Installing Software on High Performance Computing Systems

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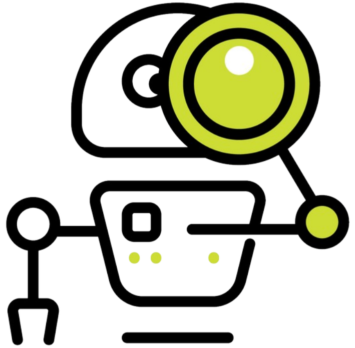
Research Technology Services
June 2021

Research Technology Services

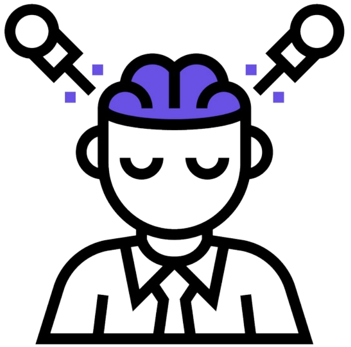
1. **Research Computing**
    - High Performance Computing: Gadi, Katana, …
    - Cloud computing: Amazon AWS, Microsoft Azure, Google
    - Code and algorithm support
2. **Research Data**
    - Data management including highly sensitive or complex data
    - Assistance with data moves, storage, planning, tools
    - Pilot scheme for publishing Open Data
    - UNSW GitHub private, public and limited-sharing repositories



Research Technology Services

3. Research Community

- Over 50 *free* training courses: Linux, Python, Matlab, R, …
- Weekly **Hacky Hour** meetings: via Microsoft Teams, on Thursdays at 3pm. Bring your problems with code, HPC, data and more!
- ResTech seminars, lunch-and-learn series, training videos, …



4. ResBaz

- Annual data and compute literacy festival/conference for researchers from all over New South Wales
- Watch this space for 2021!

Installing Software on HPC Systems

- Assumed knowledge
- Avoiding software installations
- Installing binary packages
- Installing from source code
- Creating module files
- Installing Python packages
- Installing R and RStudio libraries
- Installing Julia packages
- Questions?

Part of the Gadi cluster in Canberra, ACT
Image credit: National Computational Infrastructure

Assumed knowledge

- You have an account on a High Performance Computing system
  - Katana at UNSW
  - Gadi at NCI
- You know how to log in to that HPC system via SSH (Secure Shell)
  - See the Katana documentation or NCI Help pages for details
- You know basic Linux commands
  - See the Introduction to Linux and High Performance Computing course notes and associated recorded video
- You understand basic module commands
  - See Software Modules part 1 and part 2
- You are not afraid to try doing things yourself!

Avoiding software installations

First rule of installing software on HPC: **DON’T**

- Is your software already installed system-wide?
- Is your software already installed by your colleagues?
- Is a different version of your software already installed?
- Is a similar package already installed?
- Try asking HPC staff to install your software for you
  - For Katana: send an email to *itservicecentre@unsw.edu.au* mentioning Katana
  - For Gadi: send an email to *help@nci.org.au*

Checking if a package is installed

- Is your required package already part of the base operating system?
  - Default editors, programming languages, compilers, debuggers and libraries
  - Check using `yum list installed` (ignore any warnings about old repositories)
- Is it already installed system-wide?
  - Multiple versions of applications, all stored in `/apps` directory
  - Check using `module avail`
- Is it installed by your colleagues?
  - Ask them!

Try it now:

```
yum list installed | less      # To return to the command line, press "q" to quit
module avail |& less           # … press "q" to quit.  Note the unusual "|&"!
```

Installing binary packages

- Compiling from source code is often best
  - Allows you to use specific HPC-optimised compilers, compiler flags and libraries
- If only a binary package is available:
  - Download the binary package (avoid DEB and RPM packages): 64-bit Intel x86_64 / AMD64 architecture, CentOS 7 compatibility for Katana, CentOS 8 for Gadi
  - Start an interactive session using `qsub -I` with appropriate parameters
  - Follow the supplied instructions to install the software
  - Do *not* try to use `apt-get install`, `yum install`, `dnf install`, `su` or `sudo`!

Try it now:

```
wget -N https://ftp.zap.org.au/pub/trader/unix/binary/appimage/trader-
    7.16-x86_64.AppImage                          # Download the precompiled package
chmod a+rx ./trader-7.16-x86_64.AppImage          # Make the application executable
./trader-7.16-x86_64.AppImage --help              # Test the application
```

Installing from source code

- Download the source code
- Download source code to any library dependencies
- If possible, use the system compiler and linker (`gcc` and `ld`) and libraries
- Start an interactive session using `qsub -I` with appropriate parameters
- If necessary, load any required modules for compilers and libraries
- Follow the supplied instructions for compiling the package
- Install the software to your home directory or scratch directory (for large packages)
- With Autoconf-enabled software, often as simple as running

```
./configure --prefix=$HOME/apps/PACKAGE/VERSION
make && make install
```

Installing from source code

Try it now on Katana:

```
mkdir ~/src; cd ~/src                # Source code will be stored in $HOME/src
wget -N https://ftp.zap.org.au/pub/trader/unix/trader-7.16.tar.xz
                                     # Download the source code
tar xvf trader-7.16.tar.xz           # Unpack the source code
cd trader-7.16                       # Change to the source code directory
less README; less INSTALL            # Read the installation instructions; “q” to quit each file
qsub -l walltime=0:30:00 -l select=1:ncpus=1:mem=8GB -I
                                     # Request an interactive job (you may need to wait)
```

Once a command line prompt appears:

```
cd ~/src/trader-7.16                              # Go to the source code directory
./configure --prefix=$HOME/apps/trader/7.16           # Configure the software
make && make install                              # Compile and install the code
~/apps/trader/7.16/bin/trader --help              # Test the installed software
cd ~/src; rm -fr trader-7.16                      # Remove the source code to save space
```

Installing from source code with modules

Try it now on Gadi:

```
mkdir ~/src; cd ~/src                  # Source code will be stored in $HOME/src
wget -N https://ftp.zap.org.au/pub/trader/unix/trader-7.16.tar.xz
                                       # Download the source code
tar xvf trader-7.16.tar.xz             # Unpack the source code
qsub -l walltime=0:30:00 -l ncpus=1 -l mem=8GB -I
                                       # Request an interactive job (you may need to wait)
```

Once a command line prompt appears:

```
cd ~/src/trader-7.16                                 # Change to the source code directory
module load intel-compiler/2021.2.0                   # Use the Intel compiler (icc)
./configure --prefix=$HOME/apps/trader/7.16          # Configure the software
make && make install                                 # Compile and install the code
~/apps/trader/7.16/bin/trader --help                 # Test the installed software
cd ~/src; rm -fr trader-7.16                         # Remove the source code to save space
```

Creating module files

- The environment module system allows for multiple versions of applications
- Short “recipes” for how to modify your compute environment
  - On Katana, stored in `/apps/modules`
  - On Gadi, stored in `/apps/Modules` (note capital “M”!)
  - Sample file `/apps/modules/templates/module_file` on Katana
- Written in the TCL programming language
- Many powerful features!
  - See documentation by running `man module` and `man 4 modulefile`
- Can easily create and use your own module file recipes
  - Create a directory `~/apps/Modules`
  - Add “`module use --append $HOME/apps/Modules`” to your `~/.bashrc` file
  - Log out and log back in to enable the `module use` command

Creating module files

Try it now on Katana or Gadi:

```
mkdir ~/apps/Modules                  # Module files will be stored here
mkdir ~/apps/Modules/trader           # Module files for the Star Trader application
nano ~/apps/Modules/trader/7.16       # Create the module file
```

Enter the following text inside the Nano editor:

```
#%Module1.0

set             basepath        $env(HOME)/apps/trader
set             version         7.16
set             path            $basepath/$version

prepend-path    PATH            $path/bin
prepend-path    MANPATH         $path/share/man
```

Press **CTRL-X** to save the file and exit the editor (follow the prompts on the bottom of the screen)

Using custom module files

Try it now on Katana or Gadi:

```
module use --append ~/apps/Modules        # Custom module files are stored here
                                          # … can be added to your ~/.bashrc file

module avail trader                       # Is the Star Trader application available?
module load trader/7.16                   # Use the new module file

trader --help                             # Test the application: no need for a full path
man trader                                # Manual page is also available (“q” to quit)
```

Installing Python packages

- On Katana, many Python packages are already installed
  - Check by running `python3 -c "import PACKAGENAME"` *after* running `module load python/VERSION` (for an appropriate 3.*x*.*y* version)
  - Can also run `pip3 list` to list package version numbers
- If not available, create a Python Virtual Environment and install the required Python package
- If required, install Conda or Anaconda for yourself—these are *not* able to be installed for multiple users
- Full instructions are available in the Katana Python documentation
- Python Virtual Environments *can* be used from Katana On Demand
  - See the Katana Jupyter Notebooks documentation for details

Installing R and RStudio libraries

- On Katana, many R and RStudio libraries are already installed
  - Load the appropriate module file: `module load R/4.0.2`
  - Note that `module load R/4.0.2-clean` loads a version of R that does *not* contain additional libraries! Useful if you want to install newer versions of libraries that conflict with those in `R/4.0.2`.
  - Start R, then run `library()` to check available libraries
- To install an R library, download the package and run `install('PACKAGE_PATH')`
- Further instructions are available in the Katana R and RStudio documentation

Installing Julia packages

- Only the default Julia packages are installed
- To install or update a package, use the Julia Package Manager (`Pkg`)
  - Load the appropriate module file: `module load julia/1.6.1`
  - Start Julia from the command line: `julia`
  - Enter the package manager: Press "**]**"
  - Refresh the package list: `up`
  - Add your required packages: `add` *`PACKAGE`*
  - Exit the package manager: Press **CTRL-C**
  - Exit Julia: `exit( )`
- You can now use the new packages in your Julia code

With whom do I discuss my HPC needs?

1. Your colleagues
2. Your supervisor
3. Hacky Hour: every Thursday 3pm on Microsoft Teams (Research Technology Training, Hacky Hour channel)
4. The Research Technology Services team
   - John Zaitseff *J.Zaitseff@unsw.edu.au*
   - The whole team at UNSW *restech@unsw.edu.au*

https://restech.unsw.edu.au/

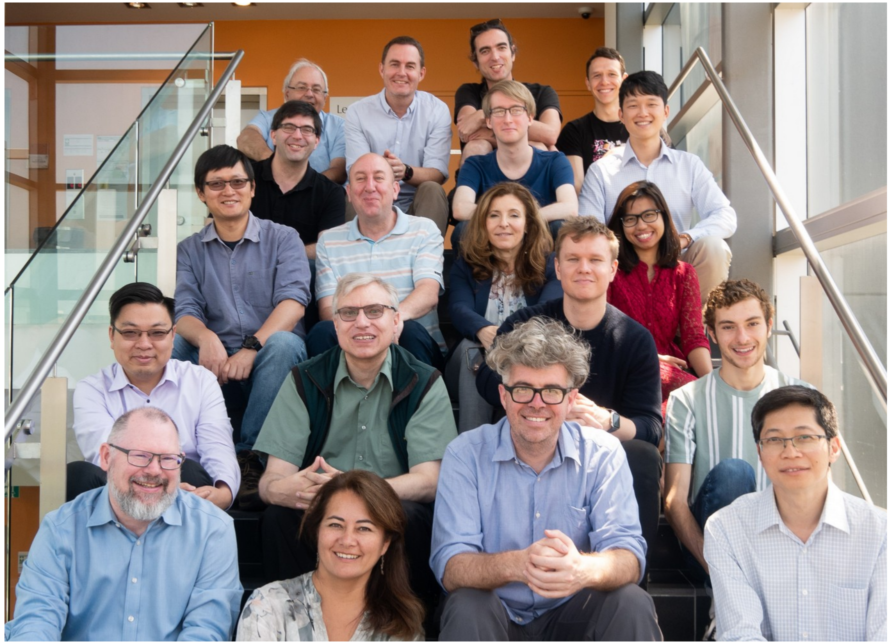


Image credit: UNSW Sydney