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Lmod is a tool for managing software packages within a shared high-performance computing environment (e.g. the ACCRE cluster). If you started using ACCRE in Winter 2017 or earlier, you can think of Lmod as a replacement for setpkgs and pkginfo. Lmod is designed to intelligently manage, negotiate, and enforce the complex dependencies between software packages and libraries in a HPC environment. This should lead to better usability of administrator-installed software packages and prevent conflicts between lower-level libraries that many packages depend on. Starting in Spring 2017, Lmod will be available for testing and general use in parallel with setpkgs and pkginfo. As the ACCRE operating system is upgraded to CentOS 7 in Summer and Fall 2017, only Lmod will be available in the new CentOS 7 environment.

- For instructions on basic Lmod usage, please start with the excellent and concise User Guide for Lmod.
- A detailed overview of using Lmod on the ACCRE cluster is also available here: Lmod Slide Deck
- There are a handful of things you must get accustomed to when transitioning from setpkgs/pkginfo to Lmod:

1 Searching for available packages

When searching for available packages, Lmod will only show you those packages that were built with a lower-level dependency (most often a compiler) that is already loaded. This means that the first time you run module avail (the equivalent of pkginfo), you will only see a handful of packages available. However, as you load packages via Lmod, additional packages will be listed when you run module avail again. For example:

\$ module avail

Anaconda2/4.3.1 IMPUTE2/2.3.2_x86_64_static
Anaconda3/4.3.1 Intel/2016.3.210-GCC-5.4.0-2.26
GCC/5.4.0-2.26 Java/1.8.0 92

Use "module spider" to find all possible modules.

```
Use "module keyword key1 key2 ..." to search for all
possible modules matching any of the "keys".
$ module load GCC/5.4.0-2.26
$ module avail
----- Applications built with GCC 5.4.0-2.26 -----
  OpenBLAS/0.2.18-LAPACK-3.6.1
  OpenMPI/1.10.3
  Perl/5.24.0
  Ruby/2.3.1
  SQLite/3.13.0
  Tc1/8.6.5
  VCFtools/0.1.14-Perl-5.24.0
----- Applications built with GCCcore 5.4.0 -----
  CMake/3.5.2
----- Core Modules -----
  Anaconda2/4.3.1 IMPUTE2/2.3.2_x86_64_static
Anaconda3/4.3.1 Intel/2016.3.210-GCC-5.4.0-2
                        Intel/2016.3.210-GCC-5.4.0-2.26
  GCC/5.4.0-2.26 (L) Java/1.8.0 92
 Where:
  L: Module is loaded
Use "module spider" to find all possible modules.
```

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

Note that additional packages are now listed under the Applications built with GCC 5.4.0-2.26 section, and can now be loaded with the module load command.

2 Searching for all installed packages

Because not all packages are shown by default, you should familiarize yourself with the module spider and module keyword commands in order to check for installed packages. For example, if you want to run R on the cluster:

| \$ | module | spider | R | | | | |
|----|--------|--------|---|------|------|------|------|
| _ | R: | | | | | | |

```
Description:
     R is a free software environment for statistical
     computing and graphics. - Homepage:
     http://www.r-project.org/
    Versions:
       R/3.2.3
    Other possible modules matches:
       GCCcore PROJ Perl Ruby Valgrind cURL ...
-----
 To find other possible module matches do:
     module -r spider '.*R.*'
_____
 For detailed information about a specific "R" module (including
 how to load the modules) use the module's full name.
 For example:
    $ module spider R/3.2.3
_____
Lmod provides a helpful suggestion for the full name of the package, which must
include the version, so let's try that:
$ module spider R/3.2.3
 R: R/3.2.3
   Description:
     R is a free software environment for statistical
     computing and graphics. - Homepage:
     http://www.r-project.org/
    Other possible modules matches:
       GCCcore, PROJ, Perl, Ruby, Valgrind, ...
   You will need to load all module(s) on any one of the
   lines below before the "R/3.2.3" module is available to load.
     GCC/5.4.0-2.26 OpenMPI/1.10.3
     Intel/2016.3.210-GCC-5.4.0-2.26 IntelMPI/5.1.3.181
   Help:
     R is a free software environment for statistical
```

```
To find other possible module matches do:
module -r spider '.*R/3.2.3.*'
```

Excellent! Lmod gives us the exact commands to run before we can load the R/3.2.3 package. Notice you have two options: the GCC-compiled version, or the Intel-compiled version. Either is fine. Intel-compiled packages tend to run a bit faster on our Intel processors, however GCC-compiled software tends to be better supported and more widely tested. In this case, let's load the GCC-compiled version of R 3.2.3. In order to do this, simply type:

\$ module load GCC/5.4.0-2.26 OpenMPI/1.10.3 R/3.2.3

Or (see point 4 below for details on default versions of packages):

\$ module load GCC OpenMPI R

To verify that you have the correct version of R loaded type:

\$ R --version

R version 3.2.3 (2015-12-10) -- "Wooden Christmas-Tree" Copyright (C) 2015 The R Foundation for Statistical Computing Platform: x86_64-pc-linux-gnu (64-bit)

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The module keyword command is also useful for getting information about available packages. For instance, if you want to see information about MPI versions available on the cluster:

\$ module keyword MPI

The following modules match your search criteria: "MPI"

GCC: GCC/5.4.0-2.26

The GNU Compiler Collection includes front ends for C, C++, Objective-C, Fortran, Java, and Ada, as well as libraries for these languages (libstdc++, libgcj,...). - Homepage: http://gcc.gnu.org/

Intel: Intel/2016.3.210-GCC-5.4.0-2.26
 Intel Cluster Toolkit Compiler Edition provides

```
Intel C,C++ and fortran compilers, Intel MPI and
    Intel MKL - Homepage:
  http://software.intel.com/en-us/intel-cluster-toolkit-compiler/
  IntelMPI: IntelMPI/5.1.3.181
    The Intel(R) MPI Library for Linux* OS is a
   multi-fabric message passing library based on ANL
   MPICH2 and OSU MVAPICH2. The Intel MPI Library for
   Linux OS implements the Message Passing Interface,
    version 2 (MPI-2) specification. - Homepage:
    http://software.intel.com/en-us/intel-mpi-library/
  OpenMPI: OpenMPI/1.10.3
    The Open MPI Project is an open source MPI-2
    implementation. - Homepage:
   http://www.open-mpi.org/
To learn more about a package enter:
   $ module spider Foo
where "Foo" is the name of a module
```

To find detailed information about a particular package you must enter the version if there is more than one version:

```
$ module spider Foo/11.1
```

The module keyword command ignores case and also supports regular expressions for filtering your searches (the same is true of the module spider command).

3 Autocompletion

Lmod supports tab autocompletion, so in order to load a package you can type module load followed by the first few letters of a package name and the <tab> key.

4 Version precedence

In the event that multiple versions of a software package are available, the default version will be noted with a (D). If you exclude the version information (e.g. module load GCC), the default version (or the only version if only a single version exists) of the software will be loaded.

5 List loaded packages

Use module list to see what packages are currently loaded in your environment:

```
# module list
No modules loaded

$ module load GCC
$ module list

Currently Loaded Modules:
   1) GCCcore/.5.4.0    3) GCC/5.4.0-2.26
   2) binutils/.2.26
```

Notice that more packages than just the GCC module were loaded. This is not unusual, so if you care about the low-level dependencies of your program it's a good idea to run module list to check.

6 Unloading specific packages

Use module unload to remove a package from your environment. For example:

```
$ module load GCC/5.4.0-2.26
$ module list

Currently Loaded Modules:
   1) GCCcore/.5.4.0   2) binutils/.2.26   3) GCC/5.4.0-2.26
$ module unload GCC/5.4.0-2.26
$ module list
No modules loaded
```

Occasionally (although not in the above example), a package's dependencies will not be removed from your environment after unloading the package via module unload. However, Lmod will remove those dependencies if they cause conflicts in a subsequent module load command.

7 Unloading all packages

Use module purge to remove all packages from your environment. For example:

```
$ module load GCC/5.4.0-2.26
```

- \$ module load OpenMPI/1.10.3
- \$ module list

Currently Loaded Modules:

- 1) GCCcore/.5.4.0 3) GCC/5.4.0-2.26
 - 5) hwloc/.1.11.3
- 2) binutils/.2.26 4) numactl/.2.0.11 6) OpenMPI/1.10.3

\$ module purge

\$ module list

No modules loaded