Lmod Tutorial

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June 12, 2014





Introduction
Software Hierarchy
Lmod
User Inspired Features to Lmod
Lessons learned and Conclusions

Introduction

- Fundamental Issues
- Environment Modules
- Software Hierarchy
- Lmod
- Conclusions





Fundamental Issues

- Software Packages are created and updated all the time.
- Some Users need new versions for new features and bug fixes.
- Other Users need older versions for stability and continuity.
- No system can support all versions of all packages.
- User programs using pre-built C++ & Fortran libraries must link with the same compiler.
- Similarly, MPI Applications must build and link with same MPI/Compiler pairing when using prebuilt MPI libraries.





Example of Lmod: Environment Modules (I)

```
$ module avail
 ------/opt/apps/modulefiles/MPI/intel/12.0/mpich2/1.4 ----------
 petsc/3.1 (default)
                    petsc/3.1-debug
                                   pmetis/4.0
                                               tau/2.20.3
       ------ /opt/apps/modulefiles/Compiler/intel/12.0 -------
 boost/1.45.0
                      gotoblas2/1.13
                                          openmpi/1.4.3
 boost/1.46.0
                      mpich2/1.3.2
                                          openmpi/1.5.1
 boost/1.46.1 (default)
                      mpich2/1.4 (default)
                                          openmpi/1.5.3 (default)
intel/11.1
 PrgEnv
                                       papi/4.1.4
 admin/admin-1.0
                  intel/12.0 (default)
                                       scite/2.28
                  lmod/lmod
                                       tex/2010
 ddt/ddt
 dmalloc/dmalloc
                  local/local (default)
                                       unix/unix (default)
 fdepend/1.2
                  mkl/mkl
                                       visit/visit
 gcc/4.4
                  noweb/2.11b
 gcc/4.5 (default)
```





Example of Lmod: Environment Modules (II)

```
$ module list
Currently Loaded Modules:
  1) PrgEnv 2) gcc/4.5 3) mpich2/1.4 4) petsc/3.1
$ module unload gcc
Inactive Modules:
  1) mpich2 2) petsc
$ module list
Currently Loaded Modules:
  1) PrgEnv
Inactive Modules:
  1) mpich2 2) petsc
$ module load intel
Activating Modules:
  1) mpich2 2) petsc
$ module swap intel gcc
Due to MODULEPATH changes the follow modules have been reloaded:
  1) mpich2 2) petsc
```





Benefits of Modules

- Users do not need to know where software is installed
- Environment Variables to interface package can be set:
 - TACC_*PACKAGE*_LIB
 - TACC_PACKAGE_INC
 - User do not need to set hardcoded paths.
- Package required variables such as LICENSE_PATH can be set automatically.





Benefits of Lmod vs. TCL/C modules

- Lmod provides all the functionality that TCL/C Modules does.
- Directly support for Software Hierarchy.
- It reads both TCL and Lua based modulefiles.
 - Lua module files have ".lua" extension.
 - TCL module files don't.
- Users can find all modules available via module spider.
- Users can set their default set of modules via module save.





Environment Modules

- The "module" command "loads" a package.
- It adds directories to PATH or LD_LIBRARY_PATH and sets other Variables.
- "module unload package" removes all packages changes: PATH, LD_LIBRARY_PATH, unset vars.
- A module file is a text file containing shell-independent commands:
 - prepend_path("PATH","/opt/apps/git/1.8/bin")
 - setenv("TACC_GIT_DIR","/opt/apps/git/1.8")





Modules and Versions

- Modules are typically named: package/version
- For example: git/1.8
- There is a default version so:
 - "module load git" load the default version.
 - "module load git/1.8" load the 1.8 version.
- Typically a module name is a directory name and the version is a file.





Sys-admin Vs. User Control of software

- Sys-admins control what versions are default.
- Users can load newer/older versions instead of the default.
- When compilers are updated, users can switch between versions, allowing for testing.
- This is the key to a flexible system.
- Users can create their own modules for personal software.





Environment Modules History

- Paper described modules in 1991 (Furlani).
- Cray used modules on Unicos mid-1990's.
- TACC has been using modules since our 1st Cray T3E in the late 90's.





Environment Modules History (II)

- At some point Environment Modules was rewritten in a TCL/C combination.
- Another module system called CMOD: www.lysator.liu.se/cmod/ (1997-1998)
- www.modules.org: TCL/C Module files written in TCL (Late '90s - now)
- A pure TCL based module system: www.modules.org (? now)
- Lmod: Lua Based Environment Module System (2008 now) (Imod.sf.net)





How could modules possibly work?

- Child processes inherit the parents environment.
- Not the other way around.
- So how does this work?





The Trick

- The module command \$LMOD CMD reads module files
- The program outputs shell dependent text.
- Second step: evaluate shell dependent text.
- In bash:

```
- module () { eval $($LMOD_CMD bash "$0")}
```

- In csh module is an alias:
 - alias module eval '\$LMOD_CMD csh \!*'





The Trick (II)

Text output of the module command:

• modulefile "foo/1.0.lua":

Output for bash:

• Output for csh:

setenv FOO_VERSION "1.0"





Interactive Playtime: Shell Startup Debug

- This is to test your VM installs
- Use VM Imod-test, login *mclay*, password: *mclay*
 - \$ cat "export SHELL_STARTUP_DEBUG=1" > \$HOME/.init.sh
 - \$ bash -1
- This is a great help in installing Lmod and tracking startup bugs.





Software Hierarchy

- TACC used modules from www.modules.org (TCL/C) modules
- Life was good at TACC until ...
- Multiple Compilers and Multiple MPI implementations.
- Pre-built C++ & Fortran libraries must link with the same compiler
- Similarly MPI Applications must build and link with same MPI/Compiler pairing when using prebuilt MPI libraries.





Introduction Software Hierarchy Lmod

User Inspired Features to Lmod Lessons learned and Conclusions

Modulefile Choices

- Flat Naming Scheme
- Hierarchical Naming Scheme





Flat Naming Scheme: PETSc

PETSc is a parallel iterative solver package:

- Compilers: GCC 4.5, Intel 11.1
- MPI Implementations: MVAPICH 1.2, Openmpi 1.5
- MPI Solver package: PETSc 4.1
- 4 versions of PETSc: 2 Compilers × 2 MPI





Flat: PETSc

- 1. PETSc-4.1-mvapich-1.2-gcc-4.5
- 2. PETSc-4.1-mvapich-1.2-intel-11.1
- 3. PETSc-4.1-openmpi-1.5-gcc-4.5
- 4. PETSc-4.1-openmpi-1.5-intel-11.1





Problems w/ Flat naming scheme

- Users have to load modules:
 - "intel/11.1"
 - "mvapich/1.2-intel-11.1"
 - "PETSc/4.1-mvapich-1.2-intel-11.1"
 - Changing compilers means unloading all three modules
 - Reloading new compiler, MPI, PETSc modules.
 - Not loading correct modules ⇒ Mysterious Failures!
 - Onus of package compatibility on users!





Hierarchical Naming Schemes

- Store modules under one tree: /opt/apps/modulefiles
- One strategy is to use sub-directories:
 - Core: Regular packages: apps, compilers, git
 - Compiler: Packages that depend on compiler: boost, MPI
 - MPI: Packages that depend on MPI/Compiler: PETSc, TAU





MODULEPATH

- MODULEPATH is a colon separated list of directories containing directories and module files.
- No modulefiles loaded ⇒ users can only load core modules.
- Loading a compiler module adds to the MODULEPATH:
 - Users can load compiler dependent modules.
 - This includes MPI implementations modules.
- Loading an MPI module adds to the MODULEPATH:
 - Users can load MPI libraries that match the MPI/compiler pairing.





Hierarchical Examples: Core

- Generic:
 - Package: /opt/apps/package/version
 - M: /opt/apps/modulefiles
 - Modulefile: \$M/Core/package/version
- Git 1.8
 - Package: /opt/apps/git/1.8Modulefile: \$M/Core/git/1.8
- Intel compilers 11.1
 - Package: /opt/apps/intel/11.1Modulefile: \$M/Core/intel/11.1
 - Modulefile adds \$M/Compiler/intel/11.1 to MODULEPATH





Introduction Software Hierarchy

Hierarchical Examples: Compiler Dependent

- Generic:
 - Package: /opt/apps/compiler-version/package/version
 - M: /opt/apps/modulefiles
 - Modulefile: \$M/Compiler/compiler/version/package/version
- Openmpi 1.5 with gcc 4.5
 - Package: /opt/apps/gcc-4_5/openmpi/1.5
 - Modulefile: \$M/Compiler/gcc/4.5/openmpi/1.5
 - Modulefile adds \$M/MPI/gcc/4.5/openmpi/1.5 to MODULEPATH
- Openmpi 1.5 with intel 11.1
 - Package: /opt/apps/intel-11_1/openmpi/1.5
 - Modulefile: \$M/Compiler/intel/11.1/openmpi/1.5
 - Modulefile adds \$M/MPI/intel/11.1/openmpi/1.5 to MODULEPATH





Hierarchical Examples: MPI/Compiler Dependent

- PETSc 4.1 (1)
 - Package: /opt/apps/intel-11_1/openmpi-1_5/petsc/4.1
 - Modulefile: \$M/MPI/intel/11.1/openmpi/1.5/petsc/4.1
- PETSc 4.1 (2)
 - Package: /opt/apps/gcc-4_5/mvapich-1_2/petsc/4.1
 - Modulefile: \$M/MPI/gcc/4.5/mvapich/1.2/petsc/4.1





Loading the correct module

- User loads "intel/11.1" module
- Can only see/load compiler dependent packages that are built with intel 11.1 compiler.
- Can not see/load package built with other versions or other compilers.
- Similar loading "openmpi/1.5" module.
- User can only load package that are built w/ intel 11.1 and openmpi 1.5 and no others.





Better but ...

- Using TCL/C modules, Users can load correct modules by using the Software Hierarchy.
- But swapping compilers or MPI stack ⇒ complicated!
- For Parallel libraries like PETSc:
 - Users must unload PETSc, MPI, compiler
 - Reload compiler, MPI, PETSc
 - Nobody got this right!
- Solution: Yet another Environment Module System: Lmod





Lmod

- Complete Rewrite of the Environment Modules System.
- Reads TCL or Lua modulefiles.
- Based on the Lua scripting language.
- Simple yet powerful with:
 - Functions are first class objects.
 - Simplifies loading/unloading of modules.
 - Tables combine array and hash seamlessly.





Key Insight (I): MODULEPATH

- Lmod remembers the current state of MODULEPATH.
- If it changes then it unloads any modules not in current search path ⇒ inactive.
- It tries to activate any inactive modules.
- It remembers inactive modules.
- It continues to attempt to activate any inactive modules on future invocations.





Key Insight (II): MODULEPATH

- Loading gcc/4.5 and boost/1.47.1
- M=/opt/apps/modulefiles
 - Adds \$M/Compiler/gcc/4.5 to MODULEPATH.
 - Boost: \$M/Compiler/gcc/4.5/boost/1.47.1
- Unloading gcc/4.5
 - Removes \$M/Compiler/gcc/4.5 from MODULEPATH.
 - Inactivates boost/1.47.1
- Loading intel/11.1
 - Adds \$M/Compiler/intel/11.1 to MODULEPATH.
 - Activates Boost: \$M/Compiler/intel/11.1/boost/1.47.1





Other Safety Features of Lmod (I)

- Users can only load one version of a package.
- "module load xyz/2.1" loads xyz version 2.1
- "module load xyz/2.2" unloads 2.1, loads 2.2





Other Safety Features of Lmod (II)

- Lmod adds a new command in modulefiles: family("name")
- All of our compiler modules have family("compiler")
- All of our MPI modules have family("MPI")
- Users can only load one compiler or MPI at a time
- Powers users can get around this restriction.





Save/Restore

- User can setup their own initially loaded modules.
 - Users simply load, unload and/or swap until happy.
 - module save saves state in "default"
 - Our login scripts do: module restore which loads the user's default.
- Users can create other collections by:
 - module save name to save it.
 - module restore name to retrieve it.
- This used to known as setdefault/getdefault.





Lmod Module Layout

- Supports Flat layouts
- Supports Hierarchical layouts
- Naming Schemes:
 - Name/Version (e.g. bowtie/2.3)
 - Category/Name/version (e.g. bio/bowtie/2.3)
 - Category/Sub/Name/version (e.g. bio/genomics/bowtie/2.3)





For those who can't type: "ml"

- ml is a wrapper:
 - With no argument: ml means module list
 - With a module name: ml foo means module load foo.
 - With a module command: ml spider means module spider.
- See ml --help for more documentation.





Interactive Playtime: Lmod example

- Use VM Imod-test, login mclay, password: mclay
 - \$ module load gcc mpich parmetis
 - \$ module list
 - \$ module avail
 - \$ module swap gcc clang
 - \$ module spider
 - \$ module spider parmetis/4.0.3





Interactive Playtime: Lmod example (II)

```
$ ml purge
$ ml gcc mpich parmetis
$ ml
$ ml -gcc clang
$ ml spider
$ ml spider parmetis/4.0.3
```





Searching for Modules

- Three ways to search for modules:
 - "module avail"
 - "module spider"
 - "module keyword"
- The "avail" command reports all "loadable" modules.
- The "spider" command reports all "possible" modules.
- The "keyword" command reports all "possible" modules that match keywords.
- What is the difference?





Module avail

- "avail" only reports modules that are loadable w/ current MPI/Compiler pairing.
- A parallel library may not be built for all possible pairings.
- Won't always show with avail.
- Not all package can be build or work with all compiler/MPI suites.





Module spider

- Reports all modules for given MODULEPATH.
- It recursively searches the tree to find all branches.
- Large systems of modules save a cache file that is saved for a day.
- Three modes:
 - module spider all possible modules no detail.
 - module spider petsc all versions of petsc, no detail.
 - module spider petsc/3.1 details.





Module keyword key1 key2 ...

• Modules can have a "whatis" description:

```
whatis("Name: Abyss")
whatis("Version: 1.2.7")
whatis("Category: computational biology, genomics")
whatis("Keywords: compbio, genomics")
whatis("URL:http://www.bcgsc.ca/platform/bioinfo/software/abyss")
whatis("Description: Assembly By Short Sequences.")
```

 module keyword key1 ... will report all modules with any of the key's.





Generic Modulefile support

- Lmod support several functions to help with generic modulefiles:
 - myModuleName() ⇒ boost, bio/bowtie
 - myModuleVersion() \Rightarrow 1.47.0
 - myModuleFullName() \Rightarrow boost/1.47.0





Generic Modulefile support: hierarchyA()

Extracting the hierarchy based on location: mpich/3.1.lua

```
local pkgName = myModuleFullName()
local hierA = hierarchyA(pkgName,1)
local comp = hierA[1]
local compDir = comp:gsub("/","-"):gsub("%.","_")
local base = pathJoin("/opt/apps", compDir, pkgName)
prepend_path("PATH", pathJoin(base,"bin"))
```

• If you use a different layout, you can provide similar functions in "SitePackage.lua"





Interactive Playtime: Generic Modulefiles

- Lets look at one way to support Generic Modulefiles:
 - \$ cd /opt/apps/modulefiles/Core; more gcc/4.8.lua
 - \$ cd ../Compiler/
 - \$ ls -R *
 - \$ cd .base/mpich/
 - \$ look at 3.1.lua
 - \$ cd ../../MPI/.base/parmetis
 - \$ look at 4.0.3.lua





Installation Overview

- Chose a place for module tree: "/opt/apps/modulefiles"
- Use configure to override default.
- Install lua and Lmod applications.
- Place module command in system shell startup.
- Possibly modify bash's startup procedure.
- Design a default set of modules for your users.





Installing Lmod (I)

- Download files from Imod.sf.net
 - lua-x.y.z.tar.gz
 - Imod-x.y.z.tar.gz
- Assume all "optional" packages are in "/opt/apps/"
- Install lua in "/opt/apps/lua/x.y.z"
- "\$ ln -s x.y.z /opt/apps/lua/lua"
- This way "/opt/apps/lua/lua/bin/lua" always points to lua independent of version.





Installing Lmod (II)

- Install Lmod in "/opt/apps/lmod/x.y.z"
- "make install" creates a symlink from "x.y.z" to lmod.
- This way "/opt/apps/lmod/lmod/..." always points to the latest Imod.





Integrating Lmod into User's Shell (I)

We must add the module alias for all user's shells by either link or copy:

- \$ ln -s /opt/apps/lmod/lmod/init/profile /etc/profile.d/z00_lmod.sh
- \$ ln -s /opt/apps/lmod/lmod/init/cshrc /etc/profile.d/z00_lmod.csh
- You may have to create "/etc/profile.d" first.





Bash Shell startup files

| | System | User |
|-----------------|--------------|---|
| login | /etc/profile | \sim /.bash_profile $\parallel \sim$ /.profile, |
| interactive | /etc/bashrc* | \sim /.bashrc |
| non-interactive | \$BASH_ENV | |

* Not always built-in! \$BASH_ENV points to a file which is run on non-interactive shells.





Csh Shell startup files

| | System | User |
|-----------------|---------------------------------|---------------------------------|
| login | /etc/csh.cshrc & /etc/csh.login | \sim /.cshrc & \sim /.login |
| interactive | /etc/csh.cshrc | \sim /.cshrc |
| non-interactive | /etc/csh.cshrc | \sim /.cshrc |





Linux /etc/profile

```
if [ -d /etc/profile.d ]; then
  for i in /etc/profile.d/*.sh; do
    if [ -r $i ]; then
        . $i
    fi
    done
fi
```





Linux /etc/bashrc

```
if ! shopt -q login_shell; then
  if [ -d /etc/profile.d ]; then
    for i in /etc/profile.d/*.sh; do
    if [ -r $i ]; then
        . $i
    fi
    done
  fi
fi
```





Linux /etc/csh.cshrc

```
if ( -d /etc/profile.d ) then
  set nonomatch
  foreach i ( /etc/profile.d/*.csh )
     if (-r $i) then
       if ($?prompt) then
         source $i
       else
         source $i >& /dev/null
       endif
    endif
  end
endif
```





Rebuilding Bash to use /etc/bashrc on non-login shells

- By default bash does not read /etc/bashrc (or similar)
- Debian and Ubuntu read /etc/bash.bashrc on interactive non-login shells.
- Red Hat, Centos, Mac OS X, don't read /etc/bashrc
- At TACC, we rebuilt bash so that it does read /etc/bashrc
- You must patch config-top.h to change bash's behavior.





Rebuilding Bash Benefits

- We want bash interactive non-login shells to behave the same as login shells.
- Fortran 90 program typically need "ulimit -s unlimited"
- MPI invokes an interactive non-login, non-prompt shell on every node.
- bash users were not getting "ulimit -s unlimited" from system /etc/profile.d/*.sh
- By rebuilding Bash we guarantee that MPI jobs source /etc/profile.d/*.sh
- We control what goes into /etc/tacc/{profile,bashrc}





Loading Default Modules

- At TACC, all users get a default set of module loaded at startup.
- In "/etc/profile.d/z96_login_modules.sh:" export LMOD_SYSTEM_DEFAULT_MODULES=TACC module --initial_load restore
- Most users get the "TACC" set of modules
- We load standard tools, a compiler, and an MPI implementation.
- Users can replace the default via "module save"





Modules and Package Management at TACC

- All of the "optional" software: compilers, MPI Stacks, Libraries, and Applications are installed via the RPM package manager.
- We create our optional RPMs with both the software and the module files.
- Uninstalling a package removes both the software and the module that access it.
- We use a single parameterized RPM spec file to build all compiler/MPI pairings.





Management of Modules

- Encourage users to use modules with their own software.
- Check modulefile syntax errors by running: module spider
- Use prereq("foo", "bar") instead of load("foo", "bar")
- Use family("compiler") and similar in your compiler and MPI module files.





Deploying Lmod

- Lmod can be tested even though your site runs TCL/C modules.
- Make sure that Lua and lua-posix and lua-filesytem are installed
- Otherwise install lua-5.1.4.8.tar.gz from lmod.sf.net
- Install Lua, Install Lmod in your account.





Deploying Lmod: Personal startup

```
if [ -z "$LMOD CMD" ]: then
  CURRENT MPATH=$MODULEPATH
  module purge 2> /dev/null
                                        # purge using old cmd
  LMOD_PKG=$HOME/pkg/lmod/lmod
  LMOD CMD=$LMOD PKG/libexec/lmod
  export BASH_ENV=$LMOD_PKG/init/bash
  . $BASH ENV
                                        # redefine module cmd
  export LMOD_SYSTEM_DEFAULT_MODULES=...
  MODULEPATH=$CURRENT_MPATH
  module --initial_load restore
fi
```





Opt-in Testing

```
    You and others can then opt-in
        if [ -d $HOME/.lmod.d ]; then
        # Use Lmod for Modules
        ...
        else
        # Use TCL/C modules
        ...
        fi
```





Opt-out deployment

• When read to deploy to users do:

```
if [ ! -f $HOME/.no.lmod ]; then
  # Use Lmod for Modules
   ...
else
  # Use TCL/C modules
   ...
fi
```





Module usage

- It is possible to record module usage:
 - Record modules loaded at logout time and/or job submission.
 - Find out what modules are not or under used. ⇒ removal or upgrade.
 - Suggest to users of one module to consider using another module
- Use "load" hook to record every loaded module via SitePackage.lua





HPC issues: Root

- Root should not define the module command or load a default set of modules during shell startup.
- No non-local path should automatically ever be in root's path.
- What if /opt/apps/ is unavailable?





HPC issues: Startup Files and Compute nodes

- At TACC: the environment variable: ENVIRONMENT is "BATCH" when on a compute node.
- When in BATCH mode:
 - The module command is defined.
 - The TACC module is NOT loaded.
 - The user's environment is passed to all processes.
 - Mvapich2: mpirun_rsh ... Var1=V1 Var2=V2 ...
 - Where Var1 ... are env. vars such as \$HOME, \$PATH ...
- This prevents every node from a users parallel job from doing "opendir("/opt/apps/modulefile/Core")"





HPC issues: Users

- Users can overwork the parallel file system.
- Encourage your users to use module save
- Or users should load their modules via ~/.bashrc or ~/.cshrc but wrap them:

```
if [ -z $_READ -a -z $ENVIRONMENT ]; then
  export _READ=1 # Put any module commands here:
  module load git
fi
```

 Otherwise each node of a user's 8192 process job will try to load modules ⇒ Parallel file system metadata servers can hang.





Version Sorting

- TCL/C module and older Lmod sorted alphabetically:
- intel/9.0 "was" newer than intel/10.0 \Rightarrow Yuck!
- Python has a clever scheme. I've re-implemented it in Lua.
- Lmod 4.1+ uses version sorting:

```
2.4dev1: 00002.00004.*@.00001.*zfinal
2.4a1: 00002.00004.*a.00001.*zfinal
2.4rc1: 00002.00004.*c.00001.*zfinal
```

2.4: 00002.00004.*zfinal

2.4-1: 00002.00004.*zfinal-.00001.*zfinal

2.4.1: 00002.00004.00001.*zfinal 3.2-static: 00003.00002.*static.*zfinal

3.2: 00003.00002.*zfinal





Load/Prereq modify functions

• In Lua modulefiles you can now do:

```
load(atleast("F00","2.3"))
load(between("BAR","7.1","10.1"))
load(latest("BAZ"))
prereg(atleast("boost","1.47.0"))
```

• I'm thinking about similar modify functions for conflict()





Module Proprieties (I)

- Modules can have properties
- At TACC, we have MIC, and GPU accelerators.
- Some libraries are MIC aware.

```
add_property("arch","mic")
```

• This is controlled by the table in Imodrc.lua





Module Properties (II)

- Some modules will be "MIC" aware: mkl, fftw3, phdf5, ...
- Lmod will decorate these modules:

```
1) unix/unix 3) ddt/ddt 5) mpich2/1.5 7) phdf5/1.8.9 (m)
2) intel/13.0 4) mkl/mkl (*) 6) petsc/3.2 8) PrgEnv

Where:
(m): module is build natively for MIC
(*): module is build natively for MIC and offload to the MIC

-----
add_property("arch", "mic") --> phdf5
add_property("arch", "mic:offload") --> mkl
```

• What properties would you like to support?





Module Properties (III): Sticky

- A module can be sticky.
- It requires "--force" to unload or purge.
 add_property("lmod", "sticky")





pushenv

- Suppose you'd like to set CC in the environment.
- setenv won't work.
- pushenv will!

• pushenv keeps an private env vars: __LMOD_STACK_NAME





always_load and always_unload

- The load() function is reversed on unload.
- The always_load() function is a no-op on unload.
- Still you may want:

```
if (not isloaded("F00")) then always_load("F00") end
```

• Which is only slightly better than:

```
if (not isloaded("F00") and mode()== "load") then
  load("F00")
end
```





prepend_path() takes priorities

• When you need to push a path to the front of the line do:

- This is great for wrapper scripts:
- "Do not use mpirun on login nodes"
- Works for append_path() as well.
- Drives paths to be last.





SitePackage.lua: Customize Behavior for your Site

- Use StandardPackage.lua as a guide for your SitePackage.lua
- Many examples of SitePackage.lua in contrib/* directories





Load hook





settarg

- Provides safety, flexibility and repeatability in a dynamic environment.
- Dynamically updates the state when modules change:

```
$ env | grep '^TARG'
TARG_BUILD_SCENARIO=dbg
TARG=OBJ/_x86_64_dbg_gcc-4.6_mpich-3.0
TARG_MPI_FAMILY=mpich
TARG_MPI=mpich-3.0
$ module swap mpich openmpi; opt; env | grep '^TARG'
TARG_BUILD_SCENARIO=opt
TARG=OBJ/_x86_64_opt_gcc-4.6_openmpi-1.6
TARG_MPI=openmpi-1.6
TARG_MPI_FAMILY=openmpi
```





settarg (II)

- Typically TARG is OBJ/\$ARCH_\$SCENARIO_\$CMPLR_\$MPI
- TARG=OBJ/_x86_64_dbg_gcc-4.6_mpich-3.0
- User can extend this with user level or directory level specialization.
- OBJ/_x86_64_dbg_intel-14.0_mpich-3.0_petsc-3.4
- A makefile can modified to write generated file into \$TARG.
- Never need to "make clobber" when switching scenario, compiler, etc.





Interactive Playtime: settarg

```
$ ml
$ cd ~/w/hello
$ ml clang mpich
$ make; mpirun -n 2 hello
$ ml -clang gcc
$ make; mpirun -n 2 hello
$ dbg
$ make; mpirun -n 2 hello
$ opt
$ make; mpirun -n 2 hello
$ cd OBJ
```





Spider Cache Advantages

- The spider cache speeds up avail and spider greatly.
- All system modulefiles have been read, properties determined.
- Lua is quite fast and reading and interpreting a single file.
- This is preferable to walking the directory tree and reading every module.
- Why is every module file read: properties.





Spider Cache Disadvantages

- There is only one: Keeping it up-to-date.
- If Lmod sees a valid cache file it assumes it is correct.
- Otherwise what's the point.
- Currently loads bypass cache but avail and spider depend on it.
- Personal modules are not effected by system cache foo.





Spider Cache Implementation

- There is a cache directory
- A time stamp file that marks the last update date.
- You can have 1 or more of these pairs.





Spider Cache Building Strategies

- Common tool to install (like losf)
 - Use it to rebuild the cache when necessary
- Using rpm or dpkg or similar to install software:
 - Wrap rpm or dpkg to update the time-stamp file
 - A cron job to rebuild the cache when necessary
- Others?





Inherit

- Imagine you are developer of a parallel library
- You are on a system deploying a software hierarchy
- How to take advantage of the system supplied layout?





Inherit (II)

- Create a personal hierarchy for each compiler and MPI stack you want to test against.
- Then copy each system compiler and MPI modulefile into your personal hierarchy.
- Then add a prepend_path("MODULEPATH",...) at the end.





Inherit Compiler Module

- Or you can "inherit" the same named module in the hierarchy.
- For a compiler modulefile it can be:

• Using \$MY_MODULE_ROOT/Compiler/C/CV





Inherit MPI Module

- Or you can "inherit" the same named module in the hierarchy.
- For a compiler modulefile it can be:

• Using \$MY_MODULE_ROOT/Compiler/C/CV/M/MV





Lessons Learned

- A very small percentage of Lmod users join the mailing list.
- Able support many requests for features but not all.
- Hardening:
 - sandbox for evaluating modulefiles
 - Checking argument types
 - checkModuleSyntax script
- Users sometimes ask the right question.
- Lmod is much better product because of its wider use.





Lessons Learned (II)

- It is hard work developing a users' communities trust.
- Some site will be managed in a way that I have never dreamed of.
- I struggle with mistakes in design that I have to live with:
 - is_spider ⇒ mode()
 - set_default, get_default ⇒ save, restore
 - duplicate paths
- Deprecating features is difficult with Lmod.
- Users would get deprecated feature reports that sys-admins must fix.





Regression Testing of Lmod

- A suite of 60+ tests each with many steps.
- No release without passing all those tests.
- These tests make Lmod re-factoring much easier.
- The github repo is generally safe.





Remote Debugging

- No software over ten lines is bug free.
- Lmod is no exception.
- Bug reports are as easy as:
 - module --config 2> config.log
 - module -D avail 2> avail.log
- Sometimes I'll create test versions with more debugging for you to test.





Recommendations for Good Site Management

- A module purge should not break things.
- Set LMOD_SYSTEM_DEFAULT_MODULES so that module restore works.
- Encourage the use of "module save" so that users can have a
 default set of modules.
- Use the family directive to protect users.
- Consider the use of "checkModuleSyntax" before installing new modules.





Follow on projects from Lmod: Lariat

- At TACC, we want to know what packages and libraries are user use.
- All parallel jobs at TACC use the script "ibrun".
- Lariat adds two tools to ibrun.
 - checkExec
 - parseLDD





CheckExec

- At TACC, your build environment and your submit environment must match.
- checkExec does an Idd of your executable looking for particular MPI libraries.
- It then uses the "reverse map" to map MPI library to MPI module and compiler module.
- It also extract your current environment to see if they match.
- It generates a warning if they don't.





ParseLDD

- The program parseLDD also does an Idd of your executable.
- It checks to see if the executable or the any of the shared libraries are TACC built modules.
- It records information for later analysis.





Lariat + ALTD \Rightarrow XALT

- Mark Fahey developed ALTD which records similar information.
- Mark and I won an NSF Grant to create XALT.
- Alpha users soon, Beta users summer of 2014.





Future Plans

- Make Lmod available as rpm and debian packages.
- How to deal with libraries and applications that do not fit neatly into the hierarchy.
- libmesh http://libmesh.sourceforge.net/
 - is a framework for solving 1D, 2D, 3D grid in parallel with support for AMR.
 - It depends on boost, petsc, trilinos, grvy, ...
 - If you are a developer how do you test it against multiple version of boost, petsc, etc.
 - I'm still thinking about how to handle this "Matrix" dependency.





Introduction Software Hierarchy Lmod User Inspired Features to Lmod Lessons learned and Conclusions

Conclusions

- Download source from: Imod.sourceforge.net (Imod.sf.net)
- Github repo: https://github.com/TACC/Imod.git
- Documentation: www.tacc.utexas.edu/tacc-projects/Imod
- Mailing list: Imod-users@lists.sourceforge.net





Projects to work on here

- Install lua-5.1.4.8.tgz in the mclay account.
- Install Lmod in mclay account
- Use your personal version of Lmod.
- Create Personal modules.
- Generic Module file discussion.
- Talk about Software install issues at your site.



