LUMI Software Stacks

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LUMI

What this talk is about…

- Software stacks on LUMI
- Some remarks about Lmod
- Creating your customised environment with EasyBuild
- Containers

Design considerations

- Very leading edge and inhomogeneous machine (new interconnect, new GPU architecture with an immature software ecosystem, some NVIDIA GPUs for visualisation, a mix of zen2 and zen3)
  - Need to remain agile
- Users that come to LUMI from 11 different channels (not counting subchannels), with different expectations
- Small central support team considering the expected number of projects and users and the tasks the support team has
  - But contributions from local support teams
- Cray Programming Environment is a key part of our system
- Need for customised setups
  - Everybody wants a central stack as long as their software is in there but not much more
  - Look at the success of conda, Python virtual environments, containers, …

The LUMI solution

- Software organised in extensible software stacks based on a particular release of the PE
  - Many base libraries and some packages already pre-installed
  - Easy way to install additional packages in project space
- Modules managed by Lmod
  - More powerful than the (old) Modules Environment which is also supported by HPE Cray
  - Powerful features to search for modules
- EasyBuild is our primary tool for software installations
  - But uses HPE Cray specific toolchains
  - Offer a library of installation recipes
  - User installations integrate seamlessly with the central stack
  - We do have a Spack setup but don’t do development in Spack ourselves

Policies

- Bring-your-own-license except for a selection of tools that are useful to a larger community
  - One downside of the distributed user management is that we do not even have the information needed to determine if a particular userid can use a particular software license
- LUST tries to help with installations of recent software but porting or bug fixing is not our work
  - Not all Linux or even supercomputer software will work on LUMI
  - We're too small a team to do all software installations, so don't count on us to do all the work
- Conda, Python installations need to go in containers
  - We offer a container-based wrapper (lumi-container-wrapper) to do that

Organisation: Software stacks

- **CrayEnv:** Cray environment with some additional tools pushed in through EasyBuild
- **LUMI** stacks, each one corresponding to a particular release of the PE
  - Work with the Cray PE modules , but accessed through a replacement for the PrgEnv-* modules
  - Tuned versions for the 3 ~~4~~ types of hardware: zen2 (login, large memory nodes), zen3 (LUMI-C compute nodes), ~~zen2 + NVIDIA GPU (visualisation partition)~~, zen3 + MI250X (LUMI-G GPU partition)
- **spack:** Install software with Spack using compilers from the PE
  - Offered as-is for users who know Spack, but we do not do development in Spack
- Distant future: Stack based on common EB toolchains as-is for LUMI-C

Accessing the Cray PE on LUMI
3 different ways

- Very bare environment available directly after login
  - What you can expect on a typical Cray system
  - Few tools as only the base OS image is available
  - User fully responsible for managing the target modules
- **CrayEnv**
  - "Enriched" Cray PE environment
  - Takes care of managing the target modules: (re)loading CrayEnv will reload an optimal set for the node you're on
  - Some additional tools, e.g., newer build tools (offered here and not in the bare environment as we need to avoid conflicts with other software stacks)
  - Otherwise used in the way discussed in this course

Accessing the Cray PE on LUMI

3 different ways

- **LUMI** software stack
  - Each stack based on a particular release of the HPE Cray PE
    - Other modules are accessible but hidden from the default view
  - Better not to use the PrgEnv modules but the EasyBuild LUMI toolchains

HPE Cray PE	LUMI toolchain	
PrgEnv-cray	cpeCray	Cray Compiler Environment
PrgEnv-gnu	cpeGNU	GNU C/C++ and Fortran
PrgEnv-aocc	cpeAOCC	AMD CPU compilers
PrgEnv-amd	cpeAMD	AMD ROCm GPU compilers (LUMI-G only)

  - Environment in which we install most software

Accessing the Cray PE on LUMI

The LUMI software stack

- The LUMI software stack uses two levels of modules
  - LUMI/21.12, LUMI/22.08: Versions of the LUMI stack
  - partition/L, partition/C, partition/G (~~and future partition/D~~): To select software optimised for the respective LUMI partition
    - partition/L is for both the login nodes and the large memory nodes (4TB)
  - Hidden partition/common for software that is available everywhere, but be careful using it for your own installs
  - When (re)loaded, the LUMI module will load the best matching partition module.
  - So be careful in job scripts: When your job starts, the environment will be that of the login nodes, but if you trigger a reload of the LUMI module it will be that of the compute node!

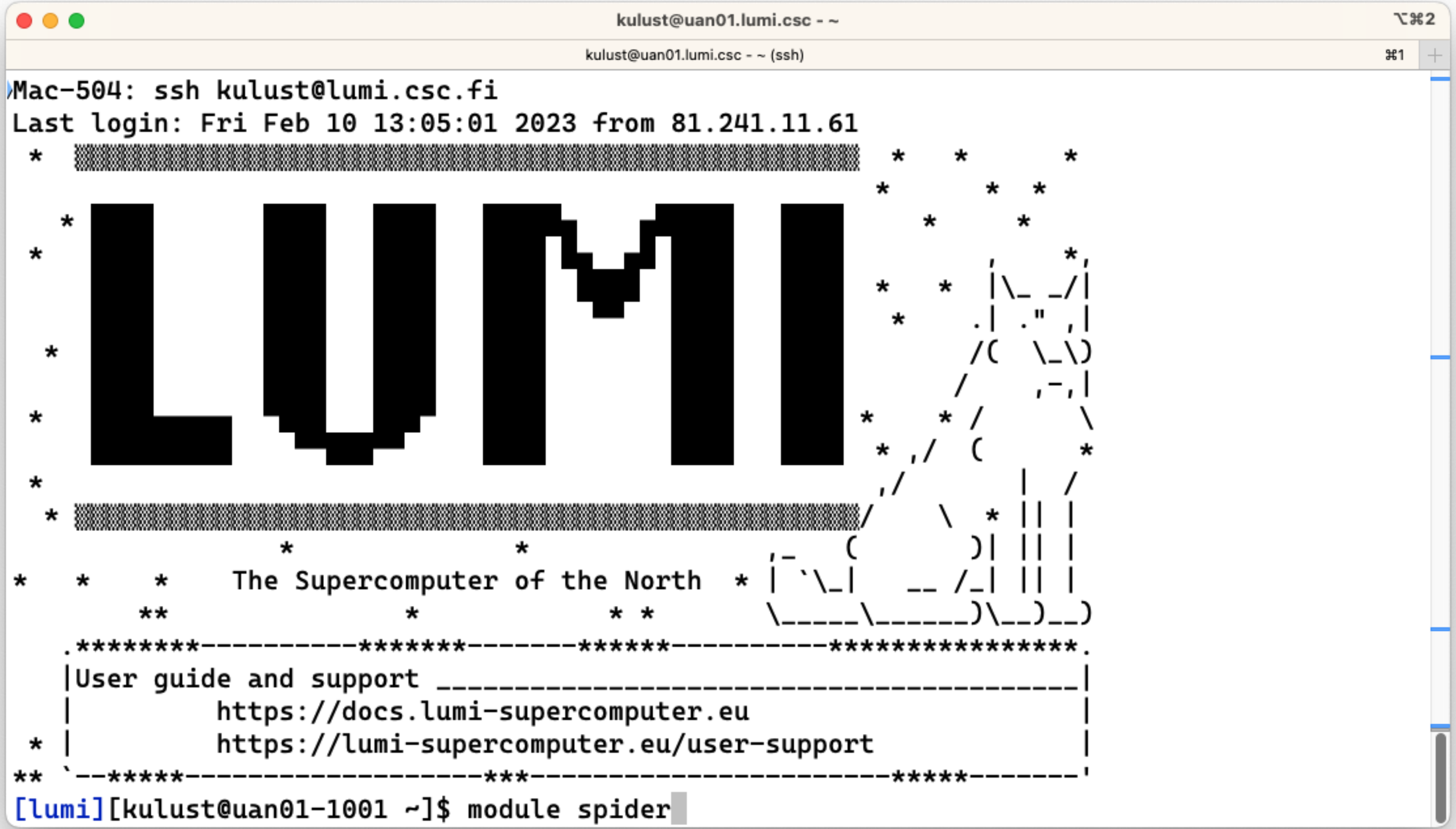
Exploring modules with Lmod

- Contrary to some other module systems, not all modules are immediately available for loading
  - Installed modules: All modules on the system that can be loaded one way or another
  - Available modules: Can be loaded without first loading another module
- Examples in the HPE Cray PE:
  - `cray-mpich` can only be loaded if a compiler module and network target module are loaded
  - Many of the performance monitoring tools only become available after loading `perftools-base`
  - `cray-fftw` only becomes available when a processor target module is loaded
- Tools
  - `module avail` is for searching in the available modules
  - `module spider` and `module keyword` are for searching in the installed modules

module spider

- `module spider` : Long list of all installed software with short description
  - Will also look into modules for "extensions" and show those also, marked with an "E"
- `module spider gnuplot` : Shows all versions of gnuplot on the system
  `module spider CMake`
- `module spider gnuplot/5.4.3-cpeGNU-22.08` : Shows help information for the specific module, including what should be done to make the module available
  - But this does not completely work with the Cray PE modules
- `module spider CMake/3.24.0` : Will tell you which module contains CMake and how to load it

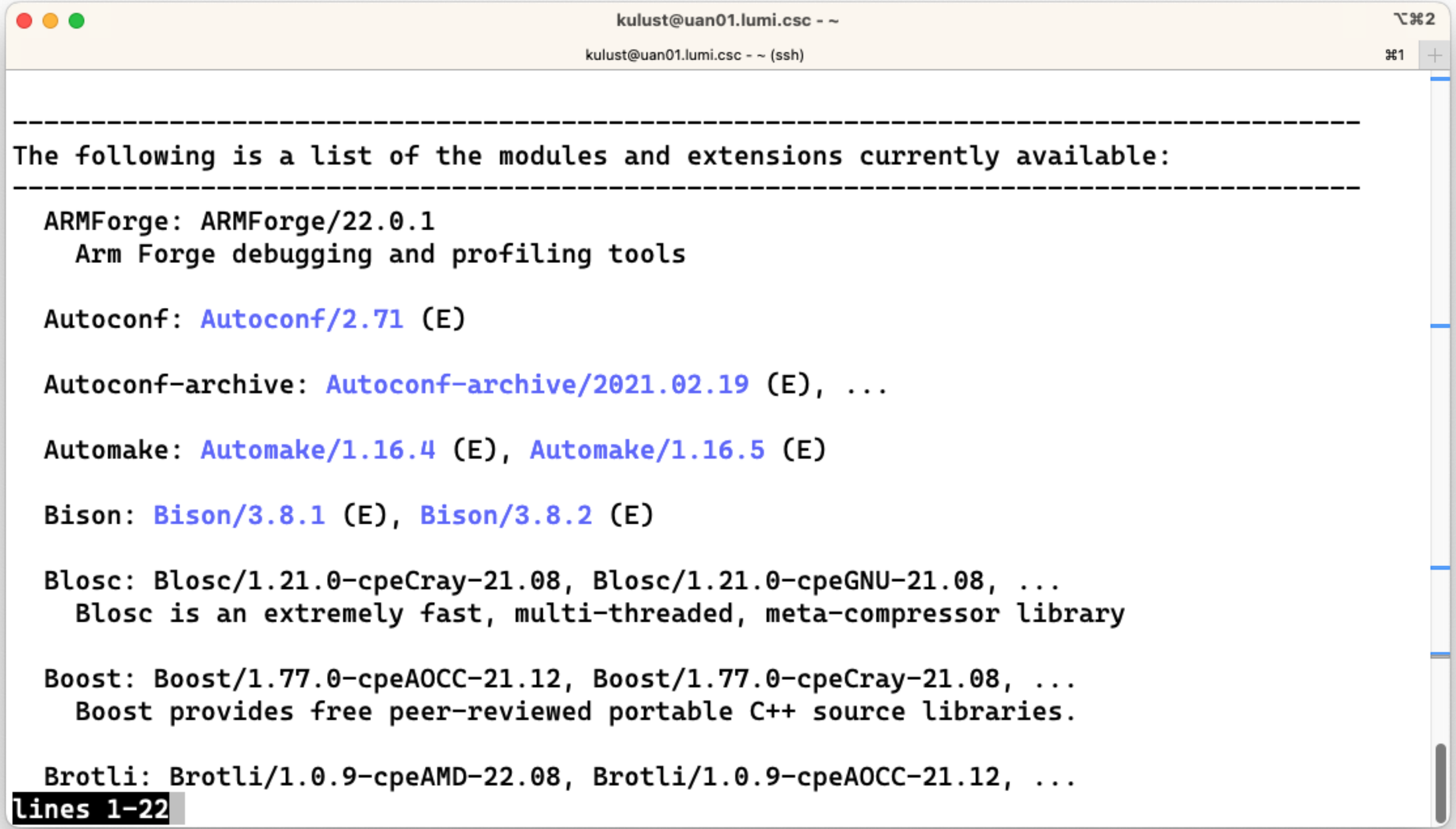
module spider (command) (1)



```
Mac-504: ssh kulust@lumi.csc.fi
Last login: Fri Feb 10 13:05:01 2023 from 81.241.11.61

*    *     *      The Supercomputer of the North  *
        **              *             * *
    .********----------*******-------******----------***************.
    |User guide and support ________________________________________|
    |         https://docs.lumi-supercomputer.eu                    |
 *  |         https://lumi-supercomputer.eu/user-support            |
**  `--*****------------------***-------------------------*****------'
[lumi][kulust@uan01-1001 ~]$ module spider
```

module spider (command) (2)

LUMI

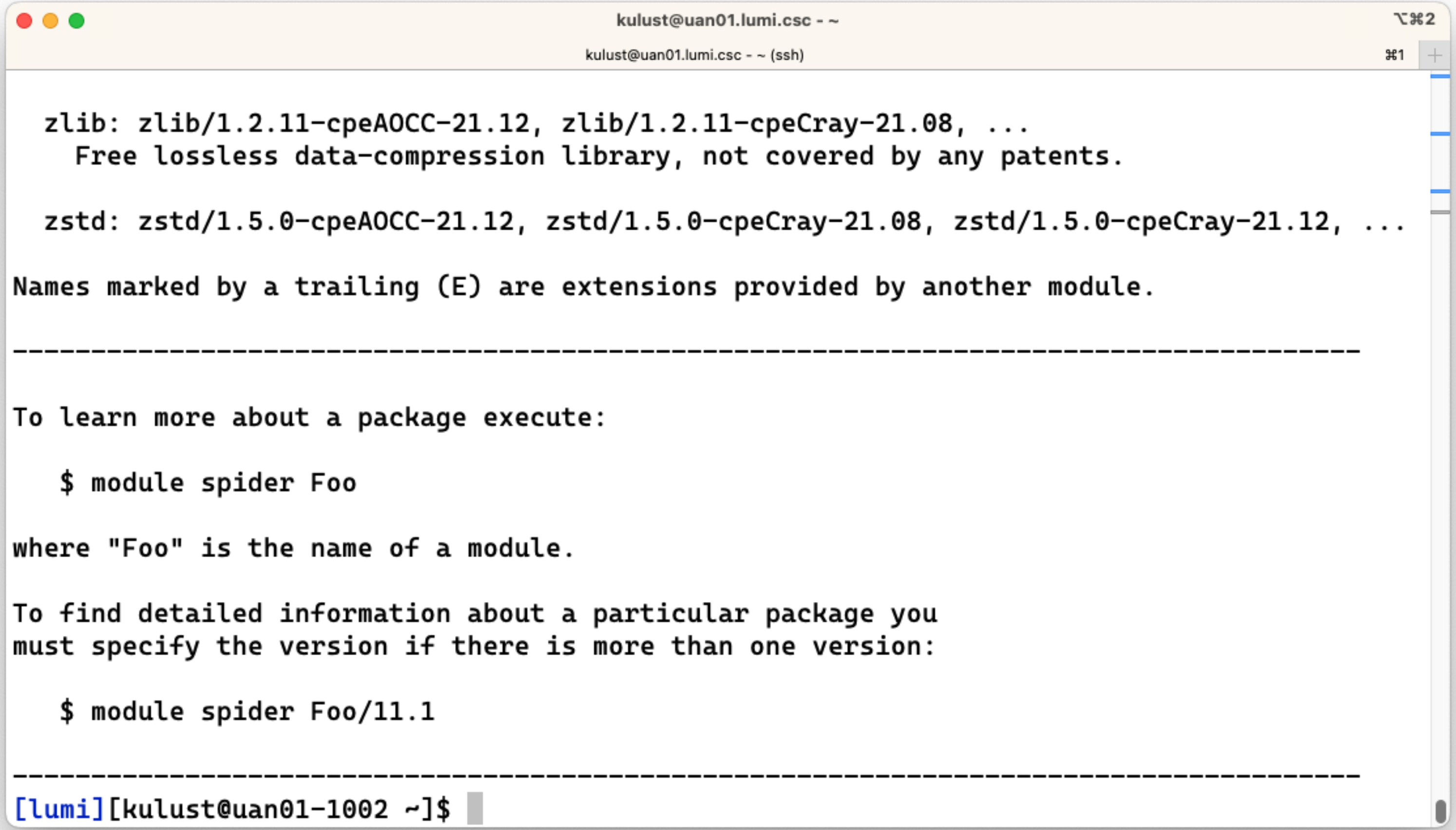


kulust@uan01.lumi.csc - ~

kulust@uan01.lumi.csc - ~ (ssh)

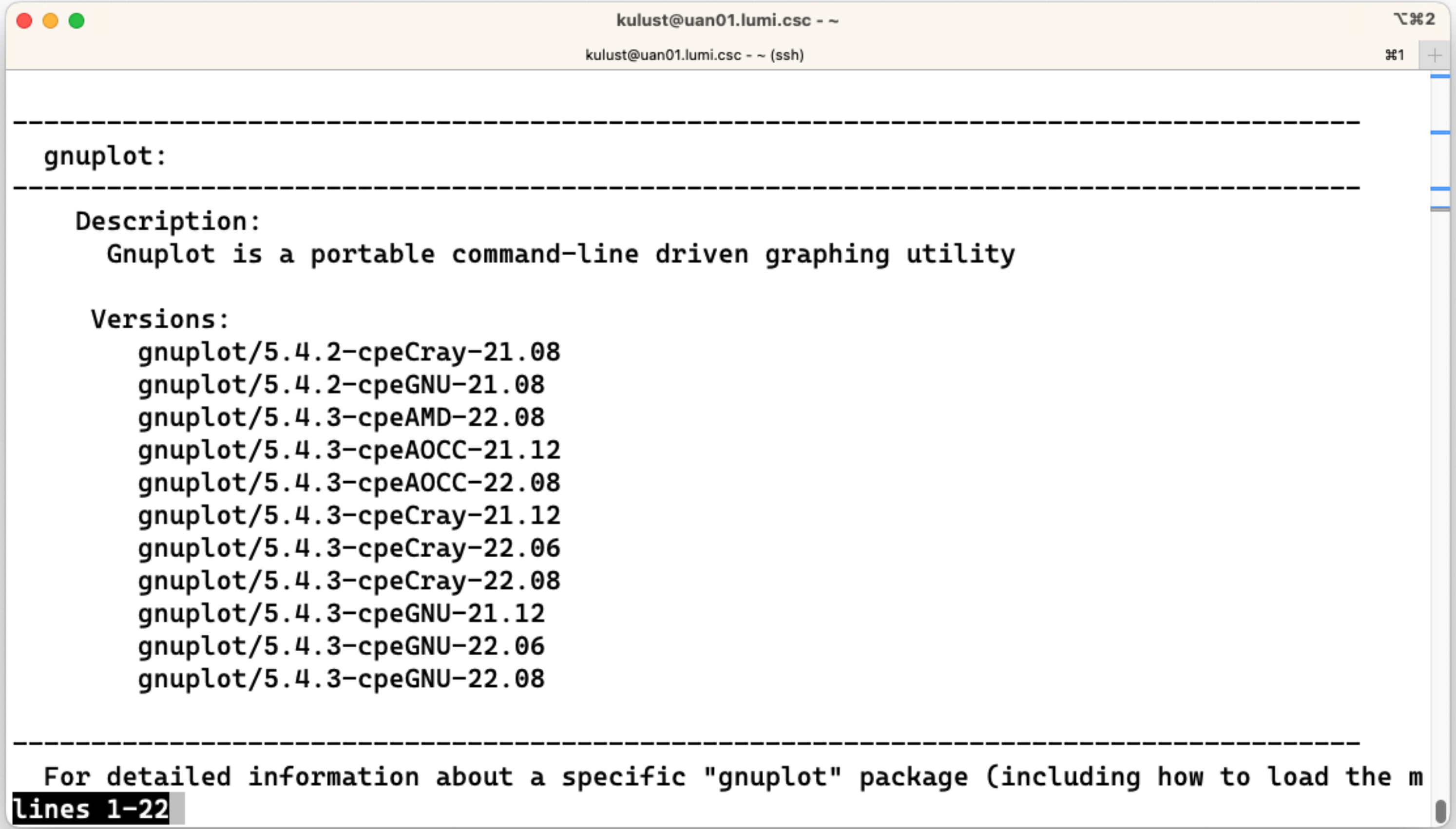
```
---------------------------------------------------------------------------------------
The following is a list of the modules and extensions currently available:
---------------------------------------------------------------------------------------
  ARMForge: ARMForge/22.0.1
    Arm Forge debugging and profiling tools

  Autoconf: Autoconf/2.71 (E)

  Autoconf-archive: Autoconf-archive/2021.02.19 (E), ...

  Automake: Automake/1.16.4 (E), Automake/1.16.5 (E)

  Bison: Bison/3.8.1 (E), Bison/3.8.2 (E)

  Blosc: Blosc/1.21.0-cpeCray-21.08, Blosc/1.21.0-cpeGNU-21.08, ...
    Blosc is an extremely fast, multi-threaded, meta-compressor library

  Boost: Boost/1.77.0-cpeAOCC-21.12, Boost/1.77.0-cpeCray-21.08, ...
    Boost provides free peer-reviewed portable C++ source libraries.

  Brotli: Brotli/1.0.9-cpeAMD-22.08, Brotli/1.0.9-cpeAOCC-21.12, ...
lines 1-22
```

module spider (command) (3)



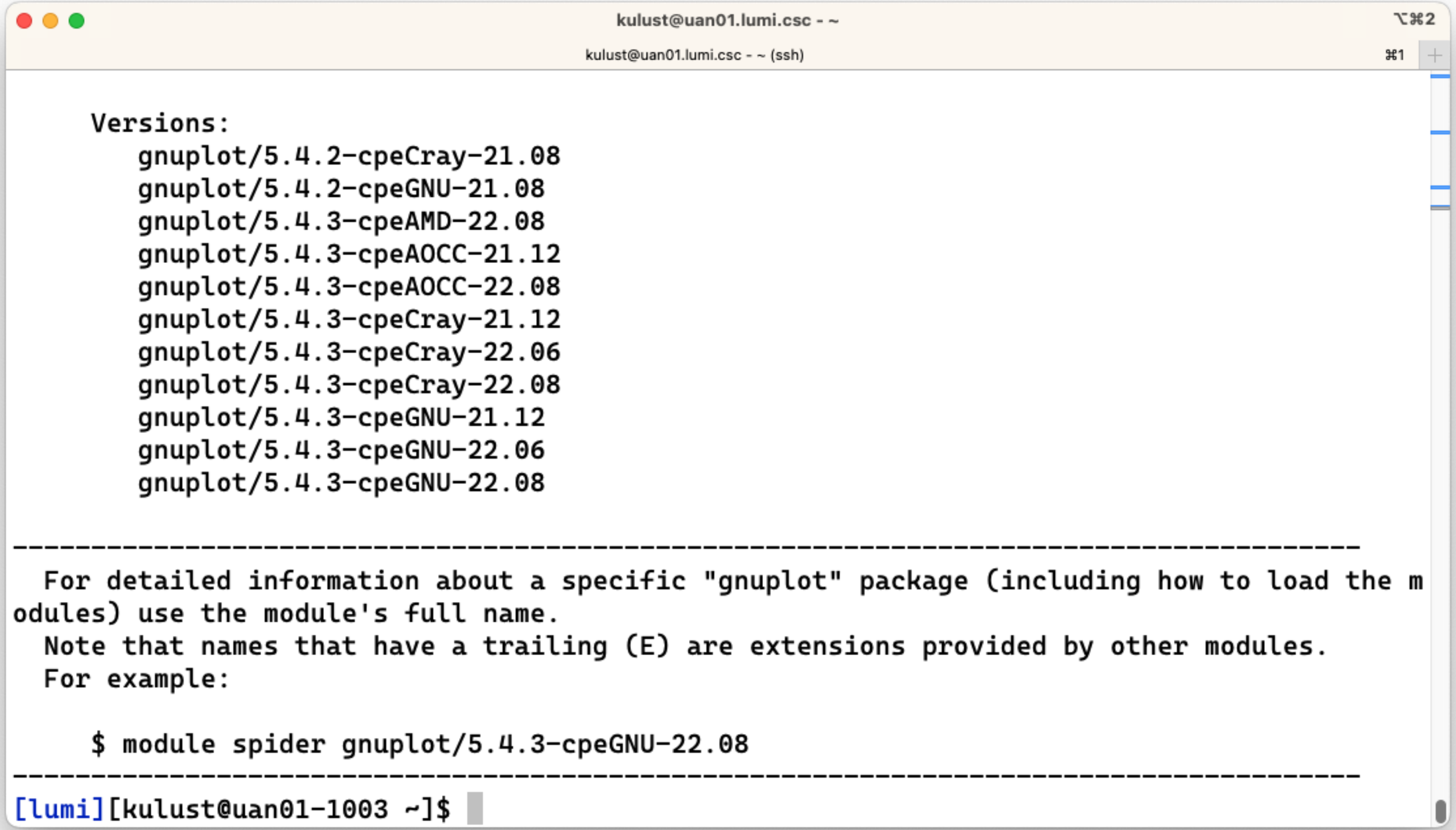
```
  zlib: zlib/1.2.11-cpeAOCC-21.12, zlib/1.2.11-cpeCray-21.08, ...
    Free lossless data-compression library, not covered by any patents.

  zstd: zstd/1.5.0-cpeAOCC-21.12, zstd/1.5.0-cpeCray-21.08, zstd/1.5.0-cpeCray-21.12, ...

Names marked by a trailing (E) are extensions provided by another module.

---------------------------------------------------------------------------------------


To learn more about a package execute:

   $ module spider Foo

where "Foo" is the name of a module.

To find detailed information about a particular package you
must specify the version if there is more than one version:

   $ module spider Foo/11.1

---------------------------------------------------------------------------------------
[lumi][kulust@uan01-1002 ~]$
```

module spider gnuplot



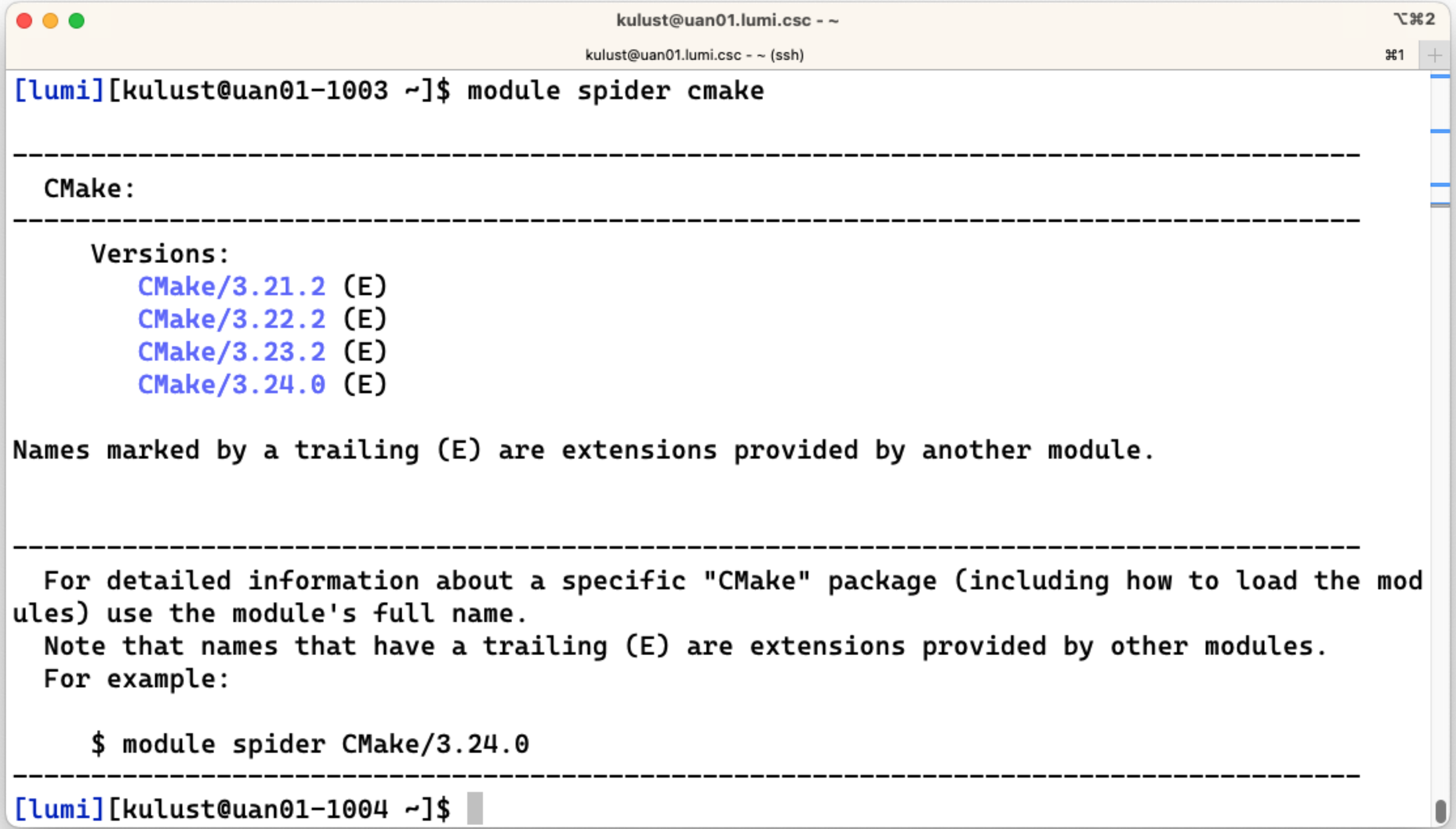
```
------------------------------------------------------------------------------
  gnuplot:
------------------------------------------------------------------------------
    Description:
      Gnuplot is a portable command-line driven graphing utility

     Versions:
        gnuplot/5.4.2-cpeCray-21.08
        gnuplot/5.4.2-cpeGNU-21.08
        gnuplot/5.4.3-cpeAMD-22.08
        gnuplot/5.4.3-cpeAOCC-21.12
        gnuplot/5.4.3-cpeAOCC-22.08
        gnuplot/5.4.3-cpeCray-21.12
        gnuplot/5.4.3-cpeCray-22.06
        gnuplot/5.4.3-cpeCray-22.08
        gnuplot/5.4.3-cpeGNU-21.12
        gnuplot/5.4.3-cpeGNU-22.06
        gnuplot/5.4.3-cpeGNU-22.08

------------------------------------------------------------------------------
  For detailed information about a specific "gnuplot" package (including how to load the m
lines 1-22
```

module spider gnuplot (2)



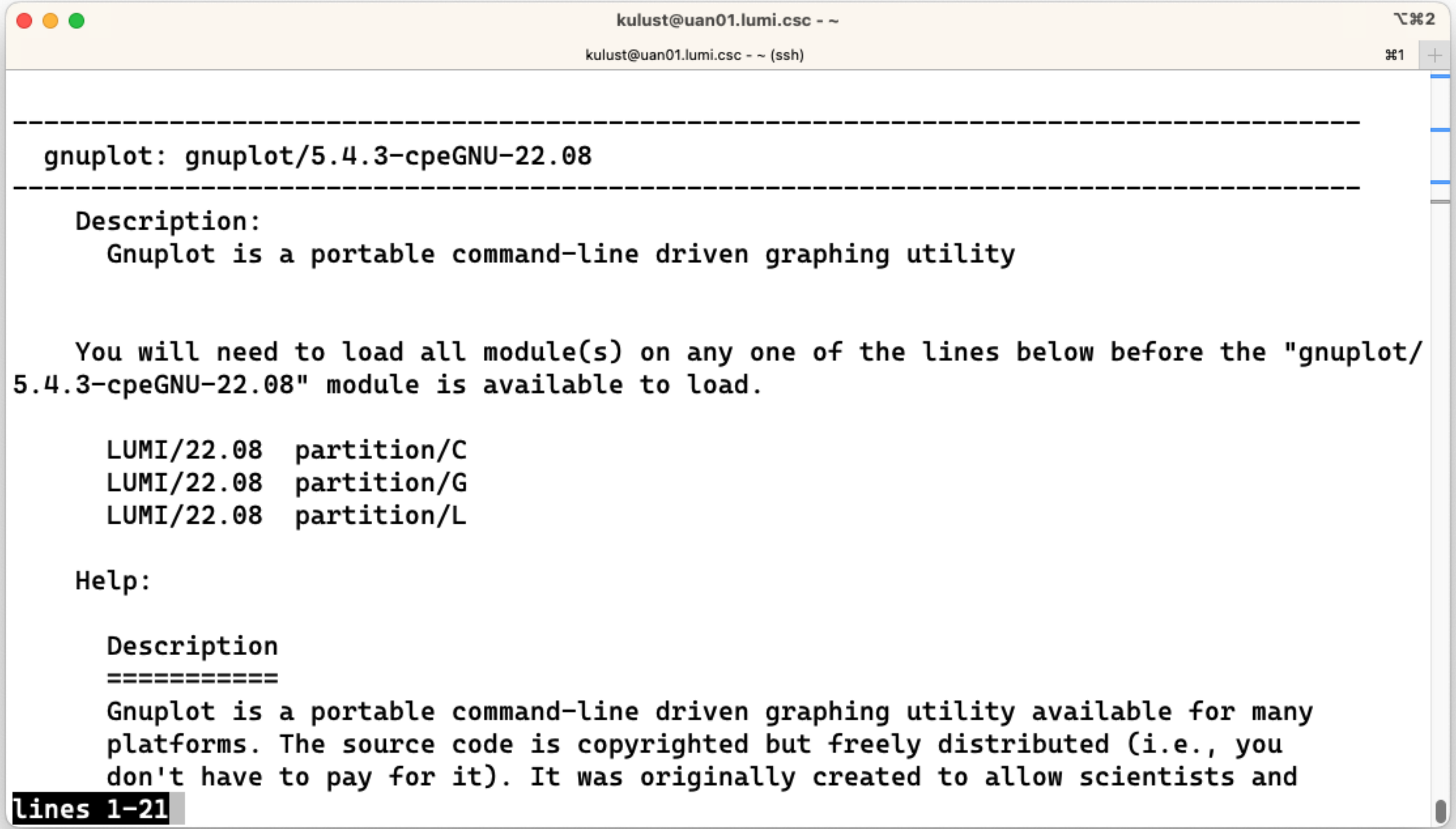
```
     Versions:
        gnuplot/5.4.2-cpeCray-21.08
        gnuplot/5.4.2-cpeGNU-21.08
        gnuplot/5.4.3-cpeAMD-22.08
        gnuplot/5.4.3-cpeAOCC-21.12
        gnuplot/5.4.3-cpeAOCC-22.08
        gnuplot/5.4.3-cpeCray-21.12
        gnuplot/5.4.3-cpeCray-22.06
        gnuplot/5.4.3-cpeCray-22.08
        gnuplot/5.4.3-cpeGNU-21.12
        gnuplot/5.4.3-cpeGNU-22.06
        gnuplot/5.4.3-cpeGNU-22.08

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

     $ module spider gnuplot/5.4.3-cpeGNU-22.08
--------------------------------------------------------------------------------------
[lumi][kulust@uan01-1003 ~]$
```

module spider cmake



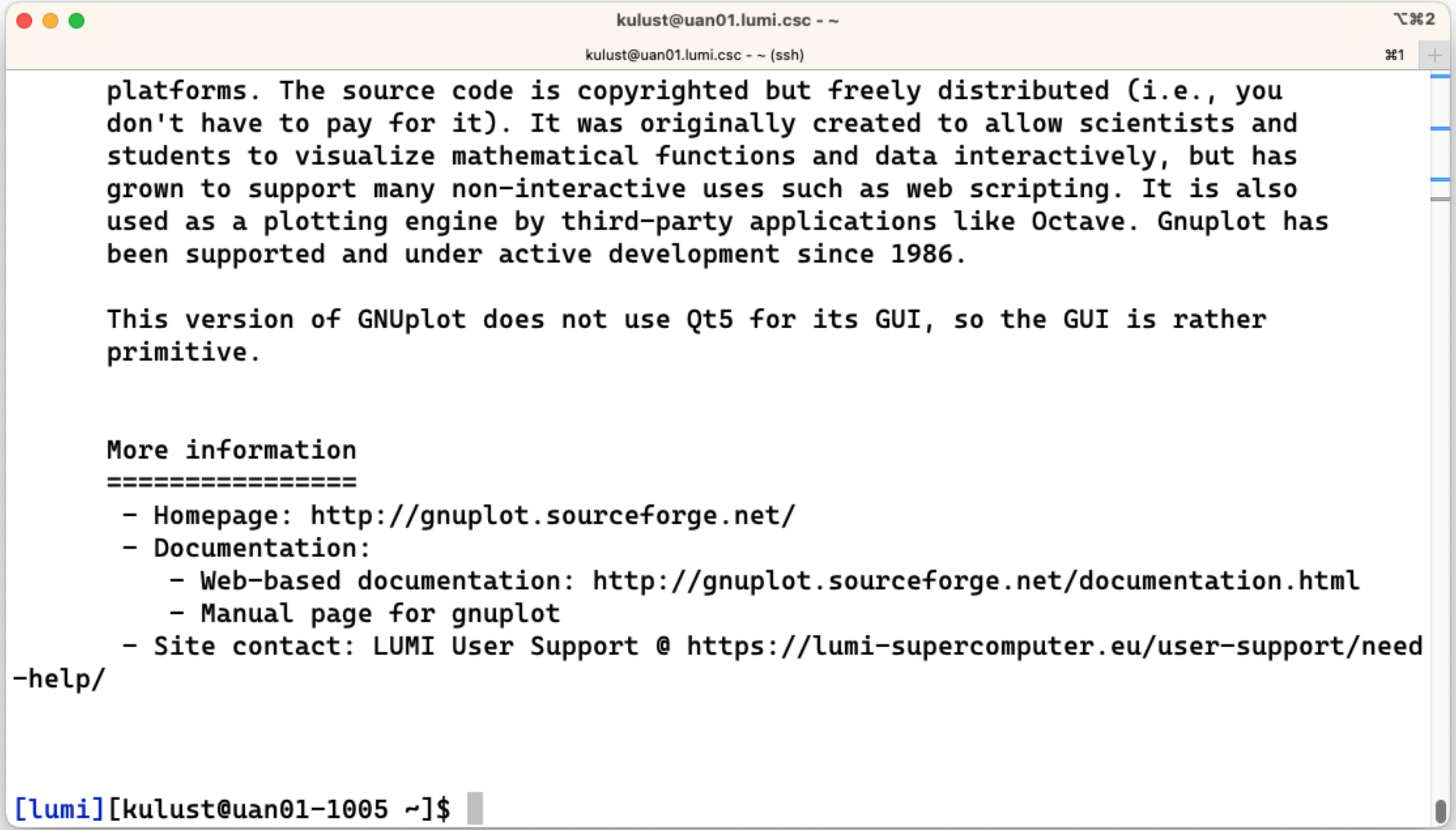
```
[lumi][kulust@uan01-1003 ~]$ module spider cmake

-----------------------------------------------------------------------------------
  CMake:
-----------------------------------------------------------------------------------

     Versions:
        CMake/3.21.2 (E)
        CMake/3.22.2 (E)
        CMake/3.23.2 (E)
        CMake/3.24.0 (E)

Names marked by a trailing (E) are extensions provided by another module.


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

     $ module spider CMake/3.24.0
-----------------------------------------------------------------------------------
[lumi][kulust@uan01-1004 ~]$
```

module spider gnuplot/5.4.3-cpeGNU-22.08



```
--------------------------------------------------------------------------------------
  gnuplot: gnuplot/5.4.3-cpeGNU-22.08
--------------------------------------------------------------------------------------
    Description:
      Gnuplot is a portable command-line driven graphing utility


    You will need to load all module(s) on any one of the lines below before the "gnuplot/
5.4.3-cpeGNU-22.08" module is available to load.

      LUMI/22.08  partition/C
      LUMI/22.08  partition/G
      LUMI/22.08  partition/L

    Help:

      Description
      ===========
      Gnuplot is a portable command-line driven graphing utility available for many
      platforms. The source code is copyrighted but freely distributed (i.e., you
      don't have to pay for it). It was originally created to allow scientists and
lines 1-21
```

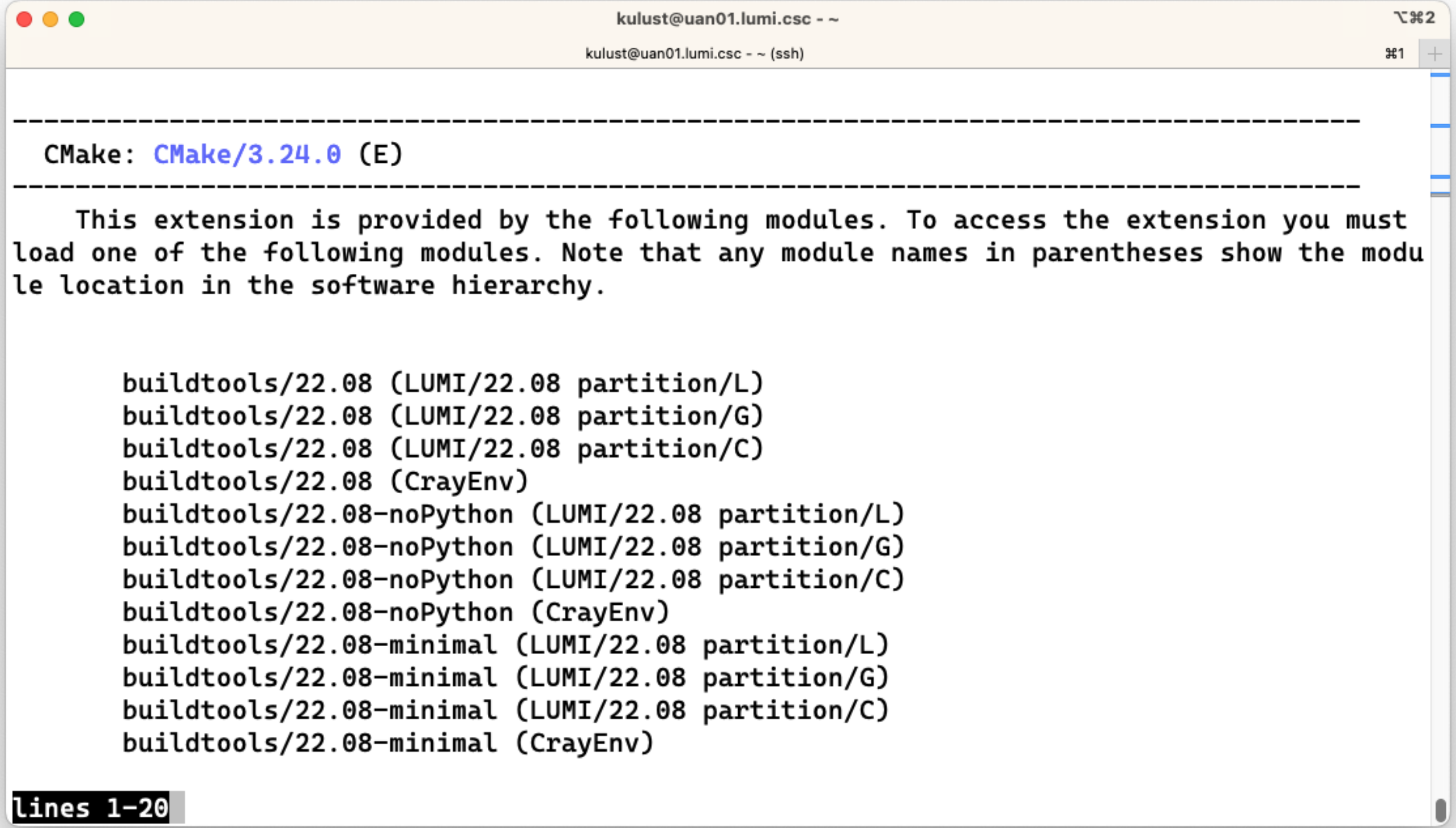
module spider gnuplot/5.4.3-cpeGNU-22.08 (2)


kulust@uan01.lumi.csc - ~

kulust@uan01.lumi.csc - ~ (ssh)

```
      platforms. The source code is copyrighted but freely distributed (i.e., you
      don't have to pay for it). It was originally created to allow scientists and
      students to visualize mathematical functions and data interactively, but has
      grown to support many non-interactive uses such as web scripting. It is also
      used as a plotting engine by third-party applications like Octave. Gnuplot has
      been supported and under active development since 1986.

      This version of GNUplot does not use Qt5 for its GUI, so the GUI is rather
      primitive.


      More information
      ================
       - Homepage: http://gnuplot.sourceforge.net/
       - Documentation:
         - Web-based documentation: http://gnuplot.sourceforge.net/documentation.html
         - Manual page for gnuplot
       - Site contact: LUMI User Support @ https://lumi-supercomputer.eu/user-support/need
-help/



[lumi][kulust@uan01-1005 ~]$
```

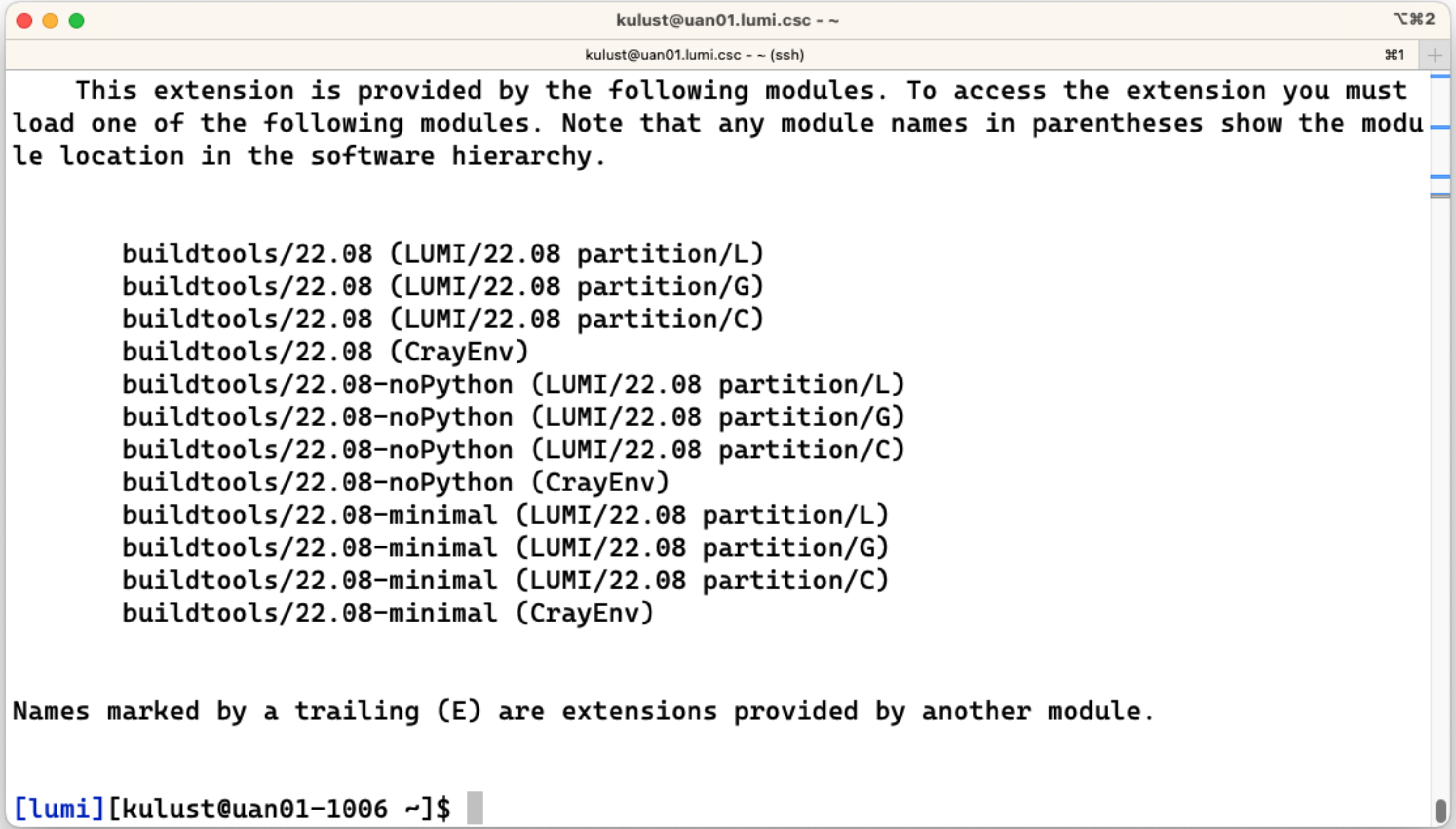
module spider CMake/3.24.0



```
--------------------------------------------------------------------------------------
  CMake: CMake/3.24.0 (E)
--------------------------------------------------------------------------------------
    This extension is provided by the following modules. To access the extension you must
load one of the following modules. Note that any module names in parentheses show the modu
le location in the software hierarchy.


       buildtools/22.08 (LUMI/22.08 partition/L)
       buildtools/22.08 (LUMI/22.08 partition/G)
       buildtools/22.08 (LUMI/22.08 partition/C)
       buildtools/22.08 (CrayEnv)
       buildtools/22.08-noPython (LUMI/22.08 partition/L)
       buildtools/22.08-noPython (LUMI/22.08 partition/G)
       buildtools/22.08-noPython (LUMI/22.08 partition/C)
       buildtools/22.08-noPython (CrayEnv)
       buildtools/22.08-minimal (LUMI/22.08 partition/L)
       buildtools/22.08-minimal (LUMI/22.08 partition/G)
       buildtools/22.08-minimal (LUMI/22.08 partition/C)
       buildtools/22.08-minimal (CrayEnv)

lines 1-20
```

module spider CMake/3.24.0

LUMI



kulust@uan01.lumi.csc - ~

kulust@uan01.lumi.csc - ~ (ssh)

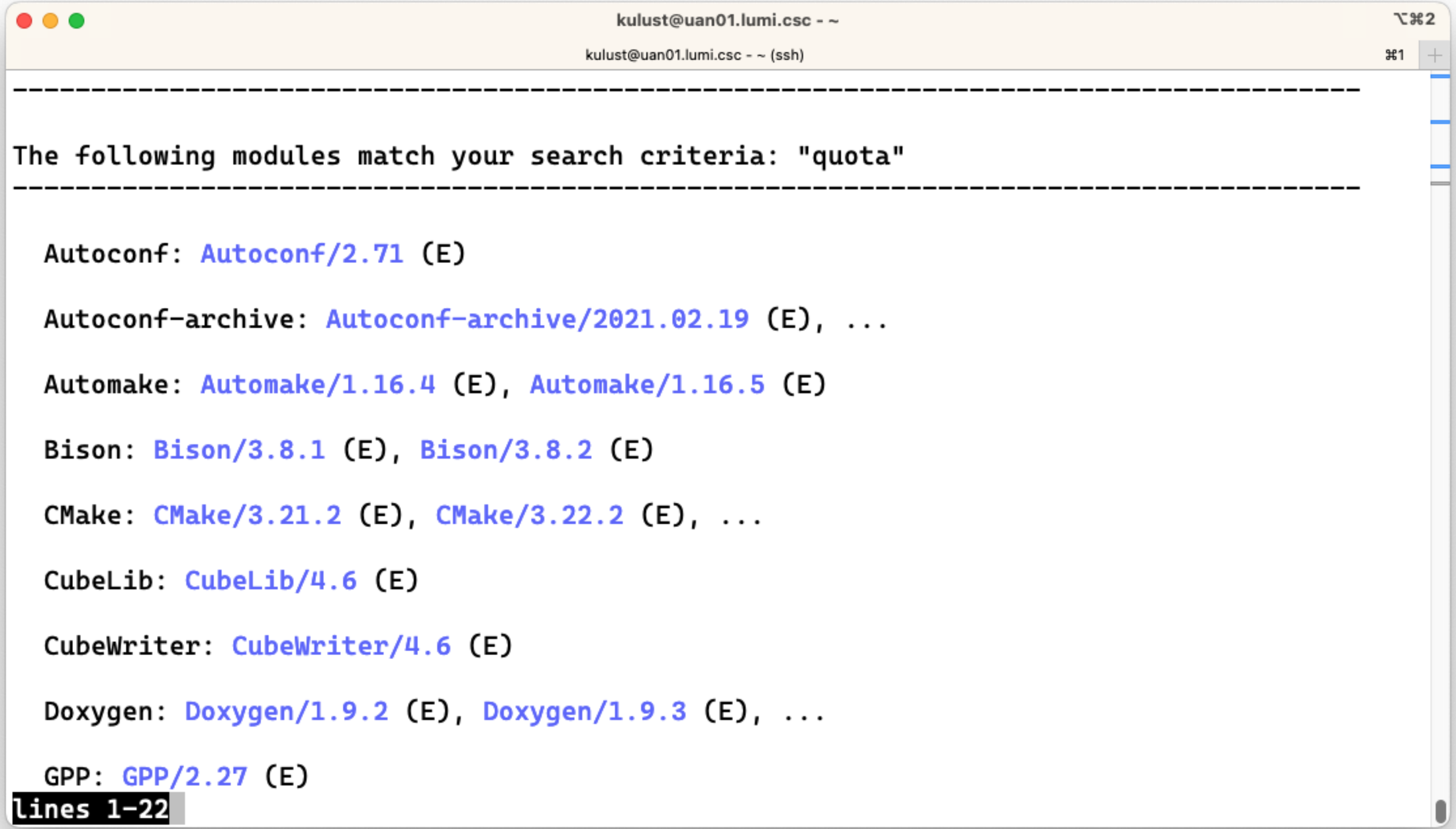
```
    This extension is provided by the following modules. To access the extension you must
load one of the following modules. Note that any module names in parentheses show the modu
le location in the software hierarchy.


       buildtools/22.08 (LUMI/22.08 partition/L)
       buildtools/22.08 (LUMI/22.08 partition/G)
       buildtools/22.08 (LUMI/22.08 partition/C)
       buildtools/22.08 (CrayEnv)
       buildtools/22.08-noPython (LUMI/22.08 partition/L)
       buildtools/22.08-noPython (LUMI/22.08 partition/G)
       buildtools/22.08-noPython (LUMI/22.08 partition/C)
       buildtools/22.08-noPython (CrayEnv)
       buildtools/22.08-minimal (LUMI/22.08 partition/L)
       buildtools/22.08-minimal (LUMI/22.08 partition/G)
       buildtools/22.08-minimal (LUMI/22.08 partition/C)
       buildtools/22.08-minimal (CrayEnv)


Names marked by a trailing (E) are extensions provided by another module.


[lumi][kulust@uan01-1006 ~]$
```

module keyword

- Currently not yet very useful due to a bug in Cray Lmod
- It searches in the module short description and help for the keyword.
  - E.g., try
    `module keyword quota`
- We do try to put enough information in the modules to make this a suitable additional way to discover software that is already installed on the system

module keyword quota

LUMI



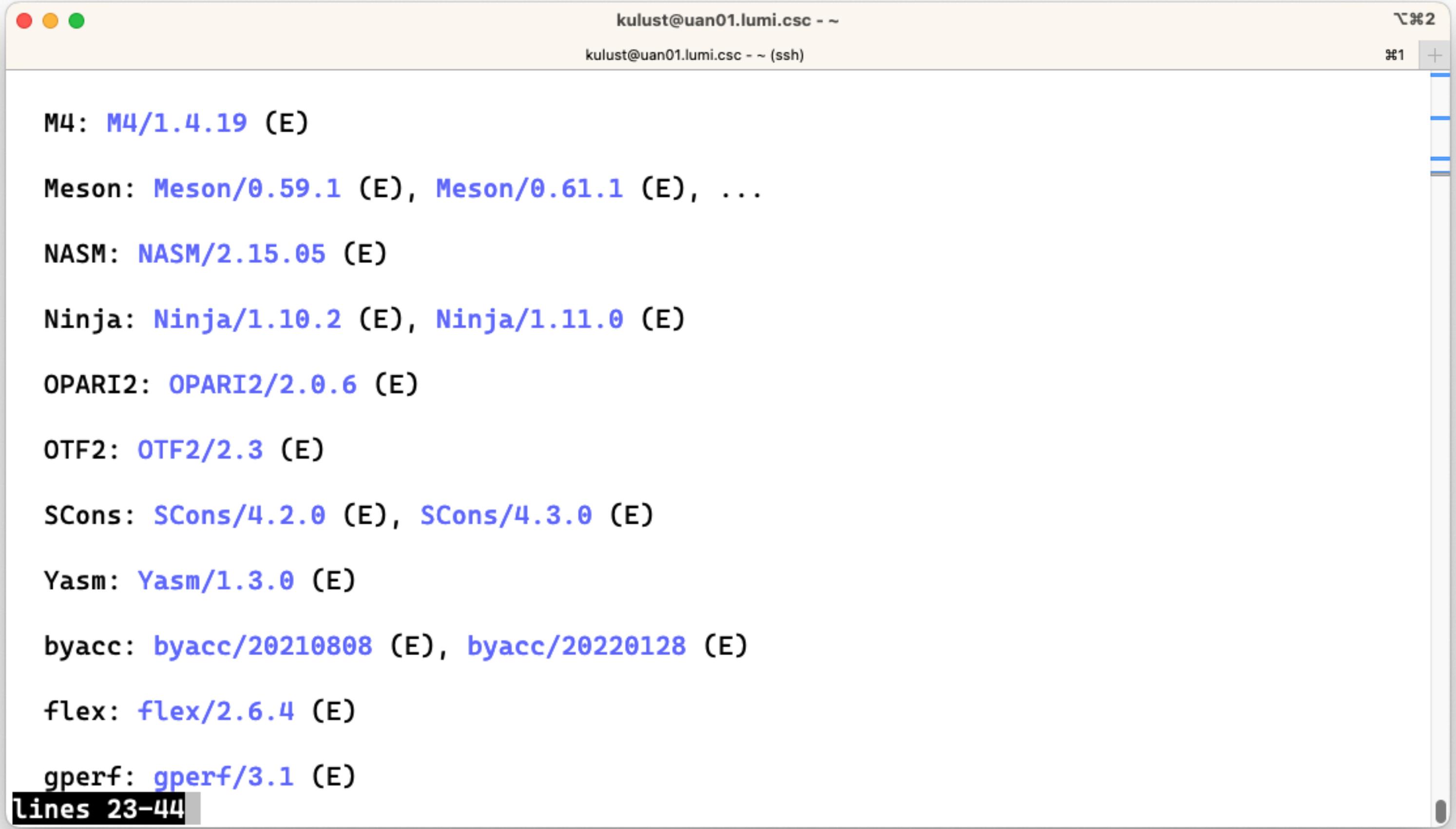
kulust@uan01.lumi.csc - ~

kulust@uan01.lumi.csc - ~ (ssh)

```
-------------------------------------------------------------------------------------

The following modules match your search criteria: "quota"
-------------------------------------------------------------------------------------

  Autoconf: Autoconf/2.71 (E)

  Autoconf-archive: Autoconf-archive/2021.02.19 (E), ...

  Automake: Automake/1.16.4 (E), Automake/1.16.5 (E)

  Bison: Bison/3.8.1 (E), Bison/3.8.2 (E)

  CMake: CMake/3.21.2 (E), CMake/3.22.2 (E), ...

  CubeLib: CubeLib/4.6 (E)

  CubeWriter: CubeWriter/4.6 (E)

  Doxygen: Doxygen/1.9.2 (E), Doxygen/1.9.3 (E), ...

  GPP: GPP/2.27 (E)
lines 1-22
```

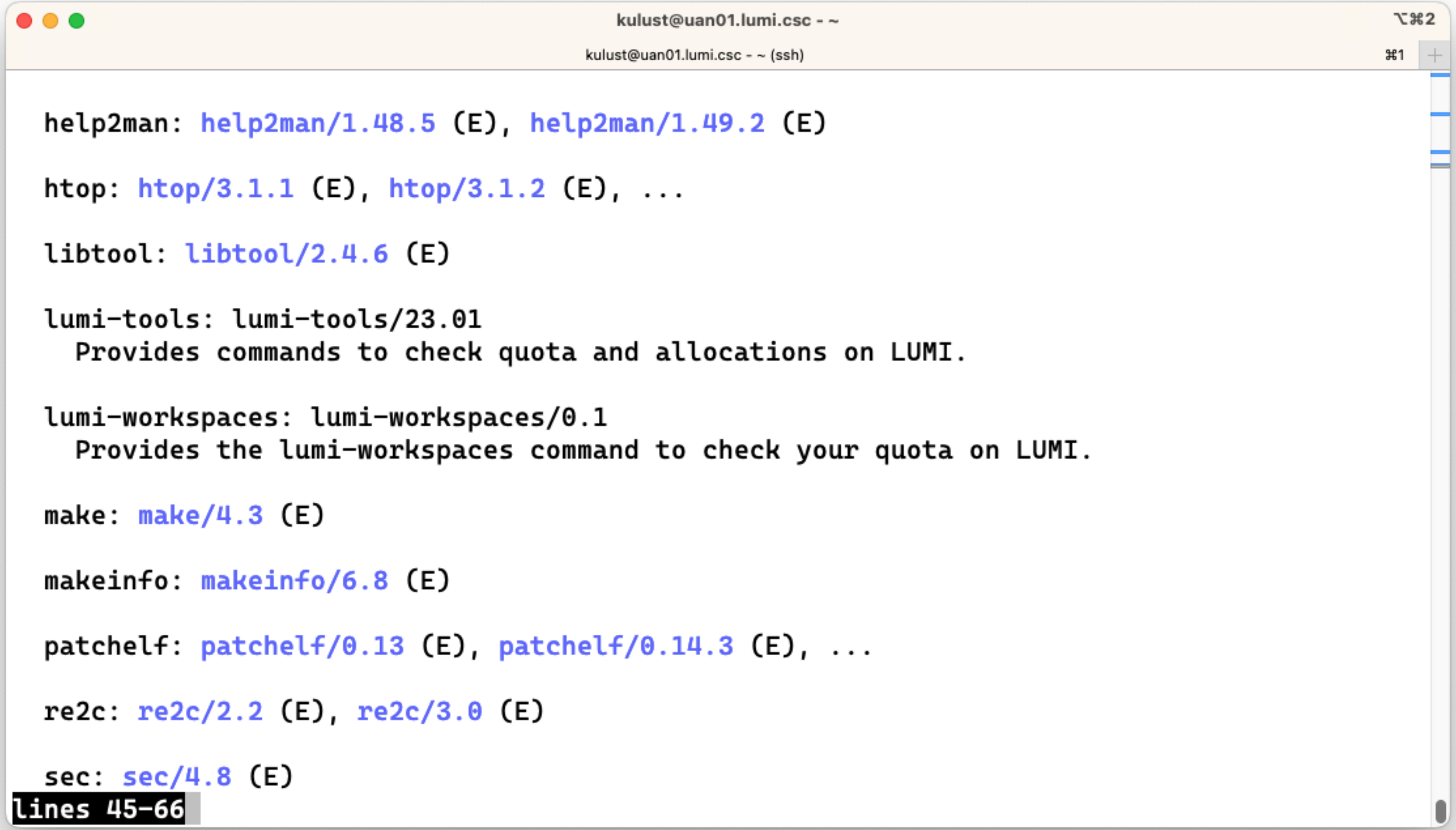
module keyword quota (2)

LUMI


kulust@uan01.lumi.csc - ~
kulust@uan01.lumi.csc - ~ (ssh)

```
M4: M4/1.4.19 (E)

Meson: Meson/0.59.1 (E), Meson/0.61.1 (E), ...

NASM: NASM/2.15.05 (E)

Ninja: Ninja/1.10.2 (E), Ninja/1.11.0 (E)

OPARI2: OPARI2/2.0.6 (E)

OTF2: OTF2/2.3 (E)

SCons: SCons/4.2.0 (E), SCons/4.3.0 (E)

Yasm: Yasm/1.3.0 (E)

byacc: byacc/20210808 (E), byacc/20220128 (E)

flex: flex/2.6.4 (E)

gperf: gperf/3.1 (E)
lines 23-44
```

module keyword quota (3)

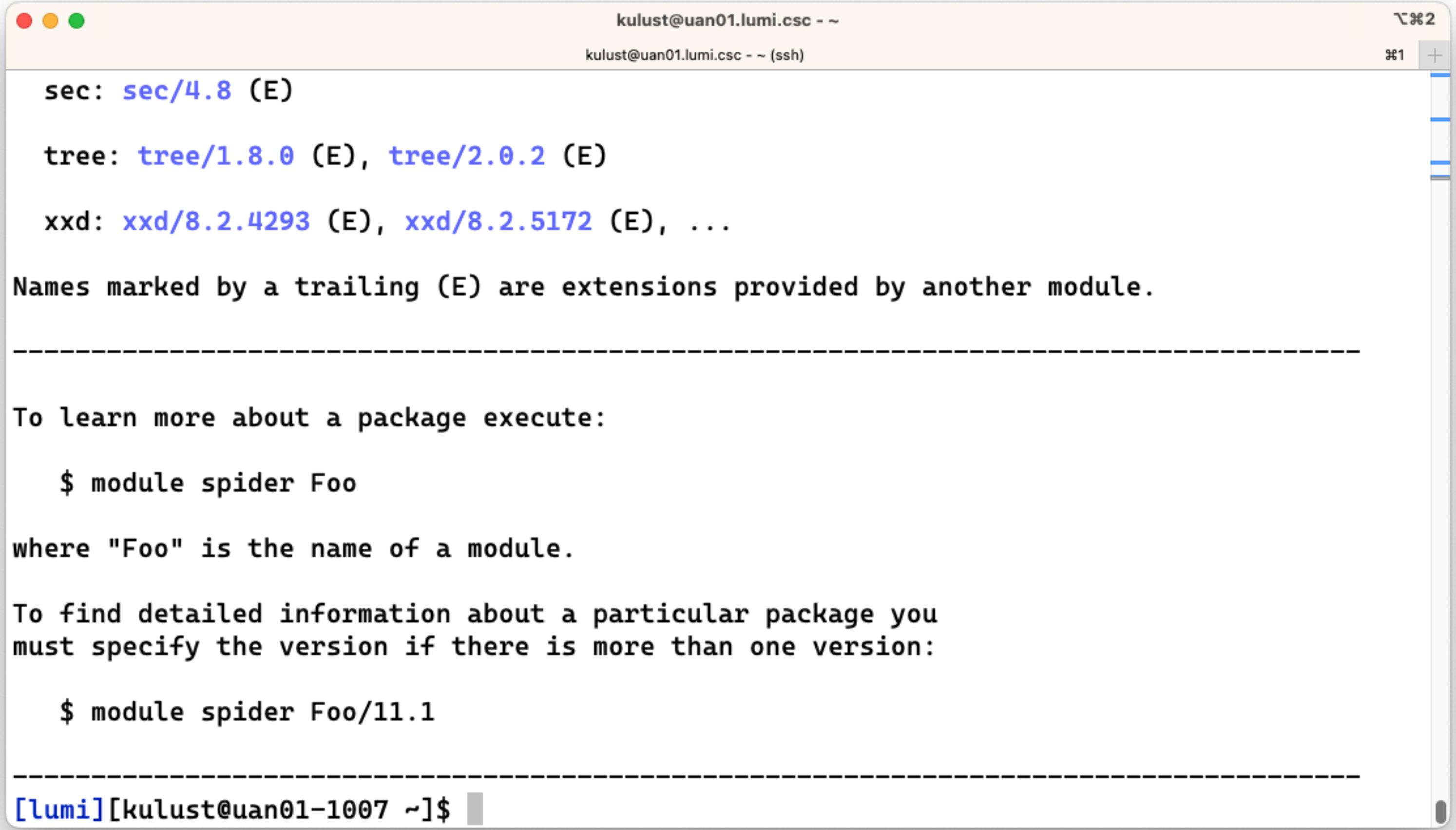


kulust@uan01.lumi.csc - ~

kulust@uan01.lumi.csc - ~ (ssh)

```
help2man: help2man/1.48.5 (E), help2man/1.49.2 (E)

htop: htop/3.1.1 (E), htop/3.1.2 (E), ...

libtool: libtool/2.4.6 (E)

lumi-tools: lumi-tools/23.01
  Provides commands to check quota and allocations on LUMI.

lumi-workspaces: lumi-workspaces/0.1
  Provides the lumi-workspaces command to check your quota on LUMI.

make: make/4.3 (E)

makeinfo: makeinfo/6.8 (E)

patchelf: patchelf/0.13 (E), patchelf/0.14.3 (E), ...

re2c: re2c/2.2 (E), re2c/3.0 (E)

sec: sec/4.8 (E)
lines 45-66
```

module keyword quota (4)

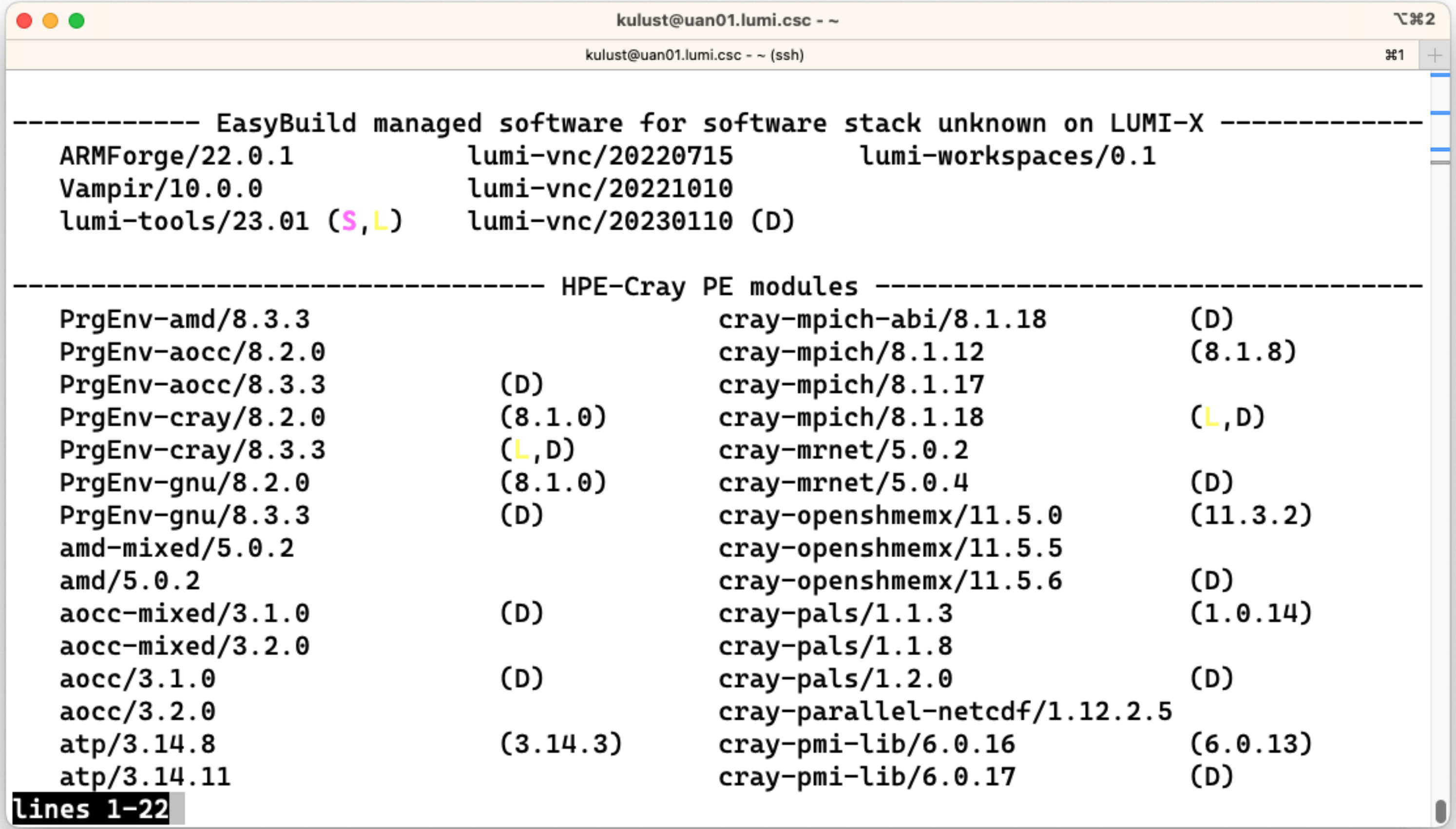


```
  sec: sec/4.8 (E)

  tree: tree/1.8.0 (E), tree/2.0.2 (E)

  xxd: xxd/8.2.4293 (E), xxd/8.2.5172 (E), ...

Names marked by a trailing (E) are extensions provided by another module.

-------------------------------------------------------------------------------------


To learn more about a package execute:

   $ module spider Foo

where "Foo" is the name of a module.

To find detailed information about a particular package you
must specify the version if there is more than one version:

   $ module spider Foo/11.1

-------------------------------------------------------------------------------------
[lumi][kulust@uan01-1007 ~]$
```

Sticky modules and module purge

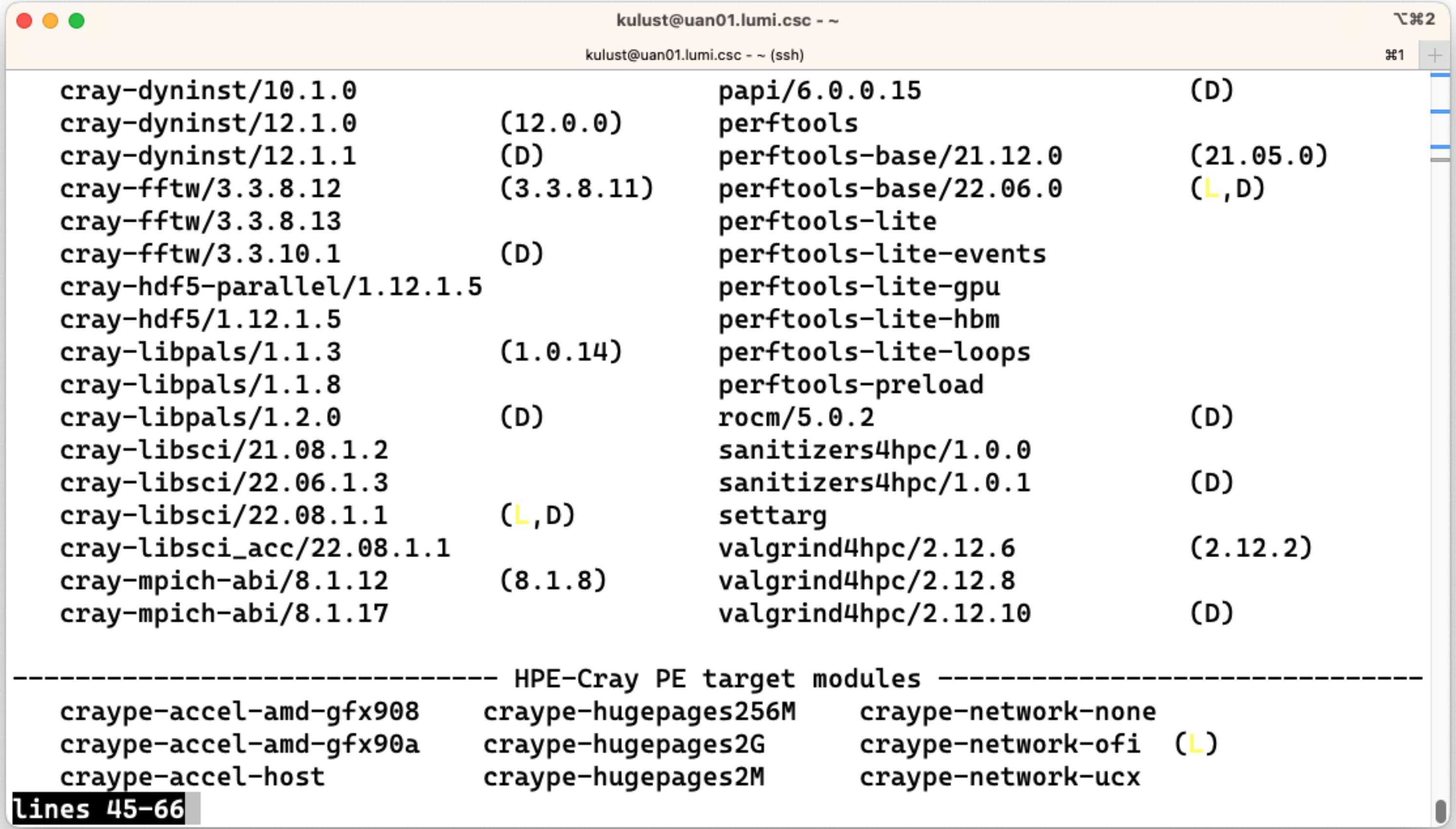
- On some systems, you will be taught to avoid `module purge` (which unloads all modules)
- Sticky modules are modules that are not unloaded by `module purge`, but reloaded.
  - They can be force-unloaded with `module --force purge` and `module --force unload`
- Used on LUMI for the software stacks and modules that set the display style of the modules
  - But keep in mind that the modules are reloaded, which implies that the target modules and partition module will be switched (back) to those for the current node.

module av


kulust@uan01.lumi.csc - ~
kulust@uan01.lumi.csc - ~ (ssh)

```
------------ EasyBuild managed software for software stack unknown on LUMI-X -------------
   ARMForge/22.0.1           lumi-vnc/20220715         lumi-workspaces/0.1
   Vampir/10.0.0             lumi-vnc/20221010
   lumi-tools/23.01 (S,L)    lumi-vnc/20230110 (D)

---------------------------------- HPE-Cray PE modules ------------------------------------
   PrgEnv-amd/8.3.3                          cray-mpich-abi/8.1.18         (D)
   PrgEnv-aocc/8.2.0                         cray-mpich/8.1.12             (8.1.8)
   PrgEnv-aocc/8.3.3              (D)        cray-mpich/8.1.17
   PrgEnv-cray/8.2.0              (8.1.0)    cray-mpich/8.1.18             (L,D)
   PrgEnv-cray/8.3.3              (L,D)      cray-mrnet/5.0.2
   PrgEnv-gnu/8.2.0               (8.1.0)    cray-mrnet/5.0.4              (D)
   PrgEnv-gnu/8.3.3               (D)        cray-openshmemx/11.5.0        (11.3.2)
   amd-mixed/5.0.2                           cray-openshmemx/11.5.5
   amd/5.0.2                                 cray-openshmemx/11.5.6        (D)
   aocc-mixed/3.1.0               (D)        cray-pals/1.1.3               (1.0.14)
   aocc-mixed/3.2.0                          cray-pals/1.1.8
   aocc/3.1.0                     (D)        cray-pals/1.2.0               (D)
   aocc/3.2.0                                cray-parallel-netcdf/1.12.2.5
   atp/3.14.8                     (3.14.3)   cray-pmi-lib/6.0.16           (6.0.13)
   atp/3.14.11                               cray-pmi-lib/6.0.17           (D)
lines 1-22
```

module av (2)

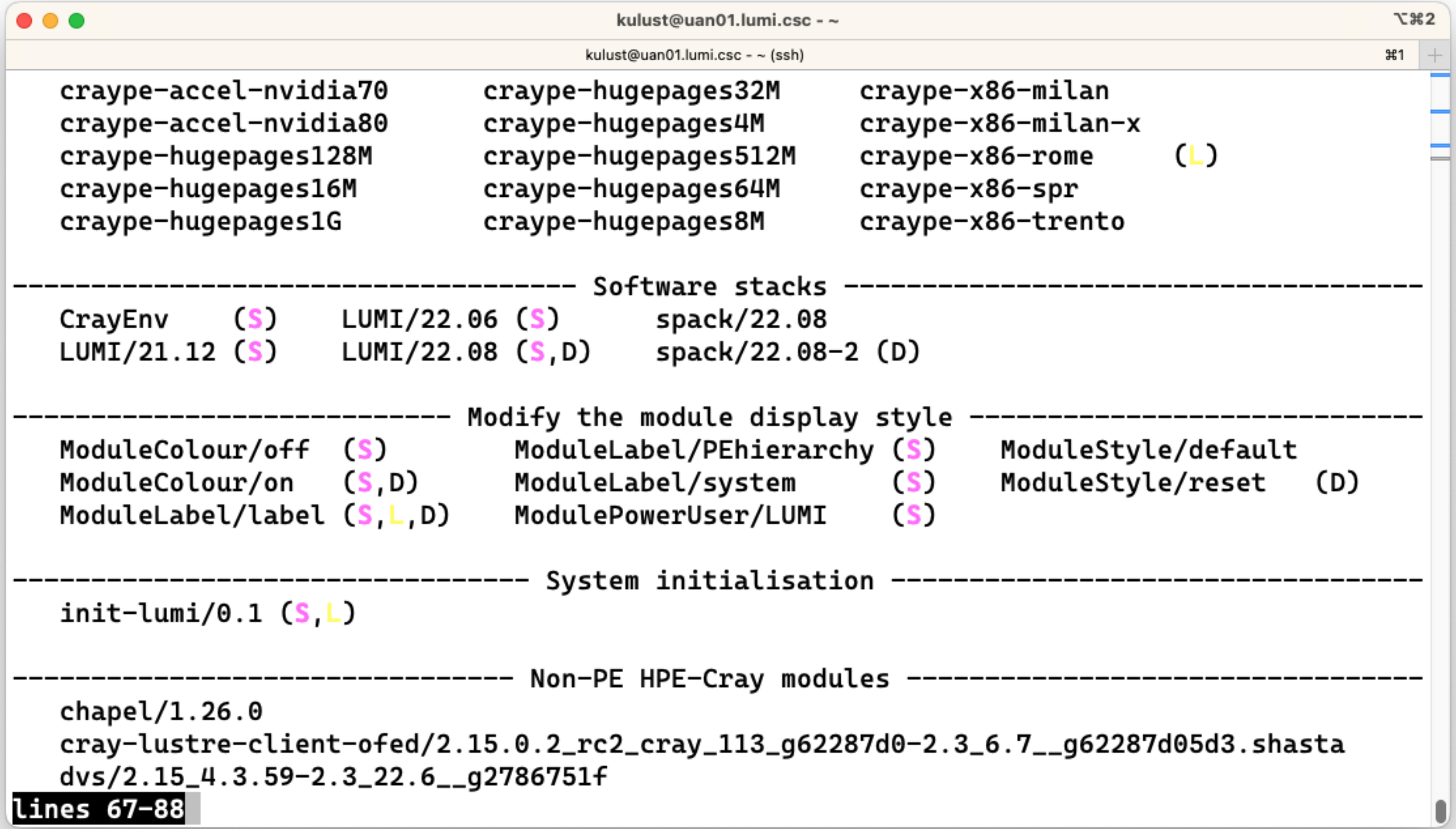

kulust@uan01.lumi.csc - ~

kulust@uan01.lumi.csc - ~ (ssh)

```
   cray-dyninst/10.1.0                        papi/6.0.0.15                (D)
   cray-dyninst/12.1.0          (12.0.0)      perftools
   cray-dyninst/12.1.1          (D)           perftools-base/21.12.0       (21.05.0)
   cray-fftw/3.3.8.12           (3.3.8.11)    perftools-base/22.06.0       (L,D)
   cray-fftw/3.3.8.13                         perftools-lite
   cray-fftw/3.3.10.1           (D)           perftools-lite-events
   cray-hdf5-parallel/1.12.1.5                perftools-lite-gpu
   cray-hdf5/1.12.1.5                         perftools-lite-hbm
   cray-libpals/1.1.3           (1.0.14)      perftools-lite-loops
   cray-libpals/1.1.8                         perftools-preload
   cray-libpals/1.2.0           (D)           rocm/5.0.2                   (D)
   cray-libsci/21.08.1.2                      sanitizers4hpc/1.0.0
   cray-libsci/22.06.1.3                      sanitizers4hpc/1.0.1         (D)
   cray-libsci/22.08.1.1        (L,D)         settarg
   cray-libsci_acc/22.08.1.1                  valgrind4hpc/2.12.6          (2.12.2)
   cray-mpich-abi/8.1.12        (8.1.8)       valgrind4hpc/2.12.8
   cray-mpich-abi/8.1.17                      valgrind4hpc/2.12.10         (D)

------------------------------- HPE-Cray PE target modules --------------------------------
   craype-accel-amd-gfx908     craype-hugepages256M    craype-network-none
   craype-accel-amd-gfx90a     craype-hugepages2G      craype-network-ofi  (L)
   craype-accel-host           craype-hugepages2M      craype-network-ucx
lines 45-66
```

module av (3)

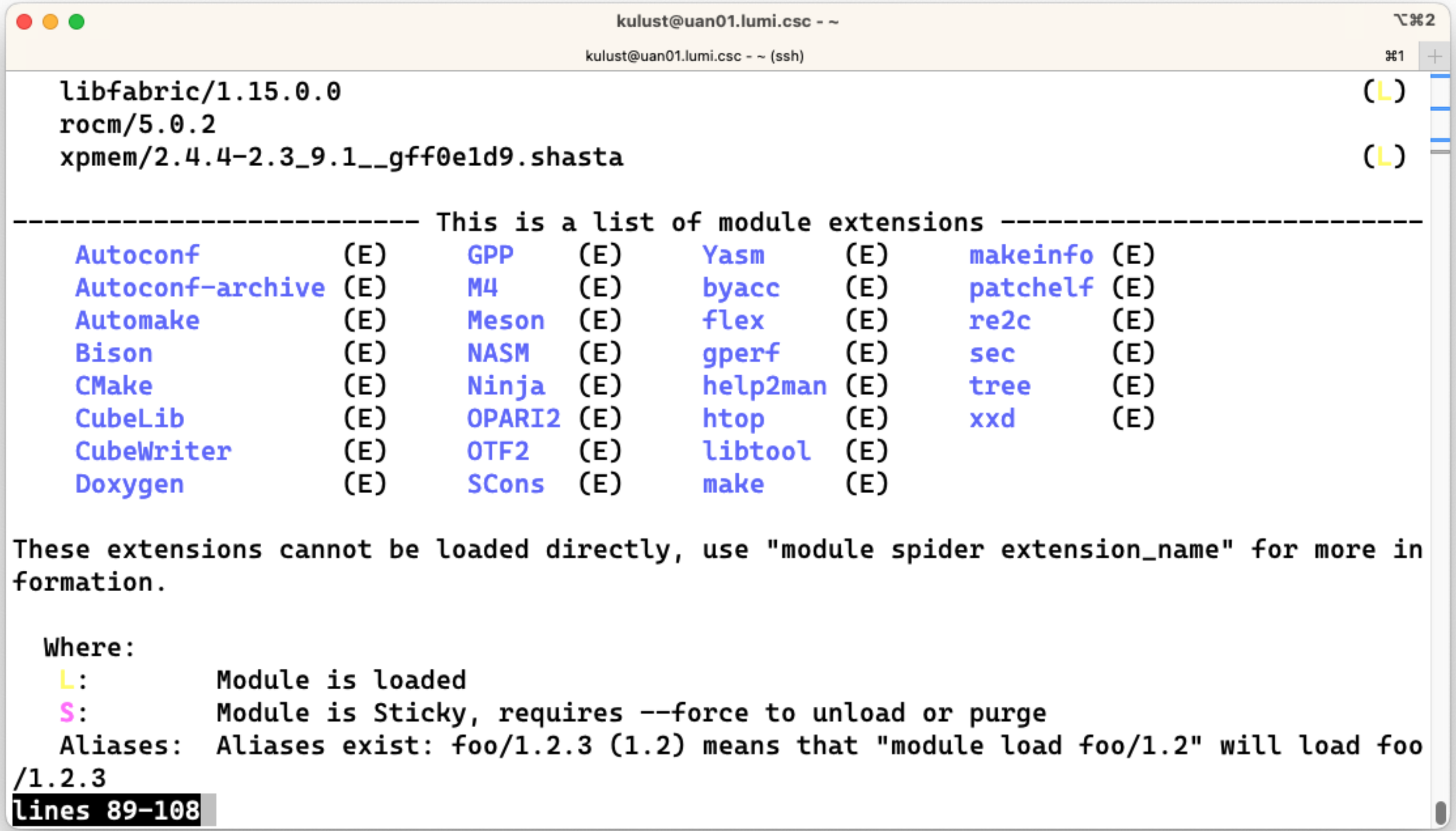
LUMI


kulust@uan01.lumi.csc - ~

kulust@uan01.lumi.csc - ~ (ssh)

```
   craype-accel-nvidia70       craype-hugepages32M     craype-x86-milan
   craype-accel-nvidia80       craype-hugepages4M      craype-x86-milan-x
   craype-hugepages128M        craype-hugepages512M    craype-x86-rome      (L)
   craype-hugepages16M         craype-hugepages64M     craype-x86-spr
   craype-hugepages1G          craype-hugepages8M      craype-x86-trento

------------------------------------ Software stacks -------------------------------------
   CrayEnv     (S)    LUMI/22.06 (S)      spack/22.08
   LUMI/21.12 (S)     LUMI/22.08 (S,D)    spack/22.08-2 (D)

---------------------------- Modify the module display style -----------------------------
   ModuleColour/off   (S)      ModuleLabel/PEhierarchy (S)    ModuleStyle/default
   ModuleColour/on    (S,D)    ModuleLabel/system      (S)    ModuleStyle/reset   (D)
   ModuleLabel/label (S,L,D)   ModulePowerUser/LUMI    (S)

--------------------------------- System initialisation ----------------------------------
   init-lumi/0.1 (S,L)

-------------------------------- Non-PE HPE-Cray modules ---------------------------------
   chapel/1.26.0
   cray-lustre-client-ofed/2.15.0.2_rc2_cray_113_g62287d0-2.3_6.7__g62287d05d3.shasta
   dvs/2.15_4.3.59-2.3_22.6__g2786751f
lines 67-88
```

module av (4)

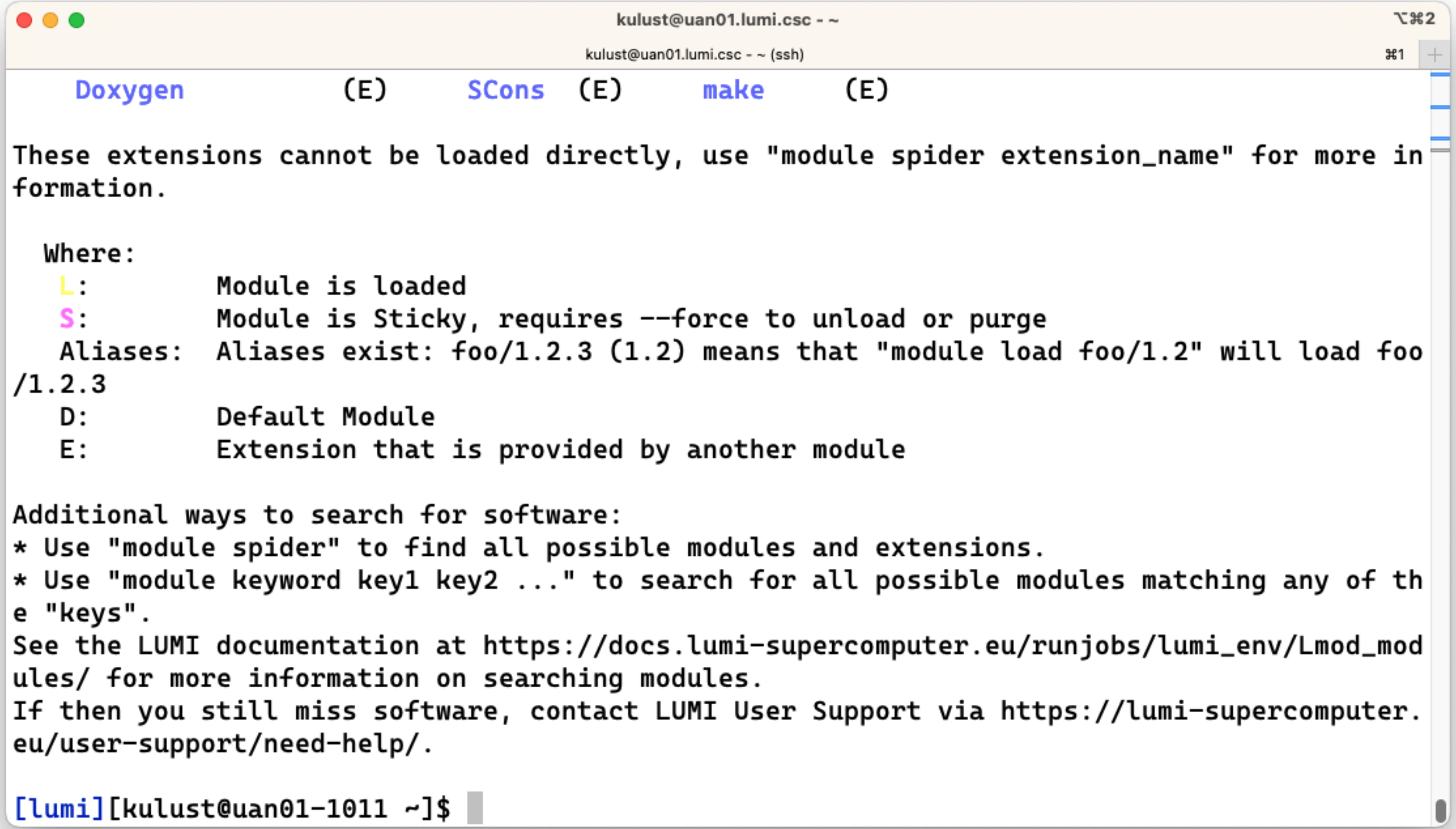


kulust@uan01.lumi.csc - ~

kulust@uan01.lumi.csc - ~ (ssh)

```
   libfabric/1.15.0.0                                                                          (L)
   rocm/5.0.2
   xpmem/2.4.4-2.3_9.1__gff0e1d9.shasta                                                        (L)

-------------------------- This is a list of module extensions ---------------------------
    Autoconf          (E)     GPP     (E)     Yasm     (E)     makeinfo (E)
    Autoconf-archive  (E)     M4      (E)     byacc    (E)     patchelf (E)
    Automake          (E)     Meson   (E)     flex     (E)     re2c     (E)
    Bison             (E)     NASM    (E)     gperf    (E)     sec      (E)
    CMake             (E)     Ninja   (E)     help2man (E)     tree     (E)
    CubeLib           (E)     OPARI2  (E)     htop     (E)     xxd      (E)
    CubeWriter        (E)     OTF2    (E)     libtool  (E)
    Doxygen           (E)     SCons   (E)     make     (E)

These extensions cannot be loaded directly, use "module spider extension_name" for more in
formation.

  Where:
   L:         Module is loaded
   S:         Module is Sticky, requires --force to unload or purge
   Aliases:   Aliases exist: foo/1.2.3 (1.2) means that "module load foo/1.2" will load foo
/1.2.3
lines 89-108
```

module av (5)



```
    Doxygen              (E)       SCons   (E)       make       (E)

These extensions cannot be loaded directly, use "module spider extension_name" for more in
formation.

  Where:
   L:         Module is loaded
   S:         Module is Sticky, requires --force to unload or purge
   Aliases:   Aliases exist: foo/1.2.3 (1.2) means that "module load foo/1.2" will load foo
/1.2.3
   D:         Default Module
   E:         Extension that is provided by another module

Additional ways to search for software:
* Use "module spider" to find all possible modules and extensions.
* Use "module keyword key1 key2 ..." to search for all possible modules matching any of th
e "keys".
See the LUMI documentation at https://docs.lumi-supercomputer.eu/runjobs/lumi_env/Lmod_mod
ules/ for more information on searching modules.
If then you still miss software, contact LUMI User Support via https://lumi-supercomputer.
eu/user-support/need-help/.

[lumi][kulust@uan01-1011 ~]$
```

Changing how the module list is displayed

- You may have noticed that you don’t see directories in the module view but descriptive texts
- This can be changed by loading a module
  - `ModuleLabel/label` : The default view
  - `ModuleLabel/PEhierarchy` : Descriptive texts, but the PE hierarchy is unfolded
  - `ModuleLabel/system` : Module directories
- Turn colour on or off using `ModuleColour/on` or `ModuleColour/off`
- Show some hidden modules with `ModulePowerUser/LUMI`
  - This will also show undocumented/unsupported modules!

Installing software on HPC systems

- Software on an HPC system is rarely installed from RPM
  - Generic RPMs not optimised for the specific CPU
  - Generic RPMs may not work with the specific LUMI environment (SlingShot interconnect, kernel modules, resource manager)
  - Multi-user system so usually no “one version fits all”
  - Need a small system image as nodes are diskless
- Spack and EasyBuild are the two most popular HPC-specific software build and installation frameworks
  - Usually install from sources to adapt the software to the underlying hardware and OS
  - Installation instructions in a way that can be communicated and executed easily
  - Make software available via modules
  - Dependency handling compatible with modules

Extending the LUMI stack with EasyBuild

- Fully integrated in the LUMI software stack
  - Load the LUMI module and modules should appear in your module view
  - EasyBuild-user module to install packages in your user space
  - Will use existing modules for dependencies if those are already on the system or in your personal/project stack
- EasyBuild built-in easyconfigs do not work on LUMI, not even on LUMI-C
  - GNU-based toolchains: Would give problems with MPI
  - Intel-based toolchains: Intel compilers and AMD CPUs are a problematic cocktail
- Library of recipes that we made in the LUMI-EasyBuild-contrib GitHub repository
  - EasyBuild-user will find a copy on the system or in your install
  - List of recipes in lumi-supercomputer.github.io/LUMI-EasyBuild-docs

EasyBuild recipes - easyconfigs

- Build recipe for an individual package
  - Relies on either a generic or a specific installation process provided by an easyblock
- Steps
  - Downloading sources and patches
  - Typical configure – build – (test) – install process
  - Extensions mechanism for perl/python/R packages
  - Some simple checks
  - Creation of the module
- All have several parameters in the easyconfig file

The toolchain concept

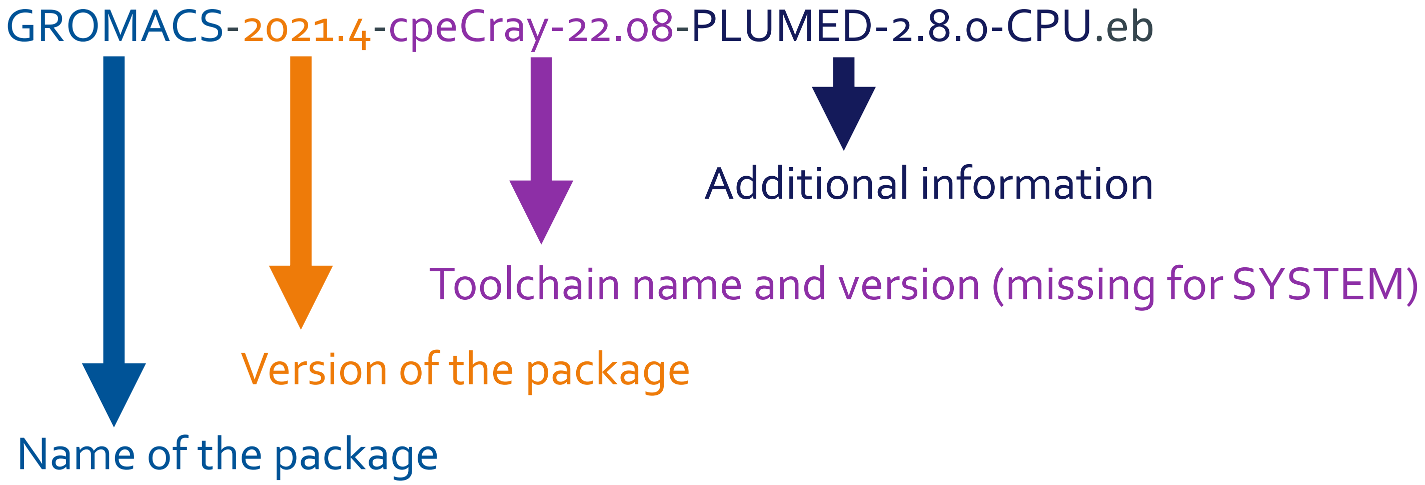
- A set of compiler, MPI implementation and basic math libraries
  - Simplified concept on LUMI as there is no hierarchy as on some other EasyBuild systems
- These are the cpeCray, cpeGNU, cpeAOCC and cpeAMD modules mentioned before!

HPE Cray PE	LUMI toolchain	
PrgEnv-cray	cpeCray	Cray Compiling Environment
PrgEnv-gnu	cpeGNU	GNU C/C++ and Fortran
PrgEnv-aocc	cpeAOCC	AMD CPU compilers
PrgEnv-amd	cpeAMD	AMD ROCm GPU compilers (LUMI-G only)

The toolchain concept (2)

- Special toolchain: SYSTEM to use the system compiler
  - Does not fully function in the same way as the other toolchains when it comes to dependency handling
  - Used on LUMI for CrayEnv and some packages with few dependencies
- It is not possible to load packages from different cpe toolchains at the same time
  - EasyBuild restriction, because mixing libraries compiled with different compilers does not always work
- Packages compiled with one cpe toolchain can be loaded together with packages compiled with the SYSTEM toolchain
  - But we do avoid mixing them when linking

easyconfig names and module names


GROMACS-2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU.eb
Additional information
Toolchain name and version (missing for SYSTEM)
Version of the package
Name of the package

Module: GROMACS/2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU

Installing
Step 1: Where to install

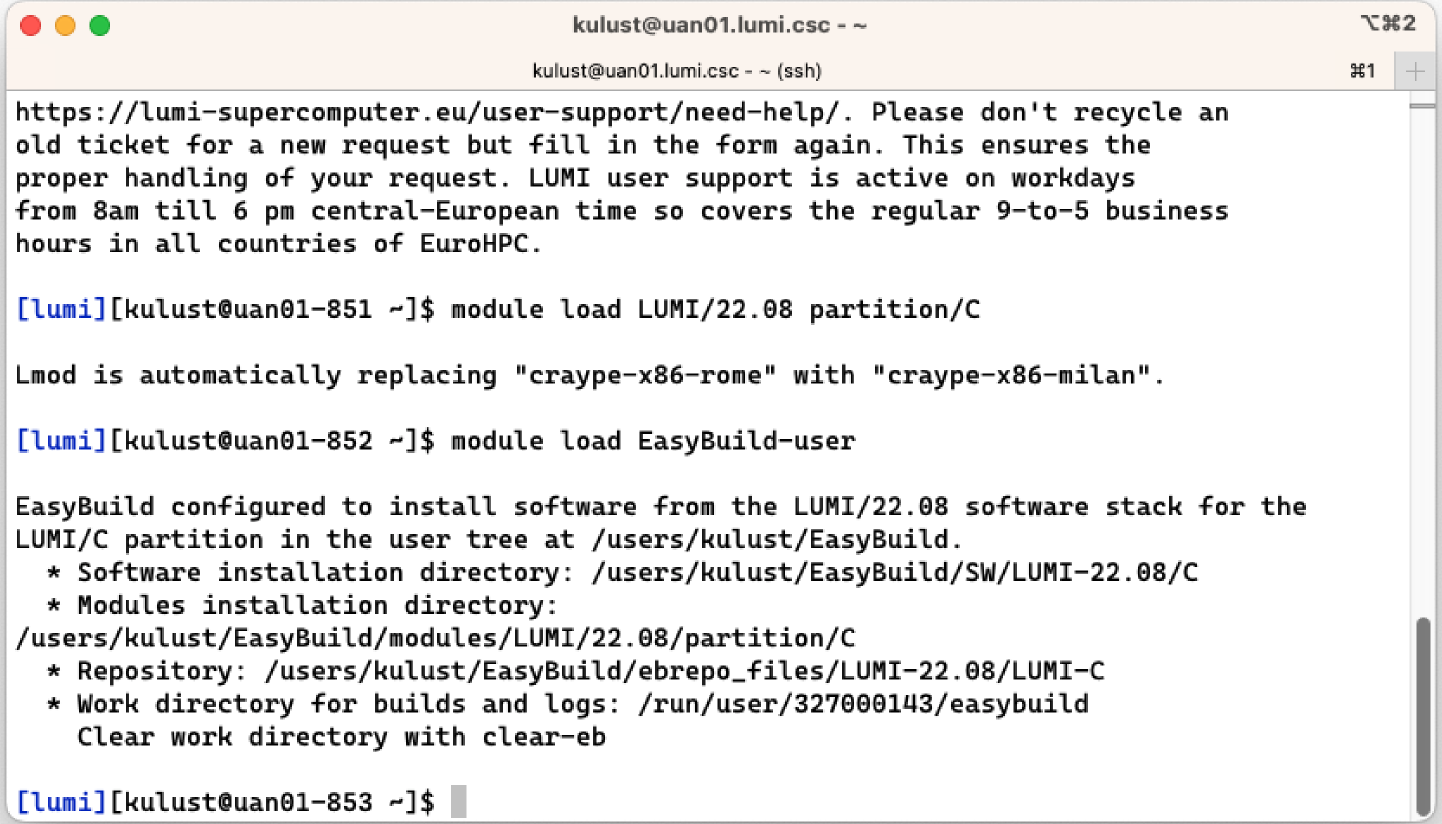
- Default location is `$HOME/EasyBuild`
- But better is to install in your project directory for the whole project
  - `export EBU_USER_PREFIX=/project/project_465000000/EasyBuild`
  - Set this *before* loading the `LUMI` module
  - All users of the software tree have to set this environment variable to use the software tree

Installing

Step 2: Configure the environment

- Load the modules for the LUMI software stack and partition that you want to use. E.g.,
  `module load LUMI/22.08 partition/C`
  - In many cases, cross-compilation is possible by loading a different partition module than the one auto-loaded by `LUMI`
  - Though cross-compilation is currently problematic for GPU code
- Load the EasyBuild-user module to make EasyBuild available and to configure it for installing software in the chosen stack and partition:
  `module load EasyBuild-user`

```
module load LUMI/22.08 partition/C
module load EasyBuild-user
```



kulust@uan01.lumi.csc - ~

kulust@uan01.lumi.csc - ~ (ssh)

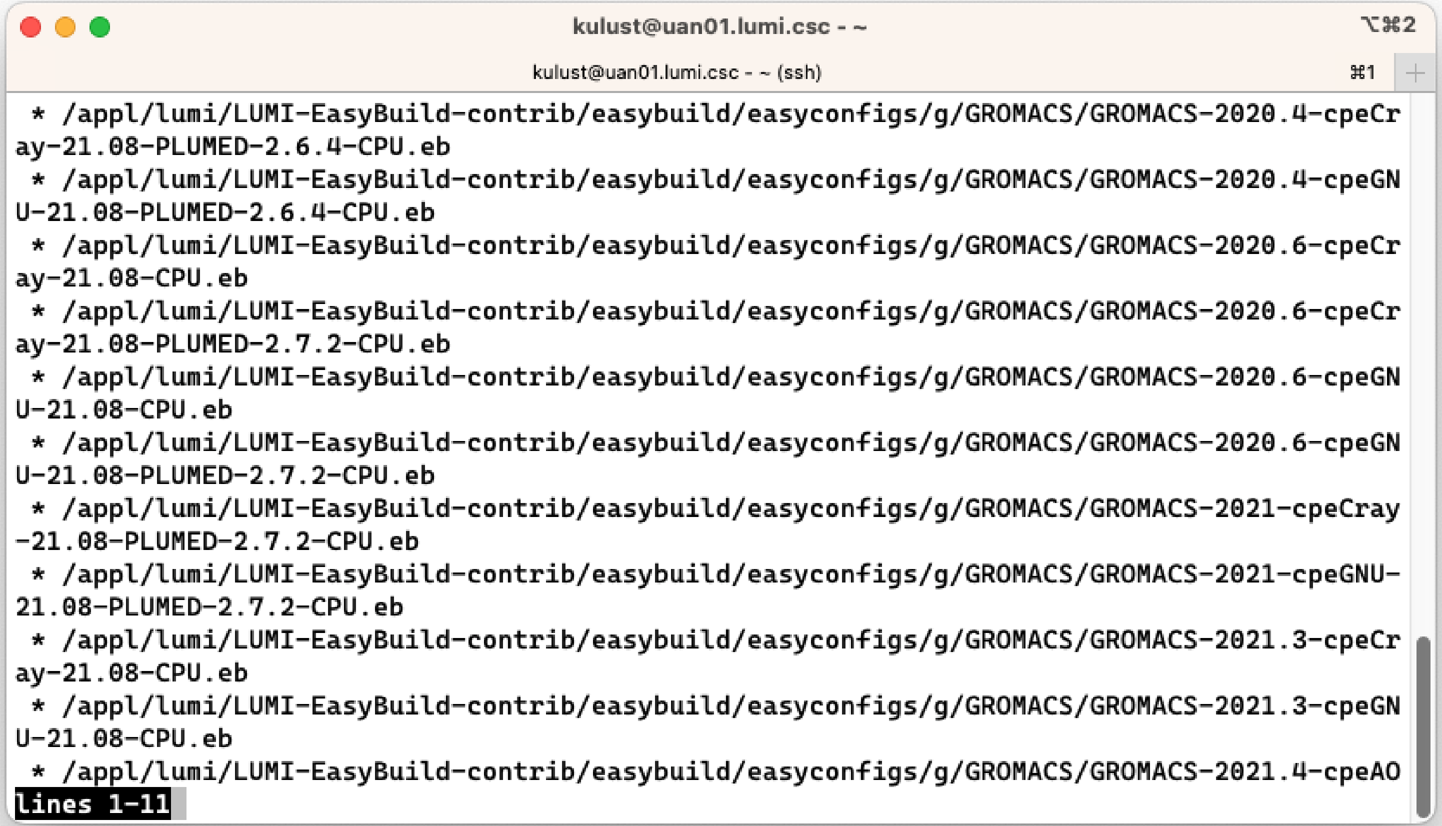
```
https://lumi-supercomputer.eu/user-support/need-help/. Please don't recycle an
old ticket for a new request but fill in the form again. This ensures the
proper handling of your request. LUMI user support is active on workdays
from 8am till 6 pm central-European time so covers the regular 9-to-5 business
hours in all countries of EuroHPC.

[lumi][kulust@uan01-851 ~]$ module load LUMI/22.08 partition/C

Lmod is automatically replacing "craype-x86-rome" with "craype-x86-milan".

[lumi][kulust@uan01-852 ~]$ module load EasyBuild-user

EasyBuild configured to install software from the LUMI/22.08 software stack for the
LUMI/C partition in the user tree at /users/kulust/EasyBuild.
  * Software installation directory: /users/kulust/EasyBuild/SW/LUMI-22.08/C
  * Modules installation directory:
/users/kulust/EasyBuild/modules/LUMI/22.08/partition/C
  * Repository: /users/kulust/EasyBuild/ebrepo_files/LUMI-22.08/LUMI-C
  * Work directory for builds and logs: /run/user/327000143/easybuild
    Clear work directory with clear-eb

[lumi][kulust@uan01-853 ~]$
```

Installing

Step 3: Install the software

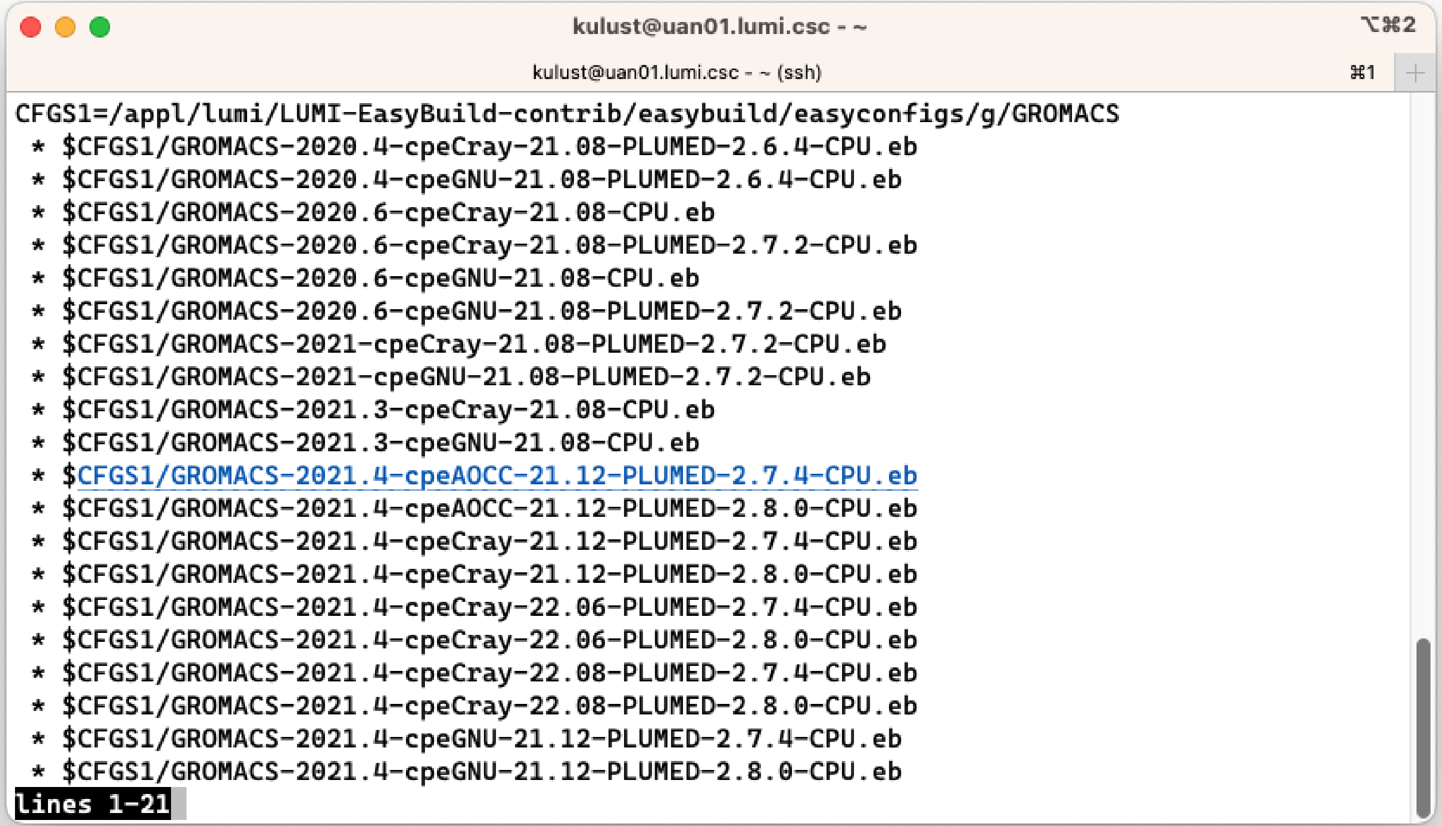
- Let's, e.g., install GROMACS
  - Search if GROMACS build recipes are available
    ```
    eb --search GROMACS
    eb –S GROMACS
    ```
    But we now also have the LUMI Software Library that lists all available software through EasyBuild.
  - Let's take GROMACS-2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU.eb:
    ```
    eb GROMACS-2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU.eb -D
    eb GROMACS-2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU.eb -r
    ```
- Now the module should be available
  ```
  module avail GROMACS
  ```

```
eb --search GROMACS | less
```

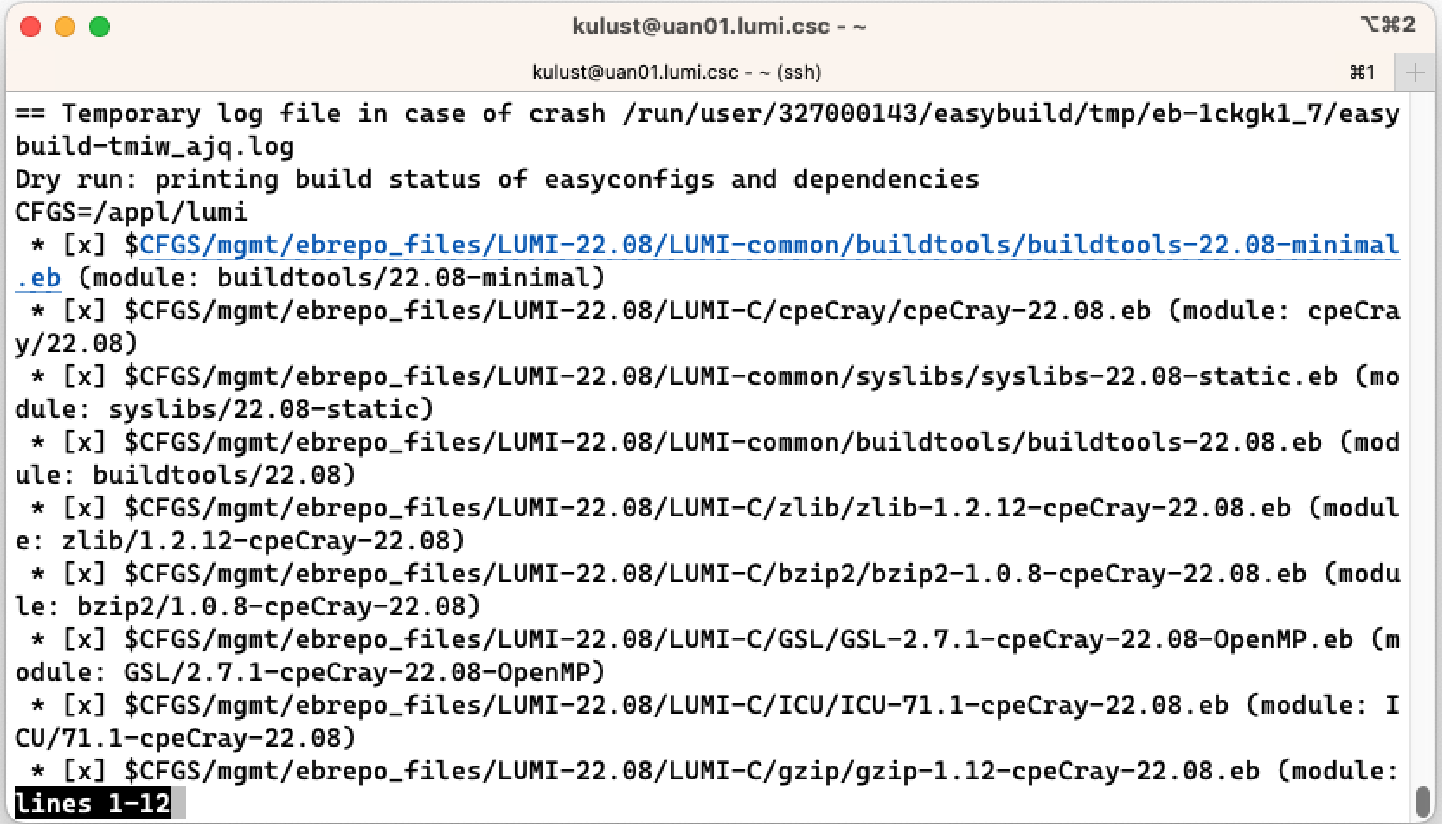


```
 * /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS/GROMACS-2020.4-cpeCr
ay-21.08-PLUMED-2.6.4-CPU.eb
 * /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS/GROMACS-2020.4-cpeGN
U-21.08-PLUMED-2.6.4-CPU.eb
 * /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS/GROMACS-2020.6-cpeCr
ay-21.08-CPU.eb
 * /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS/GROMACS-2020.6-cpeCr
ay-21.08-PLUMED-2.7.2-CPU.eb
 * /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS/GROMACS-2020.6-cpeGN
U-21.08-CPU.eb
 * /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS/GROMACS-2020.6-cpeGN
U-21.08-PLUMED-2.7.2-CPU.eb
 * /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS/GROMACS-2021-cpeCray
-21.08-PLUMED-2.7.2-CPU.eb
 * /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS/GROMACS-2021-cpeGNU-
21.08-PLUMED-2.7.2-CPU.eb
 * /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS/GROMACS-2021.3-cpeCr
ay-21.08-CPU.eb
 * /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS/GROMACS-2021.3-cpeGN
U-21.08-CPU.eb
 * /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS/GROMACS-2021.4-cpeAO
lines 1-11
```

```
eb -S GROMACS | less
```


```
CFGS1=/appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS
 * $CFGS1/GROMACS-2020.4-cpeCray-21.08-PLUMED-2.6.4-CPU.eb
 * $CFGS1/GROMACS-2020.4-cpeGNU-21.08-PLUMED-2.6.4-CPU.eb
 * $CFGS1/GROMACS-2020.6-cpeCray-21.08-CPU.eb
 * $CFGS1/GROMACS-2020.6-cpeCray-21.08-PLUMED-2.7.2-CPU.eb
 * $CFGS1/GROMACS-2020.6-cpeGNU-21.08-CPU.eb
 * $CFGS1/GROMACS-2020.6-cpeGNU-21.08-PLUMED-2.7.2-CPU.eb
 * $CFGS1/GROMACS-2021-cpeCray-21.08-PLUMED-2.7.2-CPU.eb
 * $CFGS1/GROMACS-2021-cpeGNU-21.08-PLUMED-2.7.2-CPU.eb
 * $CFGS1/GROMACS-2021.3-cpeCray-21.08-CPU.eb
 * $CFGS1/GROMACS-2021.3-cpeGNU-21.08-CPU.eb
 * $CFGS1/GROMACS-2021.4-cpeAOCC-21.12-PLUMED-2.7.4-CPU.eb
 * $CFGS1/GROMACS-2021.4-cpeAOCC-21.12-PLUMED-2.8.0-CPU.eb
 * $CFGS1/GROMACS-2021.4-cpeCray-21.12-PLUMED-2.7.4-CPU.eb
 * $CFGS1/GROMACS-2021.4-cpeCray-21.12-PLUMED-2.8.0-CPU.eb
 * $CFGS1/GROMACS-2021.4-cpeCray-22.06-PLUMED-2.7.4-CPU.eb
 * $CFGS1/GROMACS-2021.4-cpeCray-22.06-PLUMED-2.8.0-CPU.eb
 * $CFGS1/GROMACS-2021.4-cpeCray-22.08-PLUMED-2.7.4-CPU.eb
 * $CFGS1/GROMACS-2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU.eb
 * $CFGS1/GROMACS-2021.4-cpeGNU-21.12-PLUMED-2.7.4-CPU.eb
 * $CFGS1/GROMACS-2021.4-cpeGNU-21.12-PLUMED-2.8.0-CPU.eb
lines 1-21
```

eb GROMACS-2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU.eb -D



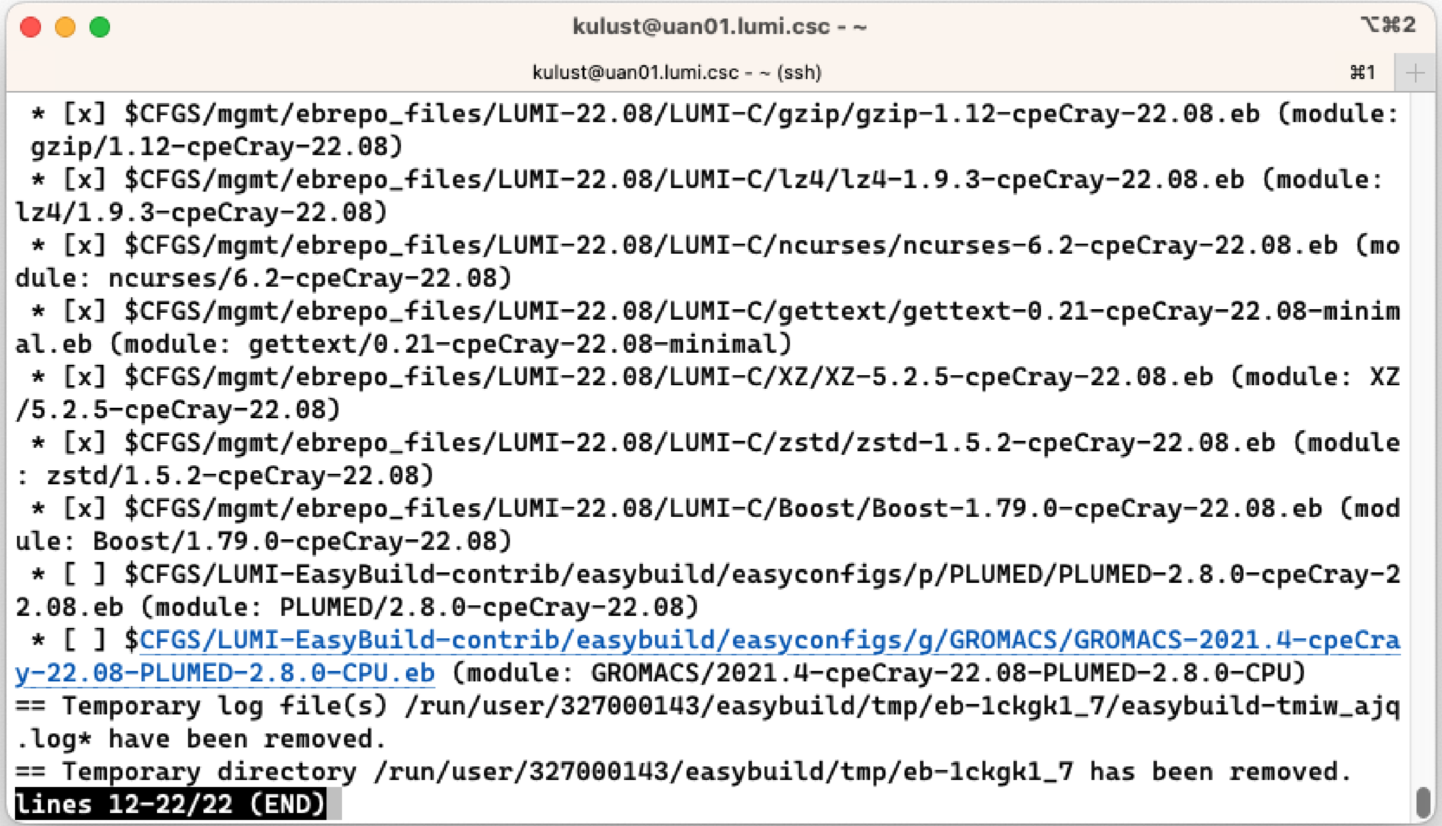
kulust@uan01.lumi.csc - ~

kulust@uan01.lumi.csc - ~ (ssh)

```
== Temporary log file in case of crash /run/user/327000143/easybuild/tmp/eb-1ckgk1_7/easy
build-tmiw_ajq.log
Dry run: printing build status of easyconfigs and dependencies
CFGS=/appl/lumi
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-common/buildtools/buildtools-22.08-minimal
.eb (module: buildtools/22.08-minimal)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-C/cpeCray/cpeCray-22.08.eb (module: cpeCra
y/22.08)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-common/syslibs/syslibs-22.08-static.eb (mo
dule: syslibs/22.08-static)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-common/buildtools/buildtools-22.08.eb (mod
ule: buildtools/22.08)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-C/zlib/zlib-1.2.12-cpeCray-22.08.eb (modul
e: zlib/1.2.12-cpeCray-22.08)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-C/bzip2/bzip2-1.0.8-cpeCray-22.08.eb (modu
le: bzip2/1.0.8-cpeCray-22.08)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-C/GSL/GSL-2.7.1-cpeCray-22.08-OpenMP.eb (m
odule: GSL/2.7.1-cpeCray-22.08-OpenMP)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-C/ICU/ICU-71.1-cpeCray-22.08.eb (module: I
CU/71.1-cpeCray-22.08)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-C/gzip/gzip-1.12-cpeCray-22.08.eb (module:
lines 1-12
```

eb GROMACS-2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU.eb -D

LUMI

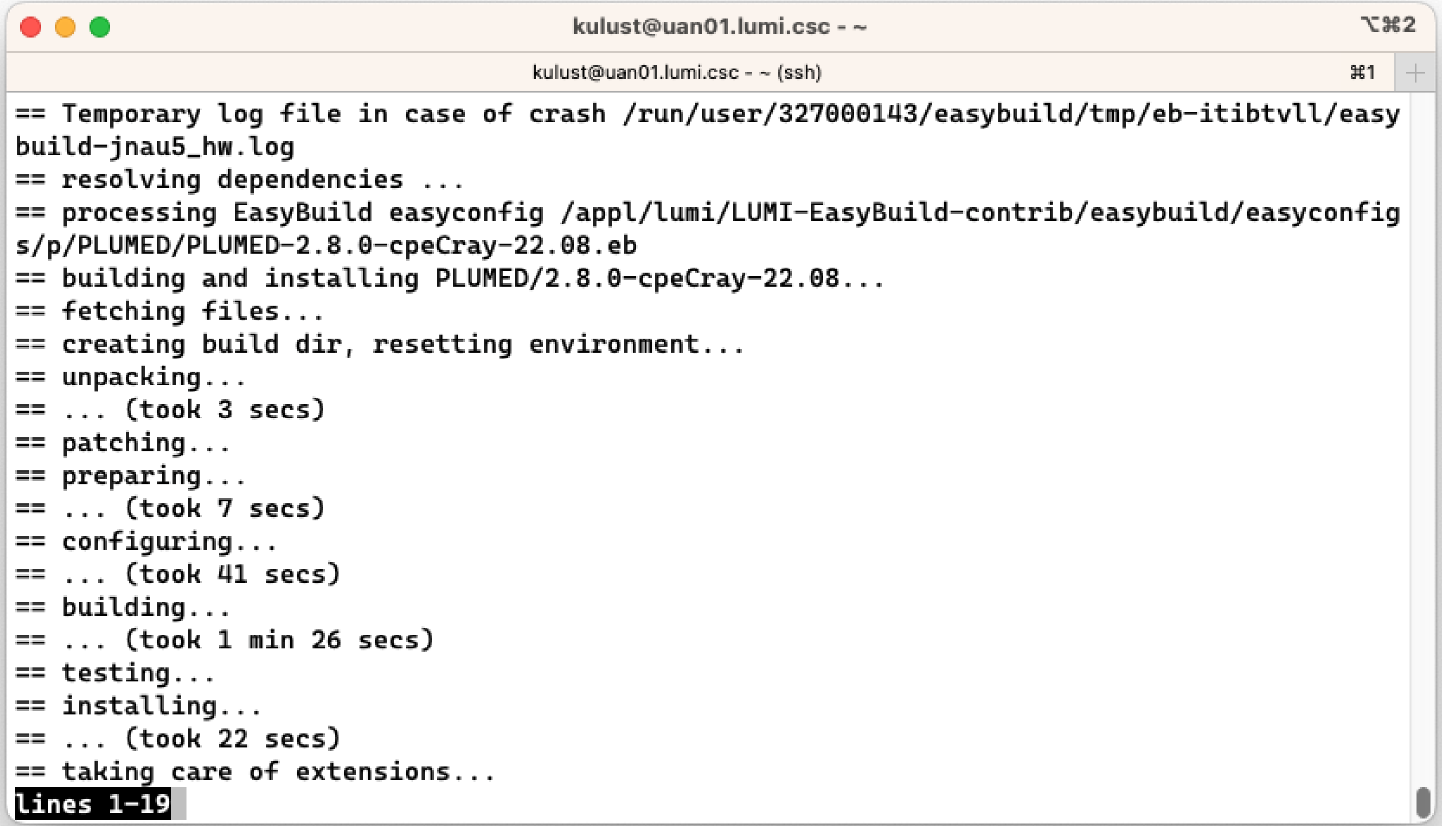


kulust@uan01.lumi.csc - ~

kulust@uan01.lumi.csc - ~ (ssh)

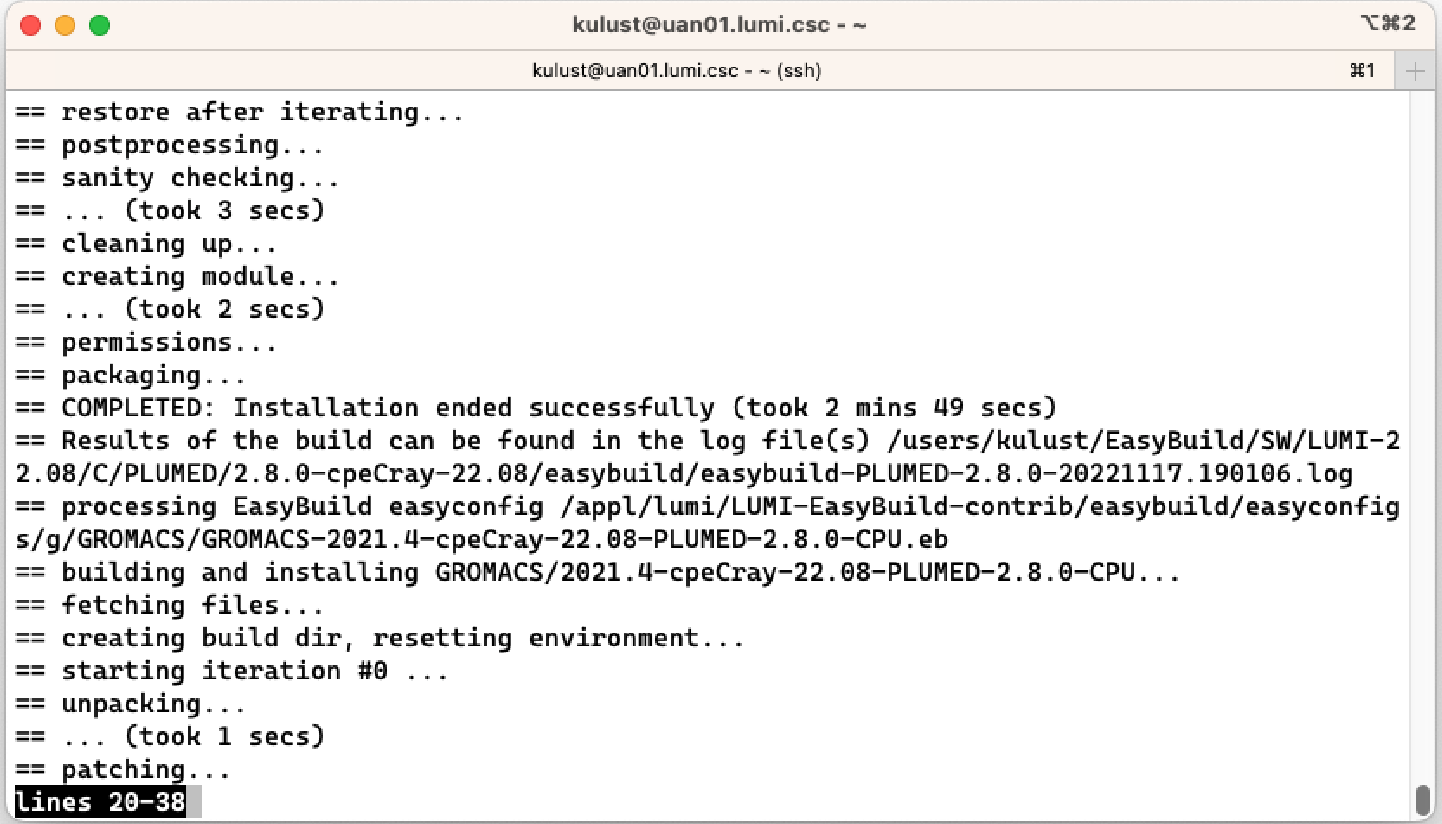
```
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-C/gzip/gzip-1.12-cpeCray-22.08.eb (module:
 gzip/1.12-cpeCray-22.08)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-C/lz4/lz4-1.9.3-cpeCray-22.08.eb (module:
lz4/1.9.3-cpeCray-22.08)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-C/ncurses/ncurses-6.2-cpeCray-22.08.eb (mo
dule: ncurses/6.2-cpeCray-22.08)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-C/gettext/gettext-0.21-cpeCray-22.08-minim
al.eb (module: gettext/0.21-cpeCray-22.08-minimal)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-C/XZ/XZ-5.2.5-cpeCray-22.08.eb (module: XZ
/5.2.5-cpeCray-22.08)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-C/zstd/zstd-1.5.2-cpeCray-22.08.eb (module
: zstd/1.5.2-cpeCray-22.08)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-C/Boost/Boost-1.79.0-cpeCray-22.08.eb (mod
ule: Boost/1.79.0-cpeCray-22.08)
 * [ ] $CFGS/LUMI-EasyBuild-contrib/easybuild/easyconfigs/p/PLUMED/PLUMED-2.8.0-cpeCray-2
2.08.eb (module: PLUMED/2.8.0-cpeCray-22.08)
 * [ ] $CFGS/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS/GROMACS-2021.4-cpeCra
y-22.08-PLUMED-2.8.0-CPU.eb (module: GROMACS/2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU)
== Temporary log file(s) /run/user/327000143/easybuild/tmp/eb-1ckgk1_7/easybuild-tmiw_ajq
.log* have been removed.
== Temporary directory /run/user/327000143/easybuild/tmp/eb-1ckgk1_7 has been removed.
lines 12-22/22 (END)
```

```
eb GROMACS-2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU.eb -r
```



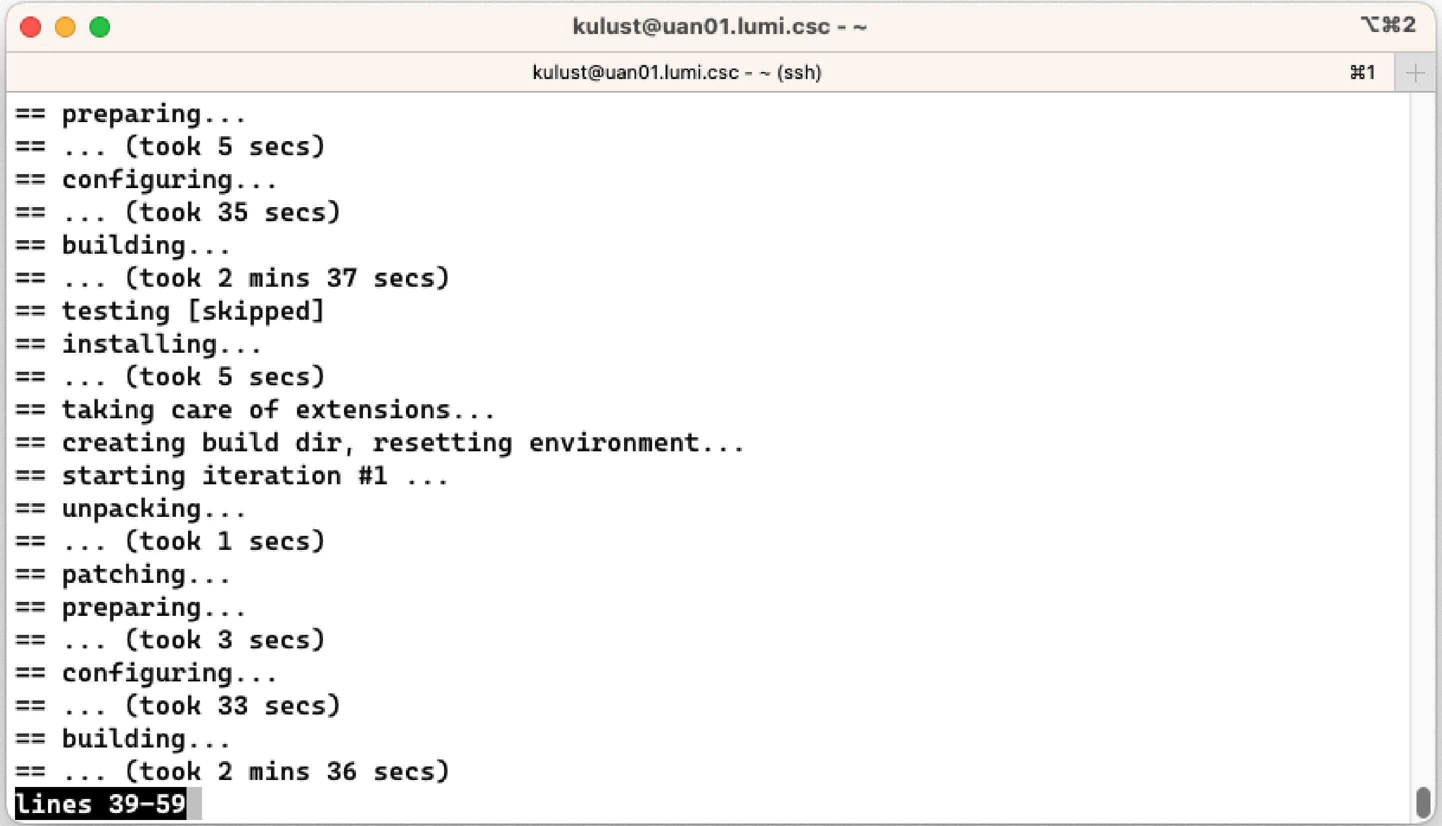
```
== Temporary log file in case of crash /run/user/327000143/easybuild/tmp/eb-itibtvll/easy
build-jnau5_hw.log
== resolving dependencies ...
== processing EasyBuild easyconfig /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfig
s/p/PLUMED/PLUMED-2.8.0-cpeCray-22.08.eb
== building and installing PLUMED/2.8.0-cpeCray-22.08...
== fetching files...
== creating build dir, resetting environment...
== unpacking...
== ... (took 3 secs)
== patching...
== preparing...
== ... (took 7 secs)
== configuring...
== ... (took 41 secs)
== building...
== ... (took 1 min 26 secs)
== testing...
== installing...
== ... (took 22 secs)
== taking care of extensions...
lines 1-19
```

```
eb GROMACS-2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU.eb -r
```



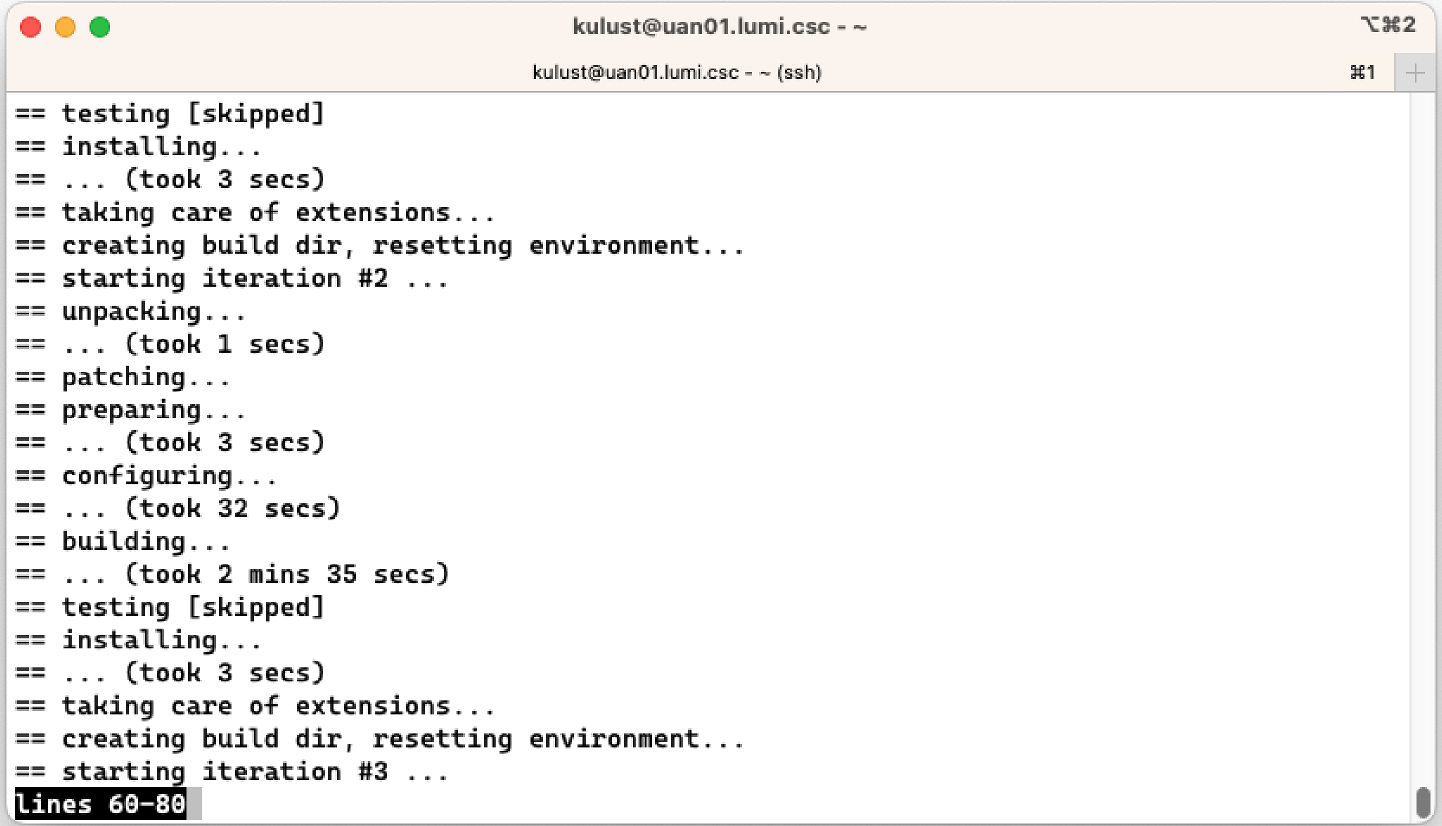
```
== restore after iterating...
== postprocessing...
== sanity checking...
== ... (took 3 secs)
== cleaning up...
== creating module...
== ... (took 2 secs)
== permissions...
== packaging...
== COMPLETED: Installation ended successfully (took 2 mins 49 secs)
== Results of the build can be found in the log file(s) /users/kulust/EasyBuild/SW/LUMI-2
2.08/C/PLUMED/2.8.0-cpeCray-22.08/easybuild/easybuild-PLUMED-2.8.0-20221117.190106.log
== processing EasyBuild easyconfig /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfig
s/g/GROMACS/GROMACS-2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU.eb
== building and installing GROMACS/2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU...
== fetching files...
== creating build dir, resetting environment...
== starting iteration #0 ...
== unpacking...
== ... (took 1 secs)
== patching...
lines 20-38
```

eb GROMACS-2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU.eb -r



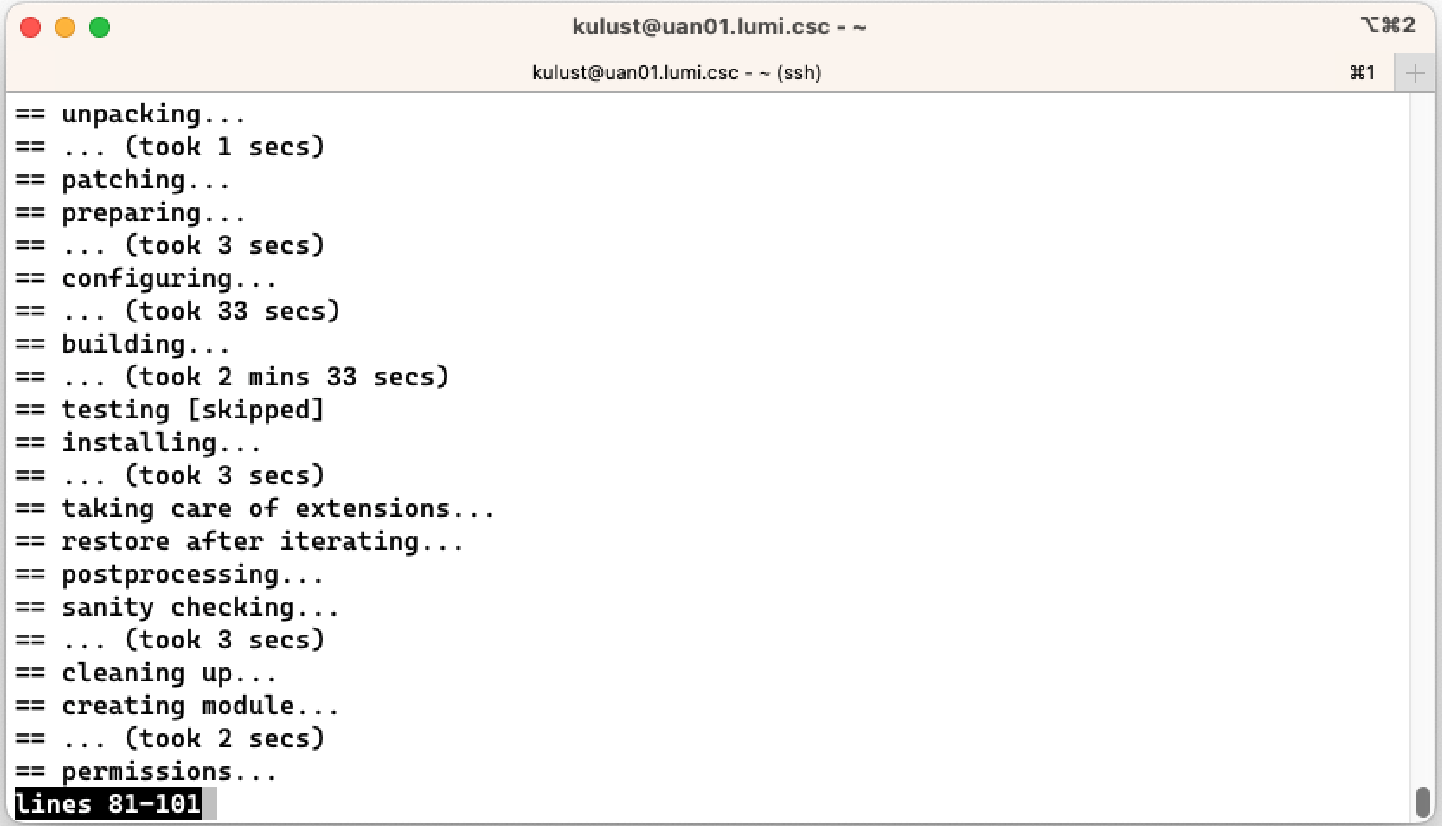
```
== preparing...
== ... (took 5 secs)
== configuring...
== ... (took 35 secs)
== building...
== ... (took 2 mins 37 secs)
== testing [skipped]
== installing...
== ... (took 5 secs)
== taking care of extensions...
== creating build dir, resetting environment...
== starting iteration #1 ...
== unpacking...
== ... (took 1 secs)
== patching...
== preparing...
== ... (took 3 secs)
== configuring...
== ... (took 33 secs)
== building...
== ... (took 2 mins 36 secs)
lines 39-59
```

```
eb GROMACS-2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU.eb -r
```



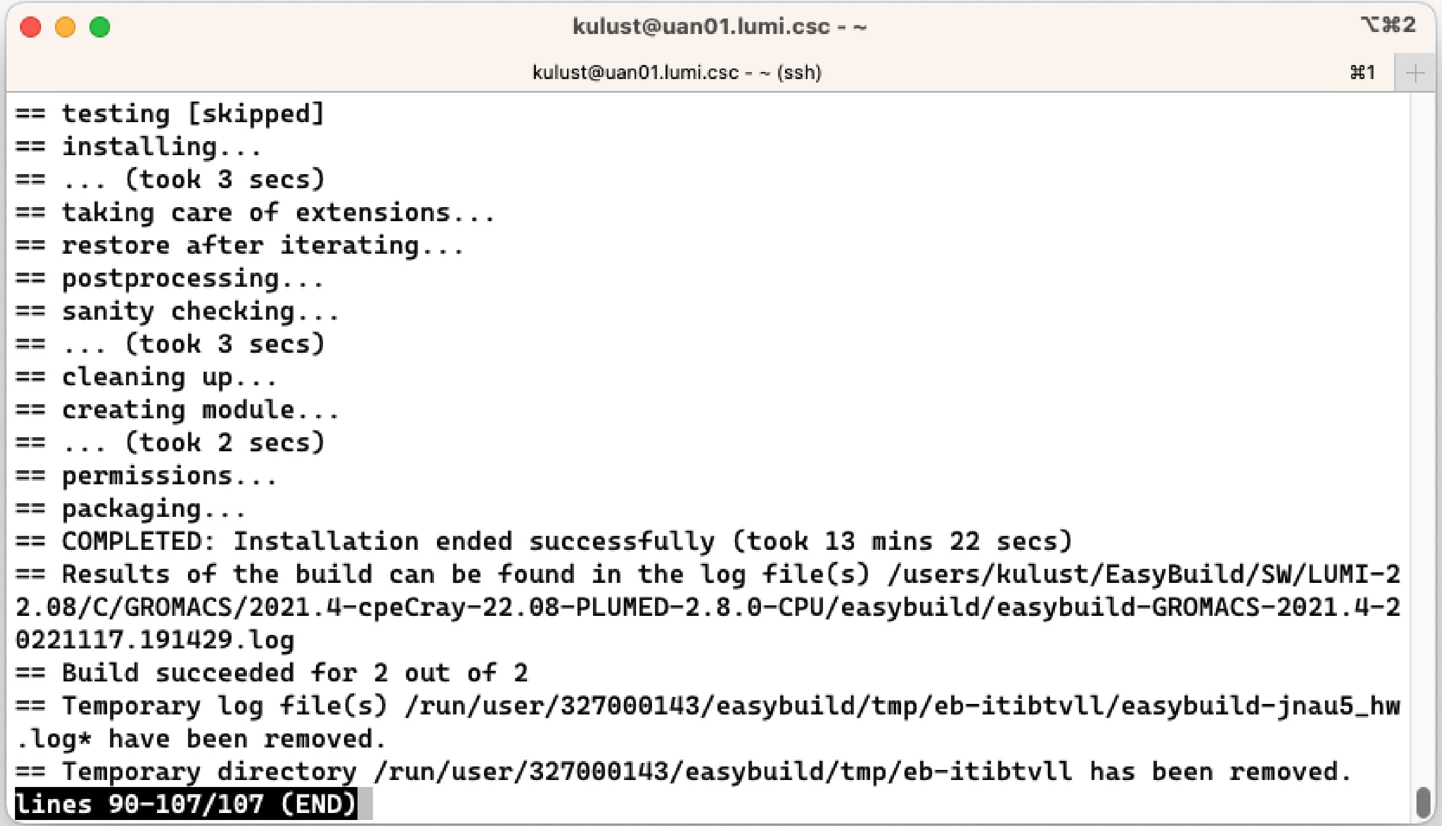
```
== testing [skipped]
== installing...
== ... (took 3 secs)
== taking care of extensions...
== creating build dir, resetting environment...
== starting iteration #2 ...
== unpacking...
== ... (took 1 secs)
== patching...
== preparing...
== ... (took 3 secs)
== configuring...
== ... (took 32 secs)
== building...
== ... (took 2 mins 35 secs)
== testing [skipped]
== installing...
== ... (took 3 secs)
== taking care of extensions...
== creating build dir, resetting environment...
== starting iteration #3 ...
lines 60-80
```

eb GROMACS-2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU.eb -r



```
== unpacking...
== ... (took 1 secs)
== patching...
== preparing...
== ... (took 3 secs)
== configuring...
== ... (took 33 secs)
== building...
== ... (took 2 mins 33 secs)
== testing [skipped]
== installing...
== ... (took 3 secs)
== taking care of extensions...
== restore after iterating...
== postprocessing...
== sanity checking...
== ... (took 3 secs)
== cleaning up...
== creating module...
== ... (took 2 secs)
== permissions...
lines 81-101
```

eb GROMACS-2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU.eb -r



```
== testing [skipped]
== installing...
== ... (took 3 secs)
== taking care of extensions...
== restore after iterating...
== postprocessing...
== sanity checking...
== ... (took 3 secs)
== cleaning up...
== creating module...
== ... (took 2 secs)
== permissions...
== packaging...
== COMPLETED: Installation ended successfully (took 13 mins 22 secs)
== Results of the build can be found in the log file(s) /users/kulust/EasyBuild/SW/LUMI-2
2.08/C/GROMACS/2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU/easybuild/easybuild-GROMACS-2021.4-2
0221117.191429.log
== Build succeeded for 2 out of 2
== Temporary log file(s) /run/user/327000143/easybuild/tmp/eb-itibtvll/easybuild-jnau5_hw
.log* have been removed.
== Temporary directory /run/user/327000143/easybuild/tmp/eb-itibtvll has been removed.
lines 90-107/107 (END)
```

Installing

Step 3: Install the software - Note

- Note: Sometimes the module does not show up immediately. This is because Lmod keeps a cache and fails to detect that the cache is outdated.
  - Remove `$HOME/.lmod.d/.cache`
    ```
    rm -rf $HOME/.lmod.d/.cache
    ```
  - We've seen rare cases where internal Lmod data structures where corrupt and logging out and in again was needed
- Installing this way is 100% equivalent to an installation in the central software tree. The application is compiled in exactly the same way as we would do and served from the same file systems.

More advanced work

- You can also install some EasyBuild recipes that you got from support and are in the current directory (preferably one without subdirectories):
  `eb my_recipe.eb -r .`
  - Note the dot after the `-r` to tell EasyBuild to also look for dependencies in the current directory (and its subdirectories)
- In some cases you will have to download the sources by hand, e.g., for VASP, which is then at the same time a way for us to ensure that you have a license for VASP. E.g.,
  - `eb --search VASP`
  - Then from the directory with the VASP sources:
    `eb VASP-6.3.2-cpeGNU-22.08.eb -r .`

More advanced work (2): Repositories

- It is possible to have your own clone of the LUMI-EasyBuild-contrib repo in your `$EBU_USER_PREFIX` subdirectory if you want the latest and greatest before it is in the centrally maintained repository

  -
    ```
    cd $EBU_USER_PREFIX
    git clone https://github.com/Lumi-supercomputer/LUMI-EasyBuild-contrib.git
    ```
- It is also possible to maintain your own repo
  - The directory should be `$EBU_USER_PREFIX/UserRepo` (but of course on GitHub the repository can have a different name)
  - Structure should be compatible with EasyBuild: easyconfig files go in `$EBU_USER_PREFIX/easybuild/easyconfigs`

More advanced work (3): Reproducibility

- EasyBuild will keep a copy of the sources in `$EBU_USER_PREFIX/sources`
- EasyBuild also keeps copies of all installed easyconfig files in two locations:
  - In `$EBU_USER_PREFIX/ebrepo_files`
    - And note that EasyBuild will use this version if you try to reinstall and did not delete this version first!
    - This ensures that the information that EasyBuild has about the installed application is compatible with what's in the module files
  - With the installed software (in `$EBU_USER_PREFIX/SW`) in a subdirectory called easybuild
    This is meant to have all information about how EasyBuild installed the application and to help in reproducing

Additional tips&tricks

- Updating version: Often some trivial changes in the EasyConfig (`.eb`) file
  - Checksums may be annoying: Use `--ignore-checksums` with the `eb` command
- Updating to a new toolchain:
  - Be careful, it is more than changing one number
  - Versions of preinstalled dependencies should be changed and EasyConfig files of other dependencies also checked
- LUMI Software Library at lumi-supercomputer.github.io/LUMI-EasyBuild-docs
  - For most packages, pointers to the license
  - User documentation gives info about the use of the package, or restrictions
  - Technical documentation aimed at users who want more information about how we build the package

EasyBuild training for advanced users and developers

- EasyBuild web site: easybuild.io
- Generic EasyBuild training materials on easybuilders.github.io/easybuild-tutorial.
- Training for CSC and local support organisations: Most up-to-date version of the training materials on klust.github.io/easybuild-tutorial.

Containers

This is about containers on LUMI-C and LUMI-G!

- What can they do and what can't they do?
- Getting containers onto LUMI
- Running containers on LUMI
- Enhancements to the LUMI environment to help you

- But remember: LUMI is an HPC infrastructure, not a container cloud!

What do containers not provide?

- **Full reproducibility** is a myth
- **Full portability**: Not every container prepared on your Ubuntu or CentOS cluster or workstation will work on LUMI.
  - Containers that rely on certain hardware, kernel modules and/or kernel versions may fail.
  - Problem cases: High-performance networking (MPI) and GPU (driver version)
- **Performance portability**:
  - A container built from sources on one CPU will not be optimal for another one.
  - Containers built from downloaded binaries may not exploit all architectural features of the CPU.
  - No support for the LUMI interconnect may lead to fall-down to slower protocol that works

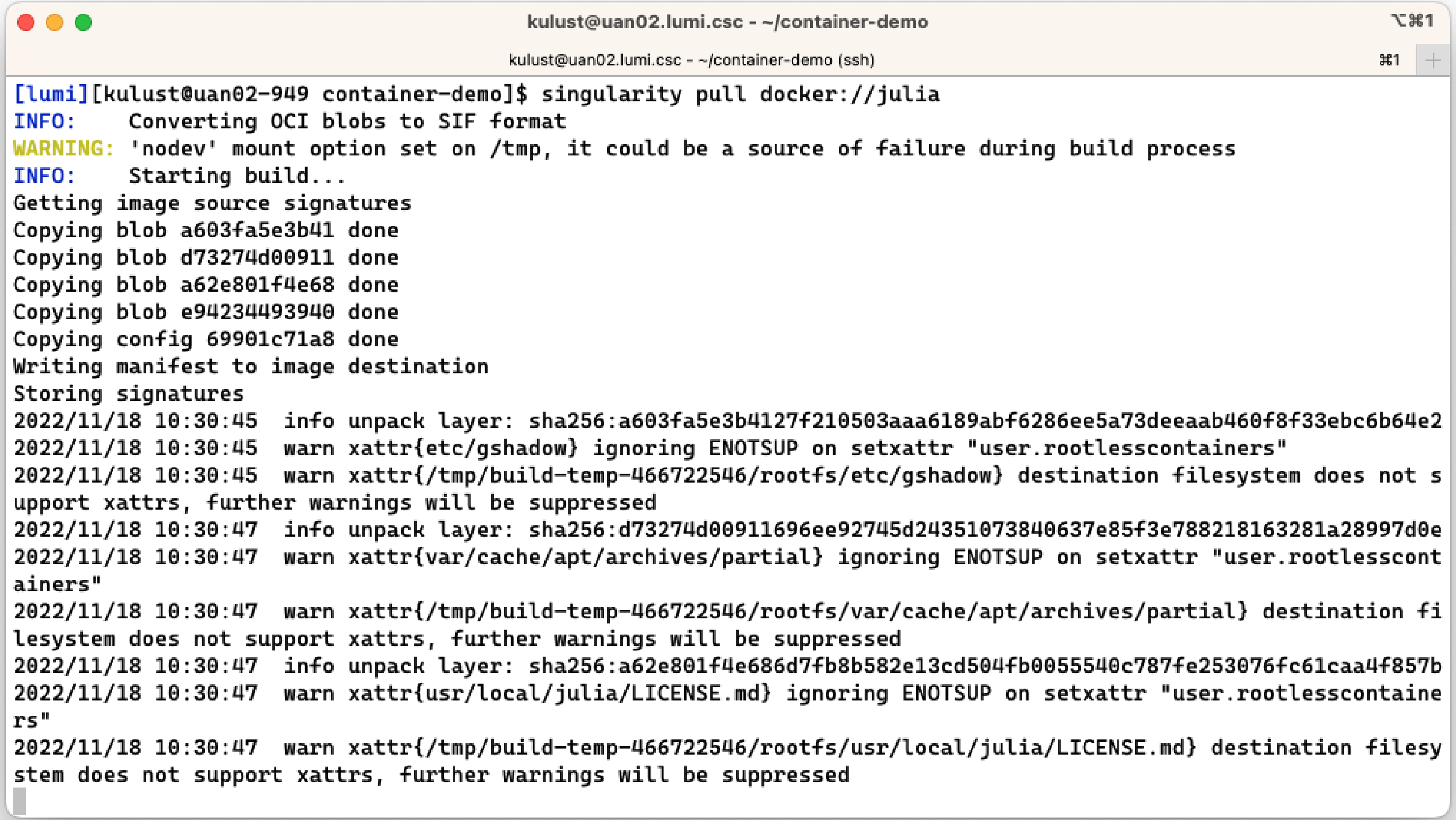
But what can they then do on LUMI?

- **Storage manageability:** Lower pressure on the filesystems (for software frameworks that access hundreds of thousands of small files) for better I/O performance and management of your disk file quota.
- **Productivity:** When not hit by the portability constraints, still useful to reproduce sophisticated user environments, e.g., Python.
- **Software installation:** Can be a way to install software with an installation process that is not aware of multi-user HPC systems and is too complicated to recompile.
- You’re the system administrator of your container, not LUST!

Managing containers

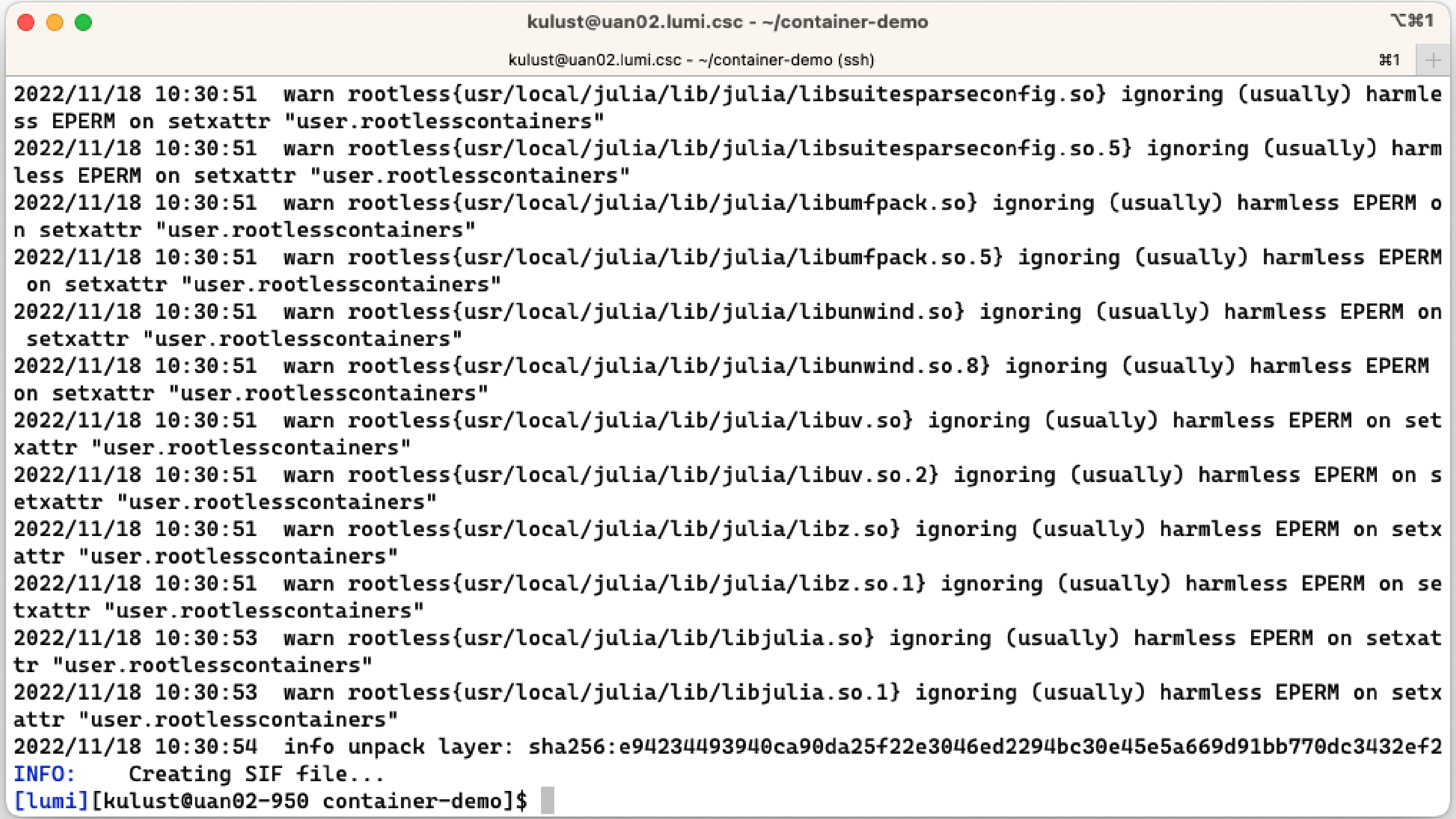
- Supported runtimes
  - Docker is **NOT** directly available from user environment
  - Singularity is natively available (as a system command) on the login and compute nodes
- Pulling containers
  - DockerHub and other registries (example: Julia container)
    `singularity pull docker://julia`
  - Singularity uses flat (single) sif file for storing container and pull command makes the conversion
  - Be carefull: cache in `.singularity` dir or `$XDG_RUNTIME_DIR` can easily exhaust your storage quota for larger images

singularity pull docker://julia


kulust@uan02.lumi.csc - ~/container-demo
⌥⌘1
kulust@uan02.lumi.csc - ~/container-demo (ssh)
⌘1

```
[lumi][kulust@uan02-949 container-demo]$ singularity pull docker://julia
INFO:    Converting OCI blobs to SIF format
WARNING: 'nodev' mount option set on /tmp, it could be a source of failure during build process
INFO:    Starting build...
Getting image source signatures
Copying blob a603fa5e3b41 done
Copying blob d73274d00911 done
Copying blob a62e801f4e68 done
Copying blob e94234493940 done
Copying config 69901c71a8 done
Writing manifest to image destination
Storing signatures
2022/11/18 10:30:45  info unpack layer: sha256:a603fa5e3b4127f210503aaa6189abf6286ee5a73deeaab460f8f33ebc6b64e2
2022/11/18 10:30:45  warn xattr{etc/gshadow} ignoring ENOTSUP on setxattr "user.rootlesscontainers"
2022/11/18 10:30:45  warn xattr{/tmp/build-temp-466722546/rootfs/etc/gshadow} destination filesystem does not s
upport xattrs, further warnings will be suppressed
2022/11/18 10:30:47  info unpack layer: sha256:d73274d00911696ee92745d24351073840637e85f3e788218163281a28997d0e
2022/11/18 10:30:47  warn xattr{var/cache/apt/archives/partial} ignoring ENOTSUP on setxattr "user.rootlesscont
ainers"
2022/11/18 10:30:47  warn xattr{/tmp/build-temp-466722546/rootfs/var/cache/apt/archives/partial} destination fi
lesystem does not support xattrs, further warnings will be suppressed
2022/11/18 10:30:47  info unpack layer: sha256:a62e801f4e686d7fb8b582e13cd504fb0055540c787fe253076fc61caa4f857b
2022/11/18 10:30:47  warn xattr{usr/local/julia/LICENSE.md} ignoring ENOTSUP on setxattr "user.rootlesscontaine
rs"
2022/11/18 10:30:47  warn xattr{/tmp/build-temp-466722546/rootfs/usr/local/julia/LICENSE.md} destination filesy
stem does not support xattrs, further warnings will be suppressed
```

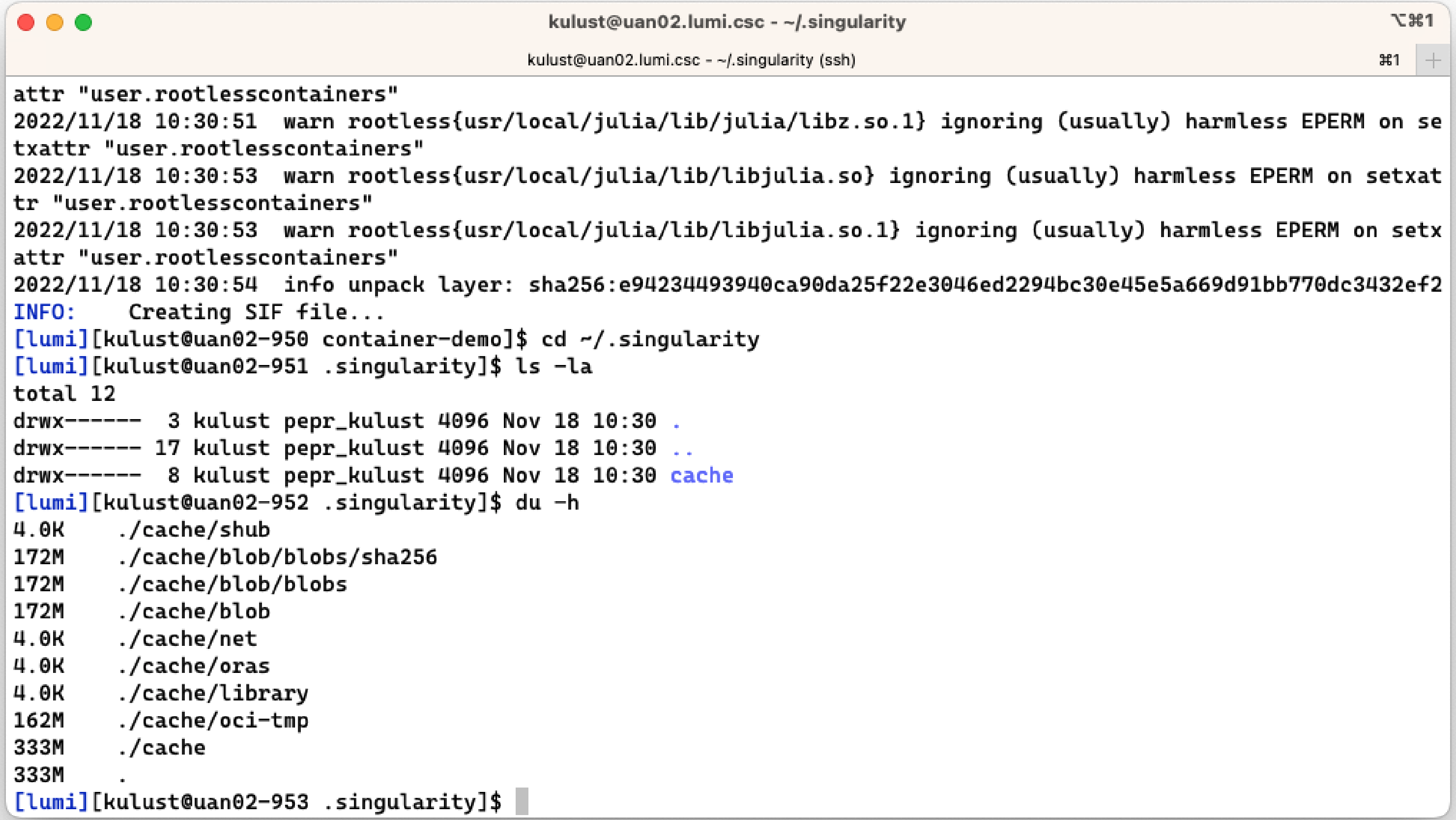
singularity pull docker://julia


kulust@uan02.lumi.csc - ~/container-demo

kulust@uan02.lumi.csc - ~/container-demo (ssh)

```
2022/11/18 10:30:51  warn rootless{usr/local/julia/lib/julia/libsuitesparseconfig.so} ignoring (usually) harmle
ss EPERM on setxattr "user.rootlesscontainers"
2022/11/18 10:30:51  warn rootless{usr/local/julia/lib/julia/libsuitesparseconfig.so.5} ignoring (usually) harm
less EPERM on setxattr "user.rootlesscontainers"
2022/11/18 10:30:51  warn rootless{usr/local/julia/lib/julia/libumfpack.so} ignoring (usually) harmless EPERM o
n setxattr "user.rootlesscontainers"
2022/11/18 10:30:51  warn rootless{usr/local/julia/lib/julia/libumfpack.so.5} ignoring (usually) harmless EPERM
 on setxattr "user.rootlesscontainers"
2022/11/18 10:30:51  warn rootless{usr/local/julia/lib/julia/libunwind.so} ignoring (usually) harmless EPERM on
 setxattr "user.rootlesscontainers"
2022/11/18 10:30:51  warn rootless{usr/local/julia/lib/julia/libunwind.so.8} ignoring (usually) harmless EPERM
on setxattr "user.rootlesscontainers"
2022/11/18 10:30:51  warn rootless{usr/local/julia/lib/julia/libuv.so} ignoring (usually) harmless EPERM on set
xattr "user.rootlesscontainers"
2022/11/18 10:30:51  warn rootless{usr/local/julia/lib/julia/libuv.so.2} ignoring (usually) harmless EPERM on s
etxattr "user.rootlesscontainers"
2022/11/18 10:30:51  warn rootless{usr/local/julia/lib/julia/libz.so} ignoring (usually) harmless EPERM on setx
attr "user.rootlesscontainers"
2022/11/18 10:30:51  warn rootless{usr/local/julia/lib/julia/libz.so.1} ignoring (usually) harmless EPERM on se
txattr "user.rootlesscontainers"
2022/11/18 10:30:53  warn rootless{usr/local/julia/lib/libjulia.so} ignoring (usually) harmless EPERM on setxat
tr "user.rootlesscontainers"
2022/11/18 10:30:53  warn rootless{usr/local/julia/lib/libjulia.so.1} ignoring (usually) harmless EPERM on setx
attr "user.rootlesscontainers"
2022/11/18 10:30:54  info unpack layer: sha256:e94234493940ca90da25f22e3046ed2294bc30e45e5a669d91bb770dc3432ef2
INFO:    Creating SIF file...
[lumi][kulust@uan02-950 container-demo]$
```

singularity pull docker://julia


kulust@uan02.lumi.csc - ~/.singularity
⌥⌘1
kulust@uan02.lumi.csc - ~/.singularity (ssh)
⌘1

```
attr "user.rootlesscontainers"
2022/11/18 10:30:51  warn rootless{usr/local/julia/lib/julia/libz.so.1} ignoring (usually) harmless EPERM on se
txattr "user.rootlesscontainers"
2022/11/18 10:30:53  warn rootless{usr/local/julia/lib/libjulia.so} ignoring (usually) harmless EPERM on setxat
tr "user.rootlesscontainers"
2022/11/18 10:30:53  warn rootless{usr/local/julia/lib/libjulia.so.1} ignoring (usually) harmless EPERM on setx
attr "user.rootlesscontainers"
2022/11/18 10:30:54  info unpack layer: sha256:e94234493940ca90da25f22e3046ed2294bc30e45e5a669d91bb770dc3432ef2
INFO:    Creating SIF file...
[lumi][kulust@uan02-950 container-demo]$ cd ~/.singularity
[lumi][kulust@uan02-951 .singularity]$ ls -la
total 12
drwx------  3 kulust pepr_kulust 4096 Nov 18 10:30 .
drwx------ 17 kulust pepr_kulust 4096 Nov 18 10:30 ..
drwx------  8 kulust pepr_kulust 4096 Nov 18 10:30 cache
[lumi][kulust@uan02-952 .singularity]$ du -h
4.0K    ./cache/shub
172M    ./cache/blob/blobs/sha256
172M    ./cache/blob/blobs
172M    ./cache/blob
4.0K    ./cache/net
4.0K    ./cache/oras
4.0K    ./cache/library
162M    ./cache/oci-tmp
333M    ./cache
333M    .
[lumi][kulust@uan02-953 .singularity]$
```

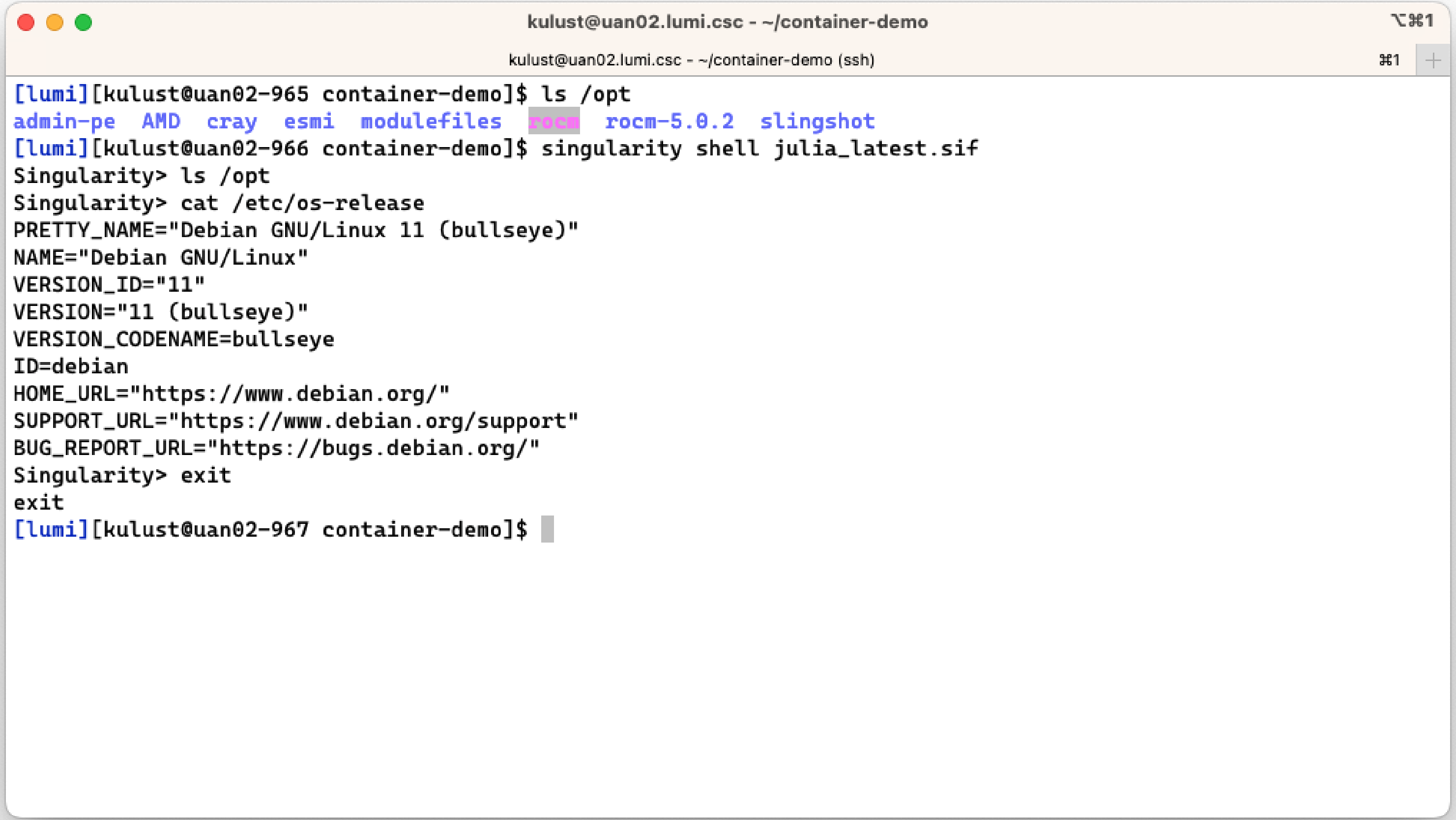
Managing containers (2)

- Building containers
  - Containers cannot be built on LUMI
  - You should either pull or copy containers from outside
  - Singularity can build from existing (base) container
  - We plan to provide a set of base LUMI images

Interacting with containers

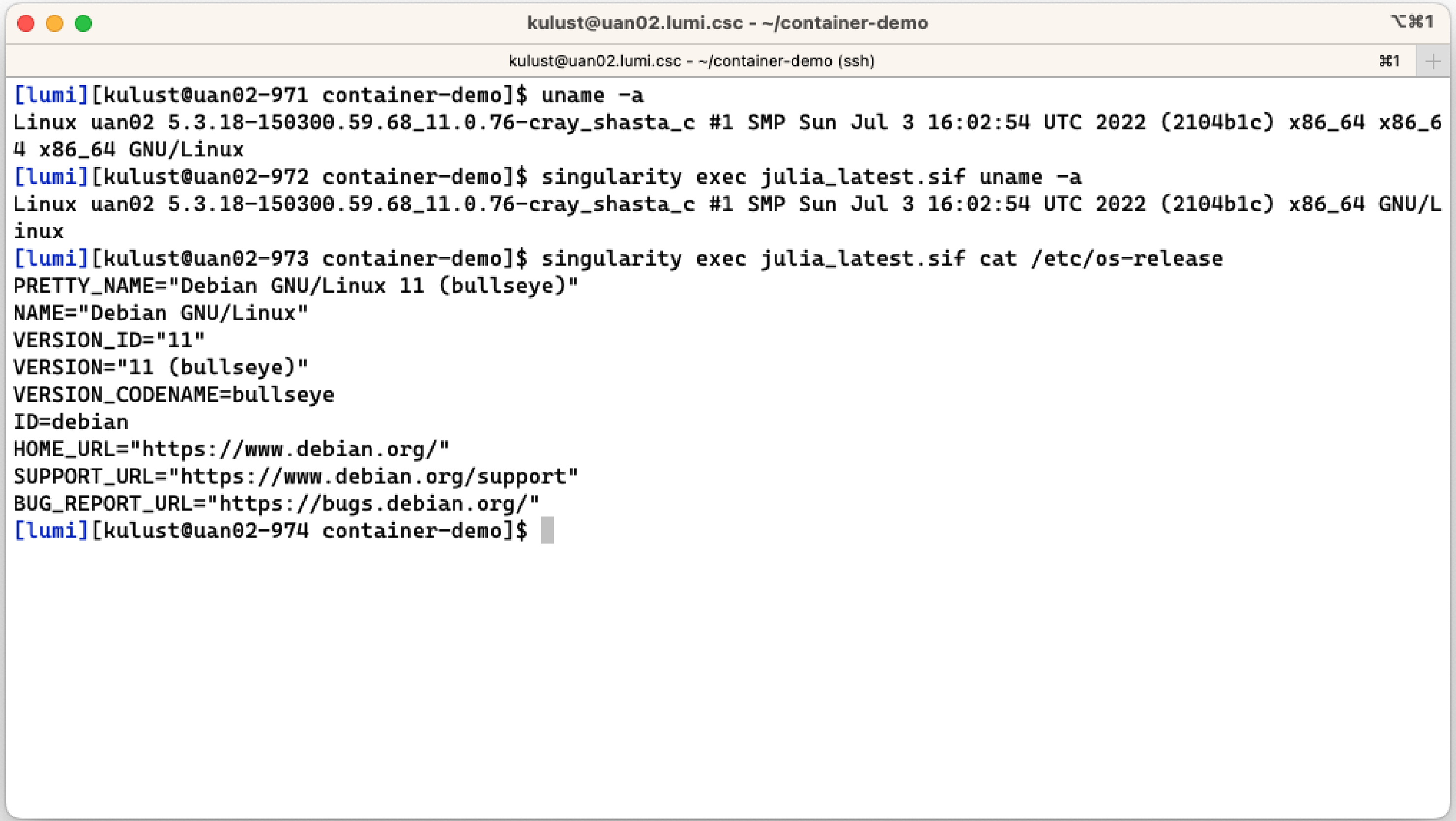
- Accessing a container with the shell command
  `singularity shell container.sif`
- Executing a command in the container with exec
  `singularity exec container.sif uname -a`
- "Running" a container
  `singularity run container.sif`
- Inspecting run definition script
  `singularity inspect --runscript container.sif`
- Accessing host filesystem with bind mounts
  - Singularity will mount `$HOME`, `/tmp`, `/proc`, `/sys`, `/dev` into container by default
  - Use `--bind src1:dest1,src2:dest2` or the `SINGULARITY_BINDPATH` environment variable to mount other host directories (like `/project` or `/appl`)

singularity shell julia_latest.sif


kulust@uan02.lumi.csc - ~/container-demo
kulust@uan02.lumi.csc - ~/container-demo (ssh)

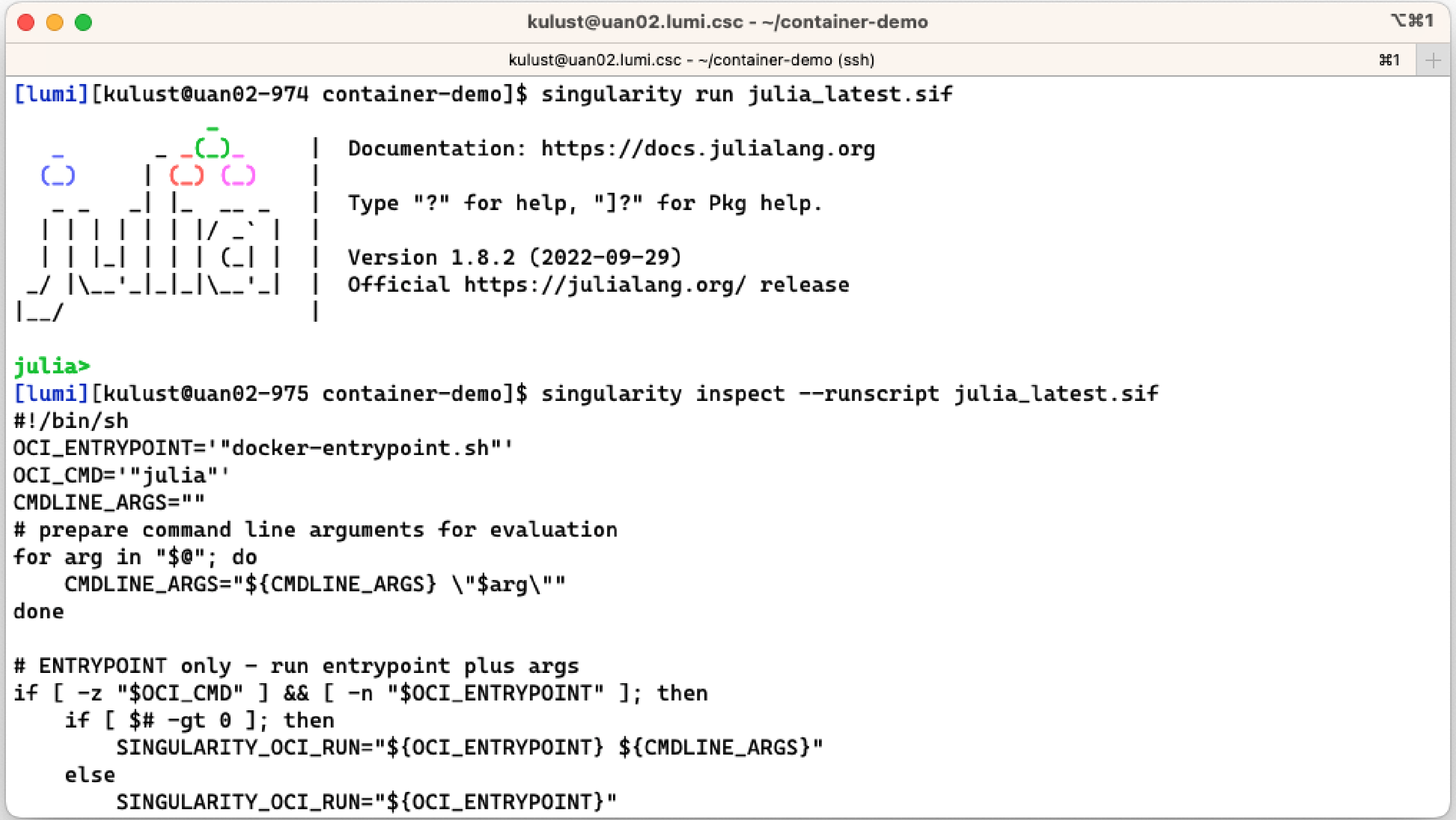
```
[lumi][kulust@uan02-965 container-demo]$ ls /opt
admin-pe  AMD  cray  esmi  modulefiles  rocm  rocm-5.0.2  slingshot
[lumi][kulust@uan02-966 container-demo]$ singularity shell julia_latest.sif
Singularity> ls /opt
Singularity> cat /etc/os-release
PRETTY_NAME="Debian GNU/Linux 11 (bullseye)"
NAME="Debian GNU/Linux"
VERSION_ID="11"
VERSION="11 (bullseye)"
VERSION_CODENAME=bullseye
ID=debian
HOME_URL="https://www.debian.org/"
SUPPORT_URL="https://www.debian.org/support"
BUG_REPORT_URL="https://bugs.debian.org/"
Singularity> exit
exit
[lumi][kulust@uan02-967 container-demo]$
```

singularity exec julia_latest.sif uname -a


kulust@uan02.lumi.csc - ~/container-demo ⌥⌘1
kulust@uan02.lumi.csc - ~/container-demo (ssh) ⌘1

```
[lumi][kulust@uan02-971 container-demo]$ uname -a
Linux uan02 5.3.18-150300.59.68_11.0.76-cray_shasta_c #1 SMP Sun Jul 3 16:02:54 UTC 2022 (2104b1c) x86_64 x86_6
4 x86_64 GNU/Linux
[lumi][kulust@uan02-972 container-demo]$ singularity exec julia_latest.sif uname -a
Linux uan02 5.3.18-150300.59.68_11.0.76-cray_shasta_c #1 SMP Sun Jul 3 16:02:54 UTC 2022 (2104b1c) x86_64 GNU/L
inux
[lumi][kulust@uan02-973 container-demo]$ singularity exec julia_latest.sif cat /etc/os-release
PRETTY_NAME="Debian GNU/Linux 11 (bullseye)"
NAME="Debian GNU/Linux"
VERSION_ID="11"
VERSION="11 (bullseye)"
VERSION_CODENAME=bullseye
ID=debian
HOME_URL="https://www.debian.org/"
SUPPORT_URL="https://www.debian.org/support"
BUG_REPORT_URL="https://bugs.debian.org/"
[lumi][kulust@uan02-974 container-demo]$
```

```
singularity run julia_latest.sif
singularity inspect –runscript julia_latest.sif
```



```
[lumi][kulust@uan02-974 container-demo]$ singularity run julia_latest.sif
               _
   _       _ _(_)_     |  Documentation: https://docs.julialang.org
  (_)     | (_) (_)    |
   _ _   _| |_  __ _   |  Type "?" for help, "]?" for Pkg help.
  | | | | | | |/ _` |  |
  | | |_| | | | (_| |  |  Version 1.8.2 (2022-09-29)
 _/ |\__'_|_|_|\__'_|  |  Official https://julialang.org/ release
|__/                   |

julia>
[lumi][kulust@uan02-975 container-demo]$ singularity inspect --runscript julia_latest.sif
#!/bin/sh
OCI_ENTRYPOINT='"docker-entrypoint.sh"'
OCI_CMD='"julia"'
CMDLINE_ARGS=""
# prepare command line arguments for evaluation
for arg in "$@"; do
    CMDLINE_ARGS="${CMDLINE_ARGS} \"$arg\""
done

# ENTRYPOINT only - run entrypoint plus args
if [ -z "$OCI_CMD" ] && [ -n "$OCI_ENTRYPOINT" ]; then
    if [ $# -gt 0 ]; then
        SINGULARITY_OCI_RUN="${OCI_ENTRYPOINT} ${CMDLINE_ARGS}"
    else
        SINGULARITY_OCI_RUN="${OCI_ENTRYPOINT}"
```

Running containers on LUMI

- Use SLURM to run containers on compute nodes
- Use srun to execute MPI containers

```
srun singularity exec --bind ${BIND_ARGS} \
${CONTAINER_PATH} my_mpi_binary ${APP_PARAMS}
```

- **Be aware your container must be compatible with Cray MPI** (MPICH ABI compatible)
  - Configure suggestion: see next slide
- Open MPI based containers need workarounds and are not well supported on LUMI at the moment (and even more problematic for the GPU)

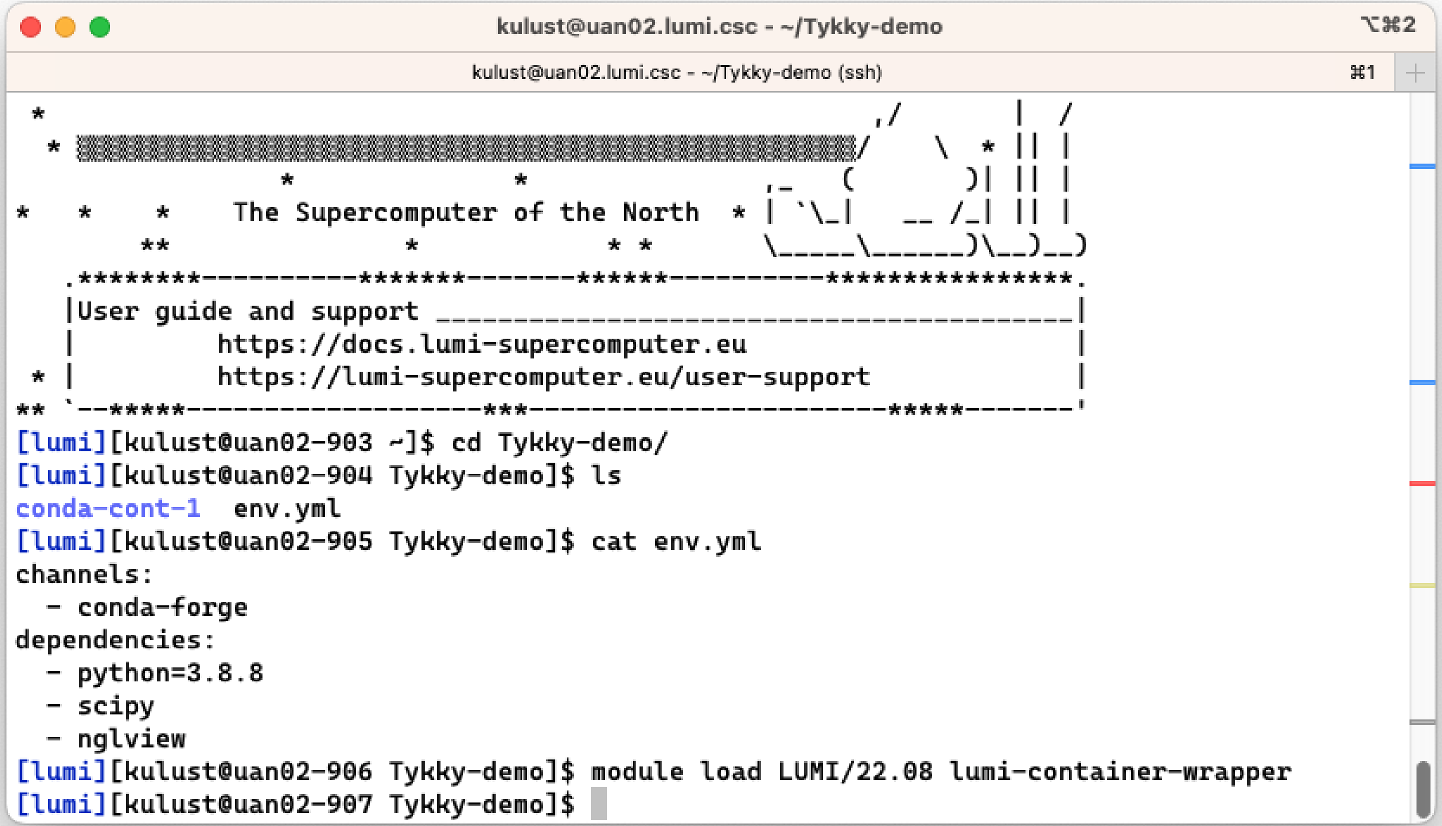
Environment enhancements

- LUMI specific tools for container interaction provided as modules
- **singularity-bindings/system** (available via easyconfig)
  - Sets the environment to use Cray MPICH provided outside the container
  - Requires a LUMI software stack
  - Use EasyBuild-user module and eb --search singularity-bindings to find the easyconfig or copy from our LUMI Software Library web site
  - Provides basic mount points for using host MPI in the container setting `SINGULARITY_BIND` and `SINGULARITY_LD_LIBRARY_PATH`

Environment enhancements (2)

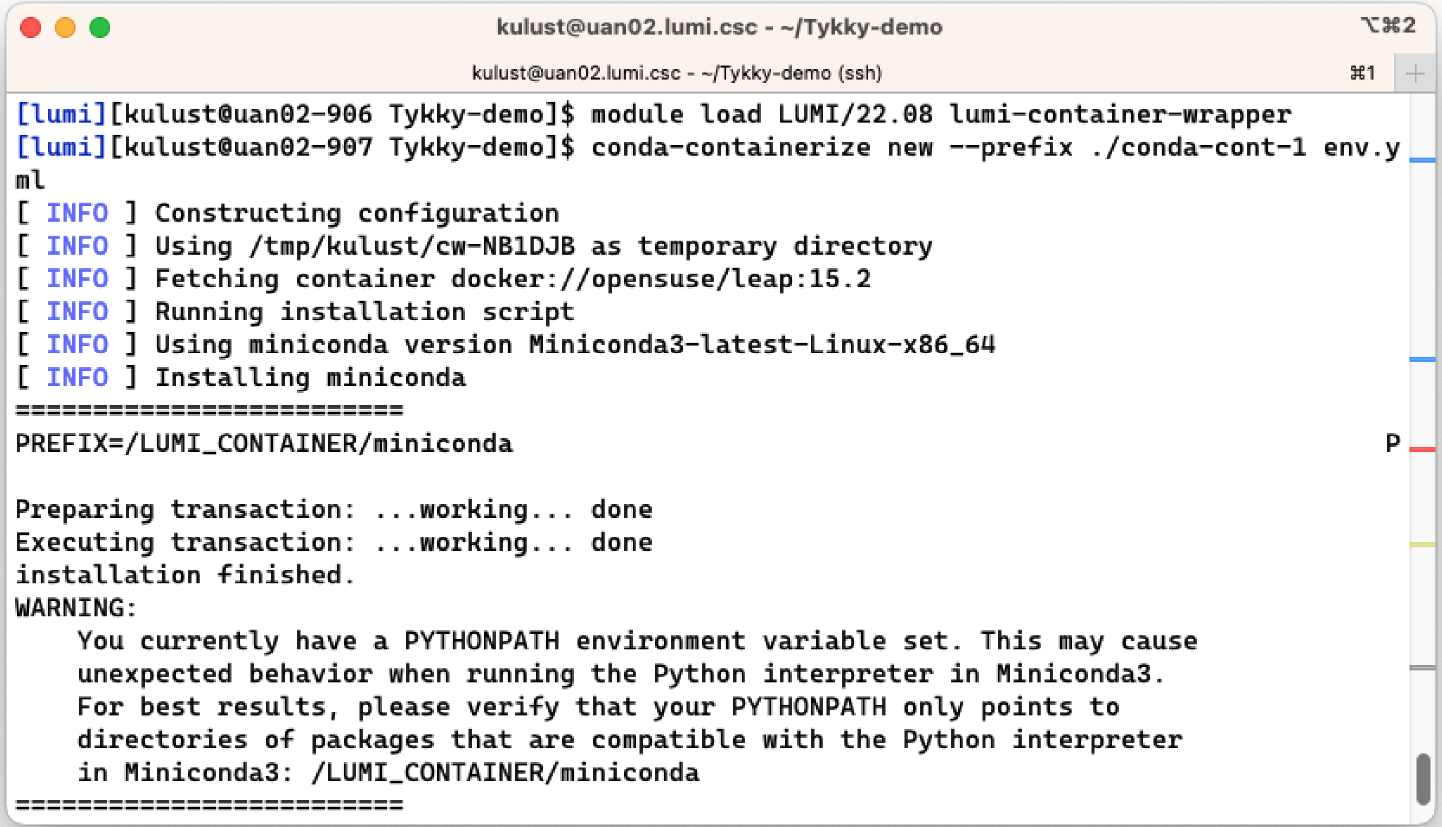
- **lumi-vnc** (LUMI and CrayEnv software stacks)
  - Provides basic VNC virtual desktop for interacting with graphical interfaces via a web browser or VNC client
- **lumi-container-wrapper** (LUMI and CrayEnv software stacks)
  - Provides wrappers to encapsulate your custom environment in the container
  - Supports conda and pip environments
  - Helps with quota on the number of files in your project and I/O performance
  - Python provided by the cray-python module (so there is an optimised NumPy etc.)

lumi-container-wrapper (1)


kulust@uan02.lumi.csc - ~/Tykky-demo
kulust@uan02.lumi.csc - ~/Tykky-demo (ssh)

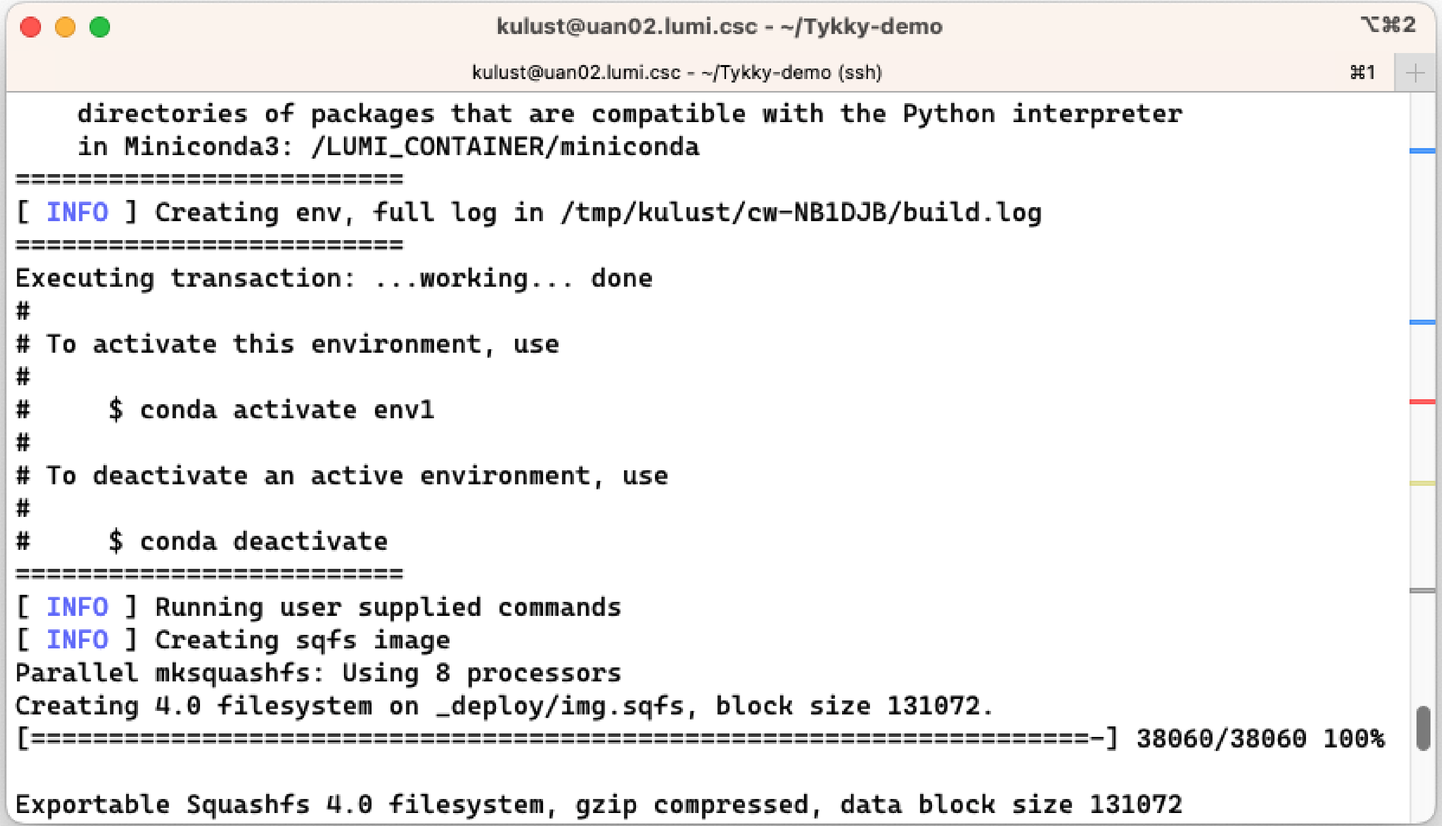
```
 *                                                                    ,/         |  /
  * ░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░/     \  * || |
            *              *               ,_   (        )| || |
*   *    *    The Supercomputer of the North  * | `\_|   __ /_| || |
       **             *            * *       \_____\______)\__)__)
   .*******----------******------******----------***************.
   |User guide and support ______________________________________|
   |         https://docs.lumi-supercomputer.eu                  |
 * |         https://lumi-supercomputer.eu/user-support          |
** `--*****-------------------***-----------------------*****-------'
[lumi][kulust@uan02-903 ~]$ cd Tykky-demo/
[lumi][kulust@uan02-904 Tykky-demo]$ ls
conda-cont-1  env.yml
[lumi][kulust@uan02-905 Tykky-demo]$ cat env.yml
channels:
  - conda-forge
dependencies:
  - python=3.8.8
  - scipy
  - nglview
[lumi][kulust@uan02-906 Tykky-demo]$ module load LUMI/22.08 lumi-container-wrapper
[lumi][kulust@uan02-907 Tykky-demo]$
```

lumi-container-wrapper (2)


kulust@uan02.lumi.csc - ~/Tykky-demo
⌥⌘2
kulust@uan02.lumi.csc - ~/Tykky-demo (ssh)
⌘1

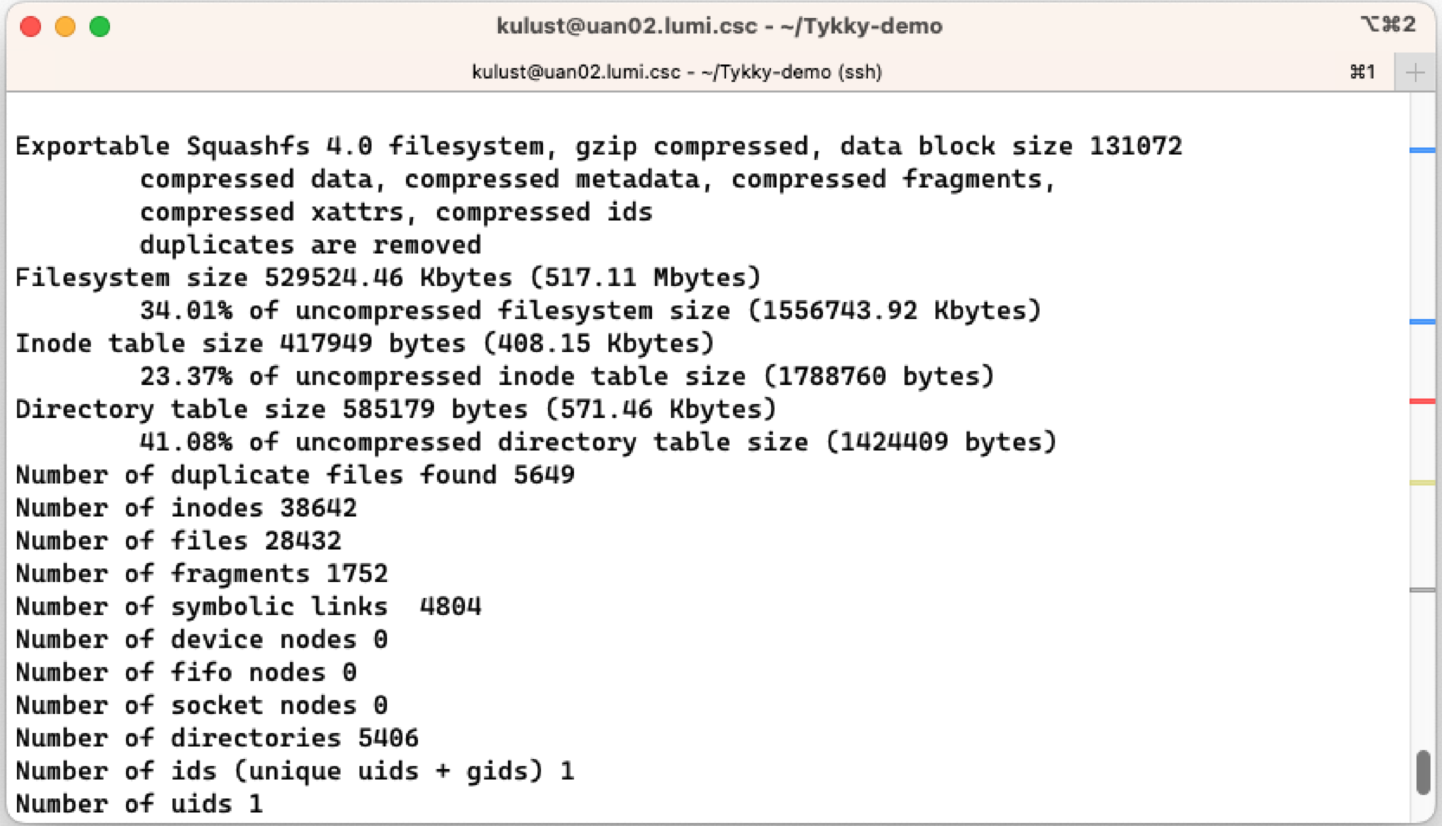
```
[lumi][kulust@uan02-906 Tykky-demo]$ module load LUMI/22.08 lumi-container-wrapper
[lumi][kulust@uan02-907 Tykky-demo]$ conda-containerize new --prefix ./conda-cont-1 env.y
ml
[ INFO ] Constructing configuration
[ INFO ] Using /tmp/kulust/cw-NB1DJB as temporary directory
[ INFO ] Fetching container docker://opensuse/leap:15.2
[ INFO ] Running installation script
[ INFO ] Using miniconda version Miniconda3-latest-Linux-x86_64
[ INFO ] Installing miniconda
=========================
PREFIX=/LUMI_CONTAINER/miniconda                                                      P

Preparing transaction: ...working... done
Executing transaction: ...working... done
installation finished.
WARNING:
    You currently have a PYTHONPATH environment variable set. This may cause
    unexpected behavior when running the Python interpreter in Miniconda3.
    For best results, please verify that your PYTHONPATH only points to
    directories of packages that are compatible with the Python interpreter
    in Miniconda3: /LUMI_CONTAINER/miniconda
=========================
```

lumi-container-wrapper (3)


kulust@uan02.lumi.csc - ~/Tykky-demo
kulust@uan02.lumi.csc - ~/Tykky-demo (ssh)

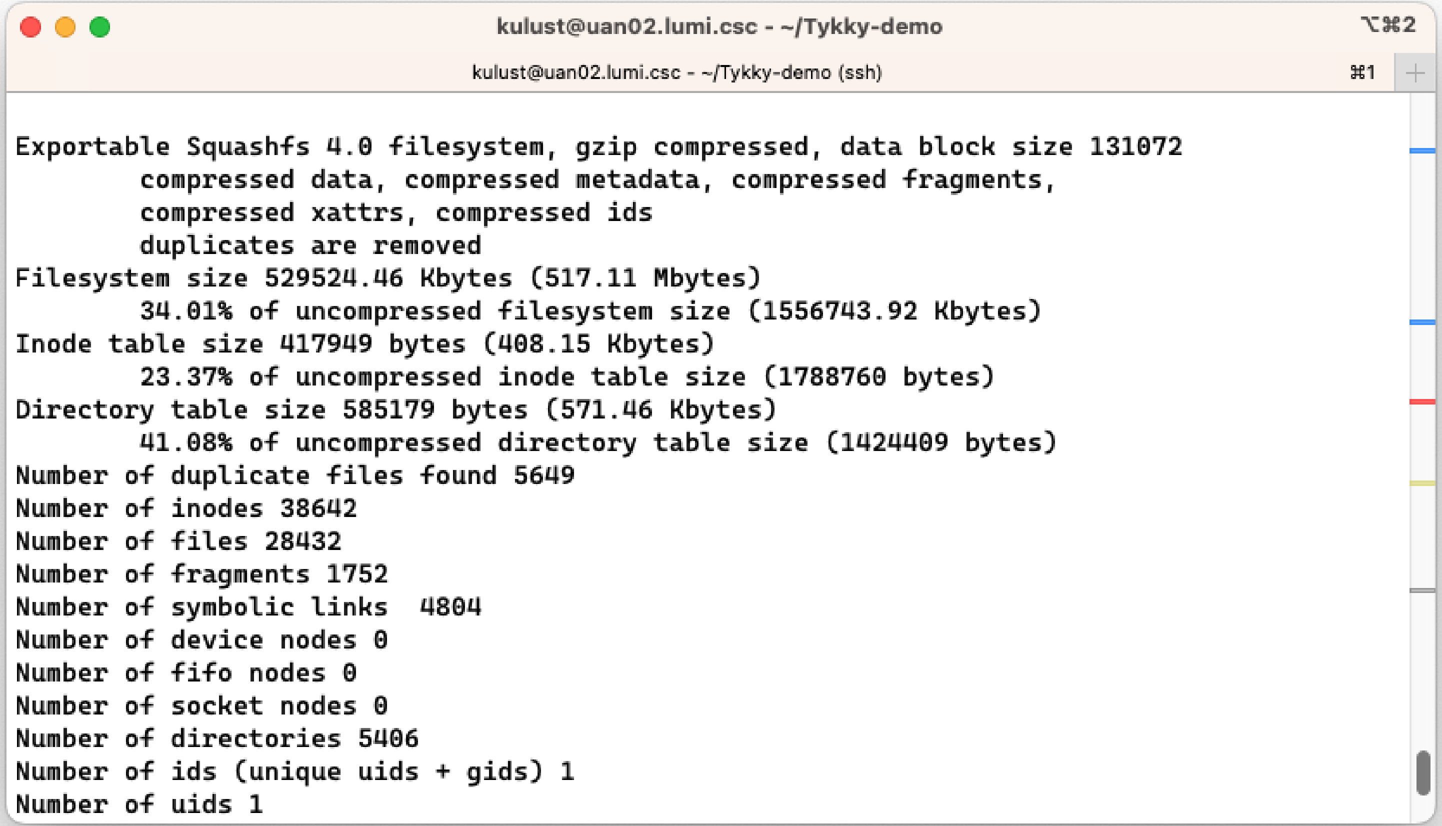
```
    directories of packages that are compatible with the Python interpreter
    in Miniconda3: /LUMI_CONTAINER/miniconda
=========================
[ INFO ] Creating env, full log in /tmp/kulust/cw-NB1DJB/build.log
=========================
Executing transaction: ...working... done
#
# To activate this environment, use
#
#     $ conda activate env1
#
# To deactivate an active environment, use
#
#     $ conda deactivate
=========================
[ INFO ] Running user supplied commands
[ INFO ] Creating sqfs image
Parallel mksquashfs: Using 8 processors
Creating 4.0 filesystem on _deploy/img.sqfs, block size 131072.
[===========================================================================-] 38060/38060 100%

Exportable Squashfs 4.0 filesystem, gzip compressed, data block size 131072
```

lumi-container-wrapper (4)


kulust@uan02.lumi.csc - ~/Tykky-demo
⌥⌘2
kulust@uan02.lumi.csc - ~/Tykky-demo (ssh)
⌘1

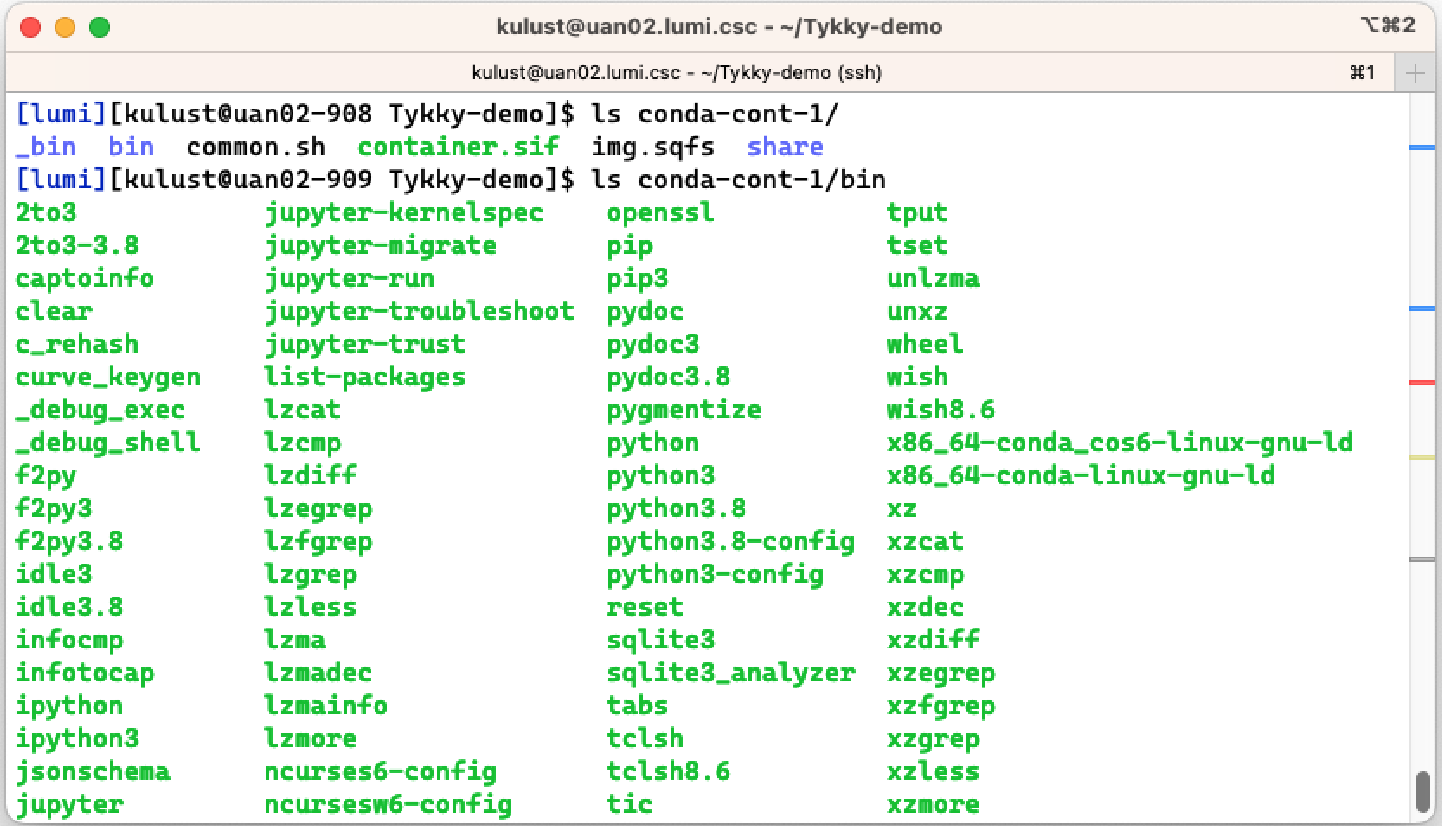
```
Exportable Squashfs 4.0 filesystem, gzip compressed, data block size 131072
        compressed data, compressed metadata, compressed fragments,
        compressed xattrs, compressed ids
        duplicates are removed
Filesystem size 529524.46 Kbytes (517.11 Mbytes)
        34.01% of uncompressed filesystem size (1556743.92 Kbytes)
Inode table size 417949 bytes (408.15 Kbytes)
        23.37% of uncompressed inode table size (1788760 bytes)
Directory table size 585179 bytes (571.46 Kbytes)
        41.08% of uncompressed directory table size (1424409 bytes)
Number of duplicate files found 5649
Number of inodes 38642
Number of files 28432
Number of fragments 1752
Number of symbolic links  4804
Number of device nodes 0
Number of fifo nodes 0
Number of socket nodes 0
Number of directories 5406
Number of ids (unique uids + gids) 1
Number of uids 1
```

lumi-container-wrapper (5)


kulust@uan02.lumi.csc - ~/Tykky-demo
⌥⌘2
kulust@uan02.lumi.csc - ~/Tykky-demo (ssh)
⌘1

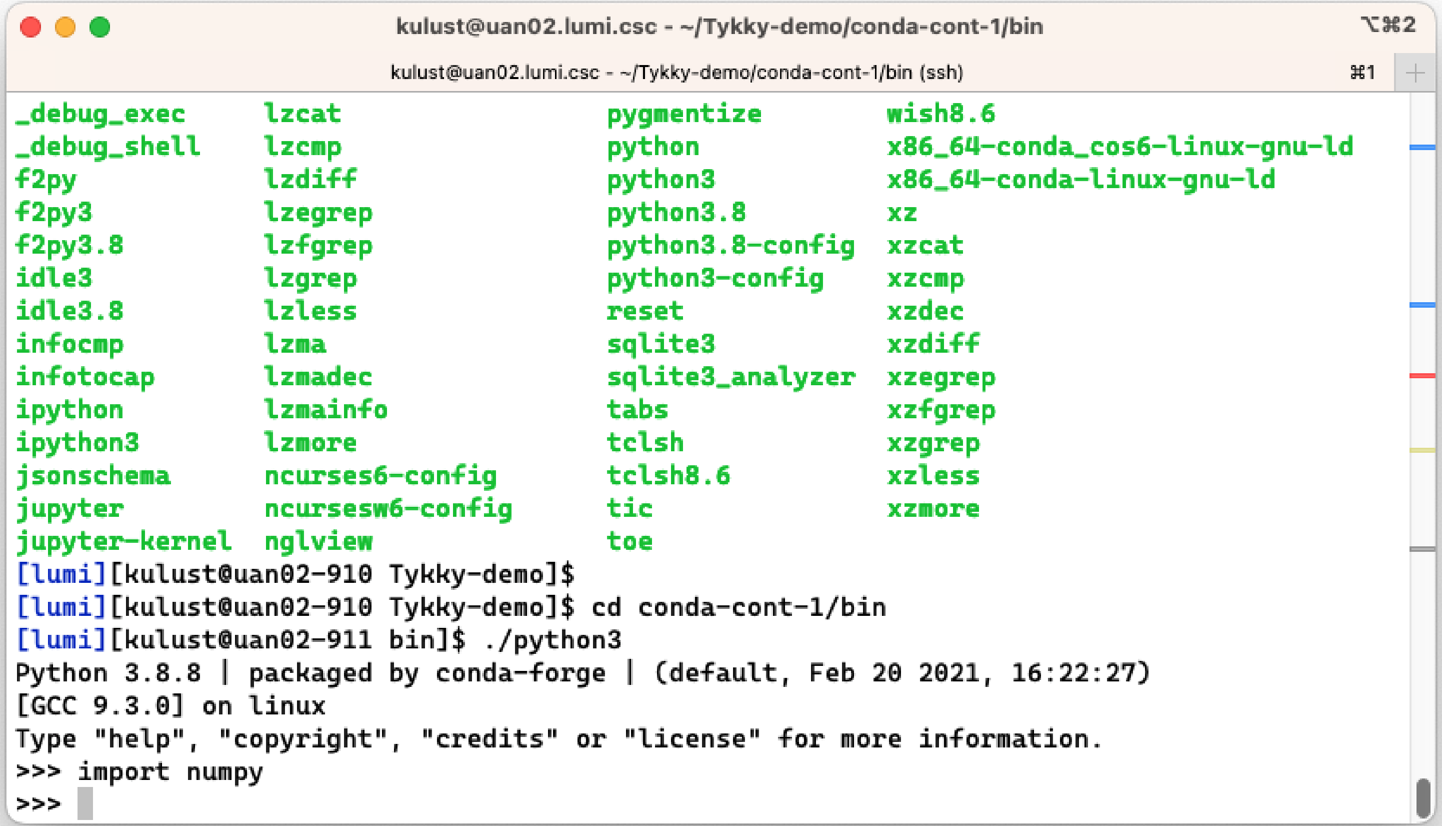
```
Exportable Squashfs 4.0 filesystem, gzip compressed, data block size 131072
        compressed data, compressed metadata, compressed fragments,
        compressed xattrs, compressed ids
        duplicates are removed
Filesystem size 529524.46 Kbytes (517.11 Mbytes)
        34.01% of uncompressed filesystem size (1556743.92 Kbytes)
Inode table size 417949 bytes (408.15 Kbytes)
        23.37% of uncompressed inode table size (1788760 bytes)
Directory table size 585179 bytes (571.46 Kbytes)
        41.08% of uncompressed directory table size (1424409 bytes)
Number of duplicate files found 5649
Number of inodes 38642
Number of files 28432
Number of fragments 1752
Number of symbolic links  4804
Number of device nodes 0
Number of fifo nodes 0
Number of socket nodes 0
Number of directories 5406
Number of ids (unique uids + gids) 1
Number of uids 1
```

lumi-container-wrapper (6)


kulust@uan02.lumi.csc - ~/Tykky-demo
⌥⌘2
kulust@uan02.lumi.csc - ~/Tykky-demo (ssh)
⌘1

```
[lumi][kulust@uan02-908 Tykky-demo]$ ls conda-cont-1/
_bin  bin  common.sh  container.sif  img.sqfs  share
[lumi][kulust@uan02-909 Tykky-demo]$ ls conda-cont-1/bin
2to3            jupyter-kernelspec     openssl              tput
2to3-3.8        jupyter-migrate        pip                  tset
captoinfo       jupyter-run            pip3                 unlzma
clear           jupyter-troubleshoot   pydoc                unxz
c_rehash        jupyter-trust          pydoc3               wheel
curve_keygen    list-packages          pydoc3.8             wish
_debug_exec     lzcat                  pygmentize           wish8.6
_debug_shell    lzcmp                  python               x86_64-conda_cos6-linux-gnu-ld
f2py            lzdiff                 python3              x86_64-conda-linux-gnu-ld
f2py3           lzegrep                python3.8            xz
f2py3.8         lzfgrep                python3.8-config     xzcat
idle3           lzgrep                 python3-config       xzcmp
idle3.8         lzless                 reset                xzdec
infocmp         lzma                   sqlite3              xzdiff
infotocap       lzmadec                sqlite3_analyzer     xzegrep
ipython         lzmainfo               tabs                 xzfgrep
ipython3        lzmore                 tclsh                xzgrep
jsonschema      ncurses6-config        tclsh8.6             xzless
jupyter         ncursesw6-config       tic                  xzmore
```

lumi-container-wrapper (7)


kulust@uan02.lumi.csc - ~/Tykky-demo/conda-cont-1/bin ⌥⌘2

kulust@uan02.lumi.csc - ~/Tykky-demo/conda-cont-1/bin (ssh) ⌘1

```
_debug_exec     lzcat             pygmentize         wish8.6
_debug_shell    lzcmp             python             x86_64-conda_cos6-linux-gnu-ld
f2py            lzdiff            python3            x86_64-conda-linux-gnu-ld
f2py3           lzegrep           python3.8          xz
f2py3.8         lzfgrep           python3.8-config   xzcat
idle3           lzgrep            python3-config     xzcmp
idle3.8         lzless            reset              xzdec
infocmp         lzma              sqlite3            xzdiff
infotocap       lzmadec           sqlite3_analyzer   xzegrep
ipython         lzmainfo          tabs               xzfgrep
ipython3        lzmore            tclsh              xzgrep
jsonschema      ncurses6-config   tclsh8.6           xzless
jupyter         ncursesw6-config  tic                xzmore
jupyter-kernel  nglview           toe
[lumi][kulust@uan02-910 Tykky-demo]$
[lumi][kulust@uan02-910 Tykky-demo]$ cd conda-cont-1/bin
[lumi][kulust@uan02-911 bin]$ ./python3
Python 3.8.8 | packaged by conda-forge | (default, Feb 20 2021, 16:22:27)
[GCC 9.3.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy
>>> 
```

Container limitations on LUMI

- Containers use the host's operating system kernel which may be different from your system.
- A generic container may not offer sufficiently good support for the SlingShot 11 interconnect on LUMI and fall back to TCP sockets resulting in poor performance, or not work at all.
  - Solution by injecting Cray MPICH, but only for containers with ABI compatibility with MPICH.
- Building containers is not supported on LUMI due to security concerns.