

Practical Python on Odyssey

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Overview

- Learn python by debugging existing code
- See common errors and their solutions
- Learn how to search for programming solutions
- Odyssey-specific lessons, including Anaconda clones

Covered subjects

Not necessarily in this order

- Structure (if/then, for, tuples, arrays, dicts, functions)
- Regular expressions, dates
- Interacting with your environment (os, environment variables, files, executing other tools)
- Packages and virtual environments (pip, python [setup.py](#), virtualenv, Anaconda, clones)
- Parallel programming (multiprocess)

Setup

- Login to Odyssey
- Get the course materials

```
[akitzmiller@holy2a ~]$ tar xvf /n/regal/informatics/workshops/python-workshop.tar.gz
```

- Check python

```
[akitzmiller@holy2a ~]$ python --version
Python 2.6.6
[akitzmiller@holy2a ~]$ which python
/usr/bin/python
```

- Hop in to the interpreter

```
[akitzmiller@holy2a ~]$ python
Python 2.6.6 (r266:84292, Jan 22 2014, 09:42:36)
[GCC 4.4.7 20120313 (Red Hat 4.4.7-4)] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

Use `ct1-d` to get out

Course materials

- `bin/hisnhers.py` - The broken script
- `bin/megaAssembler` - The high memory assembler
- `bin/hyperAssembler` - The fast, efficient assembler
- `ha/annotate.py` - The annotation module
- <https://github.com/harvardinformatics/lookkool.git> - The palindrome finder

hisnhers.py

Broken script that attempts to

1. read in a FASTQ file
2. report some information about the sequences
3. write to FASTA and feed to an assembler to create contigs
4. annotate the contigs

ha/annotate.py

Annotation module that will be called by `hisnhers.py` serially and, then, in parallel

The Python Language

- General purpose, interpreted scripting language in which everything (numbers, lists, strings, functions, classes, types) is an object.
- Code blocks (functions, loops, if/else, etc.) defined by colon and indent level
- Significant changes to the language from Python 2.x to Python 3.x
- Massive PyPI package repository (`pip install <something from PyPI>`)
- A file is a module, a directory can be a package

Run the script

```
[akitzmiller@holly2a python-workshop]$ bin/hisnhers.py
```


- Flexible interpreter path in the shebang

```
#!/usr/bin/env python
```

- Indents must match - *4 spaces, do not use tabs*

```
[akitzmiller@holy2a python-workshop]$ bin/hisnhers.py
File "bin/hisnhers.py", line 79
    seqs = []
    ^
IndentationError: unexpected indent
```

- Use a proper return value for modules named `__main__`

```
if __name__ == "__main__":  
    sys.exit(main())
```

- `import sys`

Google Interlude: Magic Variables, Magic Functions

- Meta data about a python module or package
- Double underbar (dunder) designation, e.g. `__name__`, `__ispkg__`
- [Google: python magic variables](#)
- Python objects also have magic functions that allow you to override basic behaviors (e.g. `__str__`)

imports

- A name (function, class, variable, module) cannot be used unless it is imported, defined, or a *built-in*
- You can import a module (which is a file) and use its named things

```
[akitzmiller@holy2a ~]$ ls /usr/lib64/python2.6/os.py  
/usr/lib64/python2.6/os.py
```

```
>>> import os  
>>> os.makedirs('/tmp/a/j/k')
```

- or you can import something from a module

```
[akitzmiller@holy2a ~]$ grep "def makedirs" /usr/lib64/python2.7/os.py  
def makedirs(name, mode=0777):
```

```
>>> from os import makedirs  
>>> makedirs('/tmp/a/j/k')
```

- Imports are based on paths, where path separators, / , are converted to periods

```
[akitzmiller@holy2a python-workshop]$ find ha -name "annotate.py"  
ha/annotate.py
```

```
from ha.annotate import annotateStartStopCodon
```

imports

- Valid paths depends on `sys.path` , including `PYTHONPATH`

```
[akitzmiller@holy2a ~]$ echo $PYTHONPATH
/odyssey/rc_admin/sw/admin/rcpy:

[akitzmiller@holy2a ~]$ python
Python 2.6.6 (r266:84292, Jan 22 2014, 09:42:36)
[GCC 4.4.7 20120313 (Red Hat 4.4.7-4)] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> import sys
>>> print sys.path
['', '/odyssey/rc_admin/sw/admin/rcpy', '/n/home_rc/akitzmiller',
'/usr/lib64/python26.zip', '/usr/lib64/python2.6',
'/usr/lib64/python2.6/plat-linux2', '/usr/lib64/python2.6/lib-tk',
...
'/usr/lib64/python2.6/site-packages/webkit-1.0', '/usr/lib/python2.6/site-packages',
'/usr/lib/python2.6/site-packages/setuptools-0.6c11-py2.6.egg-info']
```

- Watch out for `~/local`

os and sys modules

- os includes functions that vary between operating systems

```
# On Linux
>>> os.path.join(['usr', 'local', 'bin'])
usr/local/bin

# On Windows
>>> os.path.join(['usr', 'local', 'bin'])
usr\local\bin

# Interact with environment variables
>>> os.environ['PATH']
'/usr/local/bin:/usr/lib64/qt-3.3/bin:/usr/local/bin:/bin:/usr/bin'
>>> os.system('which module-query')
/usr/local/bin/module-query
0
>>> os.environ['PATH'] = '/n/sw/www/apps/apps/bin:%s' % os.environ['PATH']
>>> os.system('which module-query')
/n/sw/www/apps/apps/bin/module-query
0
```

- sys includes functions and data about the Python interpreter
 - ** sys.exit() exits the Python interpreter
 - ** sys.argv contains the arguments passed to the script

Fix the file reading error

```
[akitzmiller@holy2a ~]$ bin/hisnhers.py
Traceback (most recent call last):
  File "./bin/hisnhers.py", line 263, in <module>
    sys.exit(main())
  File "./bin/hisnhers.py", line 131, in main
    fastqToSequenceList(fqfilename)
  File "./bin/hisnhers.py", line 98, in fastqToSequenceList
    if fileh.closed:
AttributeError: 'str' object has no attribute 'closed'
```

- Stack trace shows you where to look

File reading error solution

```
# sys.argv == ['hisnhers.py', 'example.fq']
if len(sys.argv) < 2:
    print 'Must supply a file name'
    return 1

fqfilename = sys.argv[1]
if not os.path.exists(fqfilename):
    raise Exception('File %s does not exist' % fqfilename)

with open(fqfilename, 'r') as f:
    seqs = fastqToSequenceList(f)
```

File processing with context managers

- `f = open()` returns a file handle
- `with` block is a context manager that closes the file handle on exit

```
# Code block defined by colon and indent  
with open(fqfilename, 'r') as f:  
    seqs = fastqToSequenceList(f)
```

- `for` loop on a handle iterates over file lines

```
# Code block defined by colon and indent  
for line in fileh:  
    line = line.strip()  
    if line == '':  
        continue
```

Convert the hardcoded file name into a command argument

```
# if block defined by colon, indent  
if len(sys.argv) < 2:  
    print 'Must supply a file name'  
    return 1  
fqfilename = sys.argv[1]
```

or use argparse to handle real arguments

```
from argparse import ArgumentParser, RawDescriptionHelpFormatter  
  
parser = ArgumentParser(description='Python workshop tool', formatter_class=RawDescriptionHelpFormat  
parser.add_argument('FASTQ_FILE', help='Fastq file')  
args = parser.parse_args()  
  
fqfilename = args.FASTQ_FILE
```

Add sequence length and base counts

- Print out base frequencies and sequence length for each sequence

```
>>> print seqs[0]
('HWUSI-EAS300R_0005_FC62TL2AAXX:8:30:18447:12115#0/1',
 'CGTAGCTGTGTGTACAAGGCCCGGGAACGTATTCACCGTG',
 'acdd^aa_Z^d^ddc`^_Q_aaa`_ddc\\dfdffff\\fff')
```

Sequence 1 Length: 106 A: 4, T: 4, C: 4, G: 4

Lists and tuples

- 0 indexed list of data items that is either modifiable (lists) or unmodifiable (tuples)

```
>>> bases = ['A', 'T', 'C', 'G']
>>> bases[1]
'T'
>>> bases.append('U')
>>> bases[4]
'U'
>>> bases = ('A', 'T', 'C', 'G')
>>> bases[1]
'T'
>>> bases.append('U')
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
AttributeError: 'tuple' object has no attribute 'append'
```

Lists and tuples

- Iteration

```
for base in bases:  
    print base  
  
for i, base in enumerate(bases):  
    print base
```

- Indexing

```
>>> bases = ['A', 'T', 'C', 'G']  
>>> print bases[1:2]  
['T']  
>>> print bases[1:3]  
['T', 'C']  
>>> print bases[-1:]  
['G']
```

Lists and tuples

- Concatenating

```
allbases = dnabases + rnabases
```

- Counting

```
>>> bases
['A', 'T', 'C', 'G']
>>> len(bases)
4
>>> bases.count('A')
1
```

- Short hand list initialization by another iterable (list comprehension)

```
baselengths = [len(base) for base in bases]
complements = [dna.complement(base) for base in bases]
```

Strings

- Strings are lists of characters ...

```
>>> contig = 'ATCACTAGTCGTCG'  
>>> contig[1:3]  
'TC'
```

- ... that can be constructed with Python formatting tools

```
>>> reagent = 'SDS'  
>>> 'You will need %.2f mg of %s in %d mL' % (.565, reagent, 100)  
'You will need 0.56 mg of SDS in 100 mL'  
>>> 'You will need {reagentmass:.2f} of {reagent} in {volume} mL'.format(  
    reagentmass=0.565,  
    reagent='SDS',  
    volume=100  
)  
'You will need 0.56 of SDS in 100 mL'
```


Add sequence length and base counts

Sequence length and base count

```
# >>> seqs[0]
# ('HWUSI-EAS300R_0005_F2AAXX:8:30:18447:12115#0/1\n', 'CGTAGCTAACGTATTCACCGTG', '')
for i, seqdata in enumerate(seqs):
    seqstr = seqdata[1]
    seqlen = len(seqstr)

    basecountline = 'Sequence %d Length: %d ' % (i, seqlen)
    for base in ['A', 'T', 'C', 'G']:
        basecountline += '%s: %d ' % (base, seqstr.count(base))
    print basecountline
```

or

```
basecountstrs = ['Sequence %d Length: %d ' % (i, seqlen)]
for base in ['A', 'T', 'C', 'G']:
    basecountstrs.append('%s: %d ' % (base, seqstr.count(base)))
print ' '.join(basecountstrs)
```

Contigs file error

```
[akitzmiller@holly2a python-workshop]$ ./bin/hisnhers.py data/example.fq
Writing to data/example.fa
Traceback (most recent call last):
  File "./hisnhers.py", line 210, in <module>
    sys.exit(main())
  File "./hisnhers.py", line 135, in main
    with open(contigfilename, 'r') as c:
IOError: [Errno 2] No such file or directory: 'data/example.fa.contigs'
[akitzmiller@holly2a python-workshop]$
```

Running commands with `os.system()`

- There are about a dozen Python functions for running a command line tool, but only two of them are worth using.
- `os.system()` runs a command using the shell and returns only the return code. stdout and stderr are sent to the console. If you need to capture the contents, they must be redirected.

```
>>> os.system("echo 'hello' > hello.out")
0
>>> f = open('hello.out', 'r')
>>> print f.readlines()
['hello\n']
```

Running commands with Popen()

- `subprocess.Popen` supports all available options for synchronous execution

```
>>> import subprocess
>>> proc = subprocess.Popen(
    "echo 'hello'",
    shell=True,
    stdout=subprocess.PIPE,
    stderr=subprocess.PIPE
)
>>> stdoutstr, stderrstr = proc.communicate()
>>> print proc.returncode
0
>>> print stdoutstr
hello
```

Running commands

- Avoid bash shell processing if you need to

```
>>> args = ['/usr/bin/sed', '-i', '-e', 's/$PATH/${PATH}/', '/home/path with some spaces in it']
>>> proc = subprocess.Popen(args, shell=False)
```

- Write to stdin

```
>>> lyrics = '''
... Sundown, you better take care
... If I find you been creepin
... Down my back stair
... '''
>>> args = ['/bin/grep', 'been creepin']
>>> from subprocess import PIPE, Popen
>>> proc = Popen(args, shell=False, stdin=PIPE, stdout=PIPE, stderr=PIPE)
>>> stdout, stderr = proc.communicate(input=lyrics)
>>> stdout
'If I find you been creepin\n'
>>>
```

Running commands

- You may need to alter the environment of the subprocess
- Loading modules can work with &&

```
proc = Popen('module load bowtie2 && bowtie2 -1 m1.in.bz2 -2 m2.in.bz2', shell=True)
```

- You can set environment values in the parent

```
>>> path = os.environ.get('PATH', '')  
>>> os.environ['PATH'] = '/n/sw/fasrcsw/apps/Core/bowtie2/2.3.1-fasrc01/bin:%s' % path  
>>> proc = Popen('bowtie2 -1 m1.in.bz2 -2 m2.in.bz2', shell=True)
```

- or in the subprocess itself

```
>>> path = os.environ.get('PATH', '')  
>>> env = {'PATH' : '/n/sw/fasrcsw/apps/Core/bowtie2/2.3.1-fasrc01/bin:%s' % path}  
>>> proc = Popen('bowtie2 -1 m1.in.bz2 -2 m2.in.bz2', shell=True, env=env)
```

Replace the call to megaAssembler with a Popen-based call to hyperAssembler.

Capture return code, stdout, and stderr

Call to hyperAssembler

```
import subprocess

def runcmd(cmd):
    """
    Execute a command and return stdout, stderr, and the return code
    """
    proc = subprocess.Popen(cmd, shell=True, stdout=subprocess.PIPE, stderr=subprocess.PIPE)
    stdoutstr, stderrstr = proc.communicate()
    return (proc.returncode, stdoutstr, stderrstr)

# Run hyperAssembler with fastq file input and read the output contig
contigfilename = '%s.contigs' % fafilename
assemblerargs = [
    'hyperAssembler',
    fafilename,
]

cmd = ' '.join(assemblerargs)
returncode, stdoutstr, stderrstr = runcmd(cmd)

if returncode != 0:
    raise Exception('Error running assembler with cmd %s\nstdout: %s\nstderr: %s' % (cmd, stdoutstr, s
```

Capture stdout and parse date information

Regular expressions

- [Google: python regular expressions](#)
- Python regular expressions are a full set of processing options (character classes, capture groups, quantifiers, etc)
- Match the beginning of your string. Use a "raw" string to avoid backslash proliferation

```
>>> teststr = 'w00t!'  
>>> import re  
>>> re.match(r'[a-z]\d+.*', teststr)  
<_sre.SRE_Match object at 0x7f0e518c3098>
```

- Use `re.search` if your pattern is later in the string

```
>>> re.match(r'\d+.*', teststr)  
>>> re.search(r'\d+.*', teststr)  
<_sre.SRE_Match object at 0x7f0e518c3098>
```

Regular expressions

- Use parens to "capture" text

```
>>> segment = 'TATGCGCAAGTTACAAAAAAAAAAAAAAAAATAAGTTAAAAAAAAAAAAATGCTA'
>>> re.findall(r'(A{3,})T', segment)
['AAAAAAAAAAAAAA', 'AAAAAAAAAAAAA']
```

- Split with a regex (with or without capture group)

```
>>> re.split(r'(A{3,})T', segment)
['TATGCGCAAGTTAC', 'AAAAAAAAAAAAAA', 'AAAGTT', 'AAAAAAAAAAAAA', 'GCTA']
>>> re.split(r'A{3,}', segment)
['TATGCGCAAGTTAC', 'T', 'GTT', 'TGCTA']
```

- Process multiline text

```
>>> fasta = '''
... > transcript_1
... ATCGATCGATTACGTACAAAAAAAAATACGTAGCTAAAAAAAAATCAGCTACG
... AAAAAAAAAAAAAAAAAAACTAGTCGATGCTAGCTATCGATCGTATATATGAC
... '''
>>> re.findall(r'A{3,}', fasta)
['AAAAAAA', 'AAAAAAA', 'AAAAAAAAAAAAAAAAA']
```

Date handling

- [Google python datetime](#)
- The `datetime` and `timedelta` modules come with Python

```
>>> from datetime import datetime, timedelta
>>> datetime.now()
datetime.datetime(2017, 3, 16, 16, 52, 33, 639252)
>>> feb = datetime(2017, 2, 1)
>>> nextmonth = feb + timedelta(days=30)
>>> nextmonth
datetime.datetime(2017, 3, 3, 0, 0)
```

- `strftime` formats date objects

```
>>> nextmonth.strftime('%d/%m/%Y')
'03/03/2017'
```

- `strptime` parses dates according to a strict specification

```
>>> datetime.strptime('03/03/2017', '%d/%m/%Y')
datetime.datetime(2017, 3, 3, 0, 0)
```

- `python-dateutil` package parses whatever you throw at it

```
>>> from dateutil import parser
>>> parser.parse('03/03/2017')
datetime.datetime(2017, 3, 3, 0, 0)

>>> parser.parse('March 3, 2017')
datetime.datetime(2017, 3, 3, 0, 0)
```

Get the start and end dates from the hyperAssembler output and calculate the time

```
Assembling genome in data/example.fa
Start time: 04:01:00 PM
280
140
Finished assembling data/example.fa. Writing contigs into data/example.fa.contigs.
End time: 04:01:05 PM
```

Get the start and end dates

```
# Get the start and end time from stdout
from dateutil import parser
match = re.search(r'Start time: (.*?)\n', stdoutstr, re.MULTILINE)
if match:
    starttime = parser.parse(match.group(1))
match = re.search(r'End time: (.*?)\n', stdoutstr, re.MULTILINE)
if match:
    endtime = parser.parse(match.group(1))
if starttime and endtime:
    delta = endtime - starttime
    print 'Elapsed assembly time %d seconds' % delta.total_seconds()
```

Missing lookkool module

```
Traceback (most recent call last):
File "./bin/hisnhers.py", line 179, in <module>
    sys.exit(main())
File "./bin/hisnhers.py", line 160, in main
    annotations += annotatePalindromes(seqid, contig)
File "./ha/annotate.py", line 66, in annotatePalindromes
    from lookkool import findPalindromes
ImportError: No module named lookkool
```


Python packages

- A package is a set of Python modules and scripts (and possibly C, Fortran, etc. supporting code) that can be installed in a Python environment
- Python library called `setuptools` (son of `distutils`) allows packages of Python code to be installed in a standard fashion

```
[akitzmiller@holy2a ~]$ tar xvf mpi4py-2.0.0.tar.gz  
[akitzmiller@holy2a ~]$ cd mpi4py-2.0.0  
[akitzmiller@holy2a mpi4py-2.0.0]$ python setup.py install
```

- Avoid doing this

```
[akitzmiller@holy2a mpi4py-2.0.0]$ python setup.py install --user
```

Python packages - pip

- pip installs directly from the huge PyPI repository and recurses dependencies

```
[akitzmiller@holy2a /tmp]$ pip install Flask-Script
Collecting Flask-Script
  Downloading Flask-Script-2.0.5.tar.gz (42kB)
    100% |████████████████████████████████████████| 51kB 710kB/s
Collecting Flask (from Flask-Script)
  Downloading Flask-0.12-py2.py3-none-any.whl (82kB)
    100% |████████████████████████████████████████| 92kB 2.0MB/s
Collecting click>=2.0 (from Flask->Flask-Script)
  Downloading click-6.7-py2.py3-none-any.whl (71kB)
    100% |████████████████████████████████████████| 71kB 4.9MB/s
...
Building wheels for collected packages: Flask-Script, itsdangerous
  Running setup.py bdist_wheel for Flask-Script ... done
  Running setup.py bdist_wheel for itsdangerous ... done
Successfully built Flask-Script itsdangerous
Installing collected packages: click, Jinja2, Werkzeug, itsdangerous, Flask, Flask-Script
Successfully installed Flask-0.12 Flask-Script-2.0.5 Jinja2-2.9.5 Werkzeug-0.12.1 click-6.7 itsda
```

- Copy an entire python setup with pip

```
pip freeze > requirements.txt  
pip install -r requirements.txt
```

- Install from a git repository (including branch or tag)

```
[akitzmiller@holy2a ~]$ pip install git+https://github.com/harvardinformatics/MISO.git@slurm
```

Anaconda

- Python distribution that includes the most popular scientific and utility packages (numpy, scipy, matplotlib, etc.)
- Package management system (`conda install/remove/update`)
 - ** pip-like dependency recursion
 - ** maintains compatible versions among dependencies
 - ** may include compiled C / Fortran libraries
 - ** supports multiple "channels"
 - ** update Python itself
- Odyssey python modules are Anaconda modules

```
[akitzmiller@holy2a ~]$ module load python/2.7.11-fasrc01
```

```
[akitzmiller@holy2a ~]$ module list
```

Currently Loaded Modules:

1) Anaconda/2.5.0-fasrc01 2) python/2.7.11-fasrc01

Anaconda

- Get the latest

```
[akitzmiller@holy2a ~]$ conda install netcdf4
Fetching package metadata .....
Solving package specifications: .
```

The following NEW packages will be INSTALLED:

```
h5py:          2.6.0-np111py27_2
hdf4:          4.2.12-0
hdf5:          1.8.17-1
libnetcdf:     4.4.1-0
netcdf4:       1.2.4-np111py27_0
```

The following packages will be UPDATED:

```
astropy:       1.1.2-np110py27_0 --> 1.3-np111py27_0
bottleneck:    1.0.0-np110py27_0 --> 1.2.0-np111py27_0
curl:          7.45.0-0          --> 7.49.0-1
llvmlite:      0.9.0-py27_0      --> 0.16.0-py27_0
matplotlib:    1.5.1-np110py27_0 --> 1.5.1-np111py27_0
numba:         0.24.0-np110py27_0 --> 0.31.0-np111py27_0
numexpr:       2.5-np110py27_0 --> 2.5.2-np111py27_0
numpy:         1.10.4-py27_1     --> 1.11.0-py27_0
pandas:        0.18.0-np110py27_0 --> 0.19.2-np111py27_1
patsy:         0.4.0-np110py27_0 --> 0.4.1-py27_0
pycurl:        7.19.5.3-py27_0  --> 7.43.0-py27_0
pytables:      3.2.2-np110py27_1 --> 3.3.0-np111py27_0
scikit-image:  0.12.3-np110py27_0 --> 0.12.3-np111py27_1
scikit-learn:  0.17.1-np110py27_0 --> 0.17.1-np111py27_0
scipy:         0.17.0-np110py27_2 --> 0.17.0-np111py27_2
statsmodels:   0.6.1-np110py27_0 --> 0.8.0-np111py27_0
```

Proceed ([y]/n)?

Anaconda

- or a specific version

```
[akitzmiller@holy2a ~]$ conda install netcdf4==1.2.1
Fetching package metadata .....
Solving package specifications: .
```

Package plan **for** installation **in** environment /home/akitzmiller/anaconda2/envs/workshop:

The following NEW packages will be INSTALLED:

```
h5py:      2.6.0-np110py27_0
hdf5:      1.8.15.1-3
libnetcdf: 4.3.3.1-3
netcdf4:   1.2.1-np110py27_0
```

Proceed ([y]/n)?

Virtual environments - virtualenv

- You don't have root so you can't install to system library paths.
- You can use `install --prefix` and `PYTHONPATH`, but it is a pain and some packages are poorly behaved
- Some packages depend on mutually exclusive versions of other packages
- `virtualenv` allows you to create one or more Python environments over which you have control

```
[akitzmiller@holy2a ~]$ mkdir envs
[akitzmiller@holy2a ~]$ cd envs
[akitzmiller@holy2a envs]$ virtualenv workshop
New python executable in /n/home_rc/akitzmiller/envs/workshop/bin/python
Installing setuptools, pip, wheel...done.
[akitzmiller@holy2a envs]$ source workshop/bin/activate
(workshop) [akitzmiller@holy2a envs]$ which python
~/envs/workshop/bin/python
(workshop) [akitzmiller@holy2a envs]$ pip install -r workshop-requirements.txt
...
(workshop) [akitzmiller@holy2a envs]$ deactivate
[akitzmiller@holy2a envs]$ which python
/usr/bin/python
```

Anaconda virtual environments

- Make an environment (make sure pip is installed)

```
[akitzmiller@holy2a ~]$ module load python/2.7.13-fasrc01
[akitzmiller@holy2a ~]$ module list
Currently Loaded Modules:
  1) Anaconda/4.3.0-fasrc01   2) python/2.7.13-fasrc01
```

```
[akitzmiller@holy2a ~]$ conda create -n new pip
The following NEW packages will be INSTALLED:
```

```
openssl:    1.0.2k-1
pip:        9.0.1-py27_1
python:     2.7.13-0
...
wheel:      0.29.0-py27_0
zlib:       1.2.8-3
```

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

```
...
```

```
#
```

```
# To activate this environment, use:
```

```
# > source activate new
```

```
#
```

```
# To deactivate this environment, use:
```

```
# > source deactivate new
```

```
#
```

```
[akitzmiller@holy2a ~]$ source activate new
```

```
(new) [akitzmiller@holy2a ~]$ which python
```

```
~/conda/envs/new/bin/python
```

```
(new) [akitzmiller@holy2a ~]$ source deactivate
```

```
[akitzmiller@holy2a ~]$
```


Anaconda virtual environments

- Make a clone of the parent environment (may take a while) so that all base packages are included

```
[akitzmiller@holy2a ~] module load python/2.7.13-fasrc01
[akitzmiller@holy2a ~] conda create -n clone --clone $PYTHON_HOME
Using Anaconda Cloud api site https://api.anaconda.org
Fetching package metadata: .....
src_prefix: '/n/sw/fasrcsw/apps/Core/Anaconda/4.3.0-fasrc01/x'
dst_prefix: '/n/home_rc/akitzmiller/.conda/envs/clone'
Packages: 163
Files: 2254
Linking packages ...
[      COMPLETE      ]|#####| 100%
#
# To activate this environment, use:
# $ source activate clone
#
# To deactivate this environment, use:
# $ source deactivate
#
```

- Clone names can be a full path

```
[akitzmiller@holy2a ~] conda create -p /n/my_lab/shared/software/pyenv --clone $PYTHON_HOME
```

- Install package from Continuum

```
(clone)[akitzmiller@holy2a ~] conda install Django --yes  
Using Anaconda Cloud api site https://api.anaconda.org
```

The following packages will be downloaded:

package	build	
ca-certificates-2017.1.23	0	166 KB
django-1.10.6	py27_0	4.5 MB
Total:		4.7 MB

With some of our Anacondas, you may need to do this:

```
(clone)[akitzmiller@holy2a ~] conda remove conda-env conda-build --yes
```

- Or from a particular conda channel

```
(clone)[akitzmiller@holly2a ~] conda install --channel conda-forge tensorflow  
Using Anaconda Cloud api site https://api.anaconda.org
```

The following NEW packages will be INSTALLED:

```
ca-certificates: 2017.1.23-0  
mkl:             11.3.3-0  
mock:            2.0.0-py27_0  
numpy:           1.11.2-py27_0  
pbr:             1.10.0-py27_0  
protobuf:        3.2.0-py27_0  
scipy:           0.18.1-np111py27_0  
tensorflow:      1.0.0-py27_0
```

The following packages will be UPDATED:

```
numexpr:         2.5.2-np111py27_nomkl_1 [nomkl] --> 2.5.2-np111py27_1  
python:          2.7.11-0 --> 2.7.13-0  
scikit-learn:    0.17.1-np111py27_nomkl_1 [nomkl] --> 0.17.1-np111py27_1  
sqlite:          3.9.2-0 --> 3.13.0-0
```

Proceed ([y]/n)? n

- Or do a pip install

```
(clone)[akitzmiller@holy2a ~] pip install BioPython
Collecting BioPython
  Downloading biopython-1.68.tar.gz (14.4MB)
    100% |████████████████████████████████████████| 14.4MB 24kB/s
Building wheels for collected packages: BioPython
  Running setup.py bdist_wheel for BioPython ... done
  Stored in directory: /n/home_rc/akitzmiller/.cache/pip/wheels/a7/40/7e/cf0e1056601c97bbf42acac
Successfully built BioPython
Installing collected packages: BioPython
Successfully installed BioPython-1.68
(clone)[akitzmiller@holy2a ~]
```

- Compiled code in conda packages can be a problem

```
(clone)[akitzmiller@holy2a ~] conda install -c conda-forge tensorflow  
Using Anaconda Cloud api site https://api.anaconda.org
```

The **following NEW** packages will be **INSTALLED**:

```
...  
numpy:          1.11.2-py27_0  
pbr:            1.10.0-py27_0  
protobuf:       3.2.0-py27_0  
scipy:          0.18.1-np111py27_0  
tensorflow:     1.0.0-py27_0
```

The **following** packages will be **UPDATED**:

```
...
```

Unlinking packages ...

```
[ COMPLETE ]|#####| 100%
```

Linking packages ...

```
[ COMPLETE ]|#####| 100%
```

```
(clone)[akitzmiller@holy2a ~] python
```

```
Python 2.7.13 |Anaconda 2.5.0 (64-bit)| (default, Dec 20 2016, 23:09:15)
```

```
[GCC 4.4.7 20120313 (Red Hat 4.4.7-1)] on linux2
```

```
Type "help", "copyright", "credits" or "license" for more information.
```

```
Anaconda is brought to you by Continuum Analytics.
```

```
Please check out: http://continuum.io/thanks and https://anaconda.org
```

```
>>> import tensorflow as tf
```

```
Traceback (most recent call last):
```

```
...
```

```
File "/n/home_rc/akitzmiller/.conda/envs/clone/lib/python2.7/site-packages/tensorflow/python/p
```

```
_mod = imp.load_module('_pywrap_tensorflow', fp, pathname, description)
```

```
ImportError: /usr/lib64/libstdc++.so.6: version `GLIBCXX_3.4.19' not found (required by /n/home_
```

```
>>>
```

- Installing with pip instead of conda compiles source code, which may not be better

```
(clone)[akitzmiller@holy2a ~] pip install gattlib
Collecting gattlib
  Downloading gattlib-0.20150805.tar.gz (1.7MB)
    100% |████████████████████████████████████████| 1.7MB 170kB/s
Building wheels for collected packages: gattlib
  Running setup.py bdist_wheel for gattlib ... error
Complete output from command /n/home_rc/akitzmiller/.conda/envs/clone/bin/python -u -c "import
running bdist_wheel
running build
running build_ext
building 'gattlib' extension
creating build
...
creating build/temp.linux-x86_64-2.7/src/bluez/btio
gcc -pthread -fno-strict-aliasing -g -O2 -DNDEBUG -g -fwrapv -O3 -Wall -Wstrict-prototypes -fPIC
cc1plus: warning: command line option "-Wstrict-prototypes" is valid for Ada/C/ObjC but not for
src/gattservices.cpp:6:33: error: bluetooth/bluetooth.h: No such file or directory
src/gattservices.cpp:7:27: error: bluetooth/hci.h: No such file or directory
src/gattservices.cpp:8:31: error: bluetooth/hci_lib.h: No such file or directory
In file included from src/gattlib.h:22,
               from src/gattservices.cpp:12:
src/bluez/attrib/gatt.h:25:27: error: bluetooth/sdp.h: No such file or directory
In file included from src/gattlib.h:19,
               from src/gattservices.cpp:12:
src/bluez/lib/uuid.h:153: error: 'uint128_t' does not name a type
```

Fix the missing lookkool module by installing from the Harvard Informatics github repository into an Anaconda clone

```
pip install git+https://github.com/harvardinformatics/lookkool.git
```

Parallel Python - Multiprocessing

- The Python interpreter does not support real parallel threading
- The multiprocessing module simulates a typical threading library using forked processes
- Do something else, while a tool runs in the background

```
from multiprocessing import Process

def runAnalysis(parametersfile){
    cmd = 'OMA %s' % parametersfile
    os.system(cmd)
}
p = Process(target=runAnalysis, args=(parametersfile))
p.start()
# Do some other stuff
...
p.join()
```


Parallel Python - Multiprocessing Pool

- If you're doing a variable number of simultaneous processes, you may want to use a Pool

```
>>> from multiprocessing import Pool
>>> import os
>>> def echo(echoable):
...     os.system('echo %s && sleep 10' % echoable)
...
>>> echoables = [
...     'ajk',
...     '123',
...     'qwerty',
...     'uiop',
...     'lkjdsa',
... ]
>>> numprocs = os.environ.get('NUMPROCS', 3)
>>> pool = Pool(numprocs)
>>> result = pool.map(echo, echoables)
123
ajk
qwerty
lkjdsa
uiop
```

Parallel Python - Multiprocessing Pool

- Pool.map does not work if you have more than one argument, so iterate through and use apply_async
- You'll need to "get" the return value from the result object(s)

```
>>> from multiprocessing import Pool
>>> import os
>>> def greet(name,message):
...     os.system('echo "Hi %s, %s" && sleep 10' % (name,message))
...     return '%s was greeted' % name
...
>>> greetings = [
...     ('Aaron','What's up?'),
...     ('Bert','Where's Ernie?'),
...     ('Donald','What're you thinking?'),
...     ('folks','Chill!'),
... ]
>>> numprocs = os.environ.get('NUMPROCS',3)
>>> pool = Pool(numprocs)
>>> results = []
>>> for greeting in greetings:
...     result = pool.apply_async(greet,greeting)
...     results.append(result)
Hi Bert, Where's Ernie?
Hi Aaron, What's up?
Hi Donald, What're you thinking?
Hi folks, Chill!
>>> for result in results:
...     print result.get()
Aaron was greeted
Bert was greeted
Donald was greeted
folks was greeted
```

Analyze the contigs using a multiprocessing pool. Compare the elapsed time with the for loop version.

Analyze contigs with a multiprocessing pool.

```
starttime = time.time()
from multiprocessing import Pool
numprocs = os.environ.get('ANNOTATION_PROC_NUM', 2)
pool = Pool(numprocs)

annotations = []
results = []
for contig in contigs:
    result = pool.apply_async(annotateStartStopCodons, contig)
    results.append(result)
    result = pool.apply_async(annotatePalindromes, contig)
    results.append(result)

for result in results:
    annotations += result.get()

endtime = time.time()
```

Python dictionaries

- A dictionary is like a list, but can be indexed by non-integers (AKA hash map)
- Elements are not necessarily in the order you think

```
>>> basecounts = { 'A' : 230, 'T' : 120, 'C' : 999, 'G' : 100 }
>>> for base, count in basecounts.items():
...     print '%s: %d' % (base, count)
...
A: 230
C: 999
T: 120
G: 100
```

- OrderedDict is available in Python 2.7 and you can order output by sorting keys

```
>>> for base in sorted(basecounts.keys()):
...     print '%s: %d' % (base, basecounts[base])
...
A: 230
C: 999
G: 100
T: 120
```

- Dictionary of lists

```
# Make a dictionary keyed by contig name  
annotatedcontigs = {}  
for annotation in annotations:  
    annotatedcontigs.setdefault(annotation['seqid'], []).append(annotation)
```

Python can be used to submit Slurm jobs

- Use a "heredoc" and format method to write a Slurm script

```
>>> script = '''#!/bin/bash
... #SBATCH -p {partition}
... #SBATCH -t {time}
... #SBATCH --mem {mem}
... #SBATCH -n {cores}
... #SBATCH -N {nodes}
...
... {cmd}
... '''.format(partition='gpu',time='100',mem='500',cores='1',nodes='1',cmd='hostname')
>>> print script
#!/bin/bash
#SBATCH -p serial_requeue
#SBATCH -t 1-0:00
#SBATCH --mem 1000
#SBATCH -n 1
#SBATCH -N 1

hostname

>>>
```

- Use a subprocess to submit and monitor your job
- Catch the job id from sbatch output

```
>>> from subprocess import Popen, PIPE
>>> def submit(filename):
...     proc = Popen('sbatch %s' % filename, shell=True, stdout=PIPE, stderr=PIPE)
...     stdout, stderr = proc.communicate()
...     return stdout.strip('Submitted batch job ')
...
>>>
```

- and use it to check sacct

```
from subprocess import Popen, PIPE
def isDone(jobid):
    done = ['COMPLETED', 'CANCELLED', 'FAILED', 'TIMEOUT', 'PREEMPTED', 'NODE_FAIL']
    proc = Popen('sacct --format state --noheader -j %d' % int(jobid), shell=True, stdout=PIPE, stderr=PIPE)
    stdout, stderr = proc.communicate()
    if proc.returncode != 0:
        raise Exception('Error running sacct: %s' % stderr)
    if stdout.strip() == '':
        return False
    lines = stdout.split()
    if lines[0].strip() in done:
        return True
    return False
```


