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High Performance Computing and software environments:

Install and/or use existing software and modules

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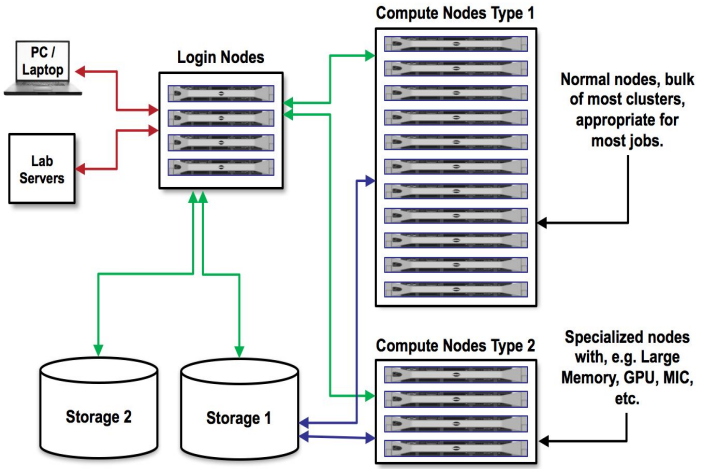
Outline

- ★ Software distribution on HPC clusters
- ★ Why modules? How to find modules?
- ★ Software stacks on Grex
- ★ How to build software from sources
  - ○ R packages
  - ○ Python packages
  - ○ Perl modules
  - ○ configure/make
  - ○ cmake/make
- ★ Singularity/Apptainer

HPC Cluster:

- Hardware
- Network
- Software



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Software distribution

Operating system package managers/repos:

- ★ **Ubuntu:** ~$ ***sudo apt-get install <package>***
- ★ **CentOS:** ~$ ***sudo yum install <package>***
- ★ **On HPC:** users do not have **sudo**!

On cloud and personal machines, users have a privilege access but not on HPC clusters.

Using a centralized HPC software stack:

- ★ **Software distributed via CVMFS:** CC software stack (CC clusters), …
- ★ **Local software:** modules, legally restricted software (VASP, Gaussian, …)

Admin

Local installation: usually to $HOME {/home/$USER} or $PROJECT

- ★ **Get the code:** download the sources/binaries: wget, git clone, … etc.
- ★ **Settings:** load dependencies, set environment variables, … etc.
- ★ **Build:** ./configure {***cmake*** ..} +opts; make; make test {***check***}; make install

End User

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Software layers

User layer: Python packages, Perl and R modules, home made codes, …

Software stacks: modules for Intel, PGI, OpenMPI, CUDA, MKL, high-level applications. Multiple architectures (sse3, avx, avx2, avx512)

Nix or gentoo: GNU libc, autotools, make, bash, cat, ls, awk, grep, etc.

Gray area: Slurm, Lustre client libraries, IB/OmniPath/InfiniPath client libraries (all dependencies of OpenMPI) in Nix {or gentoo} layer, but can be overridden using PATH & LD_LIBRARY_PATH.

OS: kernel, daemons, drivers, libcuda, anything privileged (e.g. the sudo command): always local. Some legally restricted software too (VASP).

User

Analysts

Sys. Admin

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Why modules?

★ Why modules?

https://docs.alliancecan.ca/wiki/Utiliser_des_modules/en

- Control different versions of the same program.
- Avoid conflicts between different versions and libraries.
- Set the right path to each program or library.

Lmod

```
[someuser@bison ]$  module avail
–
CCEnv (S)     GrexEnv (S,L)

Where:
   S:  Module is Sticky, requires --force to
unload or purge
   L:  Module is loaded
```

★ Useful commands for working with modules:

- module **list**; module **avail**
- module **spider** <soft>/<version>
- module **load** soft/version; module **unload {rm}** <soft>/<version>
- module **show** soft/version; module **help** <soft>/<version>
- module **purge**; module --force **purge**
- module **use** ~/modulefiles; module **unuse** ~/modulefiles

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Software stacks on Grex

- ★ Grex environment [default]: GrexEnv
  - no module loaded by default.
  - use module spider <name of the software> to search for modules
  - Compilers: {GCC, Intel}, MKL, PETSc, … etc.
  - Gaussian, ANSYS, MATLAB, … etc.
- ★ The Alliance (Compute Canada) environment [optional]: CCEnv
  - Switch to CCEnv; load a standard environment; choose the architecture[sse3, avx2, avx512], use module spider <soft>

```
~$ module load CCEnv
~$ module load StdEnv/2020
~$ module load arch/avx512
~$ module load gcc/9.3.0 geant4/10.7.3
```

```
module load StdEnv/2016.4
module load arch/sse3
module load nixpkgs/16.09 gcc/5.4.0 geant4/10.05.p01
```

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Modules on Grex

- More than 500 modules:
  - Compilers: GCC [5,7,9,11]; Intel [2014 - 2020].
  - Libraries: HDF5, PETSc, GSL, MKL, Libxc, Boost, ...
  - Gaussian, ANSYS, MATLAB, VASP, ORCA, MCR, Java, Python, R, … etc.
  - LAMMPS, GROMACS, ABINIT, QE, VMD, Molden, OpenBABEL, … etc.
- Software maintenance on Grex and Alliance clusters:
  - We install programs and update modules on request from users.
  - Search for a program using "module spider <name of your program>"
  - If not installed, ask for support "support@tech.alliancecan.ca"
  - We will install the module or update the version.
  - For commercial software, contact us before you purchase the code:
    - to check license type.
    - see if it will run under Linux environment, … etc.

Modules on Grex: GrexEnv

```
------------------------------------------------- /opt/lmod/grex/7.6/modulefiles/Core -------------------------------------------------
  admixture/1.3.0                    intel/14.0.2.144           ncl_ncarg/6.4.0                uofm/adf/2019.305-impi
  admixture/1.23              (D)    intel/15.0.5.223           ncl_ncarg/6.5.0                uofm/adf/2020-impi
  ant/1.10.11                        intel/2017.8               nodejs/4.4.7                   uofm/adf/2020.103-impi
  circos/0.69-6                      intel/2019.5        (D)    nodejs/8.12.0                  uofm/adf/2021-impi
  cmake/3.12.3                       intel/2020.4               nodejs/13.2.0           (D)    uofm/adf/2021.102-impi
  cmake/3.14.0                       j/j903                     openbabel/2.3.2                uofm/adf/2021.106-impi    (D)
  cmake/3.16.9                       jags/3.4.0                 openbabel/2.4.1                uofm/cfx/15.0
  cmake/3.23.2                (D)    jags/4.0.0                 openbabel/3.0.0                uofm/cfx/16.2
  cns/1.3                            jags/4.3.0          (D)    openbabel/3.1.1         (D)    uofm/cfx/18.2
  eigen/3.3.7                        java/jdk7u25               ovito/2.9.0                    uofm/cfx/19.2
  fastqc/0.11.9                      java/jdk7u45               ovito/3.0.0-dev502      (D)    uofm/cfx/20.1
  gaussian/g09.b01.unlim             java/jdk8u5                pandoc/2.9.2.1                 uofm/cfx/20.2
  gaussian/g09.b01                   java/jdk8u66               perl/5.14.4                    uofm/cfx/21.1             (D)
  gaussian/g09.e01.unlim             java/jdk8u92        (D)    perl/5.22.1             (D)    uofm/feko/2021.2
  gaussian/g09.e01                   java/jdk13.0.1             perl/5.28.1                    uofm/gaussian/g03
  gaussian/g16.b01                   julia/1.3.0-bin            php/5.6.40                     uofm/gaussian/g09.e01
  gaussian/g16.c01.avx2.unlim        julia/1.5.4-bin            php/7.3.12              (D)    uofm/gaussian/g09         (D)
  gaussian/g16.c01.avx2              julia/1.6.1-bin            python/2.7.12-miniconda        uofm/mathematica/11.0
  gaussian/g16.c01            (D)    julia/1.7.0-bin     (D)    python/3.6-miniconda    (D)    uofm/matlab/R2014A
  gcc/4.8                            libcerf/1.4                settarg                        uofm/matlab/R2015B
  gcc/5.2                            lmod                       singularity/3.5.2              uofm/matlab/R2017A
  gcc/7.4                     (D)    ls-prepost/4.7.13          smrtlink/6.0.0.47841           uofm/matlab/R2019B
  gcc/9.2                            mcr/mcr                    stata/14.2-fagfs               uofm/matlab/R2020B2       (D)
  gcc/11.2                           mkl/10.3.11         (D)    stata/15.0-fagfs        (D)    uofm/starccm/16.06.010
  git-lfs/3.2.0                      mkl/11.1.0                 tbb/14                         uofm/starccm/17.02.008-R8 (D)
  git/2.21.0                         mkl/2019.5                 tbb/2019.5              (D)    uofm/umcfd/2.4
  gnuplot/5.2.7                      molden/5.9                 trimmomatic/0.39               vina/1.1.2
  go/1.10.4                          multiwfn/3.8-gui           uofm/adf/2016-impi-test        vmd/1.9.3
  go/1.11.5                          multiwfn/3.8-nogui  (D)    uofm/adf/2016-impi             vncworkspace/1.1
  go/1.12.12                         nbo/6.0                    uofm/adf/2017-impi             vtune/2019.4
  go/1.13                            nbo/7.0             (D)    uofm/adf/2017.114-impi         vtune/2019.5              (D)
  go/1.13.3                   (D)    ncl_ncarg/6.2.1     (D)    uofm/adf/2018dev-impi          wine/3.0
  intel/12.1.5.339                   ncl_ncarg/6.3.0            uofm/adf/2019-impi             xtb/6.5.0-bin

------------------------------------------------------------ /opt/lmod/stacks ------------------------------------------------------------
  CCEnv (S)    GrexEnv (S,L)
```

module avail

module spider python
module spider java

module load gcc ompi
module avail

module spider <soft>
module spider <soft>/<ver>

module show <soft>
module purge

If not available:
➔ contact support
support@tech.alliancecan.ca

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Find and load Gaussian

Gaussian: restricted software; requires a registration https://docs.alliancecan.ca/wiki/Gaussian

https://um-grex.github.io/grex-docs/specific-soft/gaussian/

```
[someuser@bison ]$  module spider gaussian
---------------------------------------------------------------------------------------------------------------------------------------------------
  gaussian:
---------------------------------------------------------------------------------------------------------------------------------------------------
     Versions:
        gaussian/g09.e01
        gaussian/g16.b01
        gaussian/g16.c01.avx2
        gaussian/g16.c01
---------------------------------------------------------------------------------------------------------------------------------------------------
  For detailed information about a specific "gaussian" package (including how to load the modules) use the
module's full name. Note that names that have a trailing (E) are extensions provided by other modules.
  For example:
     $ module spider gaussian/g16.c01
---------------------------------------------------------------------------------------------------------------------------------------------------
```

```
[someuser@tatanka ~]$  module load gaussian/g16.c01
    Loading  Gaussian version 16.c01
```

Available: **Grex** [Also on **Cedar** and **Graham**]

Find and load ORCA

ORCA:

- **restricted software**
- **requires a registration**

https://docs.alliancecan.ca/wiki/ORCA
https://um-grex.github.io/grex-docs/specific-soft/orca/

[someuser@bison]$ module spider orca

[someuser@bison]$ module spider **orca/5.0.4**

---

orca:

Versions:
orca/4.2.1
orca/5.0.1
orca/5.0.2
orca/5.0.4

[someuser@bison]$ module load gcc/4.8 ompi/4.1.1 **orca/5.0.4**
Loading module: gcc/4.8
Loading module: ORCA/5.0.4

For detailed information about a specific "orca" package (including how to load the modules) use the module's full name. Note that names that have a trailing (E) are extensions provided by other modules.

For example:

$ module spider orca/5.0.4

Available: Grex and all Alliance clusters

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Find and load LAMMPS

```
[someuser@bison ]$  module spider lammps
----------------------------------------------------------------------------
  lammps:
----------------------------------------------------------------------------
     Versions:
        lammps/5Jun19
        lammps/5Nov16
        lammps/11Aug17
        lammps/23Jun22
        lammps/29Sep21
        lammps/30jul16
----------------------------------------------------------------------------
  For detailed information about a specific "lammps" package (including how to load the modules) use the
module's full name. Note that names that have a trailing (E) are extensions provided by other modules.
  For example:
     $ module spider lammps/29Sep21
----------------------------------------------------------------------------
```

```
[someuser@bison ]$  module spider lammps/29Sep21
```

```
[~@tatanka ~]$  module load intel/2019.5  ompi/3.1.4 lammps/29Sep21
Lmod is automatically replacing "gcc/7.4" with "intel/2019.5".
    Unloading module: gcc/7.4.0
    Loading module: LAMMPS/29Sep21
```

MATLAB and MCR

```
[someuser@bison ~]$  module spider matlab
```

https://um-grex.github.io/grex-docs/specific-soft/matlab/

```
----------------------------------------------------------------------------------------------------------------------
  uofm/matlab:
----------------------------------------------------------------------------------------------------------------------
     Versions:
        uofm/matlab/R2014A
        uofm/matlab/R2015B
        uofm/matlab/R2017A
        uofm/matlab/R2019B
        uofm/matlab/R2020B2
----------------------------------------------------------------------------------------------------------------------
  For detailed information about a specific "uofm/matlab" package (including how to load the modules) use
the module's full name. Note that names that have a trailing (E) are extensions provided by other modules.
  For example:
     $ module spider uofm/matlab/R2020B2
----------------------------------------------------------------------------------------------------------------------
```

```
[someuser@bison ~]$  module spider mcr
----------------------------------------------------------------------------
  mcr: mcr/mcr
----------------------------------------------------------------------------
     This module can be loaded directly: module load mcr/mcr
```

Modules from the Alliance software stack

```
---------------------------------------- MPI-dependent avx512 modules ----------------------------------------
   abinit/9.2.2        (chem)      lammps-omp/20220623       (chem,D)    plumed/2.6.2              (chem)
   abinit/9.6.2        (chem,D)    latte/1.2.1               (chem)      plumed/2.7.0              (chem)
   adol-c/2.7.2                    libcf/1.0.3                           plumed/2.7.1              (chem)
   apbs/1.3            (chem)      libgridxc-mpi/0.8.0                   plumed/2.7.3              (chem)
   berkeleygw/2.1.0    (phys)      met/9.1.1                 (phys)      plumed/2.7.4              (chem)
   berkeleygw/3.0.1    (phys,D)    mpas/7.0                              plumed/2.8.1              (chem,D)
   bigdft/1.8.3        (chem)      mpi4py/3.0.3              (t)         pnetcdf/1.9.0             (io)
   boost-mpi/1.72.0    (t)         mpi4py/3.1.2              (t)         pnetcdf/1.10.0            (io)
   boost-mpi/1.80.0    (t,D)       mpi4py/3.1.3              (t,D)       pnetcdf/1.12.2            (io,D)
   cdo/1.9.8           (geo)       mrbayes/3.2.7             (bio)       psi4/1.3.2                (chem)
   cdo/2.0.4           (geo)       mscg/1.7.3.1              (chem)      psi4/1.4                  (chem)
   cdo/2.0.5           (geo,D)     mumps-metis/5.2.1         (t)         psi4/1.5                  (chem,D)
   cfour-mpi/2.1       (chem)      mumps-parmetis/5.3.5      (t)         quantumespresso/6.5       (chem)
   cgns/3.4.1          (phys)      ncl/6.6.2                 (vis)       quantumespresso/6.6       (chem)
   cgns/4.1.0          (phys)      ncview/2.1.8              (vis)       quantumespresso/6.7       (chem)
   cgns/4.1.2          (phys,D)    nektar++/5.0.1            (math)      quantumespresso/6.8       (chem)
   combblas/1.6.2                  netcdf-c++-mpi/4.2        (io)        quantumespresso/7.0       (chem,D)
   cp2k/7.1            (chem)      netcdf-c++4-mpi/4.3.1     (io)        raxml/8.2.12              (bio)
   cp2k/8.2            (chem)      netcdf-fortran-mpi/4.5.2  (io)        ray/3.0.1                 (bio)
   cp2k/9.1            (chem,D)    netcdf-fortran-mpi/4.6.0  (io,D)      repasthpc/2.2.0           (bio)
   cpmd/4.3            (chem)      netcdf-mpi/4.7.4          (io)        repasthpc/2.3.0           (bio,D)
   cslib/20180813                  netcdf-mpi/4.9.0          (io,D)      rosetta/3.10              (chem)
   dakota/6.13         (t)         neuron/7.8.2              (bio)       rosetta/3.12              (chem)
   delft3d/62441       (chem)      neuron/8.0.0              (bio,D)     rosetta/3.13              (chem)
   dl_poly4/4.10.0     (chem)      nwchem/6.8.1              (chem)      rosetta/2019.21.60746     (chem,D)
   elpa/2020.05.001    (math)      nwchem/7.0.2-p1           (chem,D)    scalapack/2.1.0           (math)
   esmf/8.0.1          (geo)       octopus/10.1              (chem)      scotch/6.0.9              (math)
   esmf/8.2.0          (geo,D)     openfoam-extend/4.1       (phys)      shengbte/1.1.1            (phys)
   etsf_io-mpi/1.0.4               openfoam/6                (phys)      shengbte/1.5.0            (phys,D)
   fds/6.7.5                       openmolcas/20.10          (chem)      siesta/4.0.1              (chem)
   fds/6.7.6                       openmx/3.9                (chem)      siesta/4.1-b4             (chem)
   fds/6.7.7                       openmx/3.9.9              (chem,D)    siesta/4.1-MaX-3.0        (chem)
   fds/6.7.8                       osu-micro-benchmarks/5.6.2 (t)        siesta/4.1.5              (chem,D)
   fds/6.7.9           (D)         p4est/2.2                 (math)      slepc/3.14.2
   fftw-mpi/3.3.8      (math)      parallelio/2.5.4                      sundials/2.7.0
   ga/5.7.2            (t)         paraview-offscreen/5.8.0  (vis)       sundials/5.3.0            (D)
lines 1-38
```

Software stacks:

- CCEnv (S)
- GrexEnv (S,L)

On Grex:

```
module load CCEnv
module load arch/avx512
module load StdEnv/2020
module avail
```

Jobs:

- ➔ skylake partition
- ➔ largemem partition

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Example of Geant4 from CCEnv

```
[~@yak ~]$  module spider geant4
        Versions:
        geant4/9.6.p04
        geant4/10.02.p03
        geant4/10.04.p02
        geant4/10.06
        geant4/10.7.3
        geant4/11.1.0
        Other possible modules matches:
        geant4-data
  To find other possible module matches execute:
        $ module -r spider '.*geant4.*'
For detailed information about a specific "geant4" package (including how to load the modules) use the
module's full name. Note that names that have a trailing (E) are extensions provided by other modules.
  For example:
        $ module spider geant4/11.1.0
```

```
[~@yak ~]$ module load CCEnv
[~@yak ~]$ module load arch/avx512
[~@yak ~]$ module load StdEnv/2020
[~@yak ~]$ module spider geant4
[~@yak ~]$ module spider geant4/11.1.0
[~@yak ~]$ module load gcc/9.3.0 geant4/11.1.0
```

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Installing a software

as user:

What are the programs you can install locally under your account?

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Building software

- Local installation [user's directory: home, project]:
  - R packages; Julia packages, Perl modules
  - Python packages: virtual environment, conda
  - Home made programs and commercial software.
- Installation with:
  - make; make test {check}; make install
  - configure; make; make test {check}; make install
  - cmake; make; make test {check}; make install
- Java applications: jar files
- Singularity and/or Aptainer:
  - build the image and run the program from the container

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Local installation

- R packages: minimal installation
  - R as modules: users can install the packages in their home directory.
- Python as modules: python and scipy-stack
  - users can install the packages needed in their home directory.
- Perl and bioperl as modules:
  - users can install the packages needed in their home directory.
- Other software installed locally:
  - Home made programs {up to a user or a group}
  - Restricted and licensed software that can not be distributed via CVMFS.
  - Custom software: patch from a user, changing parts of the code, … etc.

https://docs.alliancecan.ca/wiki/Installing_software_in_your_home_directory

Local installation: R packages

R packages: rgdal, adegenet, stats, rjags, dplyr, … etc.

Choose a module version: module spider r

Load R and dependencies (gdal, geos, jags, gsl, udunits… etc):

module load gcc/7.3.0 r/3.6.0 gdal udunits

```
[~]$ module spider r
        Versions:
        r/4.0.0
        r/4.0.2
        r/4.0.5
        r/4.1.0
        r/4.1.2
        r/4.2.1
        r/4.2.2
```

Launch R and install the packages:

```
~$ R
> install.packages("sp")
'lib =/cvmfs/soft.computecanada.ca/easybuild/{..}/R/library"' is not writable
Would you like to use a personal library instead? (yes/No/cancel) yes
Would you like to create a personal library '~/R/{…}' to install packages into? (yes/No/cancel) yes
--- Please select a CRAN mirror for use in this session ---
> install.packages("dplyr")
```

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Local installation: Python

- ★ Load the modules:
  - module load python
- ★ Create a virtual environment
  - virtualenv ~/my_venv
- ★ Activate the virtual environment
  - source ~/my_venv/bin/activate
- ★ Update pip
  - pip install --no-index --upgrade pip
- ★ Install the packages
  - pip install pandas
  - pip install -r requirements.txt
  - python setup.py install

```
module load gcc gcc/11.2 python/3.11.2
virtualenv ~/my_venv
source ~/my_venv/bin/activate
pip install cutadapt
deactivate
```

```
module load gcc/11.2 python/3.11.2
source ~/my_venv/bin/activate
cutadapt [+options]
deactivate
```

https://docs.alliancecan.ca/wiki/Python

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Local installation: perl

Example: Hash::Merge; Logger::Simple; MCE::Mutex; threads …

Load Perl module: module load perl

Install the the first package using cpan or cpanm:

```
~$ cpan install YAML
Would you like to configure as much as possible automatically? [yes] yes
What approach do you want?  (Choose 'local::lib', 'sudo' or 'manual')
[local::lib] local::lib
Would you like me to append that to /home/$USER/.bashrc now? [yes] yes
```

Install the rest of the packages using cpan or cpanm:

```
~$ cpan install Hash::Merge
~$ cpan install Logger::Simple
~$ cpan install MCE::Mutex
```

https://docs.alliancecan.ca/wiki/Perl

Installation with make: STAR

★ Download the code {wget; curl; git clone; …}:

wget https://github.com/alexdobin/STAR/archive/refs/tags/2.7.10b.tar.gz

★ Unpack the code: tar -xvf 2.7.10b.tar.gz

★ Load GCC compiler: module load gcc

★ Compile the code:

cd STAR-2.7.10b/source

make

★ Copy the binaries and set the path:

mkdir -p ~/software/star/2.7.10b/bin

cp STAR ~/software/star/2.7.10b/bin

export PATH=$PATH:${HOME}/software/star/2.7.10b/bin

STAR: Spliced Transcripts Alignment to a Reference

~/.bash_profile

PATH=$PATH:$HOME/bin:$HOME/software/star/2.7.10b/bin
export PATH

PATHs/environment variables added to module files when the program is installed as a module. Possibility to add local modules as a user.

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Installation with configure/make

- ★ Download and unpack the code: wget, … gunzip, … etc.
- ★ Load the modules and dependencies: module load gcc ompi fftw
- ★ Configure the program
  - If configure not included, run: autoreconf -fvi [to generate it].
  - ./configure --help [to see the different options].
  - ./configure --prefix=<path to install dir> {+other options}
- ★ Compile and test:
  - make; make -j4
  - make check; make test
- ★ Install the program:
  - make install

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Installing: treemix

- Download the source files:
  wget https://bitbucket.org/nygcresearch/treemix/downloads/treemix-1.13.tar.gz
- Unpack the source files: tar -xvf treemix-1.13.tar.gz
- Change the directory: cd treemix-1.13/
- Load the modules: module load gcc boost
- Configure: ./configure --prefix=/home/$USER/software/treemix/1.13
- Compile and install: make && make install
- Set a path: export PATH=$PATH:$HOME/software/treemix/1.13/bin
- Usage in a job script:

```
module load gcc boost
export PATH=$PATH:$HOME/software/treemix/1.13/bin
treemix {+options if any}
```

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Example: ABINIT

```
module load intel ompi gsl netcdf
instdir=<path to the installation directory>

../configure --prefix=${instdir} --enable-mpi --enable-mpi-io --with-fft-flavor=fftw3-mkl
--with-linalg-flavor=mkl --with-math-flavor=gsl --enable-debug="no"
--enable-optim="standard" --enable-64bit-flags --with-linalg-libs="-L$MKLROOT/lib/intel64
-lmkl_scalapack_lp64 -lmkl_blacs_openmpi_lp64  -lmkl_intel_lp64 -lmkl_sequential
-lmkl_core -lm"  --with-fft-incs="-I$MKLROOT/include/fftw -I$MKLROOT/interfaces/fftw3xf"
--with-fft-libs="-L$MKLROOT/interfaces/fftw3xf -lfftw3xf_intel_lp64"
--with-dft-flavor="atompaw+libxc+wannier90" --with-trio-flavor="netcdf"  --enable-lotf
--enable-macroave   --enable-gw-dpc  CC=mpicc CXX=mpic++ FC=mpif90 F77=mpif77
F90=mpif90
```

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Example: PETSc

```
./configure --with-blas-lapack-dir=$MKLROOT/lib/intel64  --prefix=${instdir}  --with-cxx-dialect=C++11
--download-scalapack=yes --download-blacs=yes  --download-superlu_dist=yes
--download-mumps=yes --download-parmetis=yes --download-metis=yes --download-spooles=yes
--download-cproto=yes --download-prometheus=yes --with-mkl_pardiso=1
--with-mkl_pardiso-dir=$MKLROOT --with-mkl-sparse-optimize=1  --with-scalar-type=complex
--with-debugging=0  --with-hdf5=yes --with-hdf5-dir=$HDF5HOME  --download-suitesparse=yes
--download-fftw=${fftsrc} --download-amd=yes --download-adifor=yes  --download-superlu=yes
--download-triangle=yes --download-generator=yes  --with-64-bit-pointers=no  --with-cc=mpicc
--CFLAGS='-O2  -msse4.2 -xSSE4.2 -mp1 -I$MKLROOT/include -mkl -fPIC '  --with-cxx='mpicxx'
--CXXFLAGS='-O2 -msse4.2 -xSSE4.2 -mp1 -I$MKLROOT/include -mkl -std=c++11 -fPIC '
--with-fc='mpif90'  --FFLAGS='-O2 -msse4.2 -xSSE4.2 -mp1 -I$MKLROOT/include -mkl -fPIC '
--with-single-library=yes --with-shared-libraries=yes  --with-shared-ld=mpicc
--sharedLibraryFlags="-fpic -mkl -fPIC"  --with-mpi=yes  --with-mpi-shared=yes --with-mpirun=mpiexec
--with-mpi-compilers=yes  --with-x=yes
```

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Example with cmake/make

- ★ Download and unpack the code: wget, … gunzip, … etc.
- ★ Load the modules and dependencies: module load gcc ompi fftw
- ★ Configure the program: you may need to load cmake module
  - mkdir build && cd build
  - cmake .. --help [to see the different options].
  - cmake .. -DCMAKE_INSTALL_PREFIX=installdir {+other options}
- ★ Compile and test:
  - make; make -j8
  - make check; make test
- ★ Install the program:
  - make install

Using the GUI:

ccmake .. {+ options}

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Cmake options for GROMACS

- Download and unpack the source files
- Load modules:

  module load intel/15.0 ompi/3.1.4 fftw cmake
- configure; compile; install

  cd gromacs-5.1.4; mkdir build; cd build

  cmake -DCMAKE_INSTALL_PREFIX=<path to install dir> -DBUILD_SHARED_LIBS=off
  -DBUILD_TESTING=off -DREGRESSIONTEST_DOWNLOAD=off
  -DCMAKE_C_COMPILER=`which mpicc` -DCMAKE_CXX_COMPILER=`which mpicxx`
  -DGMX_BUILD_OWN_FFTW=on -DGMX_SIMD=SSE4.1 -DGMX_DOUBLE=off
  -DGMX_EXTERNAL_BLAS=on -DGMX_EXTERNAL_LAPACK=on
  -DGMX_FFT_LIBRARY=fftw3 -DGMX_GPU=off -DGMX_MPI=on -DGMX_OPENMP=off
  -DGMX_X11=on ../gromacs-5.1.4

  make -j4; make install

Cmake options for CERN-ROOT

- ★ Download and unpack the source files
- ★ Load modules:

  module load gcc/9.2 tbb/2019.5 gsl/2.7.1 python/3.7.5 fftw/3.3.8

  module load cfitsio/4.0.0 mkl/2019.5 cmake/3.16.9 git

  export FFTW_DIR=/global/software/cent7/fftw/3.3.8-gcc92-ompi314
- ★ configure; compile; install

```
mkdir build && cd build
cmake -DCMAKE_INSTALL_PREFIX=<path to install dir>  -DGCC_INSTALL_PREFIX=/global/software/cent7/gcc-9.2.0-rpath-76/ \
-DPYTHON_EXECUTABLE=`which python` -DGSL_CONFIG_EXECUTABLE=/global/software/cent7/gsl/2.7.1-gcc92/bin/gsl-config \
-DGSL_INCLUDE_DIR=/global/software/cent7/gsl/2.7.1-gcc92/include
-DGSL_LIBRARY=/global/software/cent7/gsl/2.7.1-gcc92/lib/libgsl.so \
-DGSL_ROOT_DIR=/global/software/cent7/gsl/2.7.1-gcc92/  -DCMAKE_C_COMPILER=`which gcc` \
-DCMAKE_CXX_COMPILER=`which g++` -DCMAKE_FORTRAN_COMPIER=`which gfortran` \
-DCFITSIO_INCLUDE_DIR=/global/software/cent7/cfitsio/4.0.0-gcc92/include \
-DCFITSIO_LIBRARY=/global/software/cent7/cfitsio/4.0.0-gcc92/lib/libcfitsio.so \
-DJEMALLOC_ROOT_DIR=/usr  -Dpython3=ON -Dpcre=ON -Dzlib=ON Dunuran=ON -Dexplicitlink=ON -Dminuit2=ON -Droofit=ON \
-DCMAKE_SKIP_RPATH=ON -Dxrootd=OFF -Dmysql=OFF -Dkrb5=OFF -Dodbc=OFF -Doracle=OFF \
-DQT_QMAKE_EXECUTABLE=/usr/bin/qmake-qt4  <path to source directory>
```

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Java applications

- ★ Download and unpack the code
- ★ Load java module: module load java
- ★ Run the code

- ★ Example: Trimmomatic
  - wget http://www.usadellab.org/cms/uploads/supplementary/Trimmomatic/Trimmomatic-0.39.zip
  - unzip Trimmomatic-0.39.zip

- ★ Run the code

```
module load java
java -jar <path to>/trimmomatic-0.39.jar {+options if any}
```

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Easybuild as package manager

All CC software stack is installed using easybuild

- ★ Software process:
  - A user request to install software: Ticket
  - Evaluation of the software: HPC analyst
  - Opening an internal ticket for software installation
    - An analyst will install the software
    - Local installation
    - Update the recipe on GitHub
    - Compile the program, push to dev and prod
  - An analyst will follow up with the user: original ticket

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Using easybuild as a user

https://github.com/ComputeCanada/easybuild-easyconfigs/tree/computecanada-main/easybuild/easyconfigs

- ➔ Search for the recipe: eb -S ont-guppy
- ➔ Copy the recipes:
  - ◆ eb ont-guppy-6.2.1.eb --try-software-version=6.4.8 --copy-ec
  - ◆ eb ont-guppy-6.2.1-gcccuda-2020a.eb --try-software-version=6.4.8 --copy-ec
- ➔ Edit the recipes and change the checksums:
  - ◆ eb ont-guppy-6.4.8.eb --force --inject-checksums
  - ◆ eb ont-guppy-6.4.8-gcccuda-2020a.eb --force --inject-checksums
- ➔ Install the modules:
  - ◆ eb ont-guppy-6.4.8.eb --force --sourcepath=./
  - ◆ eb ont-guppy-6.4.8-gcccuda-2020a.eb --force --sourcepath=./

https://docs.easybuild.io/

eb <some recipe> [+options]

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Singularity/Apptainer

Resources: Github, DockerHub, SingularityHub, Aptainer.

Singularity examples: https://github.com/singularityware/singularity/tree/master/examples

- ★ **Documentation:** https://singularityware.github.io/user-guide.html
- ★ **DockerHub:** https://hub.docker.com/explore/
- ★ **SingularityHub:** https://www.singularity-hub.org/
- ★ **Apptainer:** https://apptainer.org/docs/

https://docs.alliancecan.ca/wiki/Singularity/en
https://um-grex.github.io/grex-docs/

Access to Singularity:

- ★ **Connect to cluster:** Grex, cedar, graham, beluga or narval:
- ★ **Load a module:** module load singularity [or apptainer]
- ★ **Build the image:** convert the image from Docker to Singularity [Apptainer]
- ★ **Note:** You may need to use your own Linux machine or VM to build the image.

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Singularity/Apptainer

- ★ Alternative for running software: difficult to build from source
- ★ Possibilite to convert Docker images to singularity.
- ★ Singularity installed on all clusters {no Docker for security reasons}
- ★ Build the image:

```
module load singularity
singularity build qiime2-2021.11.sif docker://quay.io/qiime2/core:2021.11
```

- ★ Run the code via singularity:

```
singularity exec -B $PWD:/home -B /global/scratch/someuser:/outputs  \
-B /global/scratch/someuser/path/to/inputs:/inputs <path to qiime2-2021.11.sif>   \
qiime feature-classifier fit-classifier-naive-bayes \
--i-reference-reads  /outputs/some_output_feature.qza \
--i-reference-taxonomy /outputs/some_output_ref-taxonomy.qza \
--o-classifier /outputs/some_output_classifier.qza
```

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More readings

- ★ FAQ:
  - https://docs.alliancecan.ca/wiki/Frequently_Asked_Questions
- ★ Software:
  - https://docs.alliancecan.ca/wiki/Available_software
  - https://docs.alliancecan.ca/wiki/Utiliser_des_modules/en
  - https://docs.alliancecan.ca/wiki/Installing_software_in_your_home_directory
- ★ Grex: https://um-grex.github.io/grex-docs/

Thank you for your attention

Any question?