Python Best Practices on Blue Waters

Roland Haas, Victor Anisimov (NCSA)
Email: rhaas@illinois.edu

Python on Blue Waters

- HPC vendors have limited support of python on their platforms
- BWPY is NCSA supported python deployment on Blue Waters

```
$ module load bwpy
```

- Other installations, such as Anaconda in your home directory, are not supported.

- BWPY resolves typical issues with python deployment
  - Lustre filesystem does not tolerate frequent open / close
  - Using MPI on Cray is different from that on a Linux cluster
  - Compiling numerous python packages is a demanding job

BWPY versioning

- BWPY uses major.minor.patch versioning.
  - Major versions are for major changes
    - Different default python version (including minor)
    - Possibly a self-contained glibc, requiring a complete rebuild
  - Minor is for package updates
  - Patch fixes problems, mostly keeping package versions the same, unless specific package versions are broken. New packages may be added.

```
$ module load bwpy/x.y.z
```

- Current default: 1.2.4, latest: 2.0.1

BWPY submodules

`module load`

bwpy-mpi	MPI support enabled (should only be used on compute nodes!)
bwpy-libsci_mp	BWPY built with OpenMP Cray BLAS libraries (libsci_mp)
bwpy-libsci_acc	BWPY built with auto CUDA BLAS libraries (libsci_acc)
bwpy-visit	BWPY's VisIt (requires older vtk, so is a separate module)
bwpy-visit-mpi	BWPY's VisIt with MPI (only supported on compute nodes!)

Default BLAS: MKL

Available python interpreters

- CPython 2.7 (alias: python2)
- CPython 3.5 (aliases: **python**, python3)
- Cpython 3.6
- Pypy
- Pypy3

Now with much improved CPython compatibility!

Can select interpreter by setting `EPYTHON` environment variable

```
$ export EPYTHON=python2.7
$ python --version
Python 2.7.14
```

Can set the default version of python by using virtualenv (explained later)

Behind the scenes

- BWPY is a Gentoo-Linux distribution mounted as a read-only disk image
  - Use `bwpy-environ` tool to mount the image and get access to apps
  - Image appears in `/mnt/bwpy` with subdirectories `{single,mpi}` etc.
  - Image is local to each process and its children
  - Use `bwpy-environ -- program [args …]` to run a program
  - Can invoke `bwpy-environ` directly for debug purpose

What to expect

```
% which python
/usr/bin/python                    # old interpreter that comes with operating system

% module add bwpy; which python
/sw/bw/bwpy/mnt/bin/python         # wrapper around bwpy-environ

% bwpy-environ -- which python
/mnt/bwpy/single/usr/bin/python    # actual binary
```

```
% which cmake
/usr/bin/cmake                     # old cmake that comes with operating system

% module avail cmake
cmake/2.8.10.2        cmake/3.1.3(default)  cmake/3.9.4

% module add bwpy; bwpy-environ -- cmake --version
cmake version 3.11.2               # bwpy cmake
```

Things to keep in mind when using bwpy-environ

- `bwpy-environ` starts a new shell
  - ENV is lost on exit from `bwpy-environ`
  - Parent variables need to be explicitly exported to be visible
- Mounting the image is expensive, best to do multiple things at once or stay in `bwpy-environ` rather than using many Python calls
- When used with `aprun`, use `-b` switch

```
$ bwpy-environ
$ mount | grep bwpy
/mnt/a/sw/xe_xk_cle5.2UP02_pe2.3.0/images/bwpy/bwpy-2.0.1.img
on /mnt/bwpy type squashfs (ro,nosuid,nodev,noatime)

#PBS
aprun -b -n1 -- bwpy-environ -- python --version
```

Building software against BWPY

- Use with `gcc/4.9.3` (`bwpy/default`) or `gcc/5.3.0` (`bwpy/2.0.1`)
- Export these variables, so these dirs come after `-I` and `-L`

```
$ module swap PrgEnv-cray PrgEnv-gnu
$ module swap gcc gcc/4.9.3
$ export CPATH="$CPATH:$BWPY_INCLUDE_PATH"
$ export LIBRARY_PATH="$LIBRARY_PATH:$BWPY_LIBRARY_PATH"
$ export LDFLAGS="$LDFLAGS -Wl,--rpath=$BWPY_LIBRARY_PATH”
```

- Do not use LD_LIBRARY_PATH to avoid potential incompatibility issues
- Use CMake from bwpy
- Software inside of BWPY has its own include paths, e.g. `/mnt/bwpy/single/usr/include/tensorflow/` for TensorFlow’s C++ interface
- Compilation **must** be done in a `bwpy-environ` shell!

Building scipy/1.2.0 against BWPY

```
module swap PrgEnv-cray PrgEnv-gnu
module load bwpy
git clone https://github.com/scipy/scipy.git scipy
cd scipy
git tag
git checkout v1.2.0

export CPATH="$CPATH:$BWPY_INCLUDE_PATH”
export LIBRARY_PATH="$LIBRARY_PATH:$BWPY_LIBRARY_PATH”
export LDFLAGS="$LDFLAGS -Wl,--rpath=$BWPY_LIBRARY_PATH”
```

```
bwpy-environ -- setup.py build
bwpy-environ -- setup.py install –user
bwpy-environ -- pip install --user pytest
```

 # run these under bwpy-environ

```
cd $HOME
python
import pytest
import scipy
scipy.__version__
scipy.test()
```

Building a python package against BWPY

```
module swap PrgEnv-cray PrgEnv-gnu
module load fftw
module load cudatoolkit
module load bwpy
module load cray-hdf5

export CRAYPE_LINK_TYPE=dynamic
export CRAY_ADD_RPATH=yes
export CXX=CC
export CC=cc
pip freeze | grep protobuf
pip freeze | grep h5py

export CPATH="$CPATH:$BWPY_INCLUDE_PATH”
export LIBRARY_PATH="$LIBRARY_PATH:$BWPY_LIBRARY_PATH”
export LDFLAGS="$LDFLAGS -Wl,--rpath=$BWPY_LIBRARY_PATH”

mkdir build
cd build
bwpy-environ -- cmake ..
bwpy-environ -- make
```

Creating local python environment with help of Virtualenv

- BWPY (1.2.4) contains 262 python(3) packages
- Extra packages should be installed in a virtualenv to avoid version conflicts when installing in `$HOME/.local`
  - use `--sytem-site-packages` option to import the existing packages
  - Python in virtualenv is **frozen** to BWPY version active at **creation**
- Use pip to install extra packages
  - **do not** use `--user` option in virtualenv
  - use `--force-reinstall` to overwrite existing packages
  - use `pip install mypackage==x.y.z` to force specific version
  - `https+git://git-repository-with-setup.py` for git repositories

Virtualenv examples

```
$ mkdir myvirtualenv
$ cd myvirtualenv
$ virtualenv -p python2.7 --system-site-packages $PWD
$ source bin/activate
$ pip install myfavoritepackage
$ deactivate


$ export GEOS_DIR=/mnt/bwpy/single/usr/
$ pip install pyproj==1.9.3
$ pip install git+https://github.com/matplotlib/basemap

$ pip install --force-reinstall yt
```

Jupyter notebooks

- Ok to run on login nodes, within reason

```
bw$ module load bwpy
bw$ bwpy-environ -- bash -ic jupyter-notebook
The Jupyter Notebook is running at:
http://10.0.0.147:8981/
laptop% ssh -L 8888:10.0.0.147:8981 bw.ncsa.illinois.edu
laptop% open http://127.0.0.1:8888
```

- Notebook server is accessible Blue Waters wide
  - use password to protect the notebook server
  - jupyter outputs connection information to stdout on startup
  - use **second** ssh connection to the login node to forward the local port
  - jupyter auto-saves notebooks in case connection is lost (or use `screen`)

See https://bluewaters.ncsa.illinois.edu/pythonnotebooks

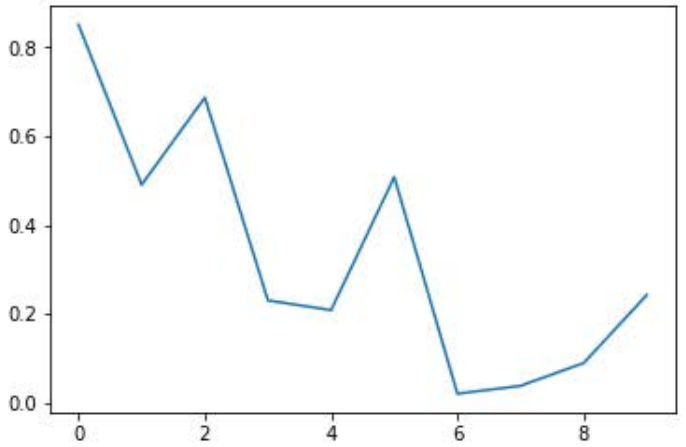
Data exploration modules

- BWPY provides large number of modules for data exploration
  - `numpy, scipy, sympy`
  - `h5py, netCDF, gdal, pandas`
  - `astropy, PostCactus`
  - `matplotlib, yt, plotly`
- use `%matplotlib notebook` to show plots

```
h2ologin3
```

In [64]:
```
import numpy as np
x = np.arange(10) ; y = np.random.rand(len(x))
```

In [65]:
```
import matplotlib.pyplot as plt
%matplotlib notebook
plt.plot(x, y);
```



In [66]:
```
import plotly
plotly.offline.init_notebook_mode()
plotly.offline.iplot([{'x': x, 'y': y}])
```


See https://bluewaters.ncsa.illinois.edu/pythonnotebooks

- BWPY includes `mpi4py` linked against Cray MPI stack
  - load as bwpy-mpi submodule
  - cannot be used on login nodes, even when using single rank
  - only one `MPI_Init()` per `aprun`, implicit in `import mpi4py.MPI`
  - use `aprun` to start Python
  - use `-d` for multi-threaded code or job bundling

```
$ cat hello.py
from mpi4py import MPI
print ("Hello from rank ", MPI.MPI_COMM_WORLD.Get_rank())
$ qsub -I -l nodes=1:ppn=32:xe -l walltime=0:30:0 -q debug
% module load bwpy
% module load bwpy-mpi
% aprun -n4 -d8 -b -- bwpy-environ -- python ./hello.py
```

Running single-threaded jobs in python

- Do not start hundreds of single-threaded python scripts via aprun
  - wasteful since each aprun claims a full node
  - slow, each aprun takes ~1min to start and finish
  - hard on the system (we will contact you if you abuse this too much)
- Use mpi4py `MPICommExecutor`
  - Put your payload code in a function taking a single argument
  - Create a list of tasks
  - Pass the list to `MPICommExecutor`
- Benefits
  - Can run multiple tasks on a single node
  - New tasks start as soon as previous ones finished
  - Pure python code

Example of job bundling

```
from mpi4py import MPI
from mpi4py.futures import MPICommExecutor

def fun(x):
    print("on %s print %g" % (MPI.COMM_WORLD.Get_rank(),x))

with MPICommExecutor(MPI.COMM_WORLD, root=0) as executor:
    jobs = range(100)
    if executor is not None:
       executor.map(fun, jobs)
```

```
aprun -n $NRANKS -d1 -b -- bwpy-environ -- python ./run.py
```

See further details in https://bluewaters.ncsa.illinois.edu/job-bundling#using_multiple_nodes_and_python

Blue Waters documentation

- https://bluewaters.ncsa.illinois.edu/python
- https://bluewaters.ncsa.illinois.edu/pythonnotebooks
- https://bluewaters.ncsa.illinois.edu/data-transfer-doc#gcli
- https://bluewaters.ncsa.illinois.edu/job-bundling#using_multiple_nodes_and_python

Questions?

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