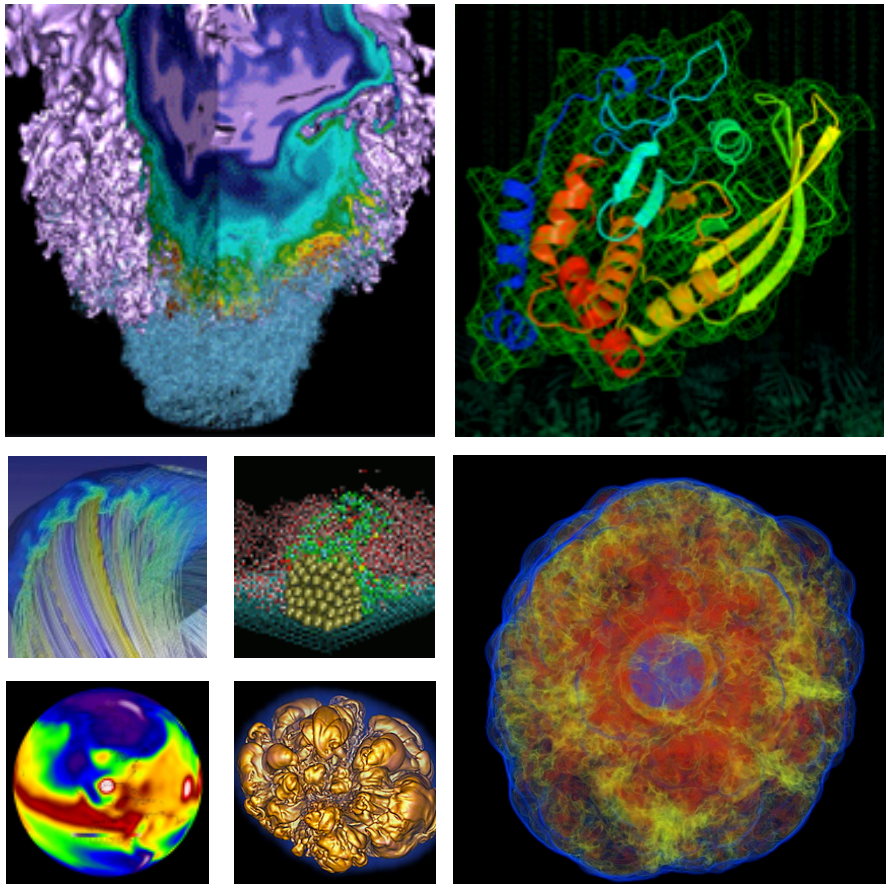
JGI Modules Tutorial



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https://bitbucket.org/TWildish/jgi-modules-tutorial.git

Introduction

- What's a module?
- Why should you use them
- Why shouldn't you use them
- Module structure
- How to build a simple module
- How to build a more complex module
- Best practices
- Exercises

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Pre-requisites

- **I assume you know basic module use:**
  - module load
  - module unload
  - module avail
  - module swap

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What's a module?

- **A module is a way of *using* software**
  - It sets up the runtime environment for installed software
    - Essentially it just sets/unsets environment variables:
    - $PATH, $LD_LIBRARY_PATH, $MANPATH, $PKG_CONFIG_PATH, $PERL5LIB, $PYTHONPATH, any others you may want
  - It allows specifying and enforcing dependencies
    - Modules X can't load without module Y etc
  - It allows specifying multiple versions of a piece of software
    - Module XYZ/1.0, XYZ/1.2, XYZ/2.0…
  - It doesn't describe how the software was built
  - It doesn't describe how the software was installed
  - it's not a version control system

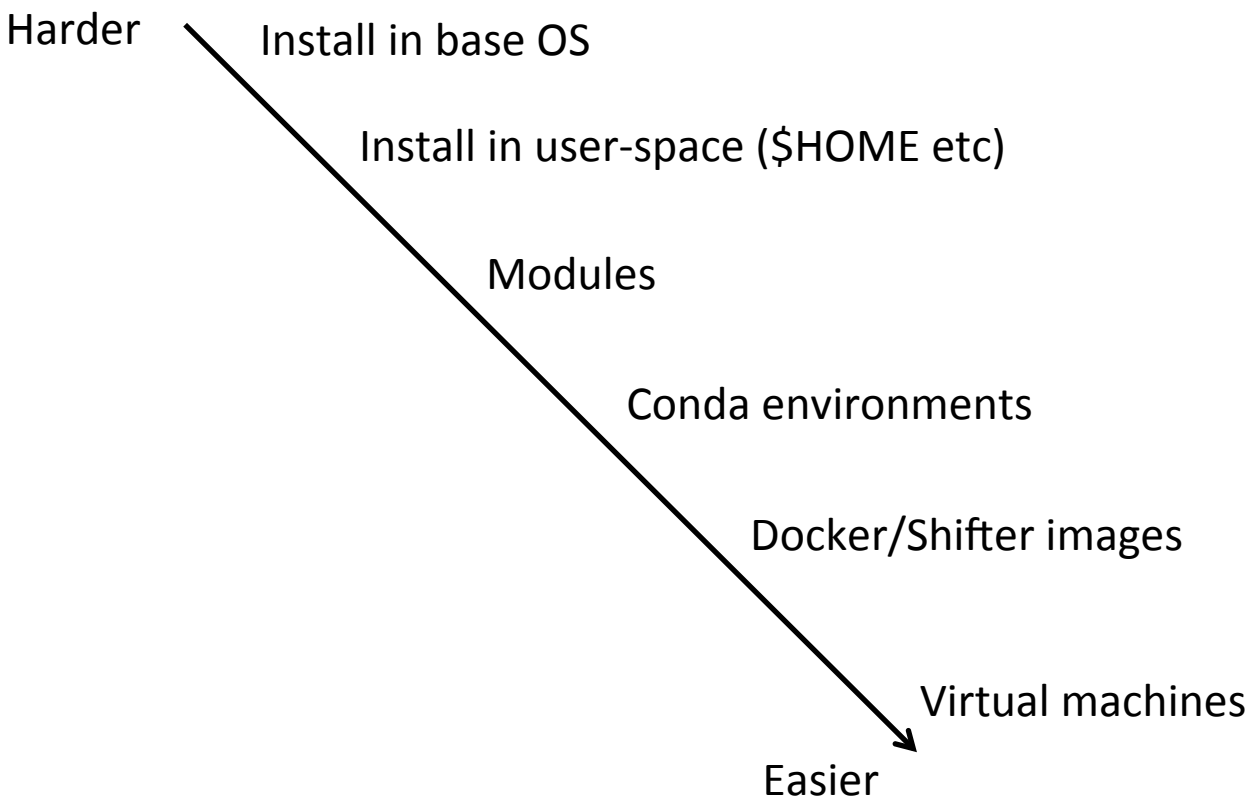
Why should you use modules?

- **Reproducibility**
  - Guarantee that your runtime environment is controlled properly
- **Flexibility**
  - Use several applications, that are built/maintained separately, in a coherent manner
- **Simplicity**
  - Module files are easy to create

Why shouldn't you use modules?

- **Reproducibility**
  - Software may be tied to the system it's built on, may not be easily portable
- **Flexibility**
  - Software that has conflicting requirements is harder to manage with modules than by other means
- **Simplicity**
  - You still have to build and install the software yourself

Portability, Flexibility



Module structure

- **To use modules you need:**
  - A directory, added to your **$MODULEPATH** (see later)
  - Subdirectories for each package
  - Version-specific *modulefiles* in each package subdirectory

- **E.g. on Denovo:**
  - **$MODULEPATH** contains **/usr/common/jgi/Modules/modulefiles**, which contains, among others: **falcon/1.8.8**

```
denovo1> module avail falcon
--------------------------- /usr/common/jgi/Modules/modulefiles ---------------------------
falcon/1.8.8
```

denovo1> cat /usr/common/jgi/Modules/modulefiles/falcon/1.8.8

```
#%Module1.0
##

## Required internal variables
set             name            falcon
set             version         1.8.8
set             root            {/usr/common/jgi/assemblers/$name/$version}

## List conflicting modules here
set mod_conflict { $name }

## List prerequisite modules here
set mod_prereq_autoload { python/2.7-anaconda }
set mod_prereq { python/2.7-anaconda }

## Source the common modules code-base
source /usr/common/usg/Modules/include/usgModInclude.tcl

## Software-specific settings exported to user environment
prepend-path    PATH            $root/fc_env/bin
prepend-path    PYTHONPATH      $root/fc_env/lib/python2.7/site-packages:$root/FALCON
setenv          FALCON_DIR      $root
setenv          PYTHONUSERBASE  $root/fc_env
setenv          FALCON_PREFIX   $root/fc_env
```

Module files are written in Tcl

N.B. This is a simplified version of the real file

```
#%Module1.0
##

## Required internal variables
set         name        falcon
set         version     1.8.8
set         root        {/usr/common/jgi/assemblers/$name/$version}

## List conflicting modules here
set mod_conflict { $name }

## List prerequisite modules here
set mod_prereq_autoload { python/2.7-anaconda }
set mod_prereq { python/2.7-anaconda }

## Source the common modules code-base
source /usr/common/usg/Modules/include/usgModInclude.tcl

## Software-specific settings exported to user environment
prepend-path    PATH        $root/fc_env/bin
prepend-path    PYTHONPATH  $root/fc_env/lib/python2.7/site-packages:$root/FALCON
setenv      FALCON_DIR      $root
setenv      PYTHONUSERBASE  $root/fc_env
setenv      FALCON_PREFIX   $root/fc_env
```

Required header

Set the **name** and **version**,
then set the **root** to point to the software installation area

```
#%Module1.0
##

## Required internal variables
set         name        falcon
set         version     1.8.8
set         root        {/usr/common/jgi/assemblers

## List conflicting modules here
set mod_conflict { $name }

## List prerequisite modules here
set mod_prereq_autoload { python/2.7-anaconda }
set mod_prereq { python/2.7-anaconda }

## Source the common modules code-base
source /usr/common/usg/Modules/include/

## Software-specific settings exported to us
prepend-path    PATH        $root/fc_en
prepend-path    PYTHONPATH  $root/
setenv      FALCON_DIR      $root
setenv      PYTHONUSERBASE  $root/fc_en
setenv      FALCON_PREFIX   $root/fc_env
```

List any module conflicts:

Most modules conflict with themselves – you won't want to use module X/1.0 and X/2.0 at the same time

List any module dependencies:

Use **mod_prereq** to prevent the module loading unless the dependencies are already loaded

Use **mod_prereq_autoload** to automatically load those dependencies

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```
#%Module1.0
##

## Required internal variables
set             name            falcon
set             version         1.8.8
set             root            {/usr/common/jgi/assemblers/$name/$version}

## List conflicting modules here
set mod_conflict { $name }

Required library functions
set mod_prereq_autoload { python/2.7-anaconda }
set mod_prereq { python/2.7-anaconda }

## Source the common modules code-base
source /usr/common/usg/Modules/include/usgModInclude.tcl

## Software-specific settings exported to user environment
prepend-path    PATH            $root/fc_env/bin
prepend-path    PYTHONPATH      $root/fc_env/lib/python2.7/site-packages:$root/FALCON
setenv          FALCON_DIR      $root
setenv          PYTHONUSERBASE  $root/fc_env
setenv          FALCON_PREFIX   $root/fc_env
```

Set **$PATH**, **$PYTHONPATH** etc, using variables defined earlier

prepend-path prefixes to $PATH-like variables

setenv simply sets a value

N.B. ***$PACKAGE*_DIR** is set to point to the base of the installation, by local convention

How to build a simple module

- **First, create a directory to hold your module files**
- **Clone the repository**

  > git clone https://bitbucket.org/TWildish/jgi-modules-tutorial.git

  > cd jgi-modules-tutorial

  > export HERE=`pwd`

- **Create a subdirectory 'Modules', add it to your $MODULEPATH**

  > mkdir Modules

  > module use $HERE/Modules

  – 'module use' adds the module to your $MODULEPATH, don't set it by hand

  – Now, modules added under that directory can be used automatically

How to build a simple module: FastTree

- **Run the build script**

  > cd examples/fasttree/build

  > ./build-fasttree-2.1.10.sh

  – That installs the binary in $HERE/examples/fasttree/2.1.10

- **Now create the module file to point to that installation**
  – There's a template file, '2.1.10', in the same directory as the build script
  – Edit it, change the definition for **root** to point to the installation root
    - 'set root { /…/jgi-modules-tutorial/examples/$name/$version }'
  – N.B. give full pathname, don't use environment variables in the module file

  – Create a 'fasttree' subdirectory in your modules directory, copy this file there
    - mkdir $HERE/Modules/fasttree
    - cp 2.1.10 $HERE/Modules/fasttree/

Recap: What did we just do?

- **We created a directory to hold module files**
  - $HERE/Modules
- **Added that directory to our MODULEPATH**
  - With the 'module use' command
- **Compiled & installed fasttree**
- **Created a module file to add the fasttree directory to the $PATH environment variable**
- **Added that module file to the module directory, in a subdirectory named for the software we installed**
  - $HERE/Modules/fasttree/2.1.10
- **Now, 'module avail fasttree' will show our module!**

A more complex module

- **The 'examples' directory contains build scripts for other tools**
  - last, mash, mummer, prodigal, vsearch, zlib
    - There's a template module file for last, you can do the others as an exercise
    - The actual module files aren't more complex, it's only the software build procedure that is more involved
- **The build scripts all run out-of-the-box on Denovo**
  - Several best-practices illustrated, please take a look at them
  - The 'last' build script, in particular, is well-documented

https://bitbucket.org/TWildish/jgi-modules-tutorial.git

Best practices: module files

- **Keep your build scripts and module templates together**
  - Can automate generating module files for most packages, ask me later if you want to do that
- **Make sure you define all the environment variables your package needs**
  - PATH, PYTHONPATH, MANPATH, package-specific variables etc
- **Keep them under version control**
  - Knowing how a module was built is essential for reproducible science
  - Makes your environment more (likely to be) portable to new platforms

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Best practices: building software

- **Build scripts require a *lot* of care to do well**
  - It's not difficult to do properly, but it is necessary for reproducibility
    - Build-scripts should be self-documenting
  - Prefer building from source over installing binaries
    - Controls dependencies better, not relying on the system so much
    - Can make a *huge* difference in performance, optimizing for modern CPU architecture (anyone using 32-bit or i386 binaries?)
  - Record the original location of the source code (the URL), so you can refer back there for more information etc
    - Document where you got the package, and how
    - Keep the source after you download it, it may disappear from the web
  - Make your scripts abort on error
    - Don't assume they will work every time
  - READ THE BUILD INSTRUCTIONS for each package
    - Don't just accept defaults without understanding what they do

Best practices: building software

- Clean the build environment, then build it up from scratch
  - Minimize dependencies on the OS (GCC, Perl, Python, graphics libraries…)
- Don't hardwire the location of the build or the installation
  - That reduces portability and flexibility, makes development harder
- Remove the installation & working directories before building
  - Don't risk incorporating stale artifacts from previous builds
- Clean up after building too, so you don't leave cruft
- If the package has built-in tests, run them before installing
  - Look for 'make check' or 'make test' targets
  - If there are no built-in tests, can you provide something minimal?
- Bonus points: add $GCC_RECORD_SWITCHES to your compilation flags
  - Set for compilers that support it, records compile options in the build products
  - Read the options back with 'readelf':
    - > readelf -p .GCC.command.line $SPADES_DIR/bin/spades

Best practices: building software

- **Building a library? Be kind to your users!**
  - Build it for all available compilers
    - Don't force the user to use a specific compiler unnecessarily
    - Use '**mod_variations**' in your module file to load the right flavor
    - See examples/zlib/build/build-zlib-1.2.11.sh
  - Add extra environment variables in your module file to make it easier to use the library
    - See examples/zlib/1.2.11, which sets ZLIB_INC, ZLIB_LIB, & others
    - See the examples for mash and vsearch for how to use them

Final comments

- **That's a lot to remember, is it worth it?**
  - Binary-only installs are OK if you can trust the person who built the software
    - Fine with Anaconda, there's a strong community
    - Docker images vary in quality, some good, some not so good
    - If you really care about the results from your applications, and the performance you get running them, you should build them yourself
- **So you've built your module, what next?**
  - You're one step away from building a container, why not try it!
    - Much less work for the container than for the original software
    - Can make the base container look like the OS you build the s/w on, then your build script should work out of the box
    - Gives you a migration path to other platforms (cloud etc) for only a little extra investment

Exercises

- **Build and install a module for each of the examples**
  - Follow the recipe from slide 14 (after preliminaries on slide 13)
  - Run the build scripts in the examples directory for each package
    - Just cd into the directory and execute the script
  - Create a module file for each package, install it
    - …/Modules/${package}/${version}
  - Verify that you can 'module load' the package and run the software
- **Bonus exercise:**
  - One of my recommended practices isn't followed by *any* of the example scripts. Can you fix them?
  - The example for metabat only provides the download link, create the build script and module file yourself.

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