

UF Research Computing

Environment Modules for trouble-free biocomputing

PBS Introduction

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Outline

◆ Environment Modules

- Need for speed i.e. reason for Env. Modules
- Introduction and basic use
- Module Tree
- Writing modulefiles

◆ HPC PBS with modules

- How to use modules in PBS pipelines

Environment Modules

The biggest ball of twine in...

App versions

Compilers

Dependencies

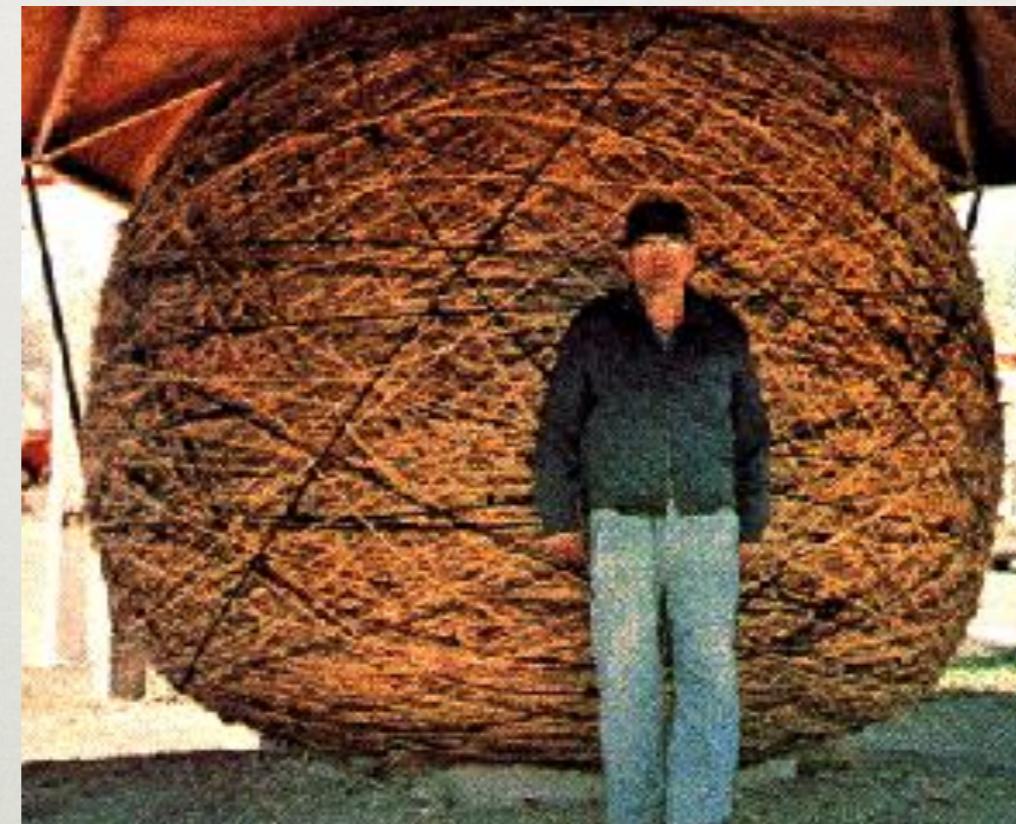
Python versions

Library versions

ENV vars

Paths

MPI implementations



The Ghost of the CLI

- Impossible to maintain many versions
- Environment setup is very complex and must be done by every user
- Things break on every upgrade
- No stable pipelines
- No way to switch Comp/MPI easily
- Hard to find the right application
- Result: the nightmare of CLI

Modules with benefits

- ◆ Users are free of the gory details
- ◆ Many application versions coexist
- ◆ Easy switching of compiler/MPI app trees
- ◆ Easy addition of dependencies
- ◆ Automated environment setup (paths, variables, licenses, etc....) and cleanup
- ◆ Powerful search and help system
- ◆ Stable pipelines

Focus on Science, not busywork

Untangle Compilers/MPIs

- ◆ mpich2_intel-1.0.8
 - ◆ mvapich2_intel-1.4.1
 - ◆ mvapich2_intel11-1.5.1
 - ◆ mvapich_intel-0.9.9
 - ◆ mvapich_intel10-0.9.9
 - ◆ openmpi_intel-1.2.7
 - ◆ openmpi_intel-1.3.4
 - ◆ openmpi_intel11-1.3.4
 - ◆ openmpi_intel11-1.4.3
- 2 Compilers
- x
- 7 MPI
implementations
- =
- Barely used beyond
the default; constant
support issues

What is a module?

- ◆ Lmod software (R. McClay, TACC)
 - <http://www.tacc.utexas.edu/tacc-projects/mclay/lmod>
- ◆ Shell environment
- ◆ Modulefiles – systemwide and user made
 - /apps/lmod/modulefiles
- ◆ Discover, evaluate, use, swap - DEUS

Module Tree

- ♦ Root of the tree - /apps/lmod/modulefiles
 - Core – does not depend on a particular Compiler/MPI combination
/apps/lmod/modulefiles/core/clustalw/2.1.lua
 - Compiler – depends on a particular compiler
/apps/lmod/modulefiles/compiler/intel/10_1/mrbayes/3.1.2.lua
 - MPI – depends on a compiler/MPI combination
/apps/lmod/modulefiles/mpi/intel10_1/openmpi_1_2/raxml/1.0.5-light.lua

Basic usage - Discover

- module spider
- module spider clu
- module spider netcdf/3.6.3
- module avail
- module avail clu (what does it find?)
- module key clu

Discover – module spider

weblogo: weblogo/3.0

generation of sequence logos

weka: weka/3.6.2

WEKA - algorithms for data mining

wgs: wgs/6.1

Celera Whole Genome Shotgun Assembler

wublast: wublast/2.0

Basic Local Alignment Search Tool - WUSTL version

Discover – module spider clu

clustalw: clustalw/2.1

Description: multiple sequence alignment software

Help: This module enables the use of the ClustalW software

Clustal is popular multiple sequence alignment software.

ClustalW produces biologically meaningful multiple sequence alignments of divergent sequences. It calculates the best match for selected sequences and lines them up, so identities, similarities, and differences can be identified.

Version 2.1

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Discover – module avail

----- /apps/lmod/modulefiles/compiler/intel/10_1 -----

amber/10	metis/4.0	mrbayes/3.1.2	openmpi/1.2.7
fftw/3.2.2	mkl/10.0	mvapich/0.9.9	openmpi/1.3.4 (default)
gromacs/4.0.7	mpich2/1.0.8	mvapich2/1.4.1	

----- /apps/lmod/modulefiles/core -----

HPC	gnuplot/4.4.3	python/2.6.4
R/2.13.1	hdf5/1.8.7	python/2.6.5
abaqus/6.9	hyphy/2.0020110824beta	python/2.7.2 (default)
add_scores/r1	hypre/2.0.0	raxml/1.0.5-light
admb/10.0	intel/10.1	raxml/7.3.0 (default)
admb/9.1 (default)	intel/11.1 (default)	repeatmasker/3.3.0
amos/3.0.0	lastz/1.02.00	rosetta/2.1.1
amos/runAmos.log (default)	lps/2.2	rosetta/2.1.2 (default)

Discover – module avail

Core:

----- /apps/lmod/modulefiles/core -----

clustalw/2.1

Compiler

----- /apps/lmod/modulefiles/compiler/intel/10_1 -----

mrbayes/3.1.2

MPI

----- /apps/lmod/modulefiles/mpi/intel10_1/openmpi_1_2 -----

amber/10 dock/64 gromacs/4.0.7 mpiblast/1.6.0 mrbayes/3.1.2 raxml/1.0.5-light

Discover – module key

- module key clu
-

The following modules match your search criteria: "clu"

clustalw: clustalw/2.1

multiple sequence alignment software

Basic usage - Evaluate

- module spider clustalw
- module whatis clustalw
- module show clustalw

Discover – module spider clustalw

clustalw: clustalw/2.1

Description: multiple sequence alignment software

Help: This module enables the use of the ClustalW software

Clustal is popular multiple sequence alignment software.

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Version 2.1

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Evaluate – module whatis clustalw

clustalw/2.1 : Name: ClustalW
clustalw/2.1 : Version: 2.1
clustalw/2.1 : Category: biology,bioinformatics,alignment
clustalw/2.1 : URL: <http://www.clustal.org/>
clustalw/2.1 : Description: multiple sequence alignment software

Evaluate – module show clustalw

Top part – like module spider clustalw

Bottom part:

```
whatis("Name: ClustalW")
```

```
whatis("Version: 2.1")
```

```
whatis("Category: biology,bioinformatics,alignment")
```

```
whatis("URL: http://www.clustal.org/")
```

```
whatis("Description: multiple sequence alignment software")
```

```
prepend_path("PATH", "/apps/clustalw/2.1/bin")
```

```
setenv("HPC_CLUSTALW_DIR", "/apps/clustalw/2.1")
```

```
setenv("HPC_CLUSTALW_BIN", "/apps/clustalw/2.1/bin")
```

```
set_alias("clustalw", "clustalw2")
```

Basic usage - Use

- module list
- module load clustalw
- module load python/2.6.5
- module add
- module del, rm, unload clustalw – pick one!
- module purge – nuclear option
- E.g. module load intel openmpi mrbayes

Use – load/unload

- module load clustalw
- module list

Currently Loaded Modules:

1) clustalw/2.1

- module unload clustalw OR module purge
- module list

Warning: No modules installed

Basic usage - Swap

- module spider mrbayes/3.1.2

This module can be loaded through the following modules:

intel/10.1, openmpi/1.2.7

intel/10.1

intel/10.1, mvapich/0.9.9

Swap – module swap

- module load intel openmpi mrbayes
- module list

Currently Loaded Modules:

1) intel/10.1 2) openmpi/1.2.7 3) mrbayes/3.1.2

- module swap openmpi mvapich

Due to MODULEPATH changes the follow modules have been reloaded:

- 1) mrbayes
- module list

Currently Loaded Modules:

1) intel/10.1 2) mvapich/0.9.9 3) mrbayes/3.1.2

Your own environment

- module list

Currently Loaded Modules:

1) intel/10.1 2) mvapich/0.9.9 3) mrbayes/3.1.2

- module setdefault mymodz1
- module listdefault

Possible defaults:

1) mymodz1 2) test1 3) pipeline2

- module getdefault mymodz1
- module list

Currently Loaded Modules:

1) intel/10.1 2) mvapich/0.9.9 3) mrbayes/3.1.2

Hands On Time

◆ Environment modules commands - module

- spider, avail
- load, add; unload
- del, rm, purge
- spider, whatis, show
- list, swap
- setdefault, listdefault, getdefault

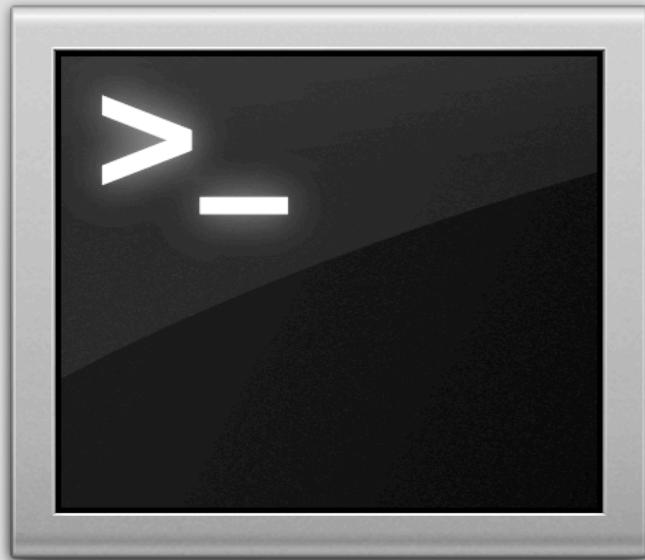
◆ E.g. module load bio

Job Scheduling and Usage

PBS

Cluster basics

Head node(s)



Login to
head
node

Scheduler



Tell the
scheduler what
you want to do

Compute
resources

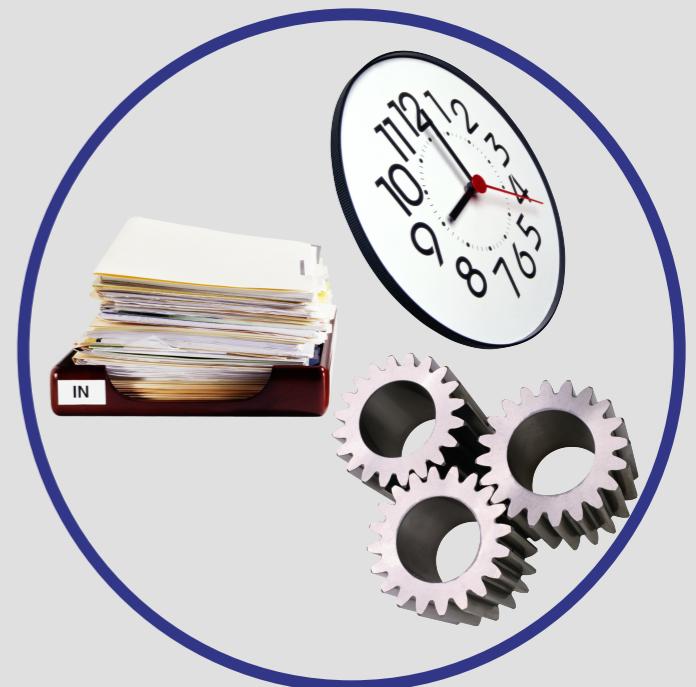


Your job
runs on the
cluster

Scheduling a job

- ♦ Need to tell scheduler what you want to do
 - Information about **how long** your job will run
 - How many **CPUs** you want and how you want them grouped
 - How much **RAM** your job will use
 - The **commands** that will be run

Scheduler



Tell the scheduler what you want to do

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♦ Ordinary Shell Script

```
#!/bin/bash  
  
pwd  
date  
hostname
```

Read the manual for
your application of
choice.

Commands typed
on the command
line can be put in a
script.

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◆ Submission Script

```
#!/bin/bash
#
#PBS -N My_Job_Name
#PBS -M Joe_Shmoef@ufl.edu
#PBS -m abe
#PBS -o My_Job_Name.log
#PBS -j oe
#PBS -l nodes=1:ppn=1
#PBS -l pmem=900mb
#PBS -l walltime=00:05:00
```

```
cd $PBS_O_WORKDIR
pwd
date
hostname
```



Scheduler



Tell the scheduler what you want to do

-l nodes=1:ppn=1

- ◆ A node is one physical computer
 - Some applications can use multiple nodes (MPI applications)
 - Others can use multiple cores as long as they are all on the same node (OpenMP, threaded, shared memory)
- ◆ **nodes=1:ppn=4** 4 cores on one node
- ◆ **nodes=2:ppn=2** 2 cores on each of 2 nodes

Node configuration

- ◆ Phase II: 2 x 2-core (4 cores/node)
 - 1316 total cores
- ◆ Phase III: 2 x 4-core (8 cores/node)
 - 872 total cores
- ◆ Phase IV: 2 x 6-core (12 cores/node)
 - 1612 total cores
- ◆ There are some additional resources, including nodes with 48 cores

-l pmem=900mb

◆ Per processor memory limit

- If your job tries to use more than this amount, it will be killed
- The scheduler reserves this amount for your job, so if you request lots more than you need you are wasting resources

Node configuration

- ◆ Phase II: 4 or 8GB (1 or 2GB / core)
 - 1316 total cores (~50% 1GB, 50% 2GB)
- ◆ Phase III: 32 or 64GB (4 or 8GB / core)
 - 872 total cores (~80% 4GB, 20% 8GB)
- ◆ Phase IV: 32GB (2.6GB / core)
 - 1612 total cores
- ◆ There are some additional resources,
including nodes with 512GB RAM

Processor equivalents

◆ Complicated formula

- Accounts for RAM usage above the per core average
- Phase IV node: 12 cores, 32GB of RAM
 - A single core job using 24GB of RAM is using ~3/4 of the resources on that node
 - It will have a PE of about 9
 - Non-investor jobs limited to 8 PEs

-l walltime=00:05:00

◆ Wall time in dd:hh:mm:ss

◆ Queues:

- long: ~10% of resources

- Investor: > 7 days (168 hrs)
 - Non-investor: > 3 days (72 hrs)

- short: ~90% of resources

◆ Keep your queue full!!!

Run a job

```
ssh <name>@submit.hpc.ufl.edu
cd /scratch/hpc/$USER
cp -r ../../galaxy/examples/blast_demo/
cd blast_demo
more BLAST.qsub
qsub BLAST.qsub
♦ Use $TMPDIR for single node jobs!
```

Job Management

- `qsub`: job submission
- `qstat`: check queue status
- `qdel`: job deletion
- `qdelmine`: delete all my jobs
- Documentation
 - http://wiki.hpc.ufl.edu/index.php/Job_Submission_Queues

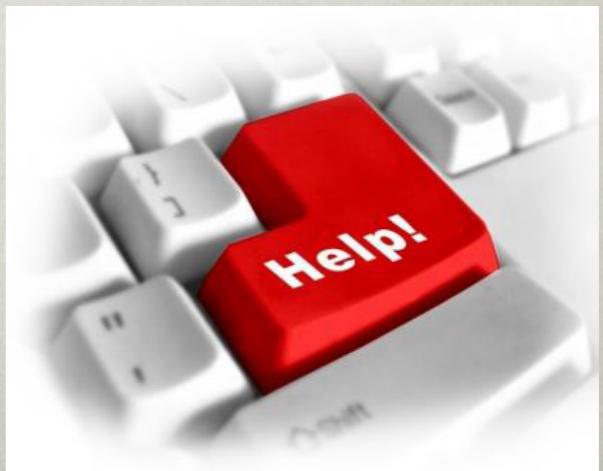
How to get help

Help!!!

How to get help

♦ Asking for help

- Support Request Tickets
 - <http://support.hpc.ufl.edu>
 - Use for everything - not just software bugs but for any questions or help requests
 - Searchable database of solutions
- When you don't have access to web
 - support@hpc.ufl.edu
 - [om@hpc.ufl.edu \(Biological Support\)](mailto:om@hpc.ufl.edu)
 - [magitz@ufl.edu \(Bio training and Q/A\)](mailto:magitz@ufl.edu)



Documentation

◆ UF HPC Encyclopedia

- <http://wiki.hpc.ufl.edu>
 - Documents on hardware and software resources
 - User guides
 - Sample submission scripts
 - Research-specific sections
- <http://hpc.ufl.edu/support>
 - Frequently Asked Questions
 - Account set up and maintenance



Training Schedule

- ✓ October 20th: Intro to UFHPC, getting started
- ✓ October 27th: Modules and basic submission scripts
- ◆ November 3rd: Galaxy overview
- ◆ November 10th: No session - Florida Genetics 2011
- ◆ November 17th: Introduction to working in Linux shell environment
- ◆ November 24th: No session – Thanksgiving
- ◆ December 1st: Working with NGS data (quality filtering, format conversion, etc.)

2011-10-27 – HPC modules

Thank
you!