Introduction to Software and modules

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Using modules

- The Cray system uses the Modules environment management package to support dynamic modification of the user environment via *modulefiles*.
- Each *modulefile* contains all the information needed to configure the shell for a particular application.
- *modulefiles* instruct the module command to alter or set shell environment variables such as PATH, MANPATH, etc.
- Modules are useful in managing different versions of applications.
- This allows environment variables, libraries, include paths to be cleanly entered and/or removed from your software environment.

Using modules

- On the Cray XT's, all applications, libraries, compilers and tools are managed via modules
- Conflicts are detected and loads that would cause conflicts are not allowed
- There are a number of basic modules loaded by default

```
$ man module

NAME
       module - command interface to the Modules package

SYNOPSIS
       module [ switches ] [ sub-command ] [ sub-command-args ]

DESCRIPTION
       module is a user interface to the Modules package.  The Modules package
       provides for the dynamic modification of  the  user's  environment  via
       modulefiles.
```

Kraken Default modules

```
lucio@krakenpf1(XT5):~> module list
Currently Loaded Modulefiles:
  1) modules/3.1.6.5
  2) torque/2.4.14
  3) moab/5.4.3.s16991
  4) /opt/cray/xt-asyncpe/default/
modulefiles/xtpe-istanbul
  5) tgusage/3.0-r2
  6) altd/1.0
  7) DefApps
  8) xtpe-target-cnl
  9) xt-service/2.2.74
 10) xt-os/2.2.74
 11) xt-boot/2.2.74
 12) xt-lustre-ss/2.2.74_1.6.5
 13) cray/job/
1.5.5-0.1_2.0202.21413.56.7
 14) cray/csa/3.0.0-1_2.0202.21426.77.7
 15) cray/account/
1.0.0-2.0202.19482.49.18
 16) cray/projdb/1.0.0-1.0202.19483.52.1
 17) Base-opts/2.2.74
 18) pgi/11.4.0
 19) xt-libsci/10.5.02
 20) pmi/2.1.4-1.0000.8596.15.1.ss
 21) xt-mpt/5.2.3
 22) xt-pe/2.2.74
 23) xt-asyncpe/4.9
 24) PrgEnv-pgi/2.2.74
 25) cray/MySQL/5.0.64-1.0202.2899.21.1
```

JaguarPF Default modules

```
dlucio@jaguarpf-login6:~$ module list
Currently Loaded Modulefiles:
  1) modules/3.1.6
  2) DefApps
  3) torque/2.4.1b1-snap.200905191614
  4) moab/5.3.6
  5) /opt/cray/xt-asyncpe/default/
modulefiles/xtpe-istanbul
  6) cray/MySQL/5.0.64-1.0000.2342.16.1
  7) xtpe-target-cnl
  8) xt-service/2.2.73
  9) xt-os/2.2.73
 10) xt-boot/2.2.73
 11) xt-lustre-ss/2.2_1.6.5
 12) cray/job/
1.5.5-0.1_2.0202.21413.56.6
 13) cray/csa/3.0.0-1_2.0202.21426.77.6
 14) cray/account/
1.0.0-2.0202.19482.49.17
 15) cray/projdb/1.0.0-1.0202.19483.52.1
 16) Base-opts/2.2.73
 17) pgi/10.9.0
 18) xt-libsci/10.5.0
 19) pmi/1.0-1.0000.8160.39.1.ss
 20) xt-mpt/5.1.3
 21) xt-pe/2.2.73
 22) xt-asyncpe/4.9
 23) PrgEnv-pgi/2.2.73
```

Using modules

Naming convention:

```
pgi/11.4.0(default)
```

application name — version number — Default version?

Many versions for the same application

```
lucio@krakenpf1(XT5):~> module avail pgi

---------------------- /opt/modulefiles -----------------------
pgi/10.5.0           pgi/11.4.0(default) pgi/7.2.5
pgi/10.6.0           pgi/11.5.0          pgi/8.0.5
pgi/10.9.0           pgi/11.6.0          pgi/8.0.6
pgi/11.2.0           pgi/11.7.0          pgi/9.0.3
pgi/11.3.0           pgi/11.8.0          pgi/9.0.4
```

HowTo use modules

More information about how to use modules can be viewed from our websites at:

http://www.nics.tennessee.edu/user-support/general-support/modules

http://www.olcf.ornl.gov/kb_articles/using-modules/

Loading commands

`module [load|unload] <my_module>`
Loads/unloads module

`module swap <module1> <module2>`
Replaces <module1> with <module2>

```
> module swap PrgEnv-pgi PrgEnv-gnu
```

Informational commands

`module help [my_module]`
Lists available commands and usage

`module show <my_module>`
Displays the actions upon loading the module <my_module>

`module list`
Displays all currently loaded modules

`module avail <name>`
Lists all modules (beginning with name)

Module Help

Using a 3rd party hdf5/1.6.7 library example

```
> module load hdf5/1.6.7
> module help hdf5/1.6.7

----------- Module Specific Help for 'hdf5/1.6.7' -----------------

Sets up environment to use serial HDF5 1.6.7 with any compiler.
Usage:  ftn test.f90 ${HDF5_FLIB}  OR  h5fc test.f90
    or   cc test.c ${HDF5_CLIB}    OR  h5cc test.c
The hdf5 module must be reloaded if you change the PrgEnv
   or you must issue a 'module update hdf5' command.
This version is deprecated and will soon be no longer available.

> cc -o myhdf5test  h5_copy18.c ${HDF5_CLIB}
```

Module Help

Using an application like NWCHEM

```
lucio@krakenpf1(XT5):~> module help nwchem

----------- Module Specific Help for 'nwchem/6.0' -----------------

Sets up environment for NWChem 6.0
Usage:   qsub -V (PBS SCRIPT)
         aprun -n (cores) -S (cores per socket) nwchem (nwchem
options)
```

Module Help

What does the *modulefile* for NWCHEM does?

```
$ module show nwchem
-------------------------------------------------------------------
/sw/xt/modulefiles/nwchem/6.0:

module-whatis          Sets up environment for NWChem 6.0
prepend-path           PATH /sw/xt/nwchem/6.0/cnl2.2_pgi11.4.0_sockpatch/nwchem-6.0/bin/LINUX64
setenv                 NWCHEM_TOP /sw/xt/nwchem/6.0/cnl2.2_pgi11.4.0_sockpatch/nwchem-6.0
setenv                 PYTHONHOME /sw/xt/python/2.5.2/sles10.1_gnu4.3.2
setenv                 PYTHONVERSION 2.5
setenv                 SHMEM_SWAP_BACKOFF 150
setenv                 MPICH_MAX_SHORT_MSG_SIZE 30000
setenv                 MPICH_UNEX_BUFFER_SIZE 100M
setenv                 CRAY_PORTALS_USE_BLOCKING_POLL 1
setenv                 NWCHEM_NWPW_LIBRARY /lustre/scratch/proj/sw/nwchem/6.0/libraryps/
setenv                 NWCHEM_BASIS_LIBRARY /lustre/scratch/proj/sw/nwchem/6.0/basis/
setenv                 HOME_NWCHEMRC /lustre/scratch/proj/sw/nwchem/6.0
-------------------------------------------------------------------
```

Using modules

The complete list of all available modules can be viewed with the command `module avail`.

The 3rd party list of all the software on Kraken and JaguarPF, can also be viewed from our websites at:

http://www.nics.tennessee.edu/user-support/software/Kraken

http://www.olcf.ornl.gov/support/software/?nccssystems=jaguar

abinit	casino	gimp	iobuf	ncview	python	tginfo
acml	cce	git	ipm	nedit	q-espresso	tgusage
adios	cdo	glib	java-jdk	netcdf	qbox	tiff
amber	charm	globalarrays	java-jre	nose	qt	tkdiff
ambertools	cmake	globus	lammps	numericpython	r	totalview
apache-ant	cpmd	gmake	lapack	numpy	ruby	trilinos
apprentice2	craypat	gnuplot	lgdb	nwchem	scalapack	udunits
apprentice2-desktop	desmond	gptl	libart	octave	scalasca	umfpack
arpack	doxygen	grace	libsci	osmesa	scientificpython	upc
atk	emacs	grads	m4	p-netcdf	scipy	valgrind
atlas	espresso	gridftp	marmot	pacman	silo	vim
atp	fastmv	gromacs	mercurial	pango	sprng	vina
autoconf	ferret	gsissh	metis	papi	srb-client	vmd
automake	fftw	gsl	mpe2	paraview	subversion	yt
aztec	fpmpi	gtk	mpip	parmetis	sundials	
bbcp	fsplit	gv	mpt	pathscale	superlu	
blacs	gamess	hdf4	mumps	petsc	superlu_dist	
blas	gcc	hdf5	namd	pgi	swig	
boost	gdlib	hypre	nano	pgplot	szip	
cairo	gempak	imagemagick	ncl	pixman	tau	
	ghostscript	intel	nco	pspline	tg-policy	