I - Installing Software

Introduction

Model, CoC and URLs

- Carpentries model: hands-on portion, aka live coding
 - Carpentries Code of Conduct
- https://github.com/SmithsonianWorkshops/
 - view *slides* or the *markdown* version

In the intro portion of the workshop you will learn:

- About downloading code
- About compiling code
- How to build a package from source code
 - configure
 - build
 - install
- What are yum, rpm, get-apt, & sudo
- How to write modules



Downloading Code

Source vs Executable

- In most cases you are better off downloading the source and building the code (aka the executable) yourself.
- Downloading an executable is easier but likely will not to work.

Downloading Executables

Some developers provide pre-built executables of their software. There are instances when available executables will run flawlessly on Hydra, but make sure that:

- 1 you can trust the origin,
- 2 you get a version compatible with Hydra,
 - i.e., CentOS 7.x for Intel/AMD CPUs (x86_64)

Remember

- Hydra configuration is specific:
 - pre-built code may need *stuff* (dependencies) not on Hydra.



Notes on Downloading Executables

Risks

- Since users on Hydra do not have elevated privileges (root access) you are very unlikely to damage the cluster, but malicious software can still damage your files.
- In rare cases it may install a Trojan horse that could exploit a known vulnerability.
 - Be vigilant and responsible.
 - In case of doubt, never hesitate to contact us.

Compiling code

Steps

Creating executable from source code is typically done as follows:

- 1 compile the source file(s) to produce object file(s),
- 2 link the object file(s) and libraries into an executable.

In Practice

- Often aided by a makefile,
- Configuring is creating such makefile or equivalent.

This will be illustrated in the hands-on section.

Building from Source

1. Configure

- Most packages come with a configuration script, a list of prerequisites (dependencies/libraries) and instructions,
- Some packages allow you to build the code without some features in case you cannot satisfy some of the prerequisites,
- You most likely need to load the right module(s) to use the appropriate tools (compilers).
- The configuration step will test if the code can be built:
 - check dependencies, versions, etc.
 - if this fails, the code cannot be built as is.

1.b Makefile only

- Other (simpler) packages come with a makefile that needs to be edited,
 - check the instructions.



Building from Source (cont'd)

2. Build

- make sure you have loaded the right modules,
- run make to compile and link (aka build) the code.

2.b Test

some packages come with the optional step of testing the built before installing it, using something like make test.

3. Install

- copy the executable(s) to the right place(s),
 - usually defined by the configuration,
- best practice is to separate build from install locations.



Basics about make and makefile

The command make

- make is a utility to maintain groups of programs.
- Uses instructions in a makefile to build targets from sources by following rules.
- written to help build & maintain code, can be used for a lot more (full Carpentries module).

Examples:

build the first target listed in the makefile:

make

- build the target "this" listed in the "makefile" file: make this
 - build "that" using "makefile.special" and set "VAR" to "val":

make -f makefile.special VAR=val that



Basics about make and makefile (cont'd)

The Makefile or makefile files

- a file that defines targets and codifies rules and dependencies to build targets;
 - dependency: has a source needed to build something changed?
- it can be very simple, but can also be quite complex.

Also

- make has implicit rules:
 - can build targets w/out a makefile or w/out rules.

This will be illustrated in the hands-on part

Setting up Your Environment to Run Your Code

Likely Needed

You likely will need to adjust your environment to run some code:

- the location of the code: path or PATH,
- the location of the libraries: LD_LIBRARY_PATH,
- 3 you may also need to set some environment variables, etc.

Easier Way: modules

This is where using a module makes things easy:

- compact, and
- works with any shell.



The yum, rpm, get-apt and sudo Soup

Definitions

- yum: is a package-management utility for CentOS
- rpm: pre-built software package
 - both are for sys-admin,
 - help handle dependencies,
 - yet ...
- get-apt: Debian's version of yum, does not work on CentOS.

Also

■ sudo: allows to run a command as 'root': you can't!

BTW

- Instructions that mention yum, rpm, apt-get or sudo
 - will not work on Hydra,
 - **yet** in most cases there is another way.



How about Hydra

Using yum

- While you cannot install packages with yum,
- you can check if we've installed a prerequisite package

In practice

- if the instructions say
 sudo yum -y install <package>
- you can run yum info <package>

Using yum info

Example

```
yum info libXt-devel
```

... stuff and may be slow the first time ...

Installed Packages

Name : libXt-devel

Arch : x86_64 Version : 1.1.5

. . .

Description: X.Org X11 libXt development package

. . .

You want the Arch: x86_64 to be listed as "Installed" not *just* "Available".

How to avoid sudo

sudo make install

- if the instructions says
- sudo make install
 - instead, set the installation directory to be under your control,
 - in most cases at the configuration step
- ./configure -prefix=/home/<username>/big-package/3.5
 - and use

make install

Replace <username> by your username.

Final Notes

Remember

- there is a way to use yum as a non privileged user
 - not recommended, unless you're an expert!
- you can always ask about a missing prerequisite,
- most of those can be built from source since Linux is an open source OS.

Hands-on Section

Hands-on

In this hands-on portion of the workshop you will

- Build and install software using best-practices,
 - trivial case,
 - simple/didactic example,
 - somewhat complex examples.
- Run the software you installed in jobs.

But first, log in to Hydra

- If you need a reminder about how to log into Hydra and how to change your password, check the *Intro to Hydra* tutorial.
 - If the link does not work:

https://github.com/SmithsonianWorkshops

- > Hydra-introduction
 - > hydra_intro.md







Let's pause here for 5-10 minutes

Hands-on - Part I

Switch to github for the Hands-on

Go to

https://github.com/SmithsonianWorkshops/advanced-hydra-workshops/

Convention

- I use % as prompt
 - your prompt might be different, like \$
 - you type what is after the prompt
 - no prompt: result from previous command.
- I where you see <genomics|sao>, you need to use either genomics or sao,
- I where you see <username>, you need to substitute your username.