Introduction to High Performance Computing Software and Lmod

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Outline

- Software distribution on HPC clusters
- How to find software packages and modules?
- Software stacks on Grex / Alliance clusters
- Hands on:
  - How to use modules to search for installed software?

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Software distribution on HPC clusters

Operating system package managers / repos:

- **Ubuntu:** ~$ *sudo apt-get install <package>*
- **CentOS:** ~$ *sudo yum install <package>*
- **On HPC:** users do not have **sudo**! [**NO NEED TO ASK FOR IT**]

Centralized software stack:

- **Software distributed via CVMFS:** software stacks and modules, …
- **Local software:** modules, restricted software (VASP, Gaussian, …)

Local installation: usually to $HOME or $PROJECT

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

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Software on HPC clusters

- Home made software: programs, scripts and tools, … etc.

  Up to a user, … Help is available!

- Free Software: GNU Public License.
- Open Source, Binaries, Libraries, Compilers, Tools, …

  Maintained by analysts and installed as modules.

- Commercial Software: restricted [VASP, STATA, …]
- Contact support and provide more details about the license, …
- We install the program & protect it with a POSIX group.

  Maintained by HPC analysts and admins.

Modules on HPC clusters

Modules:

- configuration files with instructions to modify the software environment.
- the modular architecture allows multiple versions of the same program to be installed without conflicts.
- contains instructions that modify or initialize environment variables such as PATH and LD_LIBRARY_PATH in order to use different installed programs.

Why modules?

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

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Lmod commands

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

```
[~@bison ]$  module list
Currently Loaded Modules:
SBEnv (S)
Where:
S:  Module is Sticky, requires --force to unload or purge
```

```
[~@rorqual2: ~]$ module list

Currently Loaded Modules:
  1) CCconfig            4) gcc/12.3     (t)   7) libfabric/1.18.0
10) openmpi/4.1.5    (m)  13) aocl-lapack/5.1
  2) gentoo/2023  (S)  5) hwloc/2.9.1     8) pmix/4.2.4
11) flexiblas/3.3.1      14) StdEnv/2023     (S)
  3) gcccore/.12.3 (H)  6) ucx/1.14.1      9) ucc/1.2.0
12) aocl-blas/5.1
```

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Software stacks

- ➔ A set of compilers and libraries:
  - ◆ GCC, Intel compilers, …
  - ◆ Libraries: hdf5, boost, netcdf, petsc, gsl, gdal, geos, … etc.
- ➔ Modules hierarchy:
  - ◆ arch: branch for a given architecture {~~sse3~~, avx2, avx512}
  - ◆ CUDA: any program using GPU acceleration under the same tree.
  - ◆ Core modules: java, perl, … etc.
  - ◆ Compiler:
    - ● GCC: programs compiled with gcc
    - ● Intel: compiled with Intel
  - ◆ OpenMPI: Compiler [Intel, GCC] / OpenMPI
- ➔ Possibility to maintain one or more software stack.

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Software stacks on Grex

- ➔ Grex environment [default]: SBEnv
  - ◆ no module loaded by default, two architectures: avx2/avx512
  - ◆ use module spider <software name> to search for modules
  - ◆ Compilers {GCC, Intel}, MKL, PETSc, GSL, NetCDF… etc.
  - ◆ Gaussian, ANSYS, MATLAB, … etc.

- ➔ The Alliance (CC) environment [optional]: CCEnv
  - ◆ Switch to CCEnv; load a standard environment; choose the architecture[avx2/avx512], use module spider <soft>

```
module load CCEnv
module load arch/avx512
module load StdEnv/2023
module load gcc/12.3 geant4/11.3.0
```

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Software maintenance

- ➔ Compilers/Libraries and more:
- ➔ Compilers: GCC [8.5 - 14.3]; Intel [2019, 2023], … etc.
- ➔ Libraries: HDF5, PETSc, GSL, MKL, Libxc, Boost, NetCDF, ...
- ➔ Gaussian, ANSYS, MATLAB, VASP, ORCA, MCR, Java, Python, R, … etc.
  - ◆ LAMMPS, GROMACS, OpenMM, QE, 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 and/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.

Lmod summary

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>
- module **help** <soft>
- module **purge;** module --force **purge**
- module **use** ~/modulefiles; module **unuse** ~/modulefiles

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Modules: exercises

- **List of modules:** python, java, perl, hdf5, netcdf, lammps, gromacs, cp2k, openmm, gurobi …
- Pick one module from the above list; myprogram
- Run the command: module spider myprogram
- What to expect:
  - The module does not exist {ask for support if needed}
  - One or more versions of the module are available.
    - If many, pick a version and run: module spider myprogram/<version>
    - Read the instructions, load the dependencies and the module
    - Experiment with other commands: module list, module show myprogram, module help myprogram, module whatis, module rm, …
- Run “module purge” and repeat the exercise for another program.

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More readings

Grex:

- https://um-grex.github.io/grex-docs/software/using-modules/
- https://um-grex.github.io/grex-docs/software/software-list/

Alliance clusters:

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

Modules:

- https://lmod.readthedocs.io/en/latest/010_user.html
- https://modules.readthedocs.io/en/v4.1.3/index.html
- https://lmod.readthedocs.io/en/stable/015_writing_modules.html

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Thank you for your attention

Any question?

Additional Slides

module list: narval

```
[~@narval2: ~]$ module list
Currently Loaded Modules:
1) CCconfig              5) hwloc/2.9.1        9) ucc/1.2.0                  13) StdEnv/2023 (S)
2) gentoo/2023    (S)  6) ucx/1.14.1        10) openmpi/4.1.5  (m)  14) mii/1.1.2
3) gcccore/.12.3 (H)  7) libfabric/1.18.0  11) flexiblas/3.3.1
4) gcc/12.3       (t)      8) pmix/4.2.4        12) blis/0.9.0

Where:
  S:  Module is Sticky, requires --force to unload or purge
  m:  MPI implementations / Implémentations MPI
  t:   Tools for development / Outils de développement
  H:  Hidden Module
```

module list: Grex

```
[~@bison ~]$  module list

Currently Loaded Modules:
  1) SBEnv (S)
```

CC software stack:

```
[~@bison ~]$  module load CCEnv
[~@bison ~]$  module load arch/avx512
[~@bison ~]$  module load StdEnv/2023
```

Where:

S: Module is Sticky, requires --force to unload or purge

Note:

- Before starting, make sure you have the appropriate software stack and the compilers and libraries you need.
- Use “module spider” to search for the programs.

Module example: python

```
[~@bison: ~]$ module spider python
python:
  Description:
     The Python programming language. Homepage: https://www.python.org/
  Versions:
      python/3.10.14
      python/3.10.16
      python/3.11.8
      python/3.11.11
      python/3.12.9
 For detailed information about a specific "python" 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 python/3.12.9
```

Module example: python/3.12.9

```
[~@bison: ~]$ module spider python/3.12.9
python: python/3.12.9
  Description:
  The Python programming language. Homepage: https://www.python.org/
 You will need to load all module(s) on any one of the lines below before the "python/3.12.9" module is available to load.

  arch/avx512  gcc/13.2.0
  arch/avx512  gcc/14.3.0
  arch/avx512  intel-one/2024.1
  cuda/12.4.1  arch/avx2  gcc/13.2.0

 Help:
   The Python programming language.
  Homepage: https://www.python.org/
```

We have 4 modules:

- `module load arch/avx512  gcc/13.2.0 python/3.12.9`
- `module load arch/avx512  gcc/14.3.0 python/3.12.9`
- `module load arch/avx512  intel-one/2024.1 python/3.12.9`
- `module load cuda/12.4.1 arch/avx2  gcc/13.2.0 python/3.12.9`

Use one of the above lines to load python/3.12.9

```
[~@bison: ~]$ module load arch/avx512  gcc/13.2.0 python/3.12.9
[~@bison: ~]$ module list
```

module show python/3.12.9

```
[~@bison: ~]$ module show python/3.12.9
/global/software/alma8/sb/modules/base/python/3.11.8:
prepend_path("CMAKE_PREFIX_PATH","/global/software/alma8/sb/opt/base/python/3.11.8")
prepend_path("PATH","/global/software/alma8/sb/opt/base/python/3.11.8/bin")
prepend_path("LD_LIBRARY_PATH","/global/software/alma8/sb/opt/base/python/3.11.8/lib")
prepend_path("MANPATH","/global/software/alma8/sb/opt/base/python/3.11.8/share/man")
setenv("MODULE_PYTHON_PREFIX","/global/software/alma8/sb/opt/base/python/3.11.8")
prepend_path("MODULEPATH","/global/software/alma8/sb/modules/python-3.11.8")
whatis("Description: The Python programming language. Homepage: https://www.python.org/")
family("python")
setenv("PIP_DISABLE_PIP_VERSION_CHECK","1")
setenv("PYDEVD_DISABLE_FILE_VALIDATION","1")
prepend_path("PYTHONPATH","/global/software/alma8/sb/python3/site-packages")
help([[
The Python programming language.
Homepage: https://www.python.org/
]])
```

Module example: boost

```
[~@bison: ~]$ module spider boost
boost:
 Description:
        Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well
        with the C++ Standard Library
 Versions:
        boost/1.78.0
        boost/1.85.0
        Other possible modules matches:
        xgboost
To find other possible module matches execute:
      $ module -r spider '.*boost.*'
For detailed information about a specific "boost" 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 boost/1.85.0
```

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Module example: boost

```
[~@bison: ~]$ module spider boost/1.85.0
  boost: boost/1.85.0
  Description:
     Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++
     Standard Library
  You will need to load all module(s) on any one of the lines below before the "boost/1.85.0" module is available to load.
      arch/avx512 gcc/13.2.0
      cuda/12.4.1 arch/avx2 gcc/13.2.0
```

- module load arch/avx512 gcc/13.2.0 boost/1.85.0
- module load cuda/12.4.1 arch/avx2 gcc/13.2.0 boost/1.85.0

```
Help:
      Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with
      the C++ Standard Library. Boost libraries are intended to be widely useful, and usable across a broad
      spectrum of applications. The Boost license encourages both commercial and non-commercial use.

      Homepage: http://www.boost.org
```

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Module example: boost

```
[~@bison: ~]$ module load arch/avx512  gcc/13.2.0 boost/1.85.0
[~@bison: ~]$ module show boost
/global/software/alma8/sb/modules/arch-avx512-gcc-13.2.0/boost/1.85.0:
prepend_path("CMAKE_PREFIX_PATH","/global/software/alma8/sb/opt/arch-avx512-gcc-13.2.0/boost/1.85.0")
prepend_path("CPATH","/global/software/alma8/sb/opt/arch-avx512-gcc-13.2.0/boost/1.85.0/include")
prepend_path("LIBRARY_PATH","/global/software/alma8/sb/opt/arch-avx512-gcc-13.2.0/boost/1.85.0/lib")
prepend_path("LD_LIBRARY_PATH","/global/software/alma8/sb/opt/arch-avx512-gcc-13.2.0/boost/1.85.0/lib")
setenv("MODULE_BOOST_PREFIX","/global/software/alma8/sb/opt/arch-avx512-gcc-13.2.0/boost/1.85.0")
whatis("Description: Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries
that work well with the C++ Standard Library")
whatis("Homepage: http://www.boost.org")
setenv("BOOST_ROOT","/global/software/alma8/sb/opt/arch-avx512-gcc-13.2.0/boost/1.85.0")
help([[
        Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library.
        Homepage: http://www.boost.org
]])
```

Module example: gromacs

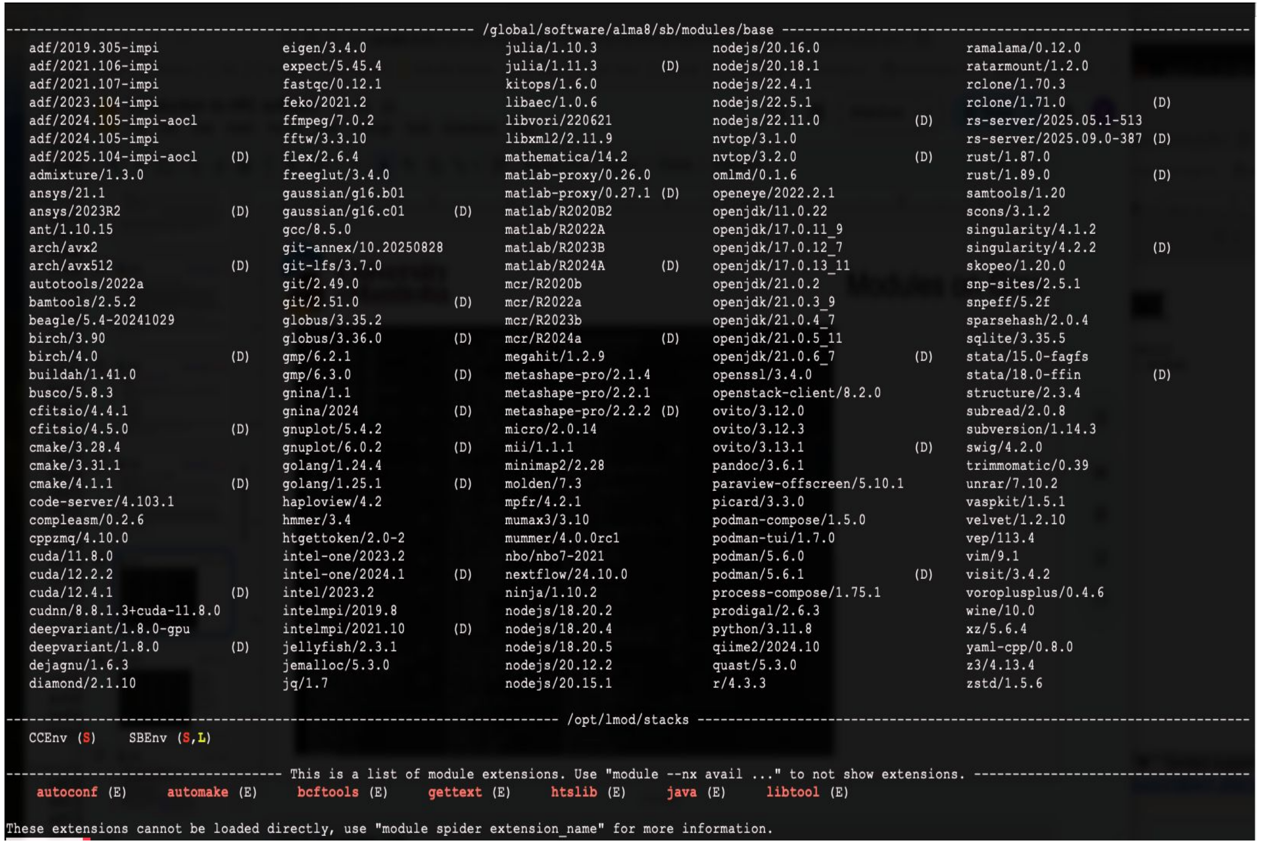
```
[~@bison: ~]$ module spider gromacs
 gromacs:
     Description:
          GROMACS (GROningen MAchine for Chemical Simulations) is a molecular dynamics package primarily
          designed for simulations of proteins, lipids and nucleic acids
    Versions:
      gromacs/2021.6
      gromacs/2022
      gromacs/2023.3
      gromacs/2024.1
      gromacs/2025.2
      gromacs/2025.3
For detailed information about a specific "gromacs" 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 gromacs/2025.3
```

Module example: gromacs

```
[~@bison: ~]$ module spider gromacs/2025.3
gromacs: gromacs/2025.3
   Description:
         GROMACS (GROningen MAchine for Chemical Simulations) is a molecular dynamics package primarily
         designed for simulations of proteins, lipids and nucleic acids
  You will need to load all module(s) on any one of the lines below before the "gromacs/2025.3" module is available to load.
         arch/avx512  gcc/13.2.0  openmpi/5.0.6
         cuda/12.4.1  arch/avx2  gcc/13.2.0
Help:
GROMACS (GROningen MAchine for Chemical Simulations) is a molecular dynamics package primarily designed for
simulations of proteins, lipids and nucleic acids. It was originally developed in the Biophysical Chemistry department of
University of Groningen, and is now maintained by contributors in universities and research centers across the world.
GROMACS is one of the fastest and most popular software packages available and can run on CPUs as well as GPUs. It is
free, open source released under the GNU General Public License. Starting from version 4.6, GROMACS is released under the
GNU Lesser General Public License.

Homepage: http://www.gromacs.org
```

Modules on Grex



```
-------------------------------------------------------------- /global/software/alma8/sb/modules/base ----------------------------------------------------------------
   adf/2019.305-impi                eigen/3.4.0                  julia/1.10.3                nodejs/20.16.0                     ramalama/0.12.0
   adf/2021.106-impi                expect/5.45.4                julia/1.11.3          (D)   nodejs/20.18.1                     ratarmount/1.2.0
   adf/2021.107-impi                fastqc/0.12.1                kitops/1.6.0                nodejs/22.4.1                      rclone/1.70.3
   adf/2023.104-impi                feko/2021.2                  libaec/1.0.6                nodejs/22.5.1                      rclone/1.71.0            (D)
   adf/2024.105-impi-aocl           ffmpeg/7.0.2                 libvori/220621              nodejs/22.11.0              (D)    rs-server/2025.05.1-513
   adf/2024.105-impi                fftw/3.3.10                  libxml2/2.11.9              nvtop/3.1.0                        rs-server/2025.09.0-387 (D)
   adf/2025.104-impi-aocl     (D)   flex/2.6.4                   mathematica/14.2            nvtop/3.2.0                 (D)    rust/1.87.0
   admixture/1.3.0                  freeglut/3.4.0               matlab-proxy/0.26.0         omlmd/0.1.6                        rust/1.89.0              (D)
   ansys/21.1                       gaussian/g16.b01             matlab-proxy/0.27.1 (D)     openeye/2022.2.1                   samtools/1.20
   ansys/2023R2               (D)   gaussian/g16.c01      (D)    matlab/R2020B2              openjdk/11.0.22                    scons/3.1.2
   ant/1.10.15                      gcc/8.5.0                    matlab/R2022A               openjdk/17.0.11_9                  singularity/4.1.2
   arch/avx2                        git-annex/10.20250828        matlab/R2023B               openjdk/17.0.12_7                  singularity/4.2.2        (D)
   arch/avx512                (D)   git-lfs/3.7.0                matlab/R2024A         (D)   openjdk/17.0.13_11                 skopeo/1.20.0
   autotools/2022a                  git/2.49.0                   mcr/R2020b                  openjdk/21.0.2                     snp-sites/2.5.1
   bamtools/2.5.2                   git/2.51.0            (D)    mcr/R2022a                  openjdk/21.0.3_9                   snpeff/5.2f
   beagle/5.4-20241029              globus/3.35.2                mcr/R2023b                  openjdk/21.0.4_7                   sparsehash/2.0.4
   birch/3.90                       globus/3.36.0         (D)    mcr/R2024a            (D)   openjdk/21.0.5_11                  sqlite/3.35.5
   birch/4.0                  (D)   gmp/6.2.1                    megahit/1.2.9               openjdk/21.0.6_7            (D)    stata/15.0-fagfs
   buildah/1.41.0                   gmp/6.3.0             (D)    metashape-pro/2.1.4         openssl/3.4.0                      stata/18.0-ffin          (D)
   busco/5.8.3                      gnina/1.1                    metashape-pro/2.2.1         openstack-client/8.2.0             structure/2.3.4
   cfitsio/4.4.1                    gnina/2024            (D)    metashape-pro/2.2.2 (D)     ovito/3.12.0                       subread/2.0.8
   cfitsio/4.5.0              (D)   gnuplot/5.4.2                micro/2.0.14                ovito/3.12.3                       subversion/1.14.3
   cmake/3.28.4                     gnuplot/6.0.2         (D)    mii/1.1.1                   ovito/3.13.1                (D)    swig/4.2.0
   cmake/3.31.1                     golang/1.24.4                minimap2/2.28               pandoc/3.6.1                       trimmomatic/0.39
   cmake/4.1.1                (D)   golang/1.25.1         (D)    molden/7.3                  paraview-offscreen/5.10.1          unrar/7.10.2
   code-server/4.103.1              haploview/4.2                mpfr/4.2.1                  picard/3.3.0                       vaspkit/1.5.1
   compleasm/0.2.6                  hmmer/3.4                    mumax3/3.10                 podman-compose/1.5.0               velvet/1.2.10
   cppzmq/4.10.0                    htgettoken/2.0-2             mummer/4.0.0rc1             podman-tui/1.7.0                   vep/113.4
   cuda/11.8.0                      intel-one/2023.2             nbo/nbo7-2021               podman/5.6.0                       vim/9.1
   cuda/12.2.2                      intel-one/2024.1      (D)    nextflow/24.10.0            podman/5.6.1                (D)    visit/3.4.2
   cuda/12.4.1                (D)   intel/2023.2                 ninja/1.10.2                process-compose/1.75.1             voroplusplus/0.4.6
   cudnn/8.8.1.3+cuda-11.8.0        intelmpi/2019.8              nodejs/18.20.2              prodigal/2.6.3                     wine/10.0
   deepvariant/1.8.0-gpu            intelmpi/2021.10      (D)    nodejs/18.20.4              python/3.11.8                      xz/5.6.4
   deepvariant/1.8.0          (D)   jellyfish/2.3.1              nodejs/18.20.5              qiime2/2024.10                     yaml-cpp/0.8.0
   dejagnu/1.6.3                    jemalloc/5.3.0               nodejs/20.12.2              quast/5.3.0                        z3/4.13.4
   diamond/2.1.10                   jq/1.7                       nodejs/20.15.1              r/4.3.3                            zstd/1.5.6

------------------------------------------------------------------------- /opt/lmod/stacks ------------------------------------------------------------------------
   CCEnv (S)    SBEnv (S,L)

------------------------------------ This is a list of module extensions. Use "module --nx avail ..." to not show extensions. ------------------------------------
    autoconf (E)    automake (E)    bcftools (E)    gettext (E)    htslib (E)    java (E)    libtool (E)

These extensions cannot be loaded directly, use "module spider extension_name" for more information.
```

module avail

module spider python
module spider java
module spider gromacs

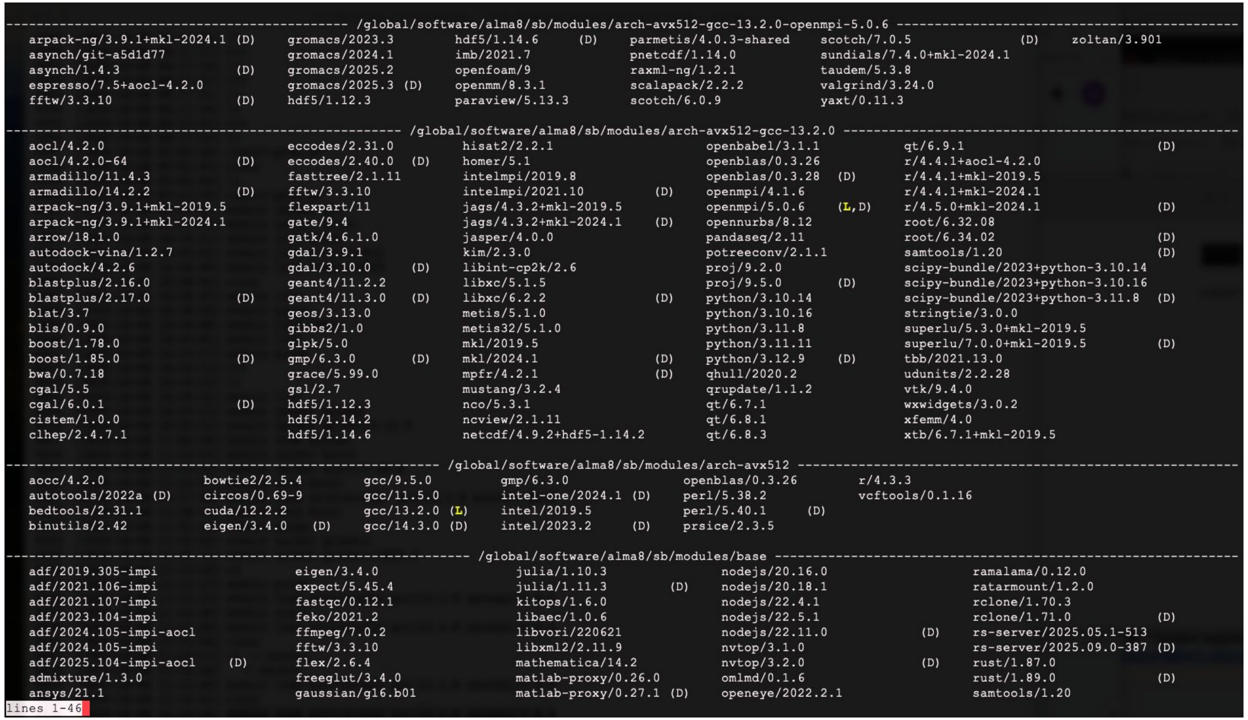
module load arch/avx512
gcc/13.2.0 openmpi/5.0.6
module avail

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

module help <soft>
module show <soft>

module purge

Modules on Grex



```
------------------------------------------- /global/software/alma8/sb/modules/arch-avx512-gcc-13.2.0-openmpi-5.0.6 -------------------------------------------
   arpack-ng/3.9.1+mkl-2024.1 (D)    gromacs/2023.3       hdf5/1.14.6    (D)    parmetis/4.0.3-shared    scotch/7.0.5             (D)    zoltan/3.901
   asynch/git-a5d1d77                gromacs/2024.1       imb/2021.7            pnetcdf/1.14.0           sundials/7.4.0+mkl-2024.1
   asynch/1.4.3               (D)    gromacs/2025.2       openfoam/9            raxml-ng/1.2.1           taudem/5.3.8
   espresso/7.5+aocl-4.2.0           gromacs/2025.3 (D)   openmm/8.3.1          scalapack/2.2.2          valgrind/3.24.0
   fftw/3.3.10                (D)    hdf5/1.12.3          paraview/5.13.3       scotch/6.0.9             yaxt/0.11.3

------------------------------------------------- /global/software/alma8/sb/modules/arch-avx512-gcc-13.2.0 -------------------------------------------------
   aocl/4.2.0                        eccodes/2.31.0       hisat2/2.2.1                    openbabel/3.1.1           qt/6.9.1                                (D)
   aocl/4.2.0-64              (D)    eccodes/2.40.0 (D)   homer/5.1                       openblas/0.3.26           r/4.4.1+aocl-4.2.0
   armadillo/11.4.3                  fasttree/2.1.11      intelmpi/2019.8                 openblas/0.3.28  (D)      r/4.4.1+mkl-2019.5
   armadillo/14.2.2           (D)    fftw/3.3.10          intelmpi/2021.10         (D)    openmpi/4.1.6             r/4.4.1+mkl-2024.1
   arpack-ng/3.9.1+mkl-2019.5        flexpart/11          jags/4.3.2+mkl-2019.5           openmpi/5.0.6    (L,D)    r/4.5.0+mkl-2024.1                      (D)
   arpack-ng/3.9.1+mkl-2024.1        gate/9.4             jags/4.3.2+mkl-2024.1    (D)    opennurbs/8.12            root/6.32.08
   arrow/18.1.0                      gatk/4.6.1.0         jasper/4.0.0                    pandaseq/2.11             root/6.34.02                            (D)
   autodock-vina/1.2.7               gdal/3.9.1           kim/2.3.0                       potreeconv/2.1.1          samtools/1.20                           (D)
   autodock/4.2.6                    gdal/3.10.0    (D)   libint-cp2k/2.6                 proj/9.2.0                scipy-bundle/2023+python-3.10.14
   blastplus/2.16.0                  geant4/11.2.2        libxc/5.1.5                     proj/9.5.0       (D)      scipy-bundle/2023+python-3.10.16
   blastplus/2.17.0           (D)    geant4/11.3.0  (D)   libxc/6.2.2              (D)    python/3.10.14            scipy-bundle/2023+python-3.11.8   (D)
   blat/3.7                          geos/3.13.0          metis/5.1.0                     python/3.10.16            stringtie/3.0.0
   blis/0.9.0                        gibbs2/1.0           metis32/5.1.0                   python/3.11.8             superlu/5.3.0+mkl-2019.5
   boost/1.78.0                      glpk/5.0             mkl/2019.5                      python/3.11.11            superlu/7.0.0+mkl-2019.5                (D)
   boost/1.85.0               (D)    gmp/6.3.0      (D)   mkl/2024.1               (D)    python/3.12.9    (D)      tbb/2021.13.0
   bwa/0.7.18                        grace/5.99.0         mpfr/4.2.1               (D)    qhull/2020.2              udunits/2.2.28
   cgal/5.5                          gsl/2.7              mustang/3.2.4                   qrupdate/1.1.2            vtk/9.4.0
   cgal/6.0.1                 (D)    hdf5/1.12.3          nco/5.3.1                       qt/6.7.1                  wxwidgets/3.0.2
   cistem/1.0.0                      hdf5/1.14.2          ncview/2.1.11                   qt/6.8.1                  xfemm/4.0
   clhep/2.4.7.1                     hdf5/1.14.6          netcdf/4.9.2+hdf5-1.14.2        qt/6.8.3                  xtb/6.7.1+mkl-2019.5

------------------------------------------------------- /global/software/alma8/sb/modules/arch-avx512 -------------------------------------------------------
   aocc/4.2.0          bowtie2/2.5.4      gcc/9.5.0         gmp/6.3.0               openblas/0.3.26        r/4.3.3
   autotools/2022a (D) circos/0.69-9      gcc/11.5.0        intel-one/2024.1 (D)    perl/5.38.2            vcftools/0.1.16
   bedtools/2.31.1     cuda/12.2.2        gcc/13.2.0 (L)    intel/2019.5            perl/5.40.1     (D)
   binutils/2.42       eigen/3.4.0   (D)  gcc/14.3.0 (D)    intel/2023.2     (D)    prsice/2.3.5

------------------------------------------------------------ /global/software/alma8/sb/modules/base ------------------------------------------------------------
   adf/2019.305-impi                 eigen/3.4.0               julia/1.10.3              nodejs/20.16.0                ramalama/0.12.0
   adf/2021.106-impi                 expect/5.45.4             julia/1.11.3       (D)    nodejs/20.18.1                ratarmount/1.2.0
   adf/2021.107-impi                 fastqc/0.12.1             kitops/1.6.0              nodejs/22.4.1                 rclone/1.70.3
   adf/2023.104-impi                 feko/2021.2               libaec/1.0.6              nodejs/22.5.1                 rclone/1.71.0                (D)
   adf/2024.105-impi-aocl            ffmpeg/7.0.2              libvori/220621            nodejs/22.11.0         (D)    rs-server/2025.05.1-513
   adf/2024.105-impi                 fftw/3.3.10               libxml2/2.11.9            nvtop/3.1.0                   rs-server/2025.09.0-387      (D)
   adf/2025.104-impi-aocl     (D)    flex/2.6.4                mathematica/14.2          nvtop/3.2.0            (D)    rust/1.87.0
   admixture/1.3.0                   freeglut/3.4.0            matlab-proxy/0.26.0       omlmd/0.1.6                   rust/1.89.0                  (D)
   ansys/21.1                        gaussian/g16.b01          matlab-proxy/0.27.1 (D)   openeye/2022.2.1              samtools/1.20
lines 1-46
```

module load arch/avx512
gcc/13.2.0 openmpi/5.0.6

module avail

module spider gromacs
module spider cp2k

If not available:

➔ contact support

support@tech.alliancecan.ca

https://um-grex.github.io/grex-docs/software/software-list/

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CVMFS on Grex

```
[~@bison ~]$  cvmfs_config probe
Probing /cvmfs/cvmfs-config.computecanada.ca... OK
Probing /cvmfs/soft.computecanada.ca... OK
Probing /cvmfs/restricted.computecanada.ca... OK
```

```
[~@bison ~]$  ls -1 /cvmfs/
cvmfs-config.computecanada.ca
restricted.computecanada.ca
soft.computecanada.ca
```

```
[~@~]$ module load CCEnv
[~@~]$ module load arch/avx512
[~@~]$ module load StdEnv/2023
[~@~]$ module spider geant4
[~@~]$ module spider geant4/11.3.0

[~@~]$ module load StdEnv/2023  gcc/12.3 geant4/11.3.0
```

```
[~@bison ~]$  ls /cvmfs/
cvmfs-config.computecanada.ca  restricted.computecanada.ca  soft.computecanada.ca
```

CVMFS on Grex: neurodesk.ardc.edu.au

```
[~@bison ~]$  ls /cvmfs/
cvmfs-config.computecanada.ca  restricted.computecanada.ca  soft.computecanada.ca

[~@bison ~]$ ls /cvmfs/neurodesk.ardc.edu.au
[~@bison ~]$ ls /cvmfs
     cvmfs-config.computecanada.ca  neurodesk.ardc.edu.au
     restricted.computecanada.ca  soft.computecanada.ca

[~@bison ~]$  ls /cvmfs/neurodesk.ardc.edu.au/neurodesk-modules
[~@bison ~]$  module use /cvmfs/neurodesk.ardc.edu.au/neurodesk-modules
[~@bison ~]$  module spider fsl
[~@bison ~]$  module spider functional_imaging/fsl/6.0.7.18
[~@bison ~]$  module load functional_imaging/fsl/6.0.7.18
[~@bison ~]$  module list
[~@bison ~]$  which fsl
/cvmfs/neurodesk.ardc.edu.au/containers/fsl_6.0.7.18_20250928/fsl
```

https://neurodesk.org/getting-started/neurocontainers/cvmfs/

Find and load Gaussian

Gaussian: restricted software; requires a registration

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

```
[~@bison ~]$  module spider gaussian
  gaussian:
      Versions:
      gaussian/g16.b01
      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
```

```
➔   [~@bison ~]$  module load gaussian
➔   [~@bison ~]$  module load gaussian/g16.c01
➔   [~@bison ~]$  module load gaussian/g16.b01
```

Find and load ORCA

ORCA: restricted software; requires a registration
https://um-grex.github.io/grex-docs/specific-soft/orca/

```
[~@bison ~]$ module spider orca
  orca:
        Versions:
         orca/5.0.4
         orca/6.0.1
  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/6.0.1
 ➔      [~@bison ~]$ module load arch/avx512 intel/2023.2  openmpi/4.1.6 orca/5.0.4
 ➔      [~@bison ~]$ module load arch/avx512 gcc/13.2.0  openmpi/4.1.6 orca/6.0.1
[~@bison ~]$  module load arch/avx512  gcc/13.2.0  openmpi/4.1.6 orca/6.0.1
      To execute ORCA, run:
          ${MODULE_ORCA_PREFIX}/orca orca.inp > orca.out
```

Find and load LAMMPS

```
[~@bison ~]$ module spider lammps
  lammps:
        Versions:
            lammps/2021-09-29
            lammps/2024-08-29p1-nep
            lammps/2024-08-29p1
```

```
[~@bison ~]$ module spider lammps/2024-08-29p1
   You will need to load all module(s) on any one of the
   lines below before the "lammps/2024-08-29p1"
   module is available to load.
 ●    arch/avx512  gcc/13.2.0  openmpi/4.1.6
 ●    arch/avx512  intel-one/2024.1  openmpi/4.1.6
 ●    cuda/12.4.1  arch/avx2  gcc/13.2.0  openmpi/4.1.6
```

```
[~@bison ~]$ module load arch/avx512  gcc/13.2.0  openmpi/4.1.6 lammps/2024-08-29p1
[~@bison ~]$ module list
Currently Loaded Modules:
   1) SBEnv       (S)   4) openmpi/4.1.6   7) fftw/3.3.10       10) zstd/1.5.6       13) gsl/2.7
   2) arch/avx512        5) kim/2.3.0       8) openblas/0.3.26  11) hdf5/1.14.2     14) lammps/2024-08-29p1
   3) gcc/13.2.0         6) ffmpeg/7.0.2    9) eigen/3.4.0      12) netcdf/4.9.2+hdf5-1.14.2
[~@bison ~]$ which lmp
/global/software/alma8/sb/opt/arch-avx512-gcc-13.2.0-openmpi-4.1.6/lammps/2024-08-29p1/bin/lmp
```

Find and load QE

```
[~@bison ~]$ module spider espresso
 espresso:
       Versions:
       espresso/7.3.1+aocl-4.2.0
       espresso/7.3.1
       espresso/7.4.1+aocl-4.2.0
       espresso/7.4.1
       espresso/7.5+aocl-4.2.0
       espresso/7.5

For detailed information about a specific "espresso" 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 espresso/7.4.1
```

➔ `[~@bison ~]$ module spider espresso/7.4.1`

➔ `[~@bison ~]$module load arch/avx512  intel/2023.2  openmpi/4.1.6 espresso/7.4.1`

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Find and load MATLAB

```
[~@bison ~]$ module spider matlab
  matlab:
    Versions:
        matlab/R2020B2
        matlab/R2022A
        matlab/R2023B
        matlab/R2024A
  For detailed information about a specific "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 matlab/R2024A
```

```
➔    [~@bison ~]$ module load matlab/R2024A
➔    [~@bison ~]$ module load matlab/R2023B
➔    [~@bison ~]$ module load matlab/R2022A
➔    [~@bison ~]$ module load matlab/R2020B2
```

Find and load MCR

```
[~@bison ~]$ module spider mcr
 mcr:
   Versions:
     mcr/R2020b
     mcr/R2022a
     mcr/R2023b
     mcr/R2024a
 For detailed information about a specific "mcr" package (including how to load the modules)
 use the module's full name.

 For example:
   $ module spider mcr/R2024a

➔    [~@bison ~]$ module load mcr/R2020b
➔    [~@bison ~]$ module load mcr/R2022a
➔    [~@bison ~]$ module load mcr/R2023b
➔    [~@bison ~]$ module load mcr/R2024a
```

Building software

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Building software

- ➔ Local installation [user’s directory: home, project]:
  - ◆ R packages; Julia packages, Perl modules
  - ◆ Python packages: virtual environment
  - ◆ 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
- ➔ Containers: Singularity, Aptainer, Podman: {separate talk}
  - ◆ build the image and run your program using the container

Building software

- ➔ R packages: minimal installation
  - ◆ R as modules: users can install the packages in their home directory.
- ➔ Python as modules: python and scipy-stack or scipy-bundle
  - ◆ users can install the packages needed in their home or project directories.
- ➔ Julia packages
- ➔ Perl as module:
  - ◆ 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
  - ◆ Custom software: patch from a user, changing parts of the code, … etc.

R packages

- ➔ R packages: rgdal, adegenet, stats, rjags, dplyr, sf, … etc.
- ➔ Choose a module version: module spider r
- ➔ Load R and dependencies (gdal, geos, jags, gsl, udunits… etc):
  - ◆ module load gcc r <+other external modules>
- ➔ Launch R and install the packages:

```
~$ R
> install.packages(”dplyr")
'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(”other packages")
```

Python packages

- ➔ Load the modules:
  - ◆ module load <deps> python <+ext>
- ➔ 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 python
virtualenv ~/my_venv
source ~/my_venv/bin/activate
pip install cutadapt
deactivate
```

```
source ~/my_venv/bin/activate
cutadapt [+options]
deactivate
```

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Perl packages

- ➔ 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
- ➔ Update the ~/.bashrc [for the first time, it asks to update ~/.bashrc]

Java applications

➔ Download and unpack the code using wget, curl, … etc.

➔ Load java module [run module spider 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}
```

STAR

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

```
wget https://github.com/alexdobin/STAR/archive/refs/tags/2.7.11b.tar.gz
```

- ➔ Unpack the code: `tar -xvf 2.7.11b.tar.gz`
- ➔ Load GCC compiler: `module load gcc`
- ➔ Compile the code:

```
cd  STAR-2.7.11b/source
make
```

- ➔ Copy the binaries and set the path:

```
mkdir -p ~/software/star/2.7.11b/bin
cp STAR  ~/software/star/2.7.11b/bin
export PATH=$PATH:${HOME}/software/star/2.7.11b/bin
```

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/$USER/software/treemix/1.13`
- ➔ Compile and install: `make && make test && make install`
- ➔ Set a path: `export PATH=$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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configure/make

- Download and unpack the code: wget, … gunzip, … etc.
- Load a compiler and dependencies: module load gcc openmpi 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
- Set the path: export PATH=${PATH}:<path to install dir>/bon

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ABINIT

```
module load intel openmpi 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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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=${fftsrc}
--download-amd=yes --download-adifor=yes  --download-superlu=yes --download-triangle=yes
--download-generator=yes   --with-64-bit-pointers=no  --with-cc=mpicc  --CFLAGS='-O2
-I$MKLROOT/include -mkl -fPIC '   --with-cxx='mpicxx'  --CXXFLAGS='-O2 -I$MKLROOT/include
-mkl -std=c++11 -fPIC '  --with-fc='mpif90'  --FFLAGS='-O2 -I$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 {+other options}
make && make install
```

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cmake/make

- Download and unpack the code: wget, … gunzip, … etc.
- Load a compiler 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

GROMACS

- Download and unpack the source files
- Load modules:

```
module load intel openmpi 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
```

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Summary

➔ Use Lmod commands to search for the modules:
- ◆ Compilers, OpenMPI, NetCDF, HDF5, PETSc, Gaussian, ANSYS, MATLAB, ORCA, MCR, Java, Python, R, … etc.

➔ Some packages require a local installation:
- ◆ Home made programs, Python, Perl, R, Julia packages, ...

➔ Software maintenance on Grex and Alliance clusters:
- ◆ 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 and/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.