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The Summit Programming Environment

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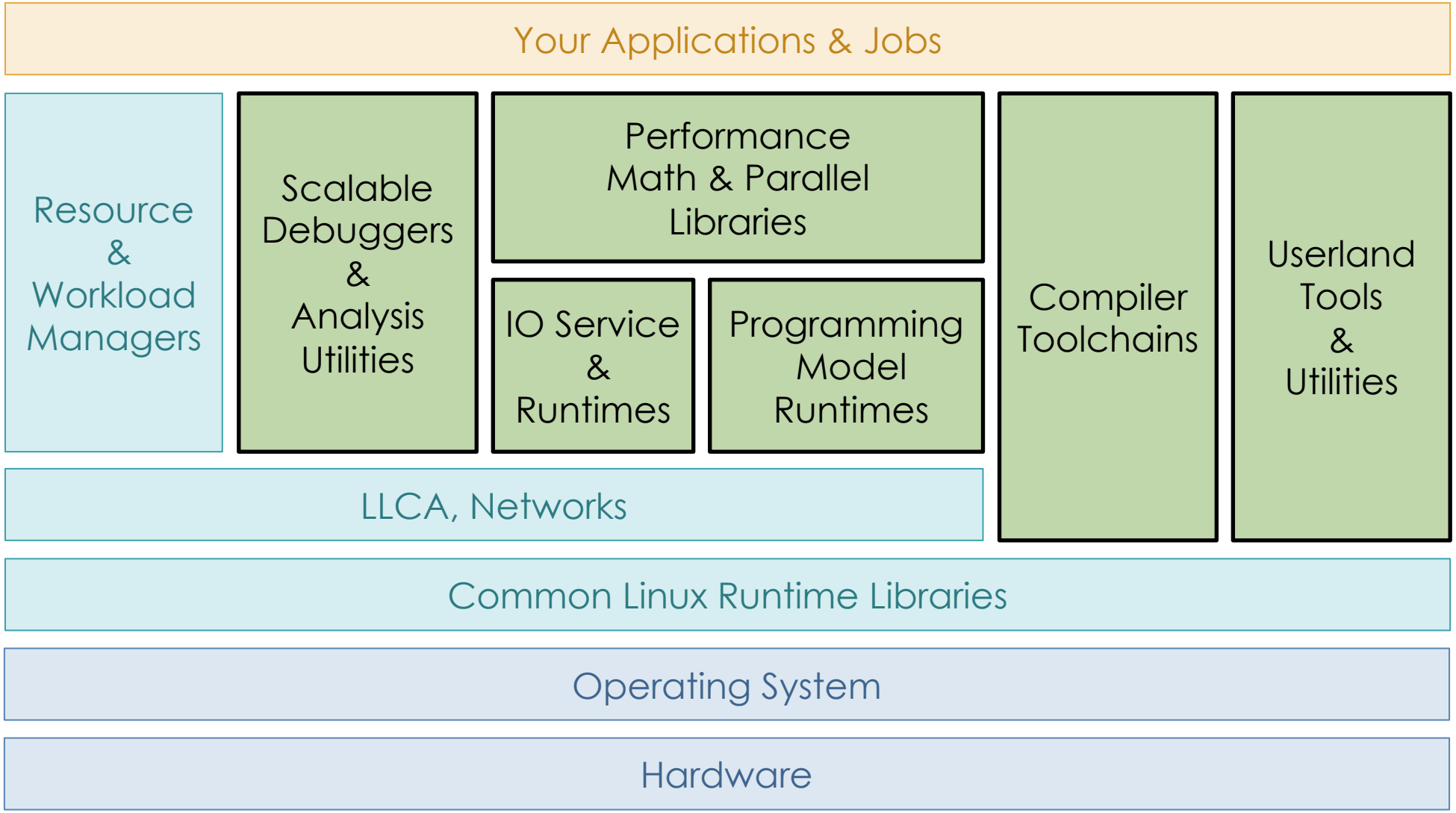
What is the Programming Environment?



Programming Environment Overview

- At the highest level, the PE is your shell's build- and run-time environment (see output of **`env`**).
- Software outside default paths (`/usr/bin`, `/usr/lib`, etc.)
- Managed via session environment variables
  - Search paths
    - `PATH`, `LD_LIBRARY_PATH`, `LIBRARY_PATH`, `PKG_CONFIG_PATH`, etc…
  - Program environment options
    - `OMPI_*`, `CC`, `FC`, ect…
- Summit uses LMOD for this purpose

LMOD Environment Modules

- Much of the available software cannot coexist simultaneously in your environment.
- Build- and runtime-environment software managed with LMOD (https://lmod.readthedocs.io)
- Usage:

```
$ module -t list                    # list loaded modules
$ module avail                      # Show modules that can be loaded given current env
$ module help <package>             # Help info for package (if provided)
$ module show <package>             # Show contents of module
$ module load <package> <package>…  # Add package(s) to environment
$ module unload <package> <package>… # Remove package(s) from environment
$ module reset                      # Restore system defaults
$ module restore <collection>       # Load a saved collection
$ module spider <package>           # Deep search for modules
$ module purge                      # Clear all modules from env.
```

Module Avail

- The `module avail` command shows **only what can be loaded given currently loaded packages.**
- Full or partial package names limit output to matches.

```
$ module avail
------------ /sw/summit/modulefiles/site/linux-rhel7-ppc64le/Core ----------
   ...
   cuda/9.1.85                      py-nose/1.3.7        (D)
   cuda/9.2.64             (D)      py-pip/9.0.1
   gcc/4.8.5               (L)      python/3.5.2
   gcc/5.4.0                        readline/6.3

  Where:
   L:  Module is loaded
   D:  Default Module

Use "module spider" to find all possible modules.
Use "module keyword key1 key2 ..." to search for all possible modules matching
any of the "keys".
```

Path in `MODULEPATH` where a module exists. Printed in order of priority.

Future labels will have explanation in legend (shown on in non-terse output)

Modulefile Priority

- Loading some modules will alter the `MODULEPATH`.
  - Compilers, MPI: Only one module in families can be loaded at a time.
- First module among duplicate `package/version` names in `MODULEPATH` will be selected:

```
$ module -t avail hdf5/1.10.0-patch1
/sw/summit/modulefiles/site/.../spectrum-mpi/10.2.0.0-20180508-riohv7q/xl/20180502:
hdf5/1.10.0-patch1
/sw/summit/modulefiles/site/.../xl/20180502:
hdf5/1.10.0-patch1
```

Example: MPI-enabled builds replace serial builds when MPI implementation is loaded.

Modulefile Priority

To override behavior, alter the `MODULEPATH` yourself:

```
$ module use /path/to/module/file/tree
$ module unuse /path/to/remove/from/search/tree
```

- Path is prepended with higher priority
- Can also provide your own custom modulefiles.
  - Complete instructions for writing modulefiles: https://lmod.readthedocs.io/en/latest/015_writing_modules.html

Searching for Modules with Spider

- Use `module spider` (not `avail`) to search for modules
  - Finds packages that cannot be loaded given current environment
  - Shows requirements needed to make package available

```
$ module -t spider hdf5/1.10.0-patch1
----------------------------------------------------------------------------
  hdf5: hdf5/1.10.0-patch1
----------------------------------------------------------------------------
    You will need to load all module(s) on any one of the lines below before
the "hdf5/1.10.0-patch1" module is available to load.
      ...
      gcc/4.8.5
      gcc/4.8.5  spectrum-mpi/10.1.0.4-20170915
      gcc/4.8.5  spectrum-mpi/10.2.0.0-20171117
      ...
```

Spider (cont'd)

- Complete listing of possible modules is only reported when searching for a specific version:
  `` `module spider <package>/<version>` ``
- Can search using limited regular expressions:
  - All modules with 'm' in their name: `module -t spider 'm'`
  - All modules starting with the letter 'm': `module -t -r spider '^m'`

Module Dependency Management

- Conflicting modules automatically reloaded or inactivated.
- Generally eliminates needs for `$ module swap PKG1 PKG2`

```
$ module load xl

Lmod is automatically replacing "gcc/4.8.5" with "xl/20180502".


Due to MODULEPATH changes, the following have been reloaded:
  1) spectrum-mpi/10.2.0.0-20180508
```

Module Dependency Management

- Check `stderr` for messages about deprecated modules.
- Modules generally only available when all dependencies are currently loaded.
  - Most provided packages use absolute RPATHs and RUNPATHs; obviates the need to actually load dependency modules.
  - Some exceptions, notably python extensions.
- Not all packages available in all compiler environments
  - Advanced approach to mix modules across compiler environments described in backup slides.

User Module Collections

- Save module collections for easy re-use

```
$ module save my_favorite_modules
Saved current collection of modules to: "my_favorite_modules", for system: "summit”

$ module reset
Resetting modules to system default

$ module restore my_favorite_modules
Restoring modules from user's my_favorite_modules, for system: "summit"

$ module savelist                # Show what collections you’ve saved
$ module describe <collection>   # Show modules in a collection
$ module disable <collection>    # Make a collection un-restorable (does not delete)
```

User Module Collections

- Modulefile updates ***may break saved collections***.
  - **To fix**: manually load desired modules, save to same name to update.
- Collection named `default` automatically loaded on login
  - Use caution with personal `default` collections due to above
- To delete a collection: `rm ~/.lmod.d/<collection>.<system>`

Default Applications

- DefApps meta module
  - XL compiler
  - SMPI
  - HSI – HPSS interface utilities
  - XAlt – Library usage
  - LSF-Tools – Wrapper utility for LSF
  - darshan-runtime – An IO profiler; unload if using other profilers.

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Compilers and Toolchains

- Compiler Environments
- Common Flags

Compiler Environments

IBM XL (default)

- `xl/16.1.1-3`
  - Older modules not recommended

LLVM/Clang

- `llvm/1.0-20190225`
  - Older modules not recommended

GCC

- `gcc/8.1.1`
  - OpenACC Capable
- `gcc/7.4.0`
  - Latest w/ CUDA10 NVCC
- `gcc/6.4.0` (default)
- `gcc/5.4.0`
- `gcc/4.8.5`
  - RHEL7 OS compiler in `/usr`
  - "Core" modulefiles

PGI

- `pgi/19.4`
- `pgi/19.1`
- `pgi/18.10` (default)
- `pgi/18.7`

New compiler releases added regularly.

IBM XL (Default toolchain)

- Base compilers `xlc`, `xlC`, `xlc++`, `xlf`
  - Many wrappers exist to apply preset flags for various language standards. Thread safe option wrappers suffixed `*_r`
  - See `${OLCF_XLC_ROOT}/etc/xlc.cfg.*` and `${OLCF_XLF_ROOT}/etc/xlf.cfg.*` for options enabled by wrappers.
- Single version in `/opt/ibm`, to reference module version, use `${OLCF_XL_ROOT}`, `${OLCF_XLC_ROOT}`, `${OLCF_XLF_ROOT}`

LLVM

- Base compilers `clang`, `gfortran` (OS)
- Build based on Clang v8, despite modulefile name
- Full software environment not provided
- Experimental, minimal support.
  - May need to use older CUDA (whichever latest release was built for) for OpenMP offload.

CUDA/NVCC

- Module `cuda/10.1.105` (default)
- Available under all compiler environments
- If you're not using the GPUs, you're not really using the machine
- Provides cuBLAS, cuDNN
  - cuBLAS located according to CUDA ≤ 9 scheme: `${OLCF_CUDA_ROOT}/{lib64,include}`
- Older modules available, but not recommended for use
  - Recompile against latest version available if possible

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Software, Libraries, and Programming Models

Provided Software

- Vendor-supplied
  - IBM: ESSL (blas/lapack**/fftw), MASS, SMPI
  - NVIDIA: CUDA, cuBLAS, cuDNN
  - Debuggers: Allinea Forge, Perf. Reports; Score-P/Vampir
- Built by OLCF
  - Built in userspace without superuser privileges.
  - Often general purpose
  - Optimized as possible while still being generally applicable
    - May not always be as optimized as you want;
      notable example: BLAS/LAPACK for CPU is mostly a reference implementation.
    - Encourage users to build own packages for special needs

MPI Implementation – IBM Spectrum-MPI

- Based on OpenMPI, similar compiler wrappers and flags
  `mpicc`, `mpic++`, `mpiCC`, `mpifort`, `mpif77`, `mpif90`, `mpixl*`
- Modules `spectrum-mpi/10.3.0.0-20190419` (Default)
  - Avoid older releases.
- Updates usually require recompilation.
- Uses `jsrun` MPI launcher (See separate talk in this series)
- Alt. implementations (OpenMPI, MPICH) unavailable

MPI environment

- When using XL, default `$OMPI_FC` is `xlf2008_r`
  - Works with standard MPI wrappers despite XL-specific wrappers `mpixlc`, `mpixlC`, `mpixlf`
  - F77 codes must use alternate xlf wrapper `` `export OMPI_FC=xlf_r` `` or set additional xlf options via `FFLAGS`, build-system, etc.
- Adaptive routing enabled by default

```
PAMI_IBV_ENABLE_OOO_AR=1
PAMI_IBV_QP_SERVICE_LEVEL=8
```

Building your own software

- Where to build?
  - Recommend `/tmp/$USER`
    - faster performance than NFS
    - doesn't leave detritus in quota's `$HOME`, `/ccs/proj` dirs.
  - GPFS also acceptable
- Where to install?
  - NFS filesystem `/ccs/proj/<PROJECTID>` preferred: not purged, RO.
  - Avoid `$HOME`, especially `~/.local/{bin,lib,share}`
    - Shared across architectures; may cause ABI or instruction set errors

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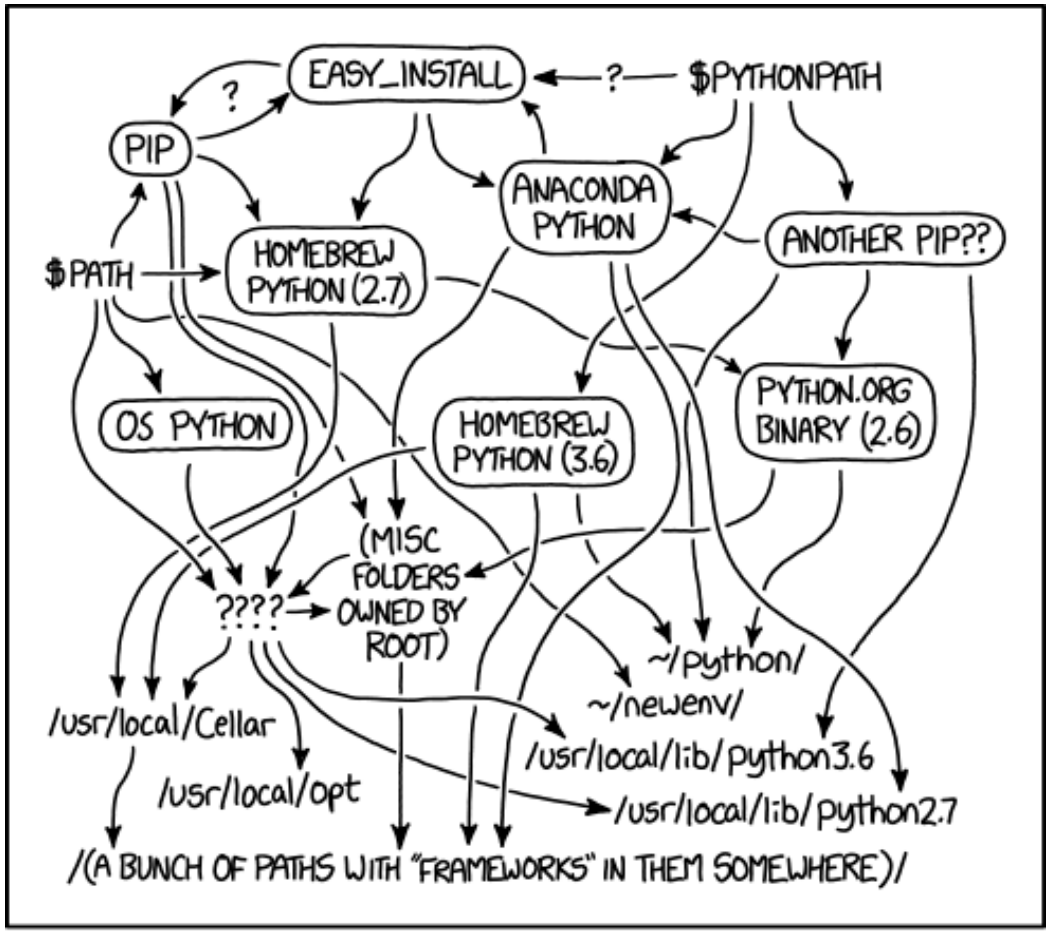
Python Runtimes and Environments

Python environments



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

supercomputer

Python environments can get messy… more so in HPC

Credit: https://xkcd.com/1987/

Provided Python Environments and Extensions

- Anaconda Distributions
  - Includes commonly used packages out-of-the box
  - Extendable/customizable with `conda` environments
- Minimal native python environment modules
  - OLCF can't feasibly provide env-modules for every extension
  - Extend the standard library with `virtualenvs`
- DIY is always an option
  - More work, but also more stable and tuned to your needs.

Anaconda

- Provided via modulefiles (default)
  - `python/{M}.{m}.{u}-anaconda{M}-{REL}`
- `PYTHONUSERBASE` set to unique location
  - Only for Anaconda loaded from modulefiles.
  - `${HOME}/.local/${HOST}/python/${MODULENAME}`
- Relies heavily on pre-compiled binaries
- Extend through `conda` environments
  - `conda` similar to `pipenv`: package manager, virtual environment all-in-one

{M}: Python Major Version
{m}: Python minor Version
{u}: Python micro Version
{REL}: Anaconda Release

Creating Conda Environments

- Pre-compiled packages pulled from *channels*
  - Generally comes with pre-compiled external dependency libraries
  - Binaries typically optimized for generic architectures
  - Pre-compiled binaries don't always work on HPC resources
  - Building packages from source possible
    - Use the OS GCC compiler

```
conda create [-c <channel>] -p <path> python=3.7 [< addt'l pkgs>...]
source activate <conda_env>
conda install numpy pyyaml [<pkg>…]
[CC=gcc MPICC=mpicc] pip install --no-binary mpi4py install mpi4py
source deactivate
```

Native Python (from environment modules)

- Provided via module files
  - `module load python/{M}.{m}.{u}`
  - Versions 3.7.0 and 2.7.15
  - 3.5.2 and 2.7.12 also on some systems

{M}: Python Major Version
{m}: Python minor Version
{u}: Python micro Version
{REL}: Anaconda Release

- Some basic packages included in root site-packages*
  - `virtualenv`, `pip`, `setuptools`, etc for setting up virtualenvs.
  - *Only for python interpreters **outside** a compiler environment: Unload all compilers to get a python environment with these pre-installed to setup a virtualenv.

Native Python (from environment modules)

- Don't rely on OLCF py-* environment modules for extensions
  - Some packages still provided by environment modules. Eg, `mpi4py`
  - Most python extension environment modules are by-products of specific site-installed software, but not intended for general use.
  - Extension env modules do not load their dependencies
    - Neither external libraries
    - Nor *extra (often required) python extensions*
- Instead, use Anaconda/conda envs or virtualenvs
  - Can also (cautiously) add self-installed extensions to `PYTHONPATH`

Thanks for listening

- Questions or comments regarding the Summit programming environment?

  Contact `help@olcf.ornl.gov`

  We're happy to help with any issues and questions you have.

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Appendix

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Appendix

Environment Modules

Sample Modulefile

```
help("GCC Compiler")
whatis("Description: ", "GCC compiler 8.1.1")

local package = "gcc”
local version = "8.1.1”
local moduleroot = myFileName():sub(1,myFileName():find(myModuleFullName(),1,true)-7)
local gccdir = "/sw/ascent/gcc/8.1.1"

-- Setup Modulepath for packages built by this compiler
prepend_path( "MODULEPATH",  pathJoin(moduleroot, package, version ) )

-- Environment Globals
prepend_path( "PATH",  pathJoin(gccdir, "bin" ) )
prepend_path( "MANPATH", pathJoin(gccdir, "share/man" ) )
prepend_path( "LD_LIBRARY_PATH", pathJoin(gccdir, "lib64") )

-- OLCF specific Environment
setenv("OLCF_GCC_ROOT",  gccdir)
```

Access to all the provided software

- Possible to use modules across compiler environments but not recommened.
- Use at your own risk
  - Modules may conflict with other software or otherwise not function
  - Read modulefile comments and build log for information about build
  - Check binaries and libraries with ldd for links against MPI version
- Modules named

```
`{PKG}-{VER}-{COMPILER}-{COMP_VER}-[{SUFFIXES}-]{HASH_STUB}`
```

```
SPACK_MODULES="/sw/summit/.swci/1-compute/share/spack/modules"
module use "${SPACK_MODULES}/20180914/linux-rhel7-ppc64le"
```

Appendix

Compilers and Toolchains

IBM XL Options and Flags

- Code standard using base compiler
  - xlc: `-std=gnu99`, `-std=gnu11`
  - xlc++: `-std=gnu++11`, `-std=gnu++1y` (partial support)
  - xlf: `-qlanglvl=90std`, `-qlanglvl=2003std`, `-qlanglvl=2008std`
  - Wrappers available for many language standards
- Default signed char: `-qchar=signed`
- Define macro: `-WF,-D`
- IBM `xlf` does not mangle Fortran symbols by default, use `-qextname` to add trailing underscores.

GNU Compiler Suite (GCC)

- Base compilers `gcc`, `g++`, `gfortran`
- OS compiler always in environment
  - Guaranteed ABI compatible with system libraries
- Code standards:
  - gcc: `-std=gnu99`, `-std=gnu11`
  - g++: `-std=gnu++11`, `-std=gnu++1y`
  - gfortran: `-std=f90`, `-std=f2003`, `-std=f2008`
- Signed char: `-fsigned-char`

PGI (Portland Group)

- Base compilers `pgcc`, `pg++`, `pgfortran`
- Code standards:
  - pgcc: `-c99`, `-c11`
  - pg++: `-std=c++11 --gnu_extensions`, `-std=c++14 --gnu_extensions`
  - Fortran code standard detected by suffix: `.F90`,`.F03`, `.F08`
- Default signed char: `-Mschar`

CUDA/NVCC Options and Flags

- C++11 support: `-std=c++11`
- host/device `lambdas` (experimental):
  `--expt-extended-lambda`
- host/device `constexpr`s (experimental):
  `--expt-relaxed-constexpr`
- Supports XL, GCC, and PGI C++ host compilers via
  `--ccbin <PATH>`
  - Some version restrictions for latest PGI, GCC toolchains

OpenACC (Version 2.5)

Supported Compiler Environments	
PGI (All Versions)	GCC 8.1.0+
`-acc -ta=nvidia:cc70`	`-fopenacc`

OpenMP

Compiler	3.1 Support	4.x Support	Enable OpenMP	Enable OpenMP 4.X Offload
IBM	FULL	PARTIAL	`-qsmp=omp`	`-qsmp=omp -qoffload`
GCC	FULL	PARTIAL	`-fopenmp`	`-fopenmp`
PGI	FULL		`-fopenmp`	

LLVM	FULL	PARTIAL	`-fopenmp`	`-fopenmp`
				`-fopenmp-targets=nvptx64-nvidia-cuda`
				`--cuda-path=${OLCF_CUDA_ROOT}`

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Appendix

Software, Libraries, and Programming Models

Detailed Information about provided software

- $OLCF_{PKG}_ROOT/.spack/build.out

```
$ head $OLCF_HDF5_ROOT/.spack/build.out
==> Executing phase: 'autoreconf'
==> Executing phase: 'configure'
==> '/autofs/nccsopen-svm1_sw/ascent/.swci/1-compute/var/spack/stage/hdf5-1.10.3-
2llvf5hpxbqzgl5agzkstjqs2xv4v4uk/hdf5-1.10.3/configure' '--prefix=/autofs/nccsopen-
svm1_sw/ascent/.swci/1-compute/opt/spack/20180914/linux-rhel7-ppc64le/xl-16.1.1-
beta5/hdf5-1.10.3-2llvf5hpxbqzgl5agzkstjqs2xv4v4uk' '--enable-unsupported' '--disable-
threadsafe' '--enable-cxx' '--enable-hl' '--enable-fortran' '--without-szlib' '--enable-
build-mode=production' '--enable-shared' 'CFLAGS=-qpic' 'CXXFLAGS=-qpic' 'FCFLAGS=-qpic'
'--enable-parallel' ...
...
checking for a BSD-compatible install... /usr/bin/install -c
checking whether build environment is sane... yes
```

Building your own software

- Recommended to rebuild with new MPI, CUDA releases
- Recommended to use common build systems and utils
  - CMake, autotools, pkgconfig, etc.
  - Many provided packages automatically alter `$CMAKE_PREFIX_PATH`, `$PKG_CONFIG_PATH`
- All center-built modules set `$OLCF_{PKG}_ROOT` vars for use in build/configure scripts

Using Spack for missing dependencies

- Spack is a homebrew-like source-build package manager (https://spack.readthedocs.io/en/latest/)
  - Used to deliver most of the packages we provide
  - Not all Spack packages written to support ppc64le... Yet
  - OLCF uses come customized packages not available upstream
- Must configure to use external SMPI, CUDA, compilers.
  - `./spack/etc/spack/packages.yaml`
- Happy to share our Spack configs and settings on request.

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Appendix

Python Environments

Native Python: Venv/Virtualenvs

- Provides isolated python environment
- python3: `python3 -m venv <path>`
- python2: `virtualenv <path>`
- Activate several ways
  - from command line: `. <path>/bin/activate; deactivate`
  - from shebang line: `#!/path/to/venv/bin/python3`
- Load all environment modules first; deactivate before changing environment modules

Building Python Packages from Source

- Can be tricky in HPC environment
- Easier to manage at a personal level than for site-provided environment modules that work for everyone
- Let `pip` do it for you:

```
[CC=gcc MPICC=mpicc] pip install \
                          -v --no-binary <pkg> <pkg>
```

- Or use distutils/setuptools: `python setup.py install`
  - Check package docs. May need to get creative passing HPC environment parameters.

General Python Guidelines

- Follow PEP394 (https://www.python.org/dev/peps/pep-0394/)
  - Call `python2` or `python3` instead of ambiguous `python`
  - Same in scripts: `#!/usr/bin/env python2` or `#!/usr/bin/python3`
- Python environments generally don't mix
  - conda envs
  - Virtualenvs
  - Native python

General Python Guidelines

- Avoid mixing virtualenvs and python extension env modules
  - Environment module changes generally conflict with virtualenvs
  - Use venv python in script shebang lines
  - eg: `#!/path/to/your/venv/bin/python3`
- Use care with `pip install --user` ...
  - Ensure `$PYTHONUSERBASE` is unique to python version and machine architecture.
  - `$HOME` is shared on a variety of architectures.

What about ML/DL?

```
module load python/3.7.0-anaconda3-5.3.0
conda create tensorflow-gpu \
             keras-gpu \
             ipython \
             -p ~/tf_conda_env
bsub -P stf007 -n1 -W 60 -Is $SHELL
source activate ~/tf_conda_env
jsrun … ~/tf_keras_test.py
```

```
#!/usr/bin/env python3
import tensorflow as tf
import keras
mnist = keras.datasets.mnist

(x_train, y_train),(x_test, y_test) = mnist.load_data()
x_train, x_test = x_train / 255.0, x_test / 255.0

model = keras.models.Sequential([
  keras.layers.Flatten(),
  keras.layers.Dense(512, activation=tf.nn.relu),
  keras.layers.Dropout(0.2),
  keras.layers.Dense(10, activation=tf.nn.softmax)
])
model.compile(optimizer='adam',
              loss='sparse_categorical_crossentropy',
              metrics=['accuracy'])

model.fit(x_train, y_train, epochs=5)
model.evaluate(x_test, y_test)
```

Matplotlib Backends

- Matplotlib backends
  - In scripts:
    ```
    import matplotlib
    matplotlib.use('tkagg')  # not case sensitive
    import matplotlib.pyplot as plt
    ```
  - Globally:
    ```
    cat ~.matplotlib/matplotlibrc
    backend : tkAgg
    ```

Changes to python code not being honored?

- Python compiles source to bytecode caches at runtime
  - Files/dirs such as `__pycache__`, `*.pyc`, `*.pyo`
- Old bytecode may be used if source changes undetected
- Solution: `export PYTHONDONTWRITEBYTECODE=1`
  - Useful when actively developing python code
  - Lesser performance, not recommended for production runs

Python Resources

- Venv/Virtualenv
  - venv (py3): https://docs.python.org/3.6/library/venv.html
  - virtualenv (py2): https://virtualenv.pypa.io/en/stable/
- Anaconda Documentation
  - conda: https://conda.io/docs/user-guide/getting-started.html
  - Installing your own: https://conda.io/docs/user-guide/install/linux.html
- Check the package documentation
  - Installation procedure in package docs is often not as simple as described when applied to an HPC environment.

Conda Initial Setup

- Setup your conda config to put conda envs on NFS filesystem.
- Recommended to use `/ccs/proj/<projid>`; not `$HOME`
- Recommended to use env names that separate project and host.

```
cat $HOME/.condarc
envs_dirs:
  - /ccs/proj/<projid>/<user>/virtualenvs/<host>...
  - /ccs/home/<user>/.local/share/virtualenvs/<host>...
```

Source Installs with `pip`

- Most python packages assume use of GCC.
- Use the `--no-binary` flag to build packages from source.
  - Comma separated list of packages or `:all:`
  - Use verbose output `-vv` to identify build errors.
- Check package documentation for configuration.
- External dependency env modules must be loaded at runtime

```
module load hdf5  # sets HDF5_DIR envvar
source /path/to/venv/bin/activate
CC=gcc HDF5_MPI="ON" HDF5_VERSION=1.10.2 pip install -v --no-binary=h5py h5py
```

Setuptools and distutils Source Builds

- Allows complex builds by
  - editing `setup.cfg` (or other, see package docs)
  - passing arguments to `setup.py configure`
- Global distutils options
  - Set in your user-config (~/.pydistutils.cfg)
  - or a temporary (preferred) site-config using `setup.py setopt` or `setup.py saveopt`
  - https://setuptools.readthedocs.io/en/latest/setuptools.html#configuration-file-options
- See `setup.py --help-commands` for build steps

Setuptools and distutils Source Builds

```
module load hdf5
. /path/to/venv/bin/activate
python setup.py configure --hdf5=$HDF5_DIR
python setup.py configure --hdf5-version=1.10.2
python setup.py configure --mpi
python setup.py install
```

Conda source builds

- Try to use conda first w/ alternate channels
  - https://conda.io/docs/user-guide/tasks/manage-pkgs.html
- Can use pip or setuptools to install PyPI packages as normal with venv
  - This doesn't use libraries provided by pre-built conda packages
- Use `conda-build` to make your own "portable" conda packages from recipes.
  - More complex; bundles dependencies into a pre-built collection for distribution, nominally from anaconda channels.
  - https://conda.io/docs/user-guide/tasks/build-packages/install-conda-build.html#install-conda-build
  - https://conda.io/docs/user-guide/tutorials/build-pkgs.html