0	149 KB
r-survival-3.5_7		r43h76d94ec_0	5.9 MB
readline-8.2		h5eee18b_0	357 KB
setuptools-69.5.1		py312h06a4308_0	1.3 MB
sqlite-3.45.3		h5eee18b_0	1.2 MB
sysroot_linux-64-2.17		h57e8cba_10	32.6 MB
tk-8.6.14		h39e8969_0	3.4 MB
tktable-2.10		h3d55465_1	96 KB
tzdata-2024a		h04d1e81_0	116 KB
wheel-0.43.0		py312h06a4308_0	142 KB
xz-5.4.6		h5eee18b_1	643 KB
zlib-1.2.13		h5eee18b_1	111 KB
zstd-1.5.5		hc292b87_2	643 KB

Total:			255.5 MB

The following NEW packages will be INSTALLED:

_libgcc_mutex	pkgs/main/linux-64::_libgcc_mutex-0.1-main
_openmp_mutex	pkgs/main/linux-64::_openmp_mutex-5.1-1_gnu
_r-mutex	pkgs/main/linux-64::_r-mutex-1.0.0-anacondar_1
_sysroot_linux-64~3-haa98f57_10	pkgs/main/noarch::_sysroot_linux-64_curr_repodata_hack-
binutils_impl_lin~h2a08ee3_1	pkgs/main/linux-64::binutils_impl_linux-64-2.38-
binutils_linux-64	pkgs/main/linux-64::binutils_linux-64-2.38.0-hc2dff05_0
blas	pkgs/main/linux-64::blas-1.0-openblas
bwidget	pkgs/main/linux-64::bwidget-1.9.16-h9eba36c_0
bzip2	pkgs/main/linux-64::bzip2-1.0.8-h5eee18b_6
c-ares	pkgs/main/linux-64::c-ares-1.19.1-h5eee18b_0
ca-certificates	pkgs/main/linux-64::ca-certificates-2024.3.11-h06a4308_0
cairo	pkgs/main/linux-64::cairo-1.16.0-hb05425b_5
curl	pkgs/main/linux-64::curl-8.7.1-hdbd6064_0
expat	pkgs/main/linux-64::expat-2.6.2-h6a678d5_0
fontconfig	pkgs/main/linux-64::fontconfig-2.14.1-h4c34cd2_2
freetype	pkgs/main/linux-64::freetype-2.12.1-h4a9f257_0
fribidi	pkgs/main/linux-64::fribidi-1.0.10-h7b6447c_0
gcc_impl_linux-64	pkgs/main/linux-64::gcc_impl_linux-64-11.2.0-h1234567_1
gcc_linux-64	pkgs/main/linux-64::gcc_linux-64-11.2.0-h5c386dc_0
gfortran_impl_lin~h1234567_1	pkgs/main/linux-64::gfortran_impl_linux-64-11.2.0-
gfortran_linux-64	pkgs/main/linux-64::gfortran_linux-64-11.2.0-hc2dff05_0
glib	pkgs/main/linux-64::glib-2.78.4-h6a678d5_0
glib-tools	pkgs/main/linux-64::glib-tools-2.78.4-h6a678d5_0
graphite2	pkgs/main/linux-64::graphite2-1.3.14-h295c915_1
gxx_impl_linux-64	pkgs/main/linux-64::gxx_impl_linux-64-11.2.0-h1234567_1
gxx_linux-64	pkgs/main/linux-64::gxx_linux-64-11.2.0-hc2dff05_0
harfbuzz	pkgs/main/linux-64::harfbuzz-4.3.0-hf52aaf7_2
icu	pkgs/main/linux-64::icu-73.1-h6a678d5_0
jpeg	pkgs/main/linux-64::jpeg-9e-h5eee18b_1
kernel-headers_li~h57e8cba_10	pkgs/main/noarch::kernel-headers_linux-64-3.10.0-
krb5	pkgs/main/linux-64::krb5-1.20.1-h143b758_1
ld_impl_linux-64	pkgs/main/linux-64::ld_impl_linux-64-2.38-h1181459_1
lerc	pkgs/main/linux-64::lerc-3.0-h295c915_0

libcurl	pkgs/main/linux-64::libcurl-8.7.1-h251f7ec_0
libdeflate	pkgs/main/linux-64::libdeflate-1.17-h5eee18b_1
libedit	pkgs/main/linux-64::libedit-3.1.20230828-h5eee18b_0
libev	pkgs/main/linux-64::libev-4.33-h7f8727e_1
libffi	pkgs/main/linux-64::libffi-3.4.4-h6a678d5_1
libgcc-devel_linu~ h1234567_1	pkgs/main/linux-64::libgcc-devel_linux-64-11.2.0-h1234567_1
libgcc-ng	pkgs/main/linux-64::libgcc-ng-11.2.0-h1234567_1
libgfortran-ng	pkgs/main/linux-64::libgfortran-ng-11.2.0-h00389a5_1
libgfortran5	pkgs/main/linux-64::libgfortran5-11.2.0-h1234567_1
libglib	pkgs/main/linux-64::libglib-2.78.4-hdc74915_0
libgomp	pkgs/main/linux-64::libgomp-11.2.0-h1234567_1
libiconv	pkgs/main/linux-64::libiconv-1.16-h5eee18b_3
libnghttp2	pkgs/main/linux-64::libnghttp2-1.57.0-h2d74bed_0
libopenblas	pkgs/main/linux-64::libopenblas-0.3.21-h043d6bf_0
libpng	pkgs/main/linux-64::libpng-1.6.39-h5eee18b_0
libssh2	pkgs/main/linux-64::libssh2-1.11.0-h251f7ec_0
libstdcxx-devel_l~ h1234567_1	pkgs/main/linux-64::libstdcxx-devel_linux-64-11.2.0-h1234567_1
libstdcxx-ng	pkgs/main/linux-64::libstdcxx-ng-11.2.0-h1234567_1
libtiff	pkgs/main/linux-64::libtiff-4.5.1-h6a678d5_0
libuuid	pkgs/main/linux-64::libuuid-1.41.5-h5eee18b_0
libwebp-base	pkgs/main/linux-64::libwebp-base-1.3.2-h5eee18b_0
libxcb	pkgs/main/linux-64::libxcb-1.15-h7f8727e_0
libxml2	pkgs/main/linux-64::libxml2-2.10.4-hfdd30dd_2
lz4-c	pkgs/main/linux-64::lz4-c-1.9.4-h6a678d5_1
make	pkgs/main/linux-64::make-4.2.1-h1bed415_1
ncurses	pkgs/main/linux-64::ncurses-6.4-h6a678d5_0
openssl	pkgs/main/linux-64::openssl-3.0.14-h5eee18b_0
pango	pkgs/main/linux-64::pango-1.50.7-h05da053_0
pcre2	pkgs/main/linux-64::pcr2-10.42-hebb0a14_1
pip	pkgs/main/linux-64::pip-24.0-py312h06a4308_0
pixman	pkgs/main/linux-64::pixman-0.40.0-h7f8727e_1
python	pkgs/main/linux-64::python-3.12.4-h5148396_1
r	pkgs/r/linux-64::r-4.3.1-r43_0
r-base	pkgs/r/linux-64::r-base-4.3.1-h1ae530e_0
r-boot	pkgs/r/noarch::r-boot-1.3_28.1-r43h6115d3f_0
r-class	pkgs/r/linux-64::r-class-7.3_22-r43h76d94ec_0
r-cluster	pkgs/r/linux-64::r-cluster-2.1.4-r43h640688f_0
r-codetools	pkgs/r/noarch::r-codetools-0.2_19-r43h6115d3f_0
r-foreign	pkgs/r/linux-64::r-foreign-0.8_85-r43h76d94ec_0
r-kernsmooth	pkgs/r/linux-64::r-kernsmooth-2.23_22-r43h640688f_0
r-lattice	pkgs/r/linux-64::r-lattice-0.22_5-r43h76d94ec_0
r-mass	pkgs/r/linux-64::r-mass-7.3_60-r43h76d94ec_0
r-matrix	pkgs/r/linux-64::r-matrix-1.6_1.1-r43h76d94ec_0
r-mgcv	pkgs/r/linux-64::r-mgcv-1.9_0-r43h76d94ec_0
r-nlme	pkgs/r/linux-64::r-nlme-3.1_163-r43h640688f_0
r-nnet	pkgs/r/linux-64::r-nnet-7.3_19-r43h76d94ec_0
r-recommended	pkgs/r/linux-64::r-recommended-4.3.1-r43_0
r-rpart	pkgs/r/linux-64::r-rpart-4.1.21-r43h76d94ec_0
r-spatial	pkgs/r/linux-64::r-spatial-7.3_17-r43h76d94ec_0
r-survival	pkgs/r/linux-64::r-survival-3.5_7-r43h76d94ec_0
readline	pkgs/main/linux-64::readline-8.2-h5eee18b_0
setuptools	pkgs/main/linux-64::setuptools-69.5.1-py312h06a4308_0
sqlite	pkgs/main/linux-64::sqlite-3.45.3-h5eee18b_0
sysroot_linux-64	pkgs/main/noarch::sysroot_linux-64-2.17-h57e8cba_10
tk	pkgs/main/linux-64::tk-8.6.14-h39e8969_0

```
tktable          pkgs/main/linux-64::tktable-2.10-h3d55465_1
tzdata           pkgs/main/noarch::tzdata-2024a-h04d1e81_0
wheel            pkgs/main/linux-64::wheel-0.43.0-py312h06a4308_0
xz               pkgs/main/linux-64::xz-5.4.6-h5eee18b_1
zlib             pkgs/main/linux-64::zlib-1.2.13-h5eee18b_1
zstd             pkgs/main/linux-64::zstd-1.5.5-hc292b87_2
```

Downloading and Extracting Packages:

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

Did Search Work?

```
(r_env) [salexan5@mblog1 ~]$ conda search tidyverse
Loading channels: done
No match found for: tidyverse. Search: *tidyverse*
# Name          Version          Build          Channel
r-tidyverse     1.0.0            r3.3.1_0      pkgs/r
...
r-tidyverse     1.3.1            r42h6115d3f_0 pkgs/r
r-tidyverse     2.0.0            r43h6115d3f_0 pkgs/r
```

Conda R related packages typically are prefixed with `r_`

Conda Install TidyVerse

TidyVerse is made up of 10s of R libraries. These dependencies are all installed.

Full Details

```
(r_env) [salexan5@mblog1 ~]$ conda install r-tidyverse=2.0.0
Channels:
- defaults
Platform: linux-64
Collecting package metadata (repodata.json): done
Solving environment: done

## Package Plan ##
```

environment location: /project/arcc/salexan5/conda/envs/r_env

added / updated specs:

- r-tidyverse=2.0.0

The following packages will be downloaded:

package	build	
pandoc-2.12	h06a4308_3	10.5 MB
r-askpass-1.2.0	r43h76d94ec_0	29 KB
r-backports-1.4.1	r43h76d94ec_0	112 KB
r-base64enc-0.1_3	r43h76d94ec_4	46 KB
r-bit-4.0.5	r43h76d94ec_0	1.0 MB
r-bit64-4.0.5	r43h76d94ec_0	480 KB
r-blob-1.2.4	r43h6115d3f_0	52 KB
r-broom-1.0.5	r43h6115d3f_0	1.7 MB
r-bslib-0.5.1	r43h6115d3f_0	4.8 MB
r-cachem-1.0.8	r43h76d94ec_0	71 KB
r-callr-3.7.3	r43h6115d3f_0	403 KB
r-cellranger-1.1.0	r43h6115d3f_0	103 KB
r-cli-3.6.1	r43h884c59f_0	1.2 MB
r-clipr-0.8.0	r43h6115d3f_0	65 KB
r-colorspace-2.1_0	r43h76d94ec_0	2.4 MB
r-conflicted-1.2.0	r43h142f84f_0	61 KB
r-cpp11-0.4.6	r43h6115d3f_0	221 KB
r-crayon-1.5.2	r43h6115d3f_0	159 KB
r-curl-5.1.0	r43h76d94ec_0	430 KB
r-data.table-1.14.8	r43h76d94ec_0	1.8 MB
r-dbi-1.1.3	r43h6115d3f_0	697 KB
r-dbplyr-2.3.4	r43h6115d3f_0	1.0 MB
r-digest-0.6.33	r43h884c59f_0	190 KB
r-dplyr-1.1.3	r43h884c59f_0	1.3 MB
r-dtplyr-1.3.1	r43h6115d3f_0	344 KB
r-ellipsis-0.3.2	r43h76d94ec_0	40 KB
r-evaluate-0.22	r43h6115d3f_0	85 KB
r-fansi-1.0.5	r43h76d94ec_0	313 KB
r-farver-2.1.1	r43h884c59f_0	1.4 MB
r-fastmap-1.1.1	r43h884c59f_0	67 KB
r-fontawesome-0.5.2	r43h6115d3f_0	1.2 MB
r-forcats-1.0.0	r43h6115d3f_0	409 KB
r-fs-1.6.3	r43h884c59f_0	481 KB
r-gargle-1.5.2	r43h142f84f_0	689 KB
r-generics-0.1.3	r43h142f84f_0	81 KB
r-ggplot2-3.4.4	r43h6115d3f_0	3.9 MB
r-glue-1.6.2	r43h76d94ec_0	146 KB
r-googledrive-2.1.1	r43h6115d3f_0	1.1 MB
r-goolesheets4-1.1.1	r43h6115d3f_0	497 KB
r-gtable-0.3.4	r43h6115d3f_0	214 KB
r-haven-2.5.3	r43h884c59f_0	356 KB
r-highr-0.10	r43h6115d3f_0	54 KB
r-hms-1.1.3	r43h6115d3f_0	102 KB
r-htmltools-0.5.6.1	r43h76d94ec_0	347 KB
r-http-1.4.7	r43h6115d3f_0	452 KB
r-ids-1.0.1	r43h142f84f_0	122 KB
r-isoband-0.2.7	r43h884c59f_0	1.5 MB

r-jquerylib-0.1.4		r43h6115d3f_0	296 KB
r-jsonlite-1.8.7		r43h76d94ec_0	618 KB
r-knitr-1.44		r43h6115d3f_0	1.2 MB
r-labeling-0.4.3		r43h6115d3f_0	64 KB
r-lifecycle-1.0.3		r43h142f84f_0	116 KB
r-lubridate-1.9.3		r43h76d94ec_0	950 KB
r-magrittr-2.0.3		r43h76d94ec_0	200 KB
r-memoise-2.0.1		r43h6115d3f_0	53 KB
r-mime-0.12		r43h76d94ec_0	49 KB
r-modelr-0.1.11		r43h6115d3f_0	211 KB
r-munsell-0.5.0		r43h6115d3f_0	236 KB
r-openssl-2.1.1		r43h76d94ec_0	619 KB
r-pillar-1.9.0		r43h6115d3f_0	591 KB
r-pkgconfig-2.0.3		r43h6115d3f_0	24 KB
r-prettyunits-1.2.0		r43h142f84f_0	158 KB
r-processx-3.8.2		r43h76d94ec_0	313 KB
r-progress-1.2.2		r43h142f84f_0	88 KB
r-ps-1.7.5		r43h76d94ec_0	301 KB
r-purrr-1.0.2		r43h76d94ec_0	469 KB
r-r6-2.5.1		r43h6115d3f_0	89 KB
r-ragg-1.2.6		r43h884c59f_0	427 KB
r-rappdirs-0.3.3		r43h76d94ec_0	50 KB
r-rcolorbrewer-1.1_3		r43h6115d3f_1	57 KB
r-readr-2.1.4		r43h884c59f_0	761 KB
r-readxl-1.4.3		r43h884c59f_0	724 KB
r-rematch-2.0.0		r43h6115d3f_0	22 KB
r-rematch2-2.1.2		r43h142f84f_0	51 KB
r-reprex-2.0.2		r43h6115d3f_0	488 KB
r-rlang-1.1.1		r43h884c59f_0	1.4 MB
r-rmarkdown-2.25		r43h6115d3f_0	1.9 MB
r-rstudioapi-0.15.0		r43h6115d3f_0	283 KB
r-rvest-1.0.3		r43h6115d3f_0	205 KB
r-sass-0.4.7		r43h884c59f_0	2.2 MB
r-scales-1.2.1		r43h6115d3f_0	577 KB
r-selectr-0.4_2		r43h6115d3f_0	404 KB
r-stringi-1.7.12		r43h884c59f_0	870 KB
r-stringr-1.5.0		r43h6115d3f_0	284 KB
r-sys-3.4.2		r43h76d94ec_0	46 KB
r-systemfonts-1.0.5		r43h884c59f_0	227 KB
r-textshaping-0.3.7		r43h884c59f_0	100 KB
r-tibble-3.2.1		r43h76d94ec_0	594 KB
r-tidyr-1.3.0		r43h884c59f_0	1.1 MB
r-tidyselect-1.2.0		r43h6115d3f_0	208 KB
r-tidyverse-2.0.0		r43h6115d3f_0	414 KB
r-timechange-0.2.0		r43h884c59f_0	175 KB
r-tinytex-0.48		r43h142f84f_0	138 KB
r-tzdb-0.4.0		r43h884c59f_0	514 KB
r-utf8-1.2.4		r43h76d94ec_0	138 KB
r-uuid-1.1_1		r43h76d94ec_0	50 KB
r-vctrs-0.6.4		r43h884c59f_0	1.2 MB
r-viridislite-0.4.2		r43h6115d3f_0	1.2 MB
r-vroom-1.6.4		r43h884c59f_0	838 KB
r-withr-2.5.1		r43h6115d3f_0	224 KB
r-xfun-0.40		r43h76d94ec_0	410 KB
r-xml2-1.3.5		r43h884c59f_0	223 KB
r-yaml-2.3.7		r43h76d94ec_0	111 KB

Total: 67.5 MB

The following NEW packages will be INSTALLED:

pandoc	pkgs/main/linux-64::pandoc-2.12-h06a4308_3
r-askpass	pkgs/r/linux-64::r-askpass-1.2.0-r43h76d94ec_0
r-backports	pkgs/r/linux-64::r-backports-1.4.1-r43h76d94ec_0
r-base64enc	pkgs/r/linux-64::r-base64enc-0.1_3-r43h76d94ec_4
r-bit	pkgs/r/linux-64::r-bit-4.0.5-r43h76d94ec_0
r-bit64	pkgs/r/linux-64::r-bit64-4.0.5-r43h76d94ec_0
r-blob	pkgs/r/noarch::r-blob-1.2.4-r43h6115d3f_0
r-broom	pkgs/r/noarch::r-broom-1.0.5-r43h6115d3f_0
r-bslib	pkgs/r/noarch::r-bslib-0.5.1-r43h6115d3f_0
r-cachem	pkgs/r/linux-64::r-cachem-1.0.8-r43h76d94ec_0
r-callr	pkgs/r/noarch::r-callr-3.7.3-r43h6115d3f_0
r-cellranger	pkgs/r/noarch::r-cellranger-1.1.0-r43h6115d3f_0
r-cli	pkgs/r/linux-64::r-cli-3.6.1-r43h884c59f_0
r-clipr	pkgs/r/noarch::r-clipr-0.8.0-r43h6115d3f_0
r-colorspace	pkgs/r/linux-64::r-colorspace-2.1_0-r43h76d94ec_0
r-conflicted	pkgs/r/noarch::r-conflicted-1.2.0-r43h142f84f_0
r-cpp11	pkgs/r/noarch::r-cpp11-0.4.6-r43h6115d3f_0
r-crayon	pkgs/r/noarch::r-crayon-1.5.2-r43h6115d3f_0
r-curl	pkgs/r/linux-64::r-curl-5.1.0-r43h76d94ec_0
r-data.table	pkgs/r/linux-64::r-data.table-1.14.8-r43h76d94ec_0
r-dbi	pkgs/r/noarch::r-dbi-1.1.3-r43h6115d3f_0
r-dbplyr	pkgs/r/noarch::r-dbplyr-2.3.4-r43h6115d3f_0
r-digest	pkgs/r/linux-64::r-digest-0.6.33-r43h884c59f_0
r-dplyr	pkgs/r/linux-64::r-dplyr-1.1.3-r43h884c59f_0
r-dtplyr	pkgs/r/noarch::r-dtplyr-1.3.1-r43h6115d3f_0
r-ellipsis	pkgs/r/linux-64::r-ellipsis-0.3.2-r43h76d94ec_0
r-evaluate	pkgs/r/noarch::r-evaluate-0.22-r43h6115d3f_0
r-fansi	pkgs/r/linux-64::r-fansi-1.0.5-r43h76d94ec_0
r-farver	pkgs/r/linux-64::r-farver-2.1.1-r43h884c59f_0
r-fastmap	pkgs/r/linux-64::r-fastmap-1.1.1-r43h884c59f_0
r-fontawesome	pkgs/r/noarch::r-fontawesome-0.5.2-r43h6115d3f_0
r-forcats	pkgs/r/noarch::r-forcats-1.0.0-r43h6115d3f_0
r-fs	pkgs/r/linux-64::r-fs-1.6.3-r43h884c59f_0
r-gargle	pkgs/r/noarch::r-gargle-1.5.2-r43h142f84f_0
r-generics	pkgs/r/noarch::r-generics-0.1.3-r43h142f84f_0
r-ggplot2	pkgs/r/noarch::r-ggplot2-3.4.4-r43h6115d3f_0
r-glue	pkgs/r/linux-64::r-glue-1.6.2-r43h76d94ec_0
r-googledrive	pkgs/r/noarch::r-googledrive-2.1.1-r43h6115d3f_0
r-googlesheets4	pkgs/r/noarch::r-googlesheets4-1.1.1-r43h6115d3f_0
r-gtable	pkgs/r/noarch::r-gtable-0.3.4-r43h6115d3f_0
r-haven	pkgs/r/linux-64::r-haven-2.5.3-r43h884c59f_0
r-highr	pkgs/r/noarch::r-highr-0.10-r43h6115d3f_0
r-hms	pkgs/r/noarch::r-hms-1.1.3-r43h6115d3f_0
r-htmltools	pkgs/r/linux-64::r-htmltools-0.5.6.1-r43h76d94ec_0
r-httptr	pkgs/r/noarch::r-httptr-1.4.7-r43h6115d3f_0
r-ids	pkgs/r/noarch::r-ids-1.0.1-r43h142f84f_0
r-isoband	pkgs/r/linux-64::r-isoband-0.2.7-r43h884c59f_0
r-jquerylib	pkgs/r/noarch::r-jquerylib-0.1.4-r43h6115d3f_0
r-jsonlite	pkgs/r/linux-64::r-jsonlite-1.8.7-r43h76d94ec_0
r-knitr	pkgs/r/noarch::r-knitr-1.44-r43h6115d3f_0
r-labeling	pkgs/r/noarch::r-labeling-0.4.3-r43h6115d3f_0
r-lifecycle	pkgs/r/noarch::r-lifecycle-1.0.3-r43h142f84f_0
r-lubridate	pkgs/r/linux-64::r-lubridate-1.9.3-r43h76d94ec_0

r-magrittr	pkgs/r/linux-64::r-magrittr-2.0.3-r43h76d94ec_0
r-memoise	pkgs/r/noarch::r-memoise-2.0.1-r43h6115d3f_0
r-mime	pkgs/r/linux-64::r-mime-0.12-r43h76d94ec_0
r-modelr	pkgs/r/noarch::r-modelr-0.1.11-r43h6115d3f_0
r-munsell	pkgs/r/noarch::r-munsell-0.5.0-r43h6115d3f_0
r-openssl	pkgs/r/linux-64::r-openssl-2.1.1-r43h76d94ec_0
r-pillar	pkgs/r/noarch::r-pillar-1.9.0-r43h6115d3f_0
r-pkgconfig	pkgs/r/noarch::r-pkgconfig-2.0.3-r43h6115d3f_0
r-prettyunits	pkgs/r/noarch::r-prettyunits-1.2.0-r43h142f84f_0
r-processx	pkgs/r/linux-64::r-processx-3.8.2-r43h76d94ec_0
r-progress	pkgs/r/noarch::r-progress-1.2.2-r43h142f84f_0
r-ps	pkgs/r/linux-64::r-ps-1.7.5-r43h76d94ec_0
r-purrr	pkgs/r/linux-64::r-purrr-1.0.2-r43h76d94ec_0
r-r6	pkgs/r/noarch::r-r6-2.5.1-r43h6115d3f_0
r-ragg	pkgs/r/linux-64::r-ragg-1.2.6-r43h884c59f_0
r-rappdirs	pkgs/r/linux-64::r-rappdirs-0.3.3-r43h76d94ec_0
r-rcolorbrewer	pkgs/r/noarch::r-rcolorbrewer-1.1_3-r43h6115d3f_1
r-readr	pkgs/r/linux-64::r-readr-2.1.4-r43h884c59f_0
r-readxl	pkgs/r/linux-64::r-readxl-1.4.3-r43h884c59f_0
r-rematch	pkgs/r/noarch::r-rematch-2.0.0-r43h6115d3f_0
r-rematch2	pkgs/r/noarch::r-rematch2-2.1.2-r43h142f84f_0
r-reprex	pkgs/r/noarch::r-reprex-2.0.2-r43h6115d3f_0
r-rlang	pkgs/r/linux-64::r-rlang-1.1.1-r43h884c59f_0
r-rmarkdown	pkgs/r/noarch::r-rmarkdown-2.25-r43h6115d3f_0
r-rstudioapi	pkgs/r/noarch::r-rstudioapi-0.15.0-r43h6115d3f_0
r-rvest	pkgs/r/noarch::r-rvest-1.0.3-r43h6115d3f_0
r-sass	pkgs/r/linux-64::r-sass-0.4.7-r43h884c59f_0
r-scales	pkgs/r/noarch::r-scales-1.2.1-r43h6115d3f_0
r-selectr	pkgs/r/noarch::r-selectr-0.4_2-r43h6115d3f_0
r-stringi	pkgs/r/linux-64::r-stringi-1.7.12-r43h884c59f_0
r-stringr	pkgs/r/noarch::r-stringr-1.5.0-r43h6115d3f_0
r-sys	pkgs/r/linux-64::r-sys-3.4.2-r43h76d94ec_0
r-systemfonts	pkgs/r/linux-64::r-systemfonts-1.0.5-r43h884c59f_0
r-textshaping	pkgs/r/linux-64::r-textshaping-0.3.7-r43h884c59f_0
r-tibble	pkgs/r/linux-64::r-tibble-3.2.1-r43h76d94ec_0
r-tidyr	pkgs/r/linux-64::r-tidyr-1.3.0-r43h884c59f_0
r-tidyselect	pkgs/r/noarch::r-tidyselect-1.2.0-r43h6115d3f_0
r-tidyverse	pkgs/r/noarch::r-tidyverse-2.0.0-r43h6115d3f_0
r-timechange	pkgs/r/linux-64::r-timechange-0.2.0-r43h884c59f_0
r-tinytex	pkgs/r/noarch::r-tinytex-0.48-r43h142f84f_0
r-tzdb	pkgs/r/linux-64::r-tzdb-0.4.0-r43h884c59f_0
r-utf8	pkgs/r/linux-64::r-utf8-1.2.4-r43h76d94ec_0
r-uuid	pkgs/r/linux-64::r-uuid-1.1_1-r43h76d94ec_0
r-vctrs	pkgs/r/linux-64::r-vctrs-0.6.4-r43h884c59f_0
r-viridislite	pkgs/r/noarch::r-viridislite-0.4.2-r43h6115d3f_0
r-vroom	pkgs/r/linux-64::r-vroom-1.6.4-r43h884c59f_0
r-withr	pkgs/r/noarch::r-withr-2.5.1-r43h6115d3f_0
r-xfun	pkgs/r/linux-64::r-xfun-0.40-r43h76d94ec_0
r-xml2	pkgs/r/linux-64::r-xml2-1.3.5-r43h884c59f_0
r-yaml	pkgs/r/linux-64::r-yaml-2.3.7-r43h76d94ec_0

Downloading and Extracting Packages:

Preparing transaction: done
 Verifying transaction: done
 Executing transaction: done

How Large is this Environment?

Confirm where this R environment is located.

```
[salexan5@mblog1 ~]$ cat .conda/environments.txt
/home/salexan5/.conda/envs/py_env
/project/arcc/salexan5/conda/envs/r_env

[salexan5@mblog2 ~a]$ cd /project/arcc/salexan5/conda

[salexan5@mblog2 conda]$ du -d 1 -h
1.2G    ./envs
526M    ./pkgs
1.7G    .
```

This R environment, and associated packages, is itself 1.7G - this is on top of the first example which still exists under the `.conda` folder in home.

Using R Environment

```
[salexan5@mblog2 ~]$ salloc -A arcc -t 10:00
salloc: Granted job allocation 786989
salloc: Nodes mba30-001 are ready for job
[salexan5@mba30-001 ~]$ module load miniconda3/24.3.0
[salexan5@mba30-001 ~]$ conda activate r_env
(r_env) [salexan5@mba30-001 ~]$ Rscript r_test.R
— Attaching core tidyverse packages

────────────────────────── tidyverse 2.0.0 ───────────────────────────
✓ dplyr      1.1.3      ✓ readr      2.1.4
...
(r_env) [salexan5@mba30-001 ~]$ conda deactivate
[salexan5@mba30-001 ~]$ exit
exit
salloc: Relinquishing job allocation 786989
```

File: `r_test.R`

```
library(tidyverse)
```

Conda Channels

Goal: What are channels and how can they be used and configured.

- [What are Channels?](#)
 - [Can't find package?](#)
 - [Additional Common Channels:](#)
 - [Add Channel](#)
 - [Search for SLiM](#)
 - [Channel Options](#)
-

What are Channels?

[Managing channels](#): Conda channels are the locations where packages are stored. They serve as the base for hosting and managing packages. Conda packages are downloaded from remote channels, which are URLs to directories containing conda packages.

Can't find package?

Example: I've heard SLiM is available to install via conda?

```
[salexan5@mblog2 ~]$ conda search slim
Loading channels: done
No match found for: slim. Search: *slim*
# Name                               Version           Build  Channel
r-slim                               0.1.1            r36h6115d3f_0  pkgs/r
...
r-waveslim                           1.8.4            r43h640688f_0  pkgs/r
```

Additional Common Channels:

- [bioconda](#): (>10K packages) Bioconda is a distribution of bioinformatics software realized as a channel for the versatile Conda package manager.
- [conda-forge](#) packages:

```
[salexan5@mblog2 ~]$ conda search bioconda::slim
Loading channels: done
No match found for: bioconda::slim. Search: bioconda::*slim*
# Name                               Version           Build  Channel
gargammel-slim                       1.1.2            h06294c5_5  bioconda
...
slimfastq                             2.04             he1b5a44_0  bioconda
...
slimm                                 0.3.4            hf1761c0_4  bioconda
[salexan5@mblog2 ~]$ conda search conda-forge::slim
Loading channels: done
```

# Name	Version	Build	Channel
slim	3.3.2	he1b5a44_0	conda-forge
...			
slim	4.2.2	h59595ed_0	conda-forge

Add Channel

```
[salexan5@mblog1 ~]$ conda config --add channels conda-forge

[salexan5@mblog1 ~]$ cat ~/.condarc
...
channels:
  - conda-forge
  - defaults
[salexan5@mblog1 ~]$ conda info
[salexan5@mblog1 ~]$ conda info
...
      channel URLs : https://conda.anaconda.org/conda-forge/linux-64
                    https://conda.anaconda.org/conda-forge/noarch
                    https://repo.anaconda.com/pkgs/main/linux-64
                    https://repo.anaconda.com/pkgs/main/noarch
                    https://repo.anaconda.com/pkgs/r/linux-64
                    https://repo.anaconda.com/pkgs/r/noarch
...

```

Search for SLiM

```
[salexan5@mblog2 ~]$ conda search slim
Loading channels: done
# Name          Version      Build      Channel
slim            3.3.2       he1b5a44_0 conda-forge
...
slim            4.2.2       h59595ed_0 conda-forge

```

No need to explicitly define the channel in the search command as it is not part of our general conda configuration.

Channel Options

The channel option can be defined within a number of other commands, such as `conda install`:

```
[salexan5@mblog2 ~]$ conda install --help
usage: conda install [-h] [--revision REVISION] [-n ENVIRONMENT | -p PATH] [-c CHANNEL] [--use-local] [--override-channels] [--repopdata-fn REPODATA_FNS]
```

```

        [--experimental {jlap,lock}] [--no-lock] [--repopdata-
use-zst | --no-repopdata-use-zst] [--strict-channel-priority] [--no-channel-
priority]
        [--no-deps | --only-deps] [--no-pin] [--copy] [--no-
shortcuts] [--shortcuts-only SHORTCUTS_ONLY] [-C] [-k] [--offline] [--json]
[-v] [-q] [-d]
        [-y] [--download-only] [--show-channel-urls] [--file
FILE] [--solver {classic,libmamba}] [--force-reinstall]
        [--freeze-installed | --update-deps | -S | --update-all
| --update-specs] [-m] [--clobber] [--dev]
        [package_spec ...]
...
Channel Customization:
  -c CHANNEL, --channel CHANNEL
        Additional channel to search for packages. These are
URLs searched in the order they are given (including local directories using
the
        'file:/' syntax or simply a path like
'/home/conda/mychan' or '../mychan'). Then, the defaults or channels from
.condarc are searched (unless
        --override-channels is given). You can use 'defaults'
to get the default packages for conda. You can also use any name and the
.condarc
        channel_alias value will be prepended. The default
channel_alias is https://conda.anaconda.org/.
...

```

Example 03: Applications: SLiM

Goals: Demonstrate using conda to install a command-line application.

- [General Process](#)
 - [Create SLiM Environment](#)
 - [Use / Activate this Environment](#)
 - [Calling the SLiM command-line](#)
-

General Process

```

[salexan5@mblog1 ~]$ cd /project/arcc/salexan5/
[salexan5@mblog1 salexan5]$ mkdir software
[salexan5@mblog1 salexan5]$ cd software
[salexan5@mblog1 software]$ pwd
/project/arcc/salexan5/software

[salexan5@mblog1 software]$ conda create -p slim_env_4.2.2
...
## Package Plan ##

```

```
environment location:
/cluster/medbow/project/arcc/salexan5/software/slim_env_4.2.2
...
# To activate this environment, use
# $ conda activate
/cluster/medbow/project/arcc/salexan5/software/slim_env_4.2.2
```

Notice we haven't performed any *activate* or *install* steps.

What do we notice about the installation location?

Create SLiM Environment

```
conda create -p ...
```

Using the `-p` option will create the environment in your current working folder.

```
[salexan5@mblog2 ~]$ conda install --help
...
-p PATH, --prefix PATH
                        Full path to environment location (i.e. prefix).
[salexan5@mblog2 ~]$ cat ~/.conda/environments.txt
/home/salexan5/.conda/envs/py_env
/project/arcc/salexan5/conda/envs/r_env
/cluster/medbow/project/arcc/salexan5/software/slim_env_4.2.2
```

Use / Activate this Environment

```
[salexan5@mblog2 ~]$ conda activate slim_env_4.2.2
EnvironmentNameNotFound: Could not find conda environment: slim_env_4.2.2
You can list all discoverable environments with `conda info --envs`.
[salexan5@mblog2 ~]$ conda info --envs
# conda environments:
#
base                                /apps/u/opt/linux/miniconda3/24.3.0

/cluster/medbow/project/arcc/salexan5/software/slim_env_4.2.2
py_env                              /home/salexan5/.conda/envs/py_env
r_env                                /project/arcc/salexan5/conda/envs/r_env
```

This environment has not 'name' and thus you must use the full path to activate.

```
[salexan5@mblog2 ~]$ conda activate
/cluster/medbow/project/arcc/salexan5/software/slim_env_4.2.2
(/cluster/medbow/project/arcc/salexan5/software/slim_env_4.2.2)
[salexan5@mblog2 ~]$
```

Calling the SLiM command-line

```
(/cluster/medbow/project/arcc/salexan5/software/slim_env_4.2.2)
[salexan5@mblog2 ~]$ slim --version
SLiM version 4.2.2, built May  5 2024 12:39:53
Git commit SHA-1: unknown (built from a non-Git source archive)

(/cluster/medbow/project/arcc/salexan5/software/slim_env_4.2.2)
[salexan5@mblog2 ~]$ which slim
/cluster/medbow/project/arcc/salexan5/software/slim_env_4.2.2/bin/slim

(/cluster/medbow/project/arcc/salexan5/software/slim_env_4.2.2)
[salexan5@mblog2 ~]$ conda deactivate

[salexan5@mblog2 ~]$ slim --version
bash: slim: command not found...
```

Reproducibility and Sharing

Goal: Introduce how conda environments can be reproduced and shared.

Based on [Managing Environments](#).

- [Clone an Environment](#)
 - [Using Cloned Environment](#)
 - [Export an Environment](#)
 - [Conda env command](#)
 - [Import an Environment](#)
-

Clone an Environment

```
[salexan5@mblog2 ~]$ conda create --help
...
options:
...
--clone ENV          Create a new environment as a copy of an existing
local environment.
...
```

Example

```
[salexan5@mblog2 software]$ conda create -p py_env2 --clone py_env
Retrieving notices: ...working... done
Source:          /home/salexan5/.conda/envs/py_env
Destination:    /cluster/medbow/project/arcc/salexan5/software/py_env2
```

```
Packages: 39
Files: 1
...
#
# To activate this environment, use
#     $ conda activate /cluster/medbow/project/arcc/salexan5/software/py_env2
▼ Full Details:
[salexan5@mblog2 software]$ pwd
/project/arcc/salexan5/software
[salexan5@mblog2 software]$ ls
slim_env_4.2.2

[salexan5@mblog2 software]$ conda create -p py_env2 --clone py_env
Retrieving notices: ...working... done
Source:      /home/salexan5/.conda/envs/py_env
Destination: /cluster/medbow/project/arcc/salexan5/software/py_env2
Packages: 39
Files: 1

Downloading and Extracting Packages:

Downloading and Extracting Packages:

Preparing transaction: done
Verifying transaction: done
Executing transaction: done
#
# To activate this environment, use
#
#     $ conda activate /cluster/medbow/project/arcc/salexan5/software/py_env2
#
# To deactivate an active environment, use
#
#     $ conda deactivate

[salexan5@mblog2 software]$ ls
py_env2  slim_env_4.2.2
```

Using Cloned Environment

Notice how you need to activate/use this cloned environment:

```
[salexan5@mblog2 ~]$ cat ~/.conda/environments.txt
/home/salexan5/.conda/envs/py_env
/project/arcc/salexan5/conda/envs/r_env
/cluster/medbow/project/arcc/salexan5/software/slim_env_4.2.2
/cluster/medbow/project/arcc/salexan5/software/py_env2
```

```
[salexan5@mblog2 ~]$ conda info --env
# conda environments:
```



```
#
base /apps/u/opt/linux/miniconda3/24.3.0

/cluster/medbow/project/arcc/salexan5/software/py_env2

/cluster/medbow/project/arcc/salexan5/software/slim_env_4.2.2
py_env /home/salexan5/.conda/envs/py_env
r_env /project/arcc/salexan5/conda/envs/r_env
```

Need to define the full path to *activate*.

```
[salexan5@mblog2 ~]$ conda activate
/cluster/medbow/project/arcc/salexan5/software/py_env2
(/cluster/medbow/project/arcc/salexan5/software/py_env2) [salexan5@mblog2 ~]$
```

Export an Environment

```
[salexan5@mblog2 ~]$ conda activate r_env
(r_env) [salexan5@mblog2 ~]$ conda env export > r_env.yml
(r_env) [salexan5@mblog2 ~]$ conda deactivate
```

```
[salexan5@mblog2 ~]$ cat r_env.yml
name: r_env
channels:
  - conda-forge
  - defaults
dependencies:
  - _libgcc_mutex=0.1=main
  ...
  - zstd=1.5.5=hc292b87_2
prefix: /project/arcc/salexan5/conda/envs/r_env
```

Conda env command

```
[salexan5@mblog2 ~]$ conda env --help
usage: conda env [-h] command ...
```

positional arguments:

command	
config	Configure a conda environment.
create	Create an environment based on an environment definition file.
export	Export a given environment
list	List the Conda environments.
remove	Remove an environment.
update	Update the current environment based on environment file.

options:

-h, --help	Show this help message and exit.
------------	----------------------------------

Import an Environment

```
[salexan5@mblog2 software]$ conda env create -p r_env2 --file r_env.yml
...
#
# To activate this environment, use
#
#     $ conda activate /cluster/medbow/project/arcc/salexan5/software/r_env2
...
```

Example 04: Application: Qiime Ecosystem

Goal: Demonstrate importing the large [qiime](#) application ecosystem.

- [Can I use a Channel](#)
 - [Using a Definition File](#)
 - [What's in this Qiime Environment?](#)
 - [How Large is this Environment?](#)
 - [Cleaning Up](#)
-

Can I use a Channel

Not from the channels I have configured.

```
[salexan5@mblog2 software]$ conda search qiime
Loading channels: done
No match found for: qiime. Search: *qiime*
# Name                               Version           Build  Channel
r-qiimer                             0.9.4            r3.3.2_0  conda-forge
...
r-qiimer                             0.9.4            r43hc72bb7e_1005  conda-forge
```

Only older versions in bioconda channel.

```
[salexan5@mblog2 software]$ conda search bioconda::qiime
Loading channels: done
# Name                               Version           Build  Channel
qiime                               1.8.0            py27_0  bioconda
...
qiime                               1.9.1            py_3  bioconda
```

Using a Definition File

[From Install QIIME2 within a conda environment:](#)

```
[salexan5@mblog1 software]$ pwd
/project/arcc/salexan5/software
[salexan5@mblog1 software]$ mkdir qiime
[salexan5@mblog1 software]$ cd qiime/
[salexan5@mblog1 qiime]$ wget https://data.qiime2.org/distro/amplicon/qiime2-
amplicon-2024.5-py38-linux-conda.yml

[salexan5@mblog1 qiime]$ conda env create -p amplicon-2024.5 --file qiime2-
amplicon-2024.5-py38-linux-conda.yml

[salexan5@mblog2 qiime]$ conda activate
(/cluster/medbow/project/arcc/salexan5/software/qiime/amplicon-2024.5
(/cluster/medbow/project/arcc/salexan5/software/qiime/amplicon-2024.5)
[salexan5@mblog2 qiime]$ qiime info
System versions
Python version: 3.9.19
QIIME 2 release: 2024.5
QIIME 2 version: 2024.5.0
q2cli version: 2024.5.0
...
```



qiime_conda_list.txt

What's in this Qiime Environment?

This environment contains qiime commands, R and libraries, Python and packages...

```
(/cluster/medbow/project/arcc/salexan5/software/qiime/amplicon-2024.5)
[salexan5@mblog2 qiime]$ which R
(/cluster/medbow/project/arcc/salexan5/software/qiime/amplicon-2024.5/bin/R
(/cluster/medbow/project/arcc/salexan5/software/qiime/amplicon-2024.5)
[salexan5@mblog2 qiime]$ R --version
R version 4.3.3 (2024-02-29) -- "Angel Food Cake"
```

```
(/cluster/medbow/project/arcc/salexan5/software/qiime/amplicon-2024.5)
[salexan5@mblog2 qiime]$ which python
/cluster/medbow/project/arcc/salexan5/software/qiime/amplicon-
2024.5/bin/python
(/cluster/medbow/project/arcc/salexan5/software/qiime/amplicon-2024.5)
[salexan5@mblog2 qiime]$ python --version
Python 3.9.19
```

```
(/cluster/medbow/project/arcc/salexan5/software/qiime/amplicon-2024.5)
[salexan5@mblog2 qiime]$ pip list -v
Package          Version          Location
Installer
-----
altair           5.3.0
/cluster/medbow/project/arcc/salexan5/software/qiime/amplicon-
2024.5/lib/python3.9/site-packages conda
anyio            4.3.0
/cluster/medbow/project/arcc/salexan5/software/qiime/amplicon-
2024.5/lib/python3.9/site-packages conda
...
```

How Large is this Environment?

```
[salexan5@mblog2 qiime]$ du -d 1 -h
4.6G    ./amplicon-2024.5
4.6G    .
```

This is just the qiime environment. It does not include all the packages that were downloaded.

What about all the other environments we have created?

```
[salexan5@mblog2 software]$ du -d 1 -h
1.2G    ./py_env2
4.6G    ./qiime
1.1G    ./r_env2
11M     ./slim_env_4.2.2
6.8G    .
```

```
[salexan5@mblog2 conda]$ du -d 1 -h
1.2G    ./envs
8.3G    ./pkgs
9.5G    .
```

With just a few environments we are using >15G of storage - do you want this within your home folder?

The `.pkgs` folder can be cleaned up, and packages will just be downloaded again if needed.

Cleaning Up

Conda provides the [clean](#) command: Remove unused packages and caches.

```
[salexan5@mblog1 ~]$ module load miniconda3/24.3.0
[salexan5@mblog1 ~]$ conda clean -a
Will remove 947 (2.00 GB) tarball(s).
Will remove 1 index cache(s).
Will remove 32 (10.0 MB) package(s).
There are no tempfile(s) to remove.
There are no logfile(s) to remove.
[salexan5@mblog1 ~]$
[salexan5@mblog2 conda]$ du -d 1 -h
0          ./empty
1.2G       ./envs
6.0G       ./pkgs
```

We managed to clean up 2.3G of packages.

Conda with salloc and sbatch

Goal: Demonstrate best practices using Conda environments with `salloc` and `sbatch`.

- [Conda with salloc and sbatch: Best Practice](#)
-

Conda with salloc and sbatch: Best Practice

As indicated in the [Modules and using salloc and sbatch: Best Practice](#) we recommend to perform a `module purge` when starting an interactive session or submitting a job.

After performing a `conda activate` on a login node, typically the related set environment variables will be inherited after performing an `salloc`. But, notice what happens to the command-line prompt:

```
[salexan5@mblog1 ~]$ conda activate py_env
(py_env) [salexan5@mblog1 ~]$ python --version
Python 3.12.4

(py_env) [salexan5@mblog1 ~]$ salloc -A arcc -t 10:00
salloc: Granted job allocation 1243597
salloc: Nodes mbcpu-025 are ready for job
[salexan5@mbcpu-025 ~]$ python --version
```

Python 3.12.4

Which conda environment is currently active?

We would suggest, as with performing a `module purge`, to `conda activate` environments explicitly after performing an `salloc`, and within you scripts that you `sbatch`.

```
[salexan5@mblog1 ~]$ salloc -A arcc -t 10:00
salloc: Granted job allocation 1243600
salloc: Nodes mbcpu-025 are ready for job
[salexan5@mbcpu-025 ~]$ module purge
[salexan5@mbcpu-025 ~]$ module load miniconda3
[salexan5@mbcpu-025 ~]$ conda activate py_env
(py_env) [salexan5@mbcpu-025 ~]$ python --version
Python 3.12.4
```

Again, since this is now detailed within an `sbatch`-ed script, ARCC can see and replicate exactly what you are doing when there is an issue.

Conda Workshop: Summary

Goal: Summarize the concepts covered across the workshop.

Summary

Looked at:

- What Conda is and the various distributions that provide it, basic terminology, and how to use miniconda3 on the cluster.
 - Creating various environments, based on languages, and application based.
 - Detailing how to configure conda to update where environments are created, packages are cached, and using channels.
 - Reproducing and sharing environments by cloning, exporting and importing.
 - Environments, packages and caches can take up Gs of storage, we looked at how we can *clean* our environments.
 - Best practices when using `salloc` and `sbatch`.
-

Use the following link to provide feedback on this training:
<https://forms.gle/fuRnwt5rGUaDgzYB6> or use the QR code below.

