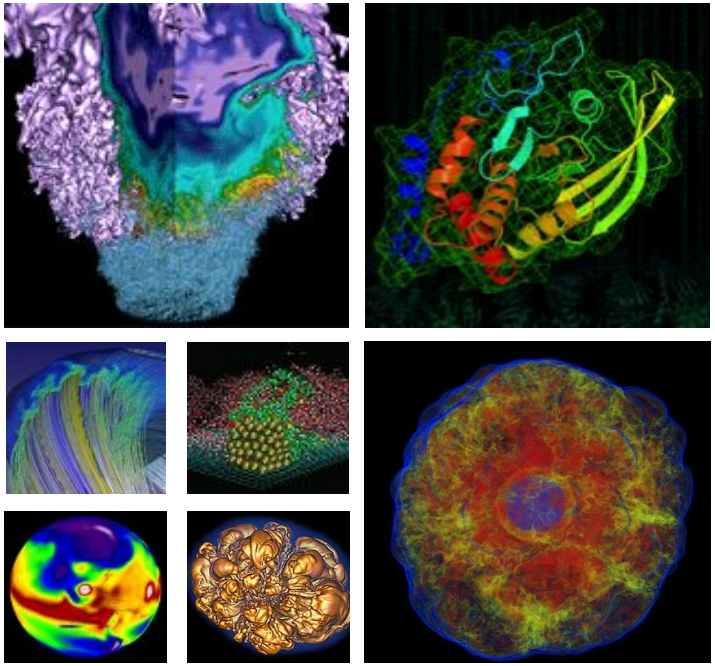
Advanced Anaconda Training



Dan Udwary and Mario Melara
DSEG / UEG

Joint Genome Institute - June 7th, 2018

NERSC

U.S. DEPARTMENT OF ENERGY | Office of Science

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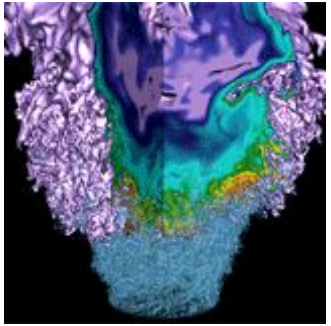
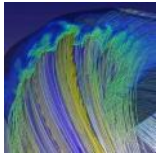
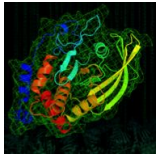
Agenda

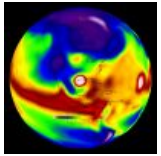
- **Conda Basics and Concepts Recap**
  - A quick overview of the basics and some concepts to get everyone on the same page
- **Tips and Tricks**
  - Ways to effectively use Anaconda
- **Packaging**
  - A run through of how to create packages for some of your tools
- **Discussion**
  - JGI software policy

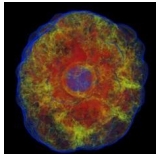
Conda Basics and Concepts Recap

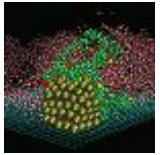












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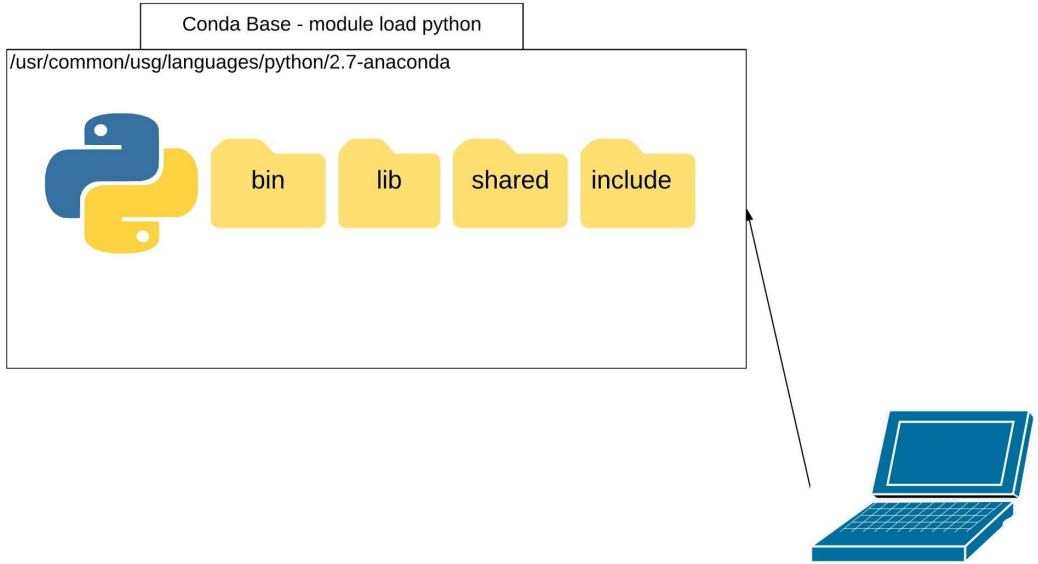
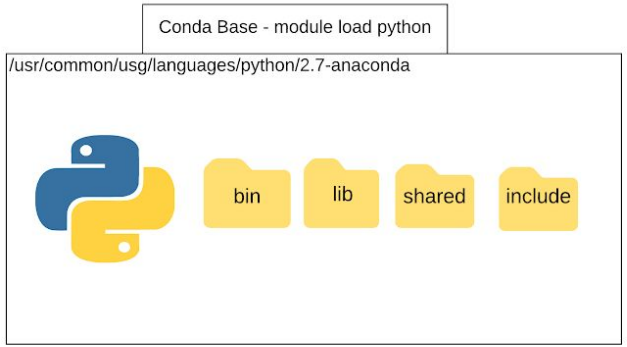
Conda Basics Recap

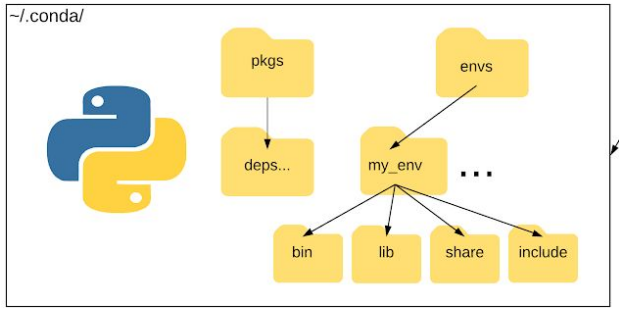
- Python provided at NERSC on Denovo via modules
  - `module avail python`
    - `python/2.7-anaconda(default)`
    - `python/3.5-anaconda`
    - `python/3.6-anaconda`
- Can use Miniconda
  - Anaconda - conda, Python, 200 packages
  - Miniconda - conda, Python
- Installing packages
  - `conda install numpy`
  - `conda install numpy=1.13(other e.g => == |)`
- Creating environments
  - `conda create --name my_env numpy`

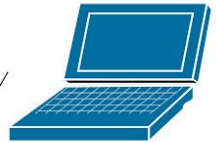
Conda Environments



Conda Environments







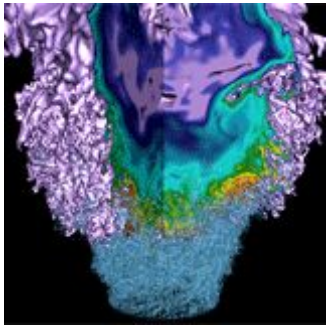
$ conda create --name my_env numpy
$ source activate my_env

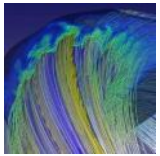
PATH=~/.conda/envs/my_env/bin:$PATH

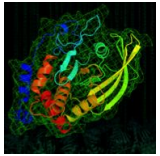
Conda Channels

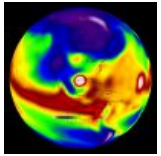
- Channels are URLs where packages are fetched
  - https://repo.continuum.io/pkgs/ (first looked here)
  - Forge
  - BioConda
- Channels can be set in .condarc
  - Useful for maintaining own private packages
- `conda install -c bioconda scikit-learn`

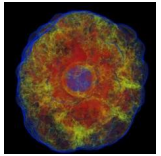
Tips and Tricks

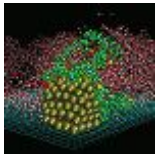












Installing Packages

- Install all your packages at once
- **REMEMBER:** All your packages are installed under ~/.conda/envs/[env]
  - If you have a lot of environments, it will eat up space in $HOME
  - If you're using the virtualenv for a massively parallel job, you're going to have a bad time (and so will everyone else)
- Recommendation:
  - *$HOME* - testing
  - */project/projectdirs/* - permanent
  - Sandbox - permanent
  - *$BSCRATCH* - good for one-off large experiments
  - `conda create --prefix=/where/you/want/env`

Exporting/Cloning Environment

- Want to share environment or move it to another machine?
  - `conda env export > my_environment.yml`
  - `conda env create -f environment.yml`
- Want to create a clone of an environment?
  - `conda create --name [new_env] --clone [other_env]`
- Consider how to incorporate version control with your environment.
  - Anaconda doesn't have vc built in at the moment.

Saving Environment Variables

- Conda allows your to save environment variables
  - Good if you need to store secret keys
- To save these variables do the following:

```
cd /path/to/anaconda/envs/myEnv
mkdir -p ./etc/conda/activate.d
mkdir -p ./etc/conda/deactivate.d
touch
./etc/conda/activate.d/env_vars.sh
touch
./etc/conda/deactivate.d/env_vars.sh
```

```
#!/bin/sh
# in activate.d/env_vars

export MY_KEY=”secret_key”
```

```
#!/bin/sh
# in deactivate.d/env_vars

unset MY_KEY
```

Clean Environment with `conda clean`

- Conda has cache files
  - Index cache
  - Lock files
  - Tarballs
  - Unused cache packages
  - Source cache

- Clean everything with a `conda clean --all`
- If you're left in a bad state -- try clearing caches

Miniconda and Anaconda

- Miniconda allows you full control of your environments and packages
- **Don’t use Miniconda and then load a Anaconda-Python module**
  - Issues can arise if you source activate an environment while trying to use Miniconda
- Unset PYTHONSTARTUP
  - Environment variable mainly relevant to system python. We don’t want users to use system Python

Conda and Pip

- Conda doesn't track pip installed pkgs
- Causes duplication
  - Env degraded
- Dependency problems
- Try as best to install conda only pkgs
- Use pip as last resort
- Fix incoming down the road
  - As of this presentation (5/7/18)

Anaconda v5.0.0
conda v4.3.27
bleach v2.1.3
html5lib 0.999999999 (9x)

↓

`pip install tensorflow`
Requires:
tensorboard,
html5lib 0.9999999 (x7)
bleach=1.5.0

→

```
bleach            2.1.3      py36_0
bleach            1.5.0      <pip>
html5lib          0.999999999
py36ha09blf3_0
html5lib          0.9999999  <pip>
numpy              1.14.0    py36ha8a80b8c
numpy              1.13.3    <pip>
setuptools        38.2.4     <pip>
setuptools        36.5.0     py36h2134326_0
tensorflow        1.4.0      <pip>
tensorflow-tensorboard 0.4.0rc3  <pip>
Werkzeug          0.13       <pip>
werkzeug          0.12.2     py36h16efa1_0
```

.condarc

- Customize how conda acts when you're installing packages and creating envs.
- `conda config --describe`
  - Shows all the options that you can tweak.
- Useful configurations:

```
create_default_packages:
    - pip
    - ipython
    - scipy
```

```
envs_dirs:
  -   $BSCRATCH/.conda/envs
```

```
pkgs_dirs:
  -   $BSCRATCH/.conda/pkgs
```

- Don't see a .condarc already in your $HOME?
  - `conda config --describe > ~/.condarc`

.condarc - adding values

- `conda config --add|--append [key] [value]`
  - For list entries
- `conda config --set [key] [value]`
- Examples:

```
conda config --add channel [channel]
conda config --append channel [channel]
```

```
conda config --set always_yes true
```

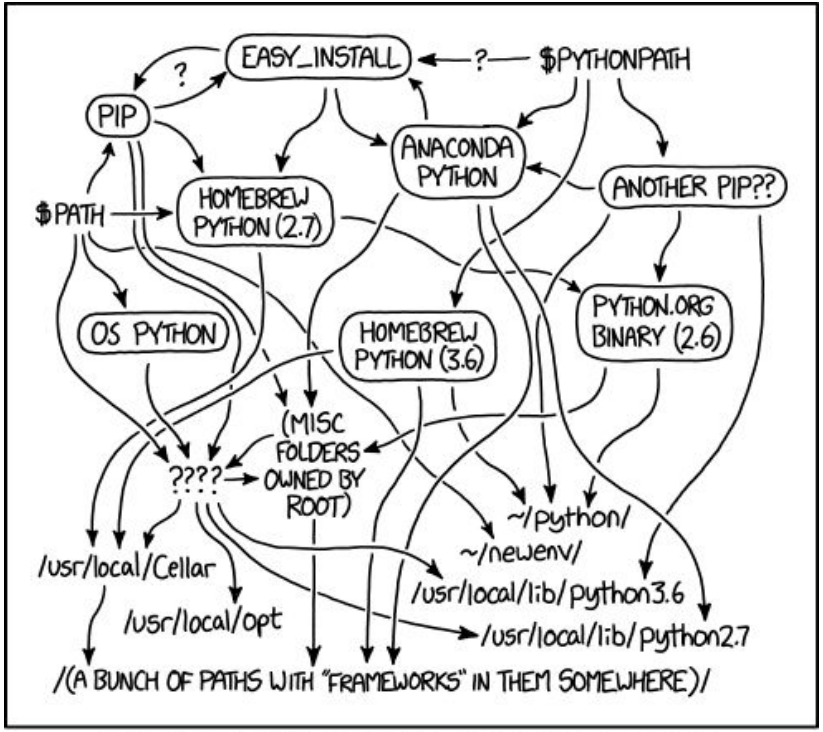
If You Want to Learn More!

RTFM: https://conda.io/docs/

Check out videos - Anaconda Youtube

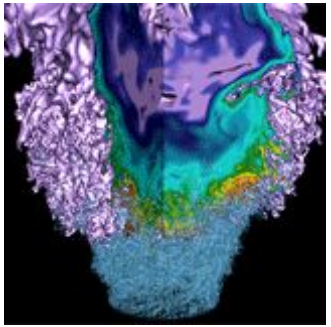
Read NERSC docs - Anaconda Python

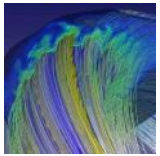
Keep It Simple

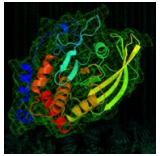


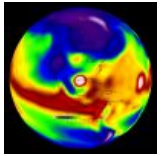
MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

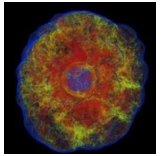
Packaging Your Own Stuff

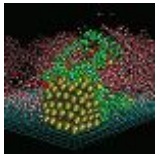












Building Your Own Anaconda Packages

- **Some caveats:**
  - Remember that Anaconda can pull down anything – it's not just a Python package manager
    - So, you can provide libraries, executables, code in other languages
  - There's more than we can cover in an hour
    - Though, the basics are pretty simple and straightforward
    - Use working examples! Don't reinvent the wheel!
    - What can NERSC do to help? Workshop? Hands-on?
  - What should JGI's software strategy be?
    - Public channel(s)? Local repo? Git repo to pull from?
    - Anaconda Cloud purchase required for private channels
    - That's all going to be up to JGI, not NERSC.

Prerequisites and Requirements

```
$ conda install anaconda-client
$ conda install conda-build
```

- **Know where your pkgs and conda-bld directories are located**
  - Typically: $HOME/conda-bld (created first time you use “conda build”)
    $HOME/.conda/pkgs (pkgs installed for virtual envs)
    $PYTHON_DIR/pkgs (central installation)
- **Note: conda-build and client is already installed and available to you within NERSC python modules.**
  - You’ll probably only need to do this if you’re using Miniconda, or building/testing/experimenting on your computers

Four simple steps to building your package

1. **Have your source code in a version-controlled repo**
   - Bitbucket, Github, GitLab, ftp – anything with a url
   - You can use local files, but seriously don't be that kind of person
2. **Prepare a recipe**
   - meta.yaml and a build.sh script (and/or bld.bat for Windows)
3. **"Conda build" your package**
   - You'll build locally.
   - Might need to make decisions about what platforms to build for if compiling
4. **Conda upload to an Anaconda channel**
   - You don't have to upload, and can "conda install" from a local directory

Step 1 - Put your source somewhere

Are you really not already using a version controlled repo?

Step 2 – Make your recipe

A simple example meta.yaml:

```yaml
package:
  name: pyinstrument
  version: "0.13.1"

source:
  git_rev: v0.13.1
  git_url: https://github.com/joerick/pyinstrument.git

requirements:
  build:
    - python
    - setuptools
  run:
    - python

test:
  imports:
    - pyinstrument

about:
  home: https://github.com/joerick/pyinstrument
  license: BSD
  license_file: LICENSE
```

Simple build.sh example:

```
$PYTHON setup.py install \
--single-version-externally-managed \
--record=record.txt
```

meta.yaml contains metadata, source locations, dependencies, tests

build.sh is the commands needed to build the software on your machine(s)

Example meta.yaml for bioconda's Blast

```yaml
package:
    name: blast
    version: 2.7.1
source:
    fn: ncbi-blast-2.7.1+-src.tar.gz
    patches:
        - boost_106400.patch
    sha256: 10a78d3007413a6d4c983d2acbf03ef84b622b82bd9a59c6bd9fbdde9d0298ca
    url: https://ftp.ncbi.nlm.nih.gov/blast/executables/blast+/2.7.1/ncbi-blast-2.7.1+-src.tar.gz
build:
    noarch: ''
    noarch_python: false
    number: '3'
    string: boost1.64_3
requirements:
    build:
        - boost 1.64.0 py36_4
        - boost-cpp 1.64.0 1
        - bzip2 1.0.6 1
        - ca-certificates 2018.1.18 0
        - certifi 2018.1.18 py36_0
        - gettext 0.19.8.1 0
        - gmp 6.1.2 0
        - gnutls 3.5.17 0
        - icu 58.2 0
        - intel-openmp 2018.0.0 8
        - libgfortran 3.0.1 h93005f0_2
        - libidn11 1.33 0
        - mkl 2018.0.2 1
        - mkl_fft 1.0.1 py36_1
        - mkl_random 1.0.1 py36_0
        - ncurses 5.9 10
        - nettle 3.3 0
        - numpy 1.14.2 py36ha9ae307_1
        - openssl 1.0.2n 0
        - pcre 8.41 1
        - pip 9.0.1 py36_1
        - python 3.6.4 0
        - readline 7.0 0
        - setuptools 39.0.1 py36_0
        - sqlite 3.20.1 2
        - time 1.7 0
        - tk 8.6.7 0
        - wheel 0.30.0 py36_2
        - xz 5.2.3 0
        - zlib 1.2.11 0
    run:
        - boost 1.64*
        - zlib 1.2.11*
        - bzip2 1.0*
        - gnutls
        - nettle 3.3|3.3.*
        - pcre
        - perl
        - perl-list-moreutils
        - perl-archive-tar
test:
    commands:
        - blastn -help
        - blastp -help
        - makeblastdb -help
        - touch libstdc++.so.6; LD_LIBRARY_PATH=. makeblastdb -help && rm libstdc++.so.6
        - update_blastdb.pl --help
    files:
        - test.fa
        - testdatabase.fa
about:
    home: http://blast.ncbi.nlm.nih.gov/Blast.cgi?PAGE_TYPE=BlastDocs
    license: Public Domain
    summary: BLAST+ is a new suite of BLAST tools that utilizes the NCBI C++ Toolkit.
extra:
    final: true
```

Example build.sh for Blast

```
$ more build.sh
#!/bin/bash

cd $SRC_DIR/c++/

export CFLAGS="$CFLAGS -O2"
export CXXFLAGS="$CXXFLAGS -O2"
export CPPFLAGS="$CPPFLAGS -I$PREFIX/include"
export LDFLAGS="$LDFLAGS -L$PREFIX/lib"

if test x"`uname`" = x"Linux"; then
    # only add things needed; not supported by OSX ld
    LDFLAGS="$LDFLAGS -Wl,-as-needed"
fi

LIB_INSTALL_DIR=$PREFIX/lib/ncbi-blast+

./configure \
    --with-dll \
    --with-mt \
    --without-autodep \
    --without-makefile-auto-update \
    --with-flat-makefile \
    --without-caution \
    --without-dbapi \
    --without-lzo \
    --with-hard-runpath \
    --with-runpath=$LIB_INSTALL_DIR \
    --without-debug \
    --with-strip \
    --without-vdb \
    --with-z=$PREFIX \
    --with-bz2=$PREFIX \
    --with-boost=$PREFIX \
```

Any files created by build.sh that are written to its directory will become part of the package.tar.bz2

```
    --without-openssl \
    --without-gcrypt \
    --with-gnutls=$PREFIX \
    --with-nettle=$PREFIX \
    --without-krb5

projects="algo/blast/ app/ objmgr/ objtools/align_format/ objtools/blast/"
cd ReleaseMT

# The "datatool" binary needs the libs at build time, create
# link from final install path to lib build dir:
ln -s $SRC_DIR/c++/ReleaseMT/lib $LIB_INSTALL_DIR

cd build
make -j${CPU_COUNT} -f Makefile.flat all_projects="$projects"

# remove temporary link
rm $LIB_INSTALL_DIR

mkdir -p $PREFIX/bin $LIB_INSTALL_DIR
rm $SRC_DIR/c++/ReleaseMT/bin/*_unit_test
cp $SRC_DIR/c++/ReleaseMT/bin/* $PREFIX/bin/
cp $SRC_DIR/c++/ReleaseMT/lib/* $LIB_INSTALL_DIR

chmod +x $PREFIX/bin/*
sed -i.bak '1 s|^.*$|#!/usr/bin/env perl|g' $PREFIX/bin/update_blastdb.pl
```

Step 3 – Build your package

```
$ conda build yourpackagedir
```

- Conda-build will pick up the meta.yaml file and run the build script
- Output will be a package.tar.bz2 file
  - typically to be found in $HOME/conda-bld/linux-64

- **Can directly install that package.tar.bz2 file**

  $ conda install --use-local /path/to/package.tar.bz2

- **Many additional options for setting up your meta.yaml and build.sh:**

https://conda.io/docs/user-guide/tasks/build-packages/define-metadata.html

Step 4 – Upload to Anaconda

- **Register an account on Anaconda Cloud**
  - http://anaconda.org
  - Free is fine for your own public channel
  - Paid for private channels and collaborative groups

```
$ anaconda login
$ anaconda upload /path/to/yourpackage.tar.bz2
```

Now your package is available to everyone

- For better or worse
- $ anaconda search packagename

```
conda-forge/pyinstrument  |    2.0.2 | conda          | linux-64, win-32, win-64, osx-64 | py36_0, py34_0, py35_0, py27_0
                                     : A call stack profiler for Python. Inspired by Apple's Instruments.app
conda-forge/pyinstrument_cext |    0.1.2 | conda          | linux-64, win-32, win-64, osx-64 | py36_0, py35_0, py27_0
                                     : A CPython extension supporting pyinstrument
danudwaryjgi/pyinstrument |    2.0.2 | conda          | linux-64        | py27_0
                                     : A call stack profiler for Python. Inspired by Apple's Instruments.app
davidliwei/pyinstrument   |   0.13.1 | conda          | osx-64          | py34_0
                                     : A call stack profiler for Python. Inspired by Apple's Instruments.app
```

Some helpful resources on packaging

- Anaconda's documentation on "Working With Packages"
  https://docs.anaconda.com/anaconda-cloud/user-guide/tasks/work-with-packages

- A tutorial on building conda packages directly from PyPI packages
  https://conda.io/docs/user-guide/tutorials/build-pkgs-skeleton.html

- A more extensive hands-on training from Anacondacon 2018. Covers some history of python package management, provides suggestions on third-party packaging tools, and has several exercises.

Thank You