LUMI Software Stacks

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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
  - Even for software on the system, users remain responsible for checking the 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, (large) 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
- Far 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 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)

  - Environment in which we install most software (mostly with EasyBuild)

Accessing the Cray PE on LUMI

The LUMI software stack

- The LUMI software stack uses two levels of modules
  - LUMI/22.08, LUMI/22.12, LUMI/23.03: 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!

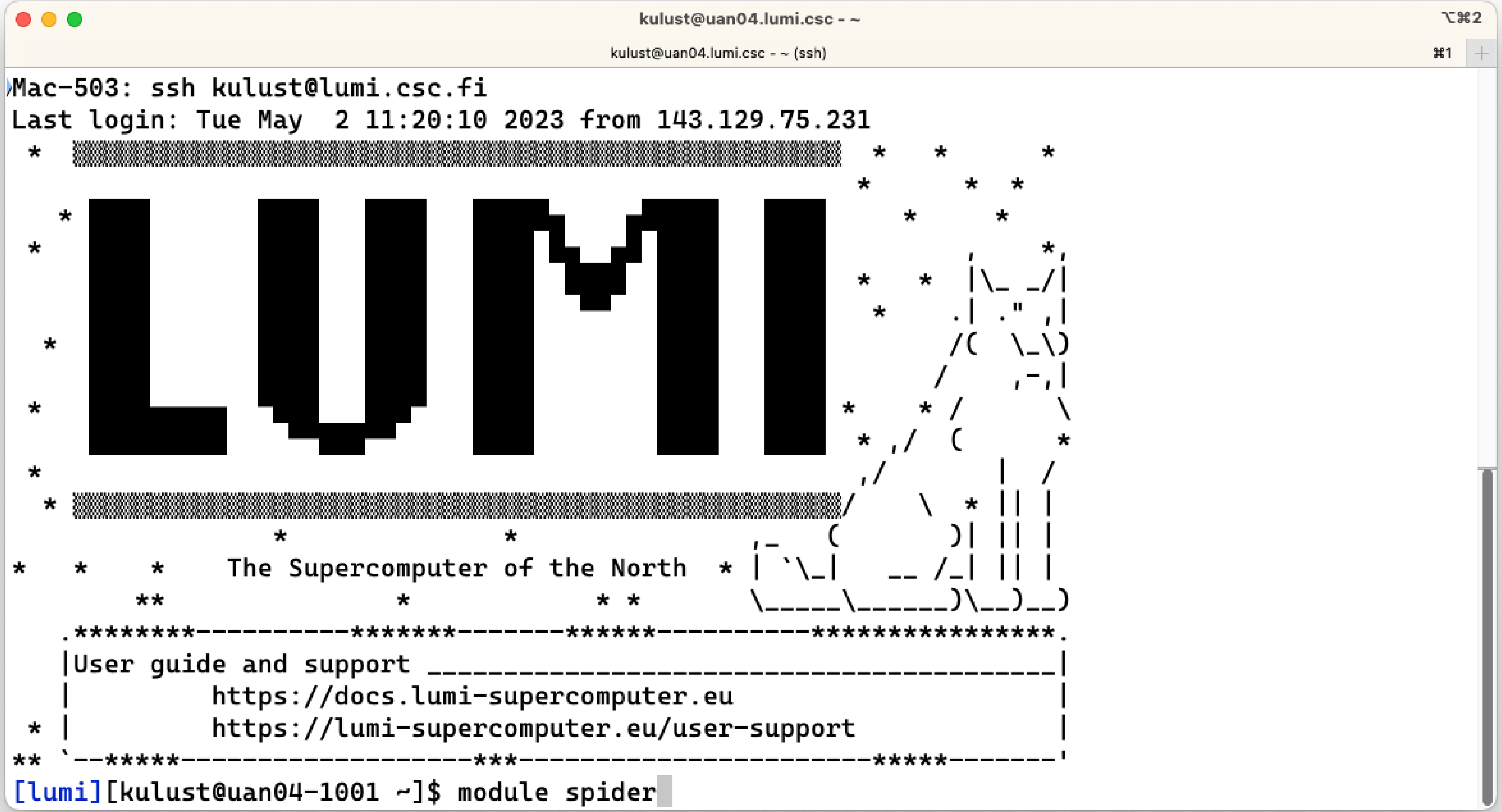
Exploring modules with Lmod

- 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` requires a compiler module and network target module first
  - Many of the performance monitoring tools require `perftools-base` first
  - `cray-fftw` only becomes available when a processor target module is loaded
- Tools
  - `module avail` searches in the available modules
  - `module spider` and `module keyword` search 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/5.4.6-cpeGNU-22.12` : 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/3.25.2` : Will tell you which module contains CMake and how to load it

module spider (command) (1)



```
Mac-503: ssh kulust@lumi.csc.fi
Last login: Tue May  2 11:20:10 2023 from 143.129.75.231
 *  ░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░░  *   *      *
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                *              *                ,_    (       )| || |
*   *    *    The Supercomputer of the North  * | `\_|   __ /_| || |
       **               *            * *      \_____\______)\__)__)
   .********----------*******-------******----------****************.
   |User guide and support ___________________________________________|
   |         https://docs.lumi-supercomputer.eu                        |
 * |         https://lumi-supercomputer.eu/user-support                |
** `--*****-------------------***-----------------------*****-------'
[lumi][kulust@uan04-1001 ~]$ module spider
```
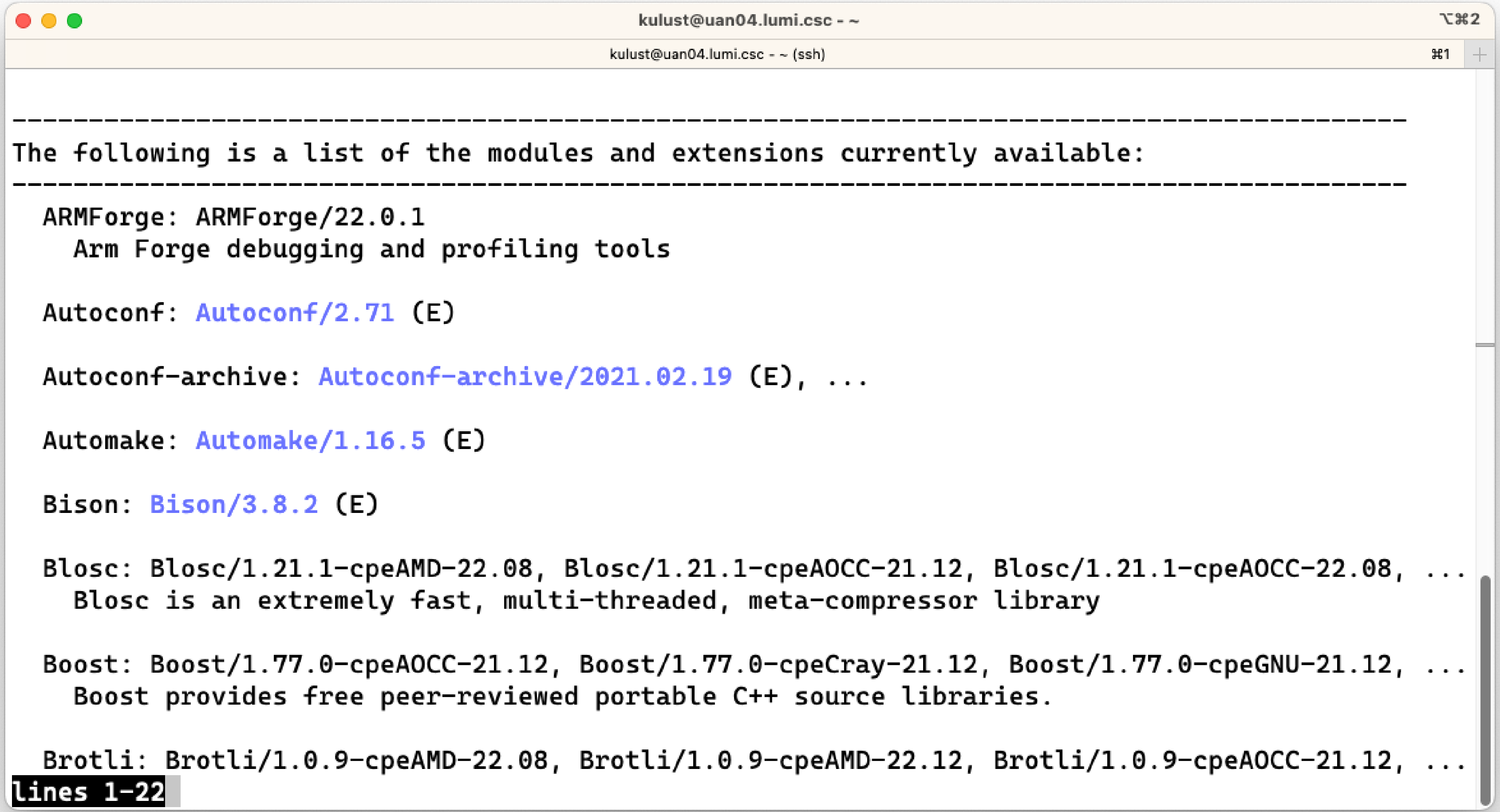
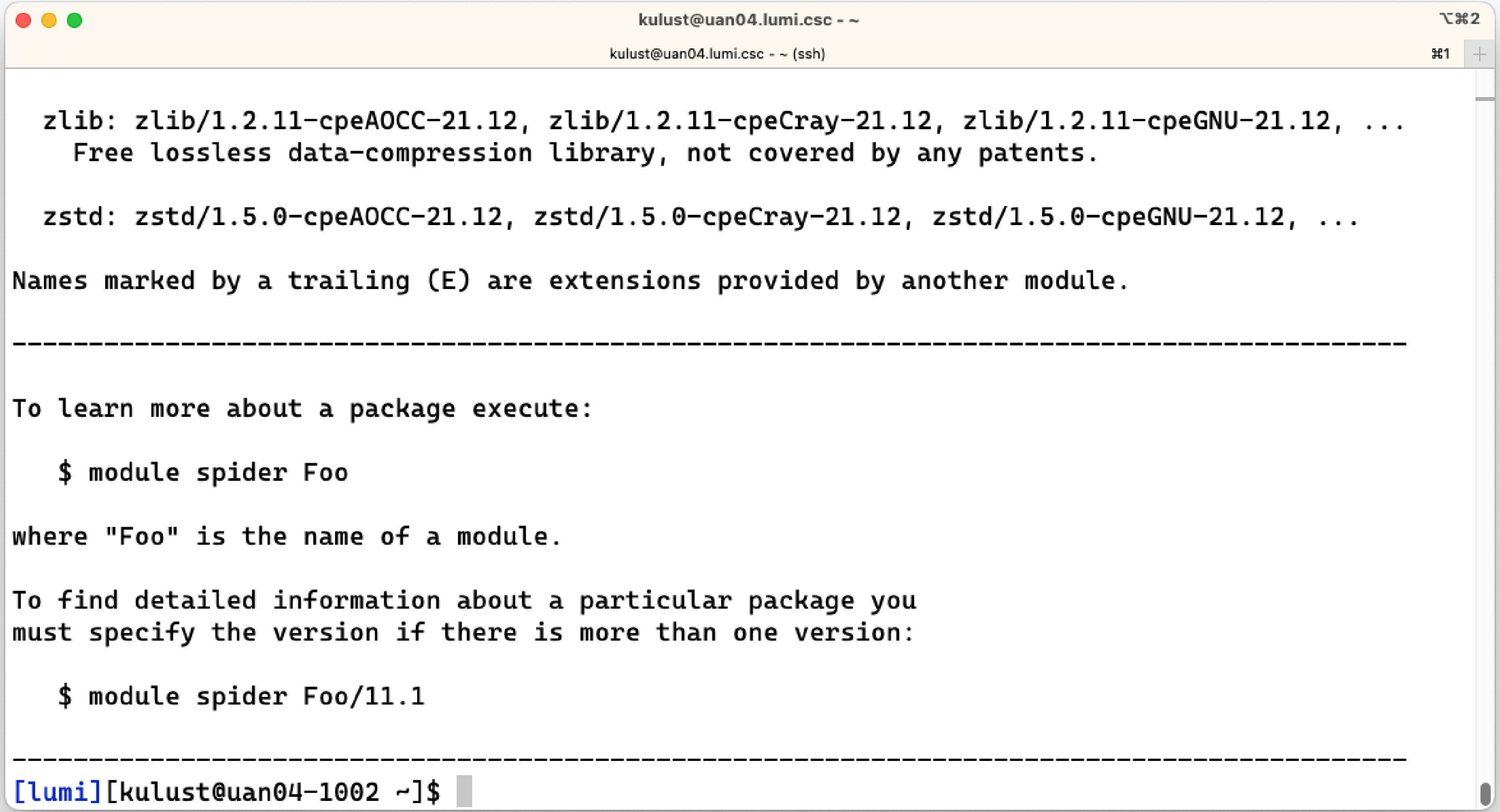

module spider (command) (2)



```
-----------------------------------------------------------------------------------------
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/1.16.5 (E)

  Bison: Bison/3.8.2 (E)

  Blosc: Blosc/1.21.1-cpeAMD-22.08, Blosc/1.21.1-cpeAOCC-21.12, Blosc/1.21.1-cpeAOCC-22.08, ...
    Blosc is an extremely fast, multi-threaded, meta-compressor library

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

  Brotli: Brotli/1.0.9-cpeAMD-22.08, Brotli/1.0.9-cpeAMD-22.12, Brotli/1.0.9-cpeAOCC-21.12, ...
lines 1-22
```

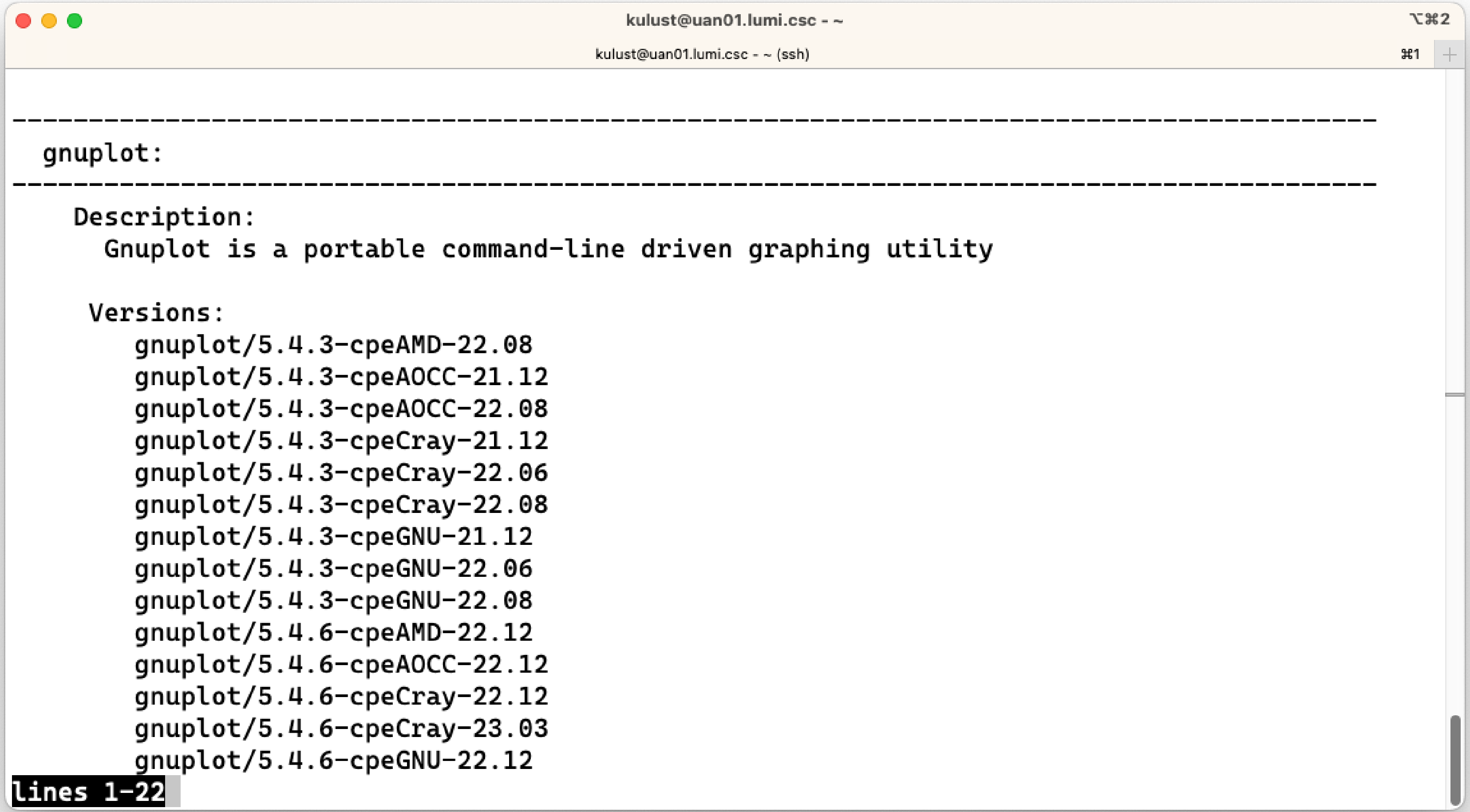
module spider (command) (3)


kulust@uan04.lumi.csc - ~

kulust@uan04.lumi.csc - ~ (ssh)

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

  zstd: zstd/1.5.0-cpeAOCC-21.12, zstd/1.5.0-cpeCray-21.12, zstd/1.5.0-cpeGNU-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@uan04-1002 ~]$
```

module spider gnuplot

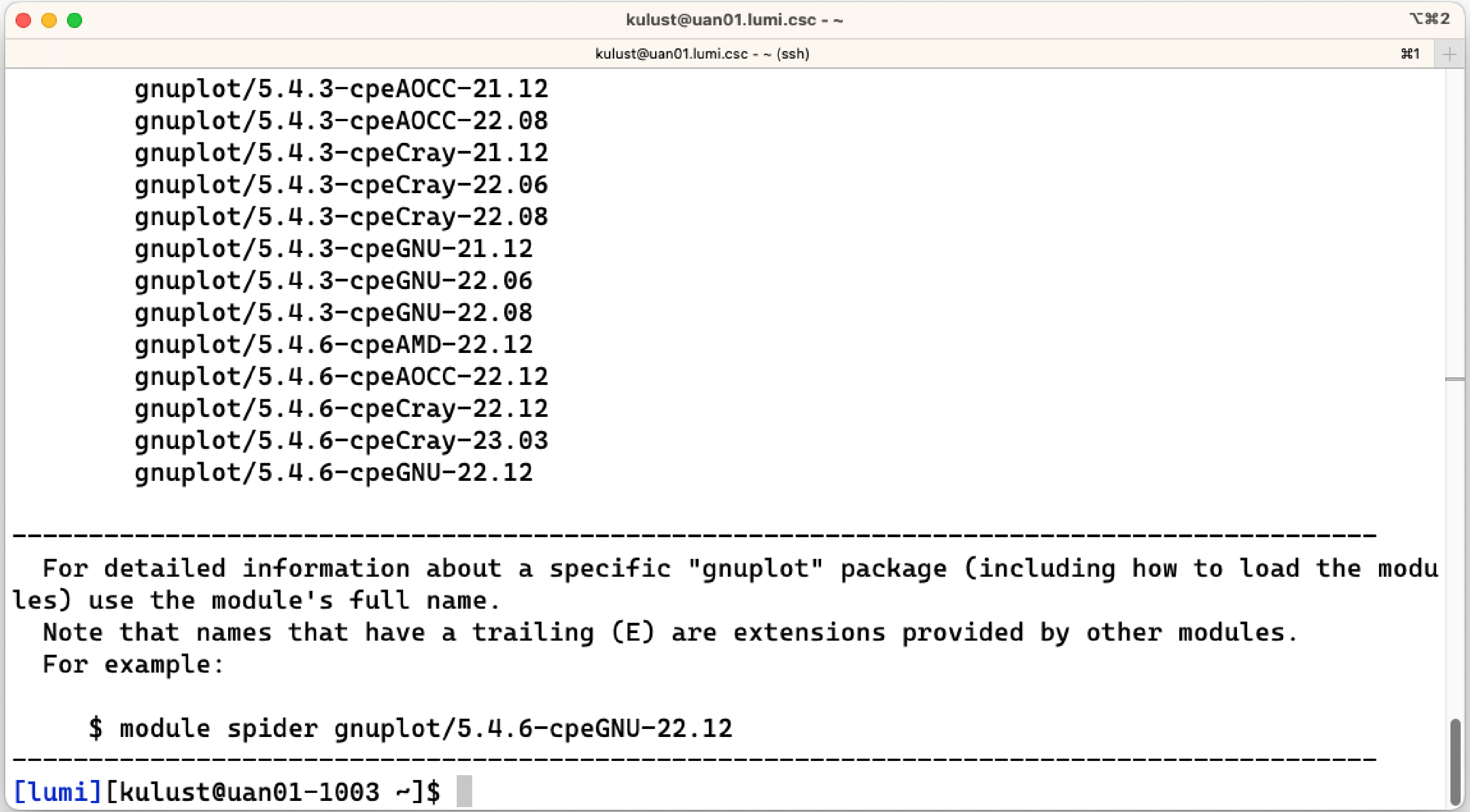


kulust@uan01.lumi.csc - ~

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

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

     Versions:
        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
        gnuplot/5.4.6-cpeAMD-22.12
        gnuplot/5.4.6-cpeAOCC-22.12
        gnuplot/5.4.6-cpeCray-22.12
        gnuplot/5.4.6-cpeCray-23.03
        gnuplot/5.4.6-cpeGNU-22.12
lines 1-22
```

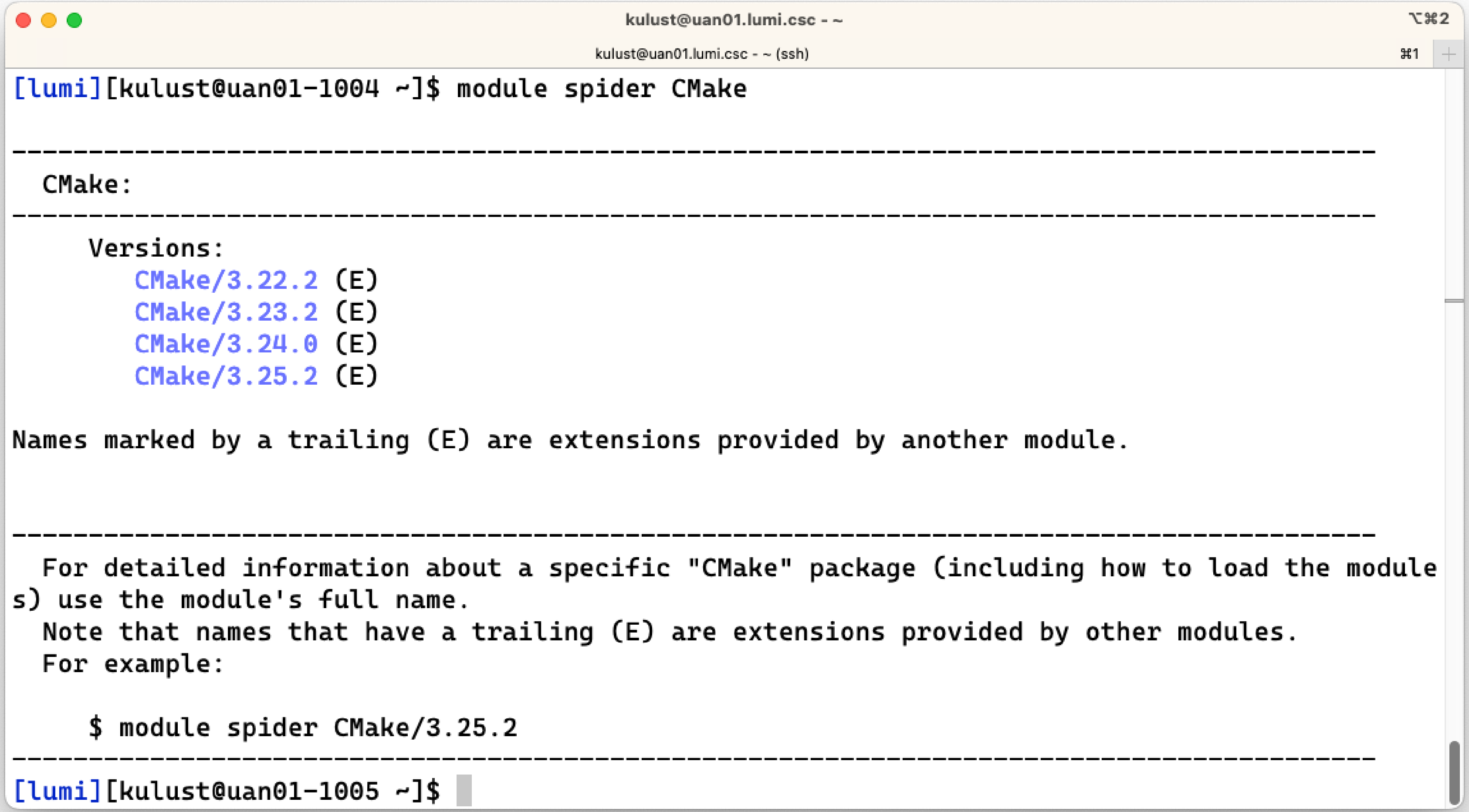
module spider gnuplot (2)


kulust@uan01.lumi.csc - ~

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

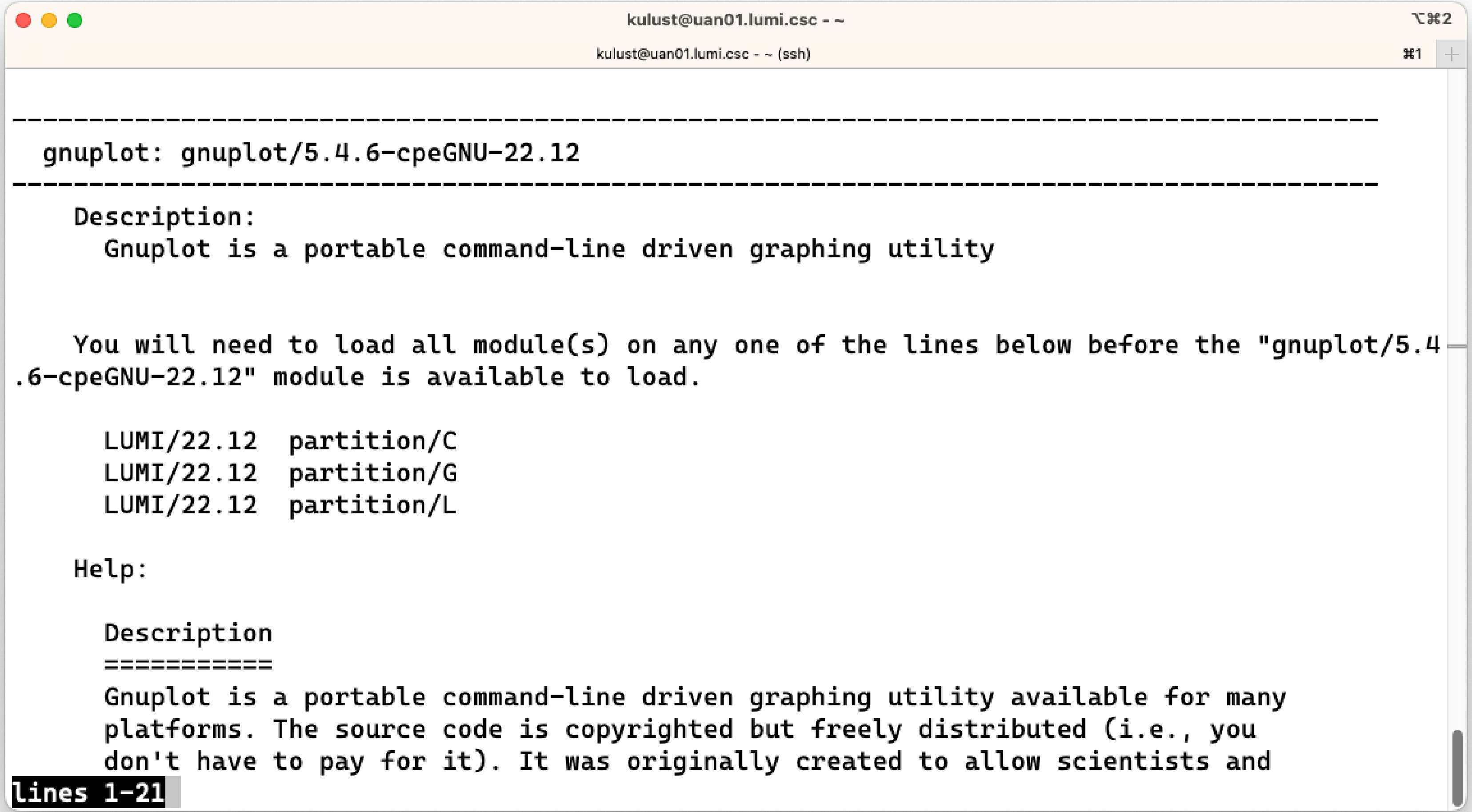
```
        gnuplot/5.4.3-cpeAOCC-21.12
        gnuplot/5.4.3-cpeAOCC-22.08
        gnuplot/5.4.3-cpeCray-21.12
        gnuplot/5.4.3-cpeCray-22.06
        gnuplot/5.4.3-cpeCray-22.08
        gnuplot/5.4.3-cpeGNU-21.12
        gnuplot/5.4.3-cpeGNU-22.06
        gnuplot/5.4.3-cpeGNU-22.08
        gnuplot/5.4.6-cpeAMD-22.12
        gnuplot/5.4.6-cpeAOCC-22.12
        gnuplot/5.4.6-cpeCray-22.12
        gnuplot/5.4.6-cpeCray-23.03
        gnuplot/5.4.6-cpeGNU-22.12


-----------------------------------------------------------------------------
  For detailed information about a specific "gnuplot" package (including how to load the modu
les) 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/5.4.6-cpeGNU-22.12
-----------------------------------------------------------------------------
[lumi][kulust@uan01-1003 ~]$
```

module spider CMake



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

----------------------------------------------------------------------------
  CMake:
----------------------------------------------------------------------------
     Versions:
        CMake/3.22.2 (E)
        CMake/3.23.2 (E)
        CMake/3.24.0 (E)
        CMake/3.25.2 (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 module
s) 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/3.25.2
----------------------------------------------------------------------------
[lumi][kulust@uan01-1005 ~]$ 
```

module spider gnuplot/5.4.6-cpeGNU-22.12

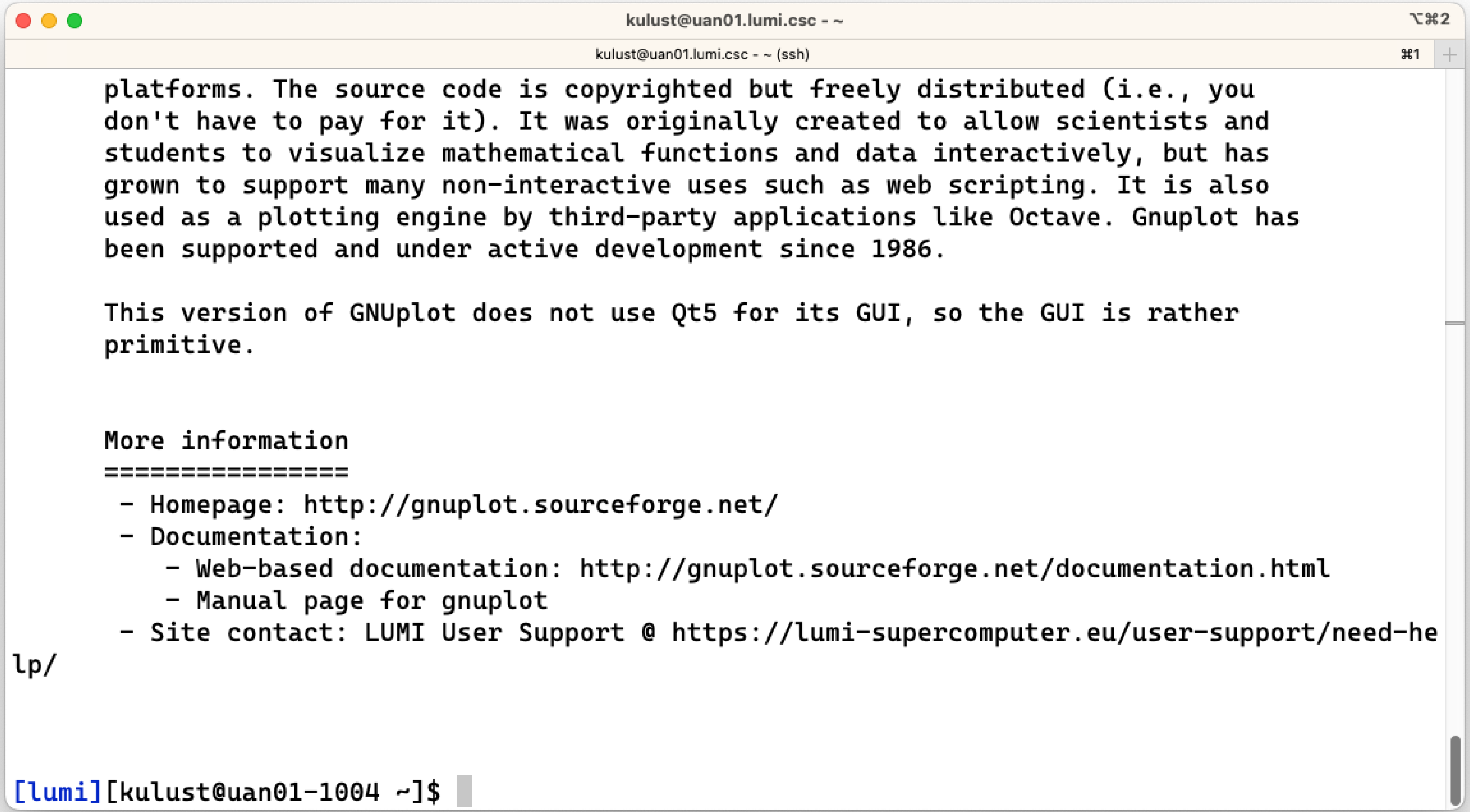


kulust@uan01.lumi.csc - ~

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

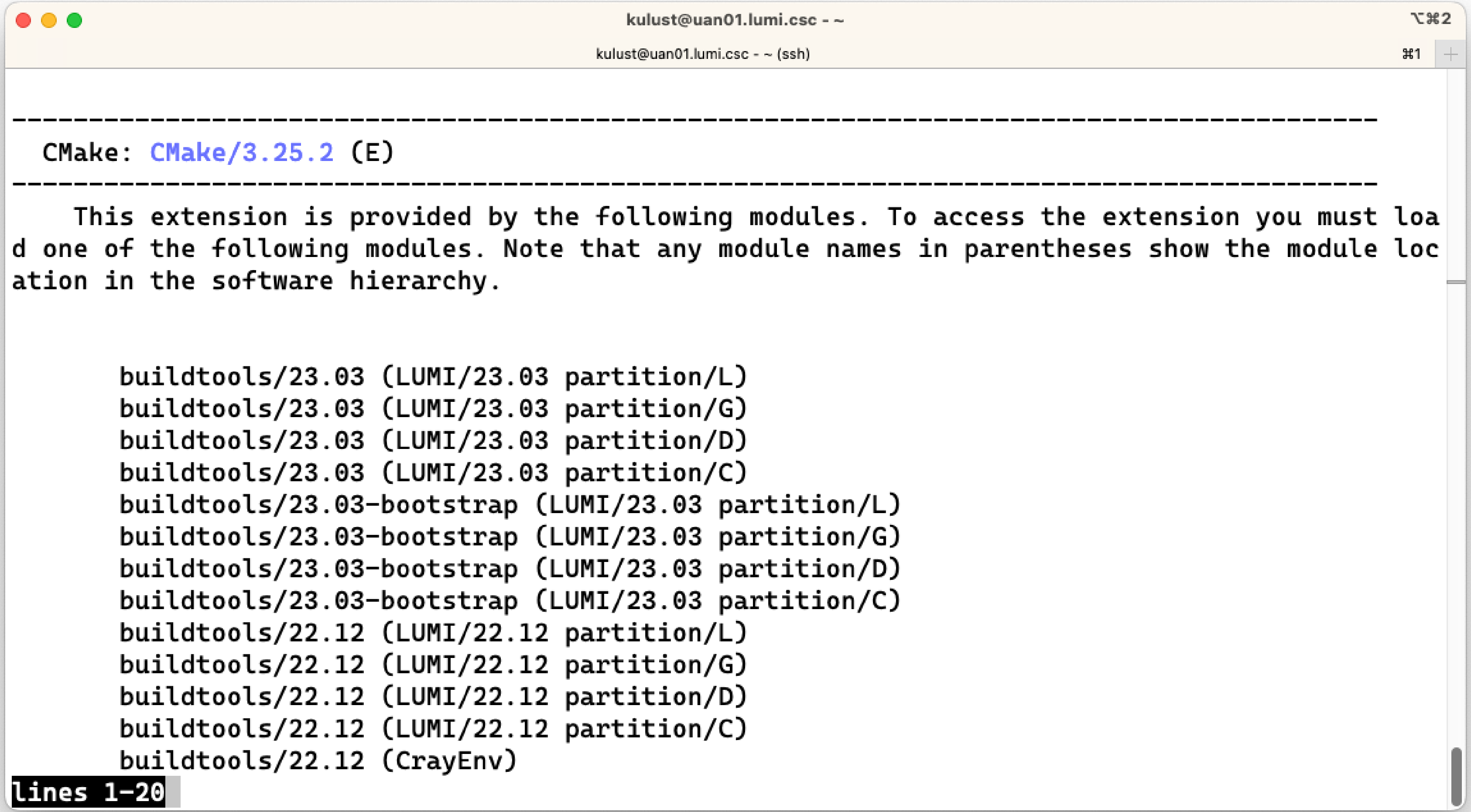
```

-----------------------------------------------------------------------------------
  gnuplot: gnuplot/5.4.6-cpeGNU-22.12
-----------------------------------------------------------------------------------
    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
.6-cpeGNU-22.12" module is available to load.

      LUMI/22.12  partition/C
      LUMI/22.12  partition/G
      LUMI/22.12  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/5.4.6-cpeGNU-22.12 (2)



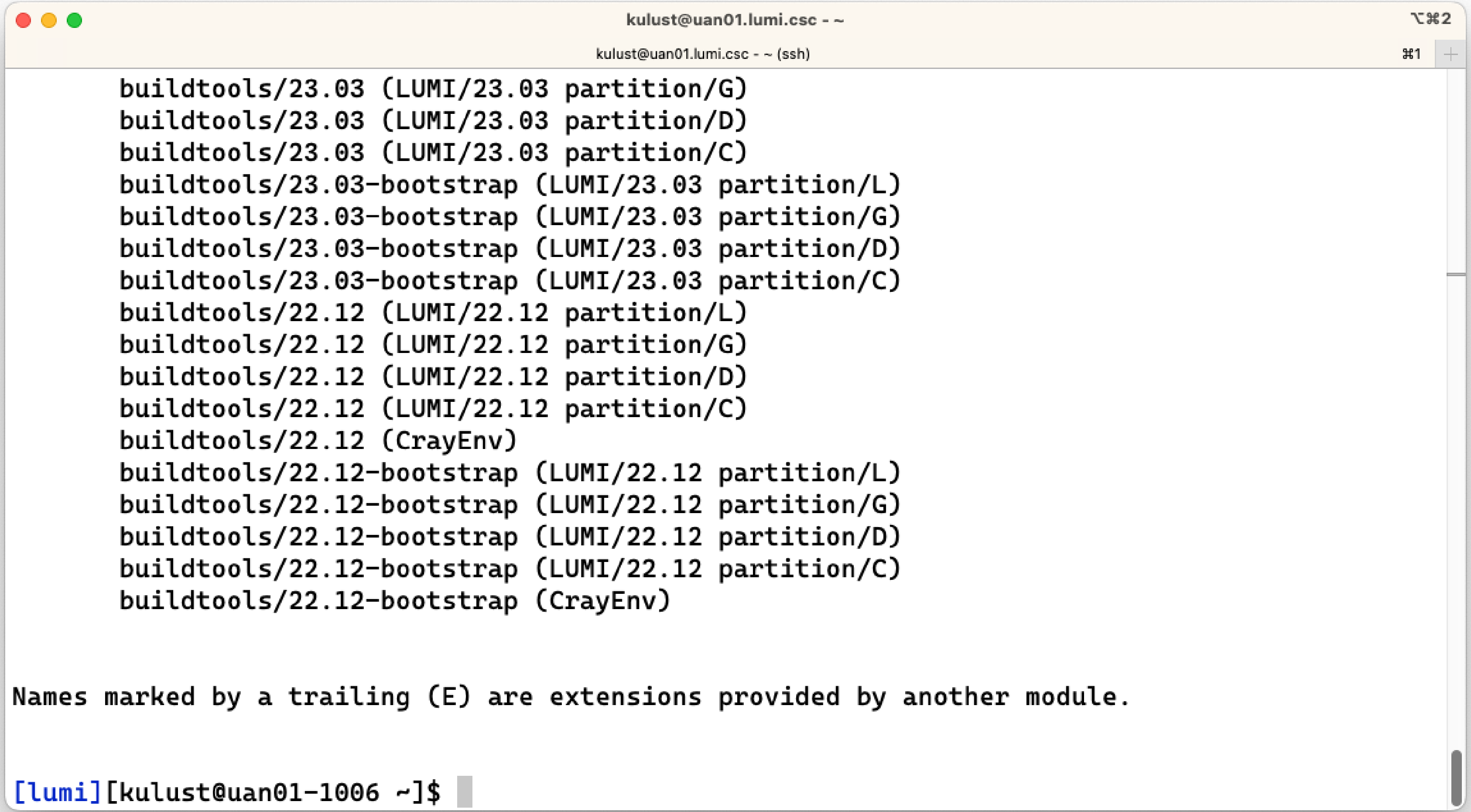
```
      platforms. The source code is copyrighted but freely distributed (i.e., you
      don't have to pay for it). It was originally created to allow scientists and
      students to visualize mathematical functions and data interactively, but has
      grown to support many non-interactive uses 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-he
lp/



[lumi][kulust@uan01-1004 ~]$
```

module spider CMake/3.25.2



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

-----------------------------------------------------------------------------------------
  CMake: CMake/3.25.2 (E)
-----------------------------------------------------------------------------------------
    This extension is provided by the following modules. To access the extension you must loa
d one of the following modules. Note that any module names in parentheses show the module loc
ation in the software hierarchy.


       buildtools/23.03 (LUMI/23.03 partition/L)
       buildtools/23.03 (LUMI/23.03 partition/G)
       buildtools/23.03 (LUMI/23.03 partition/D)
       buildtools/23.03 (LUMI/23.03 partition/C)
       buildtools/23.03-bootstrap (LUMI/23.03 partition/L)
       buildtools/23.03-bootstrap (LUMI/23.03 partition/G)
       buildtools/23.03-bootstrap (LUMI/23.03 partition/D)
       buildtools/23.03-bootstrap (LUMI/23.03 partition/C)
       buildtools/22.12 (LUMI/22.12 partition/L)
       buildtools/22.12 (LUMI/22.12 partition/G)
       buildtools/22.12 (LUMI/22.12 partition/D)
       buildtools/22.12 (LUMI/22.12 partition/C)
       buildtools/22.12 (CrayEnv)
lines 1-20
```

module spider CMake/3.25.2


kulust@uan01.lumi.csc - ~

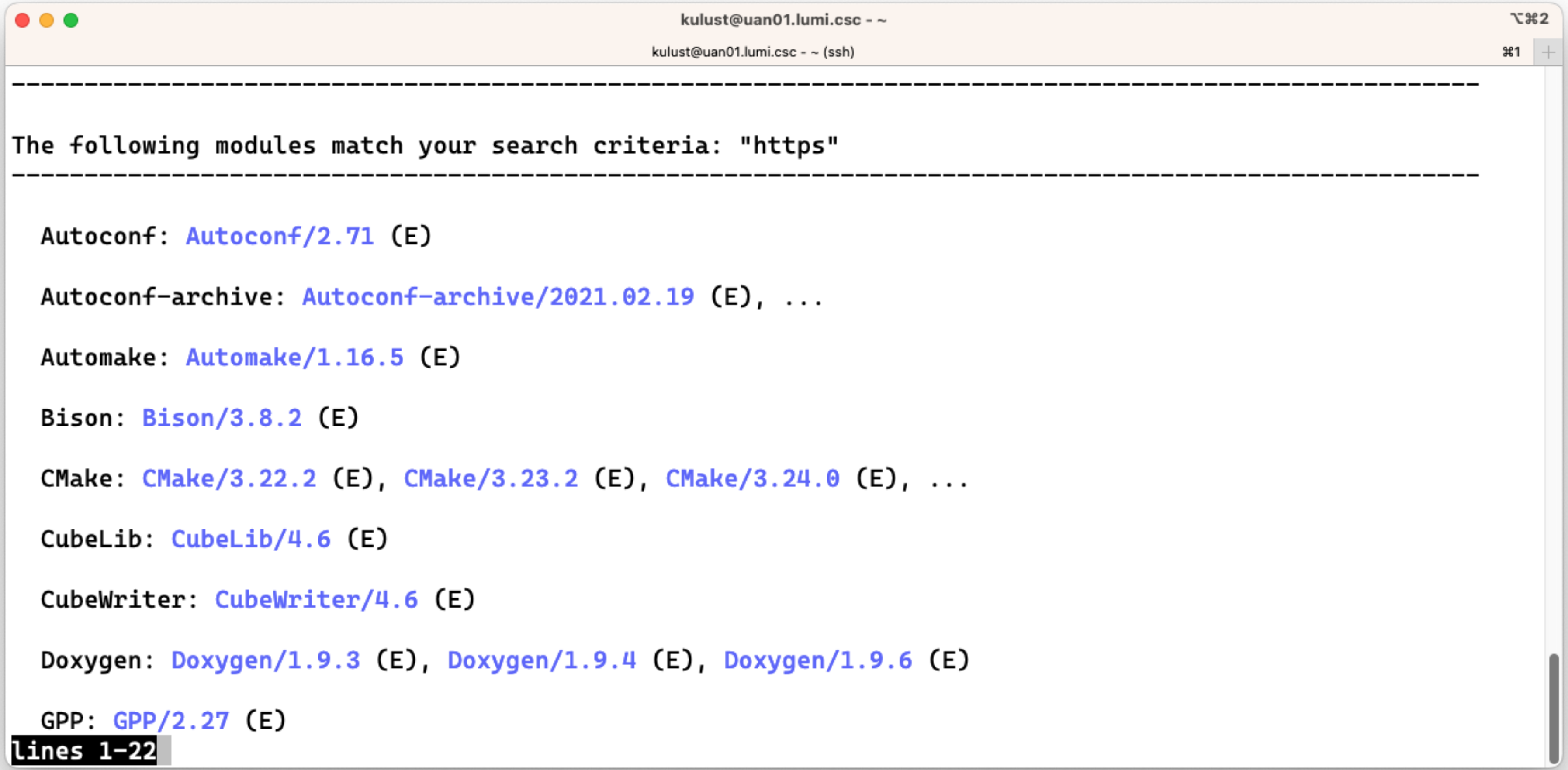
kulust@uan01.lumi.csc - ~ (ssh)

```
        buildtools/23.03 (LUMI/23.03 partition/G)
        buildtools/23.03 (LUMI/23.03 partition/D)
        buildtools/23.03 (LUMI/23.03 partition/C)
        buildtools/23.03-bootstrap (LUMI/23.03 partition/L)
        buildtools/23.03-bootstrap (LUMI/23.03 partition/G)
        buildtools/23.03-bootstrap (LUMI/23.03 partition/D)
        buildtools/23.03-bootstrap (LUMI/23.03 partition/C)
        buildtools/22.12 (LUMI/22.12 partition/L)
        buildtools/22.12 (LUMI/22.12 partition/G)
        buildtools/22.12 (LUMI/22.12 partition/D)
        buildtools/22.12 (LUMI/22.12 partition/C)
        buildtools/22.12 (CrayEnv)
        buildtools/22.12-bootstrap (LUMI/22.12 partition/L)
        buildtools/22.12-bootstrap (LUMI/22.12 partition/G)
        buildtools/22.12-bootstrap (LUMI/22.12 partition/D)
        buildtools/22.12-bootstrap (LUMI/22.12 partition/C)
        buildtools/22.12-bootstrap (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 https`
- 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 https

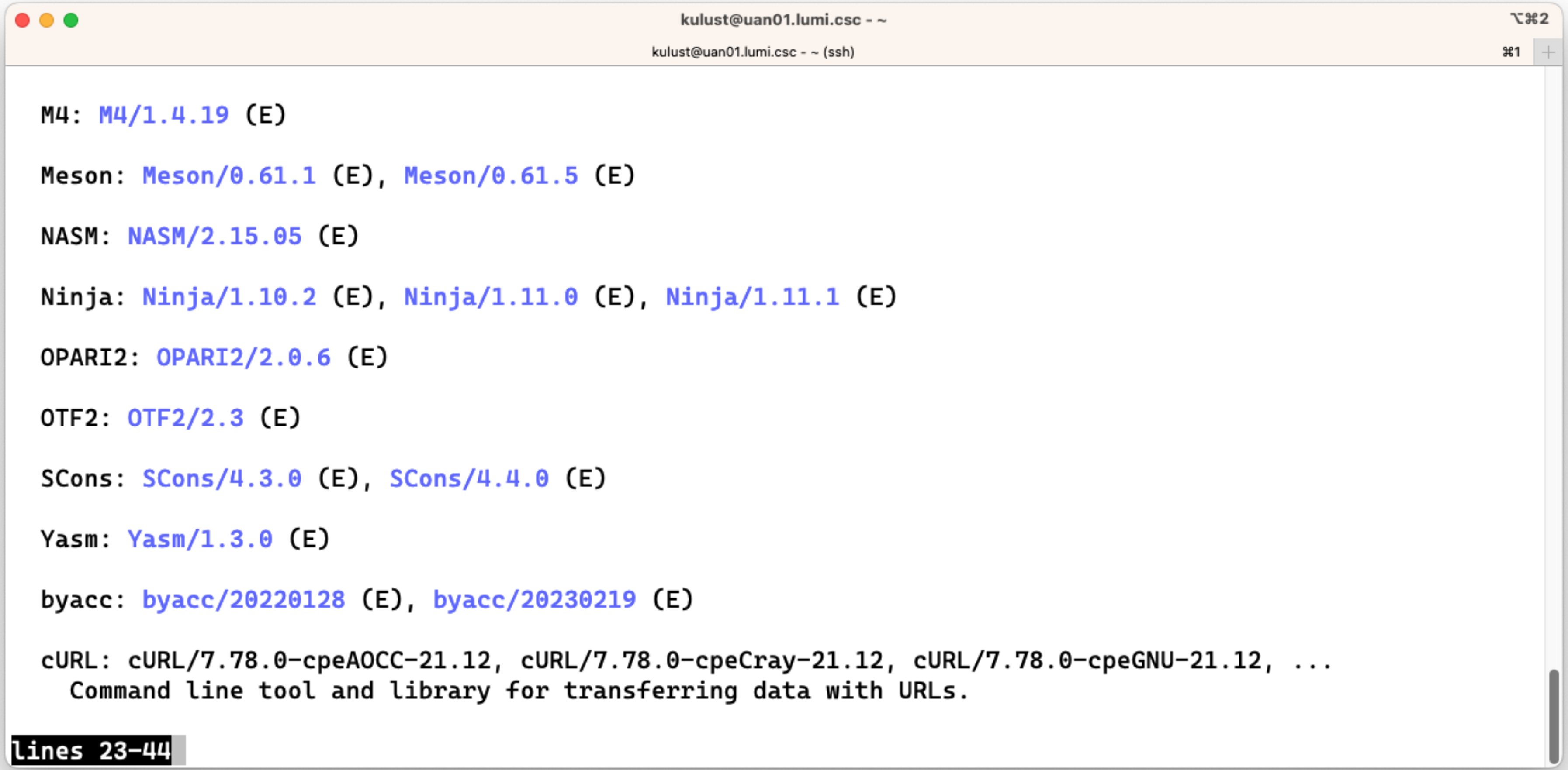


kulust@uan01.lumi.csc - ~

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

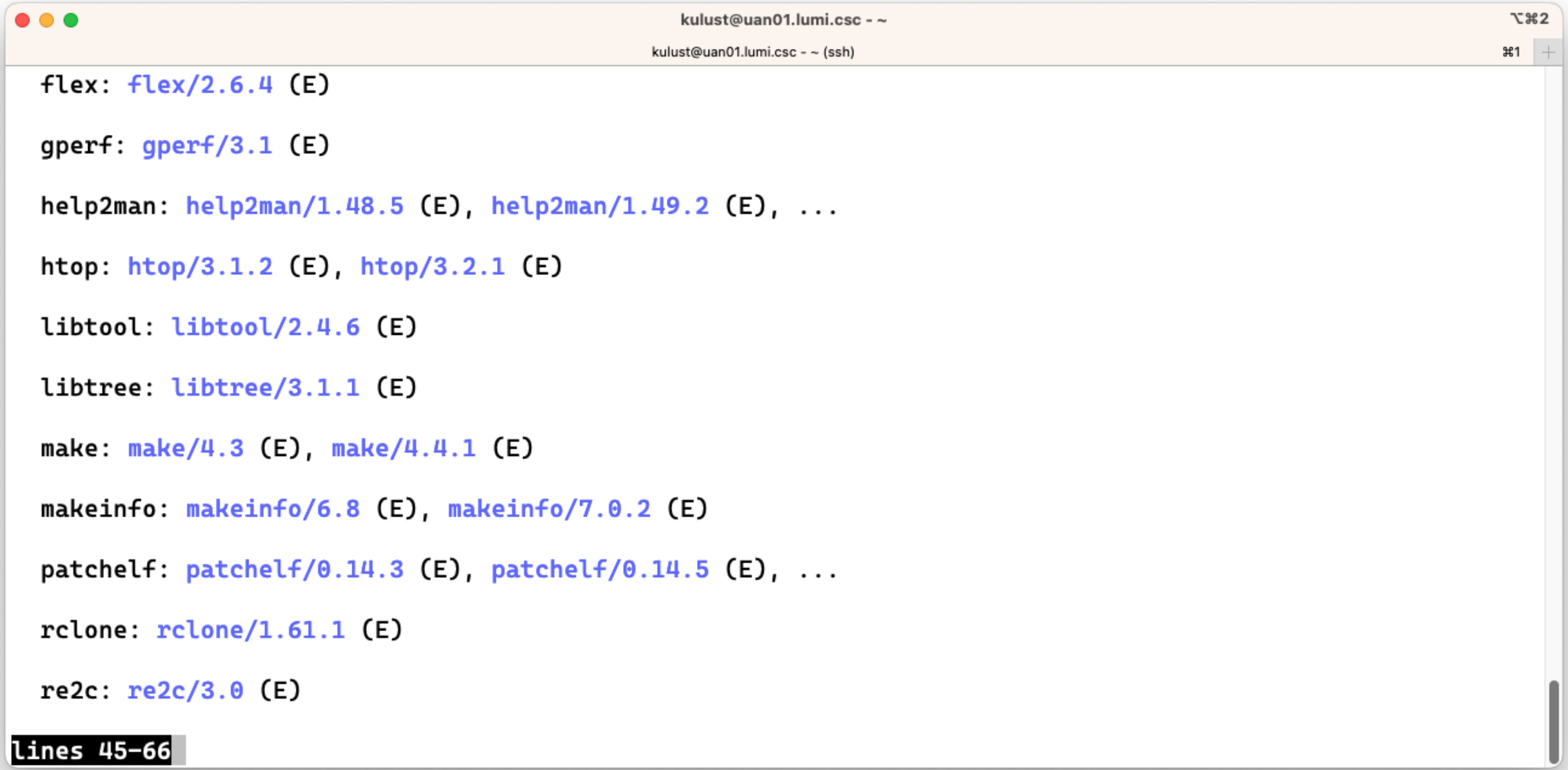
```
-----------------------------------------------------------------------------------------

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

  Autoconf: Autoconf/2.71 (E)

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

  Automake: Automake/1.16.5 (E)

  Bison: Bison/3.8.2 (E)

  CMake: CMake/3.22.2 (E), CMake/3.23.2 (E), CMake/3.24.0 (E), ...

  CubeLib: CubeLib/4.6 (E)

  CubeWriter: CubeWriter/4.6 (E)

  Doxygen: Doxygen/1.9.3 (E), Doxygen/1.9.4 (E), Doxygen/1.9.6 (E)

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

module keyword https (2)



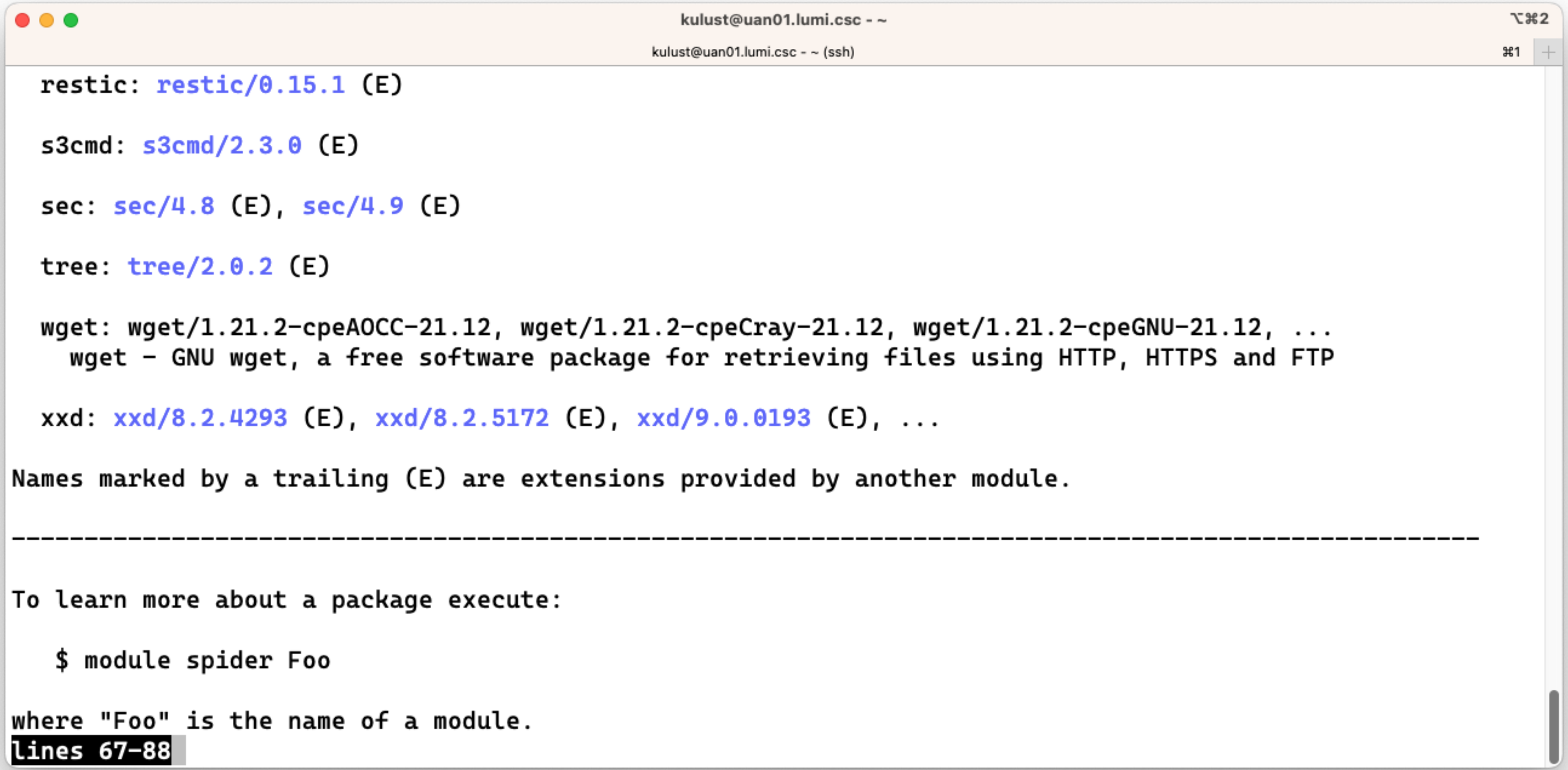
```
M4: M4/1.4.19 (E)

Meson: Meson/0.61.1 (E), Meson/0.61.5 (E)

NASM: NASM/2.15.05 (E)

Ninja: Ninja/1.10.2 (E), Ninja/1.11.0 (E), Ninja/1.11.1 (E)

OPARI2: OPARI2/2.0.6 (E)

OTF2: OTF2/2.3 (E)

SCons: SCons/4.3.0 (E), SCons/4.4.0 (E)

Yasm: Yasm/1.3.0 (E)

byacc: byacc/20220128 (E), byacc/20230219 (E)

cURL: cURL/7.78.0-cpeAOCC-21.12, cURL/7.78.0-cpeCray-21.12, cURL/7.78.0-cpeGNU-21.12, ...
  Command line tool and library for transferring data with URLs.

lines 23-44
```

module keyword https (3)



```
  flex: flex/2.6.4 (E)

  gperf: gperf/3.1 (E)

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

  htop: htop/3.1.2 (E), htop/3.2.1 (E)

  libtool: libtool/2.4.6 (E)

  libtree: libtree/3.1.1 (E)

  make: make/4.3 (E), make/4.4.1 (E)

  makeinfo: makeinfo/6.8 (E), makeinfo/7.0.2 (E)

  patchelf: patchelf/0.14.3 (E), patchelf/0.14.5 (E), ...

  rclone: rclone/1.61.1 (E)

  re2c: re2c/3.0 (E)

lines 45-66
```

module keyword https (4)

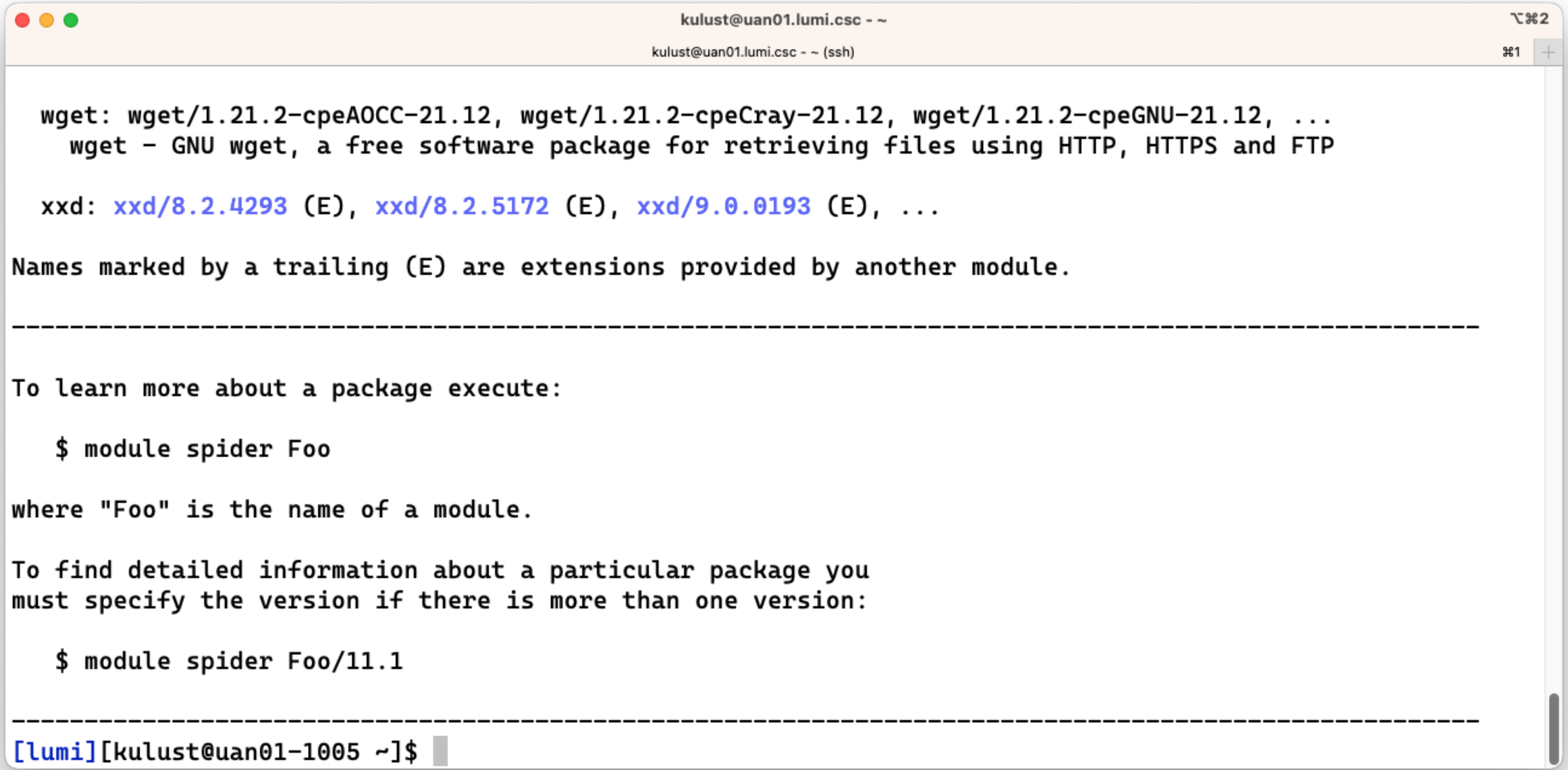


kulust@uan01.lumi.csc - ~

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

```
  restic: restic/0.15.1 (E)

  s3cmd: s3cmd/2.3.0 (E)

  sec: sec/4.8 (E), sec/4.9 (E)

  tree: tree/2.0.2 (E)

  wget: wget/1.21.2-cpeAOCC-21.12, wget/1.21.2-cpeCray-21.12, wget/1.21.2-cpeGNU-21.12, ...
    wget - GNU wget, a free software package for retrieving files using HTTP, HTTPS and FTP

  xxd: xxd/8.2.4293 (E), xxd/8.2.5172 (E), xxd/9.0.0193 (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.
lines 67-88
```

module keyword https (5)

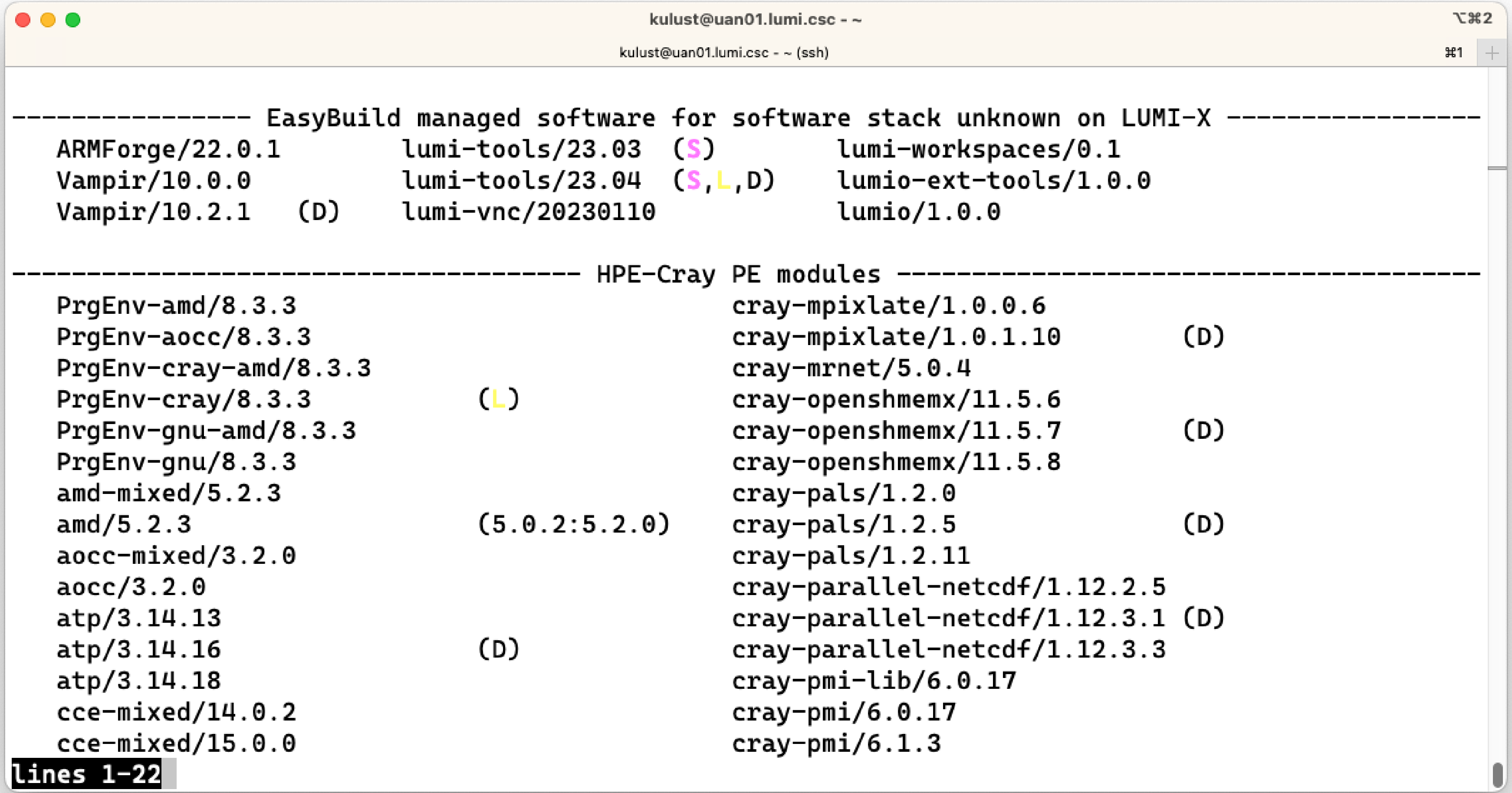


```
  wget: wget/1.21.2-cpeAOCC-21.12, wget/1.21.2-cpeCray-21.12, wget/1.21.2-cpeGNU-21.12, ...
    wget - GNU wget, a free software package for retrieving files using HTTP, HTTPS and FTP

  xxd: xxd/8.2.4293 (E), xxd/8.2.5172 (E), xxd/9.0.0193 (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@uan01-1005 ~]$
```

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, so the target modules and partition module will be switched (back) to those for the current node.

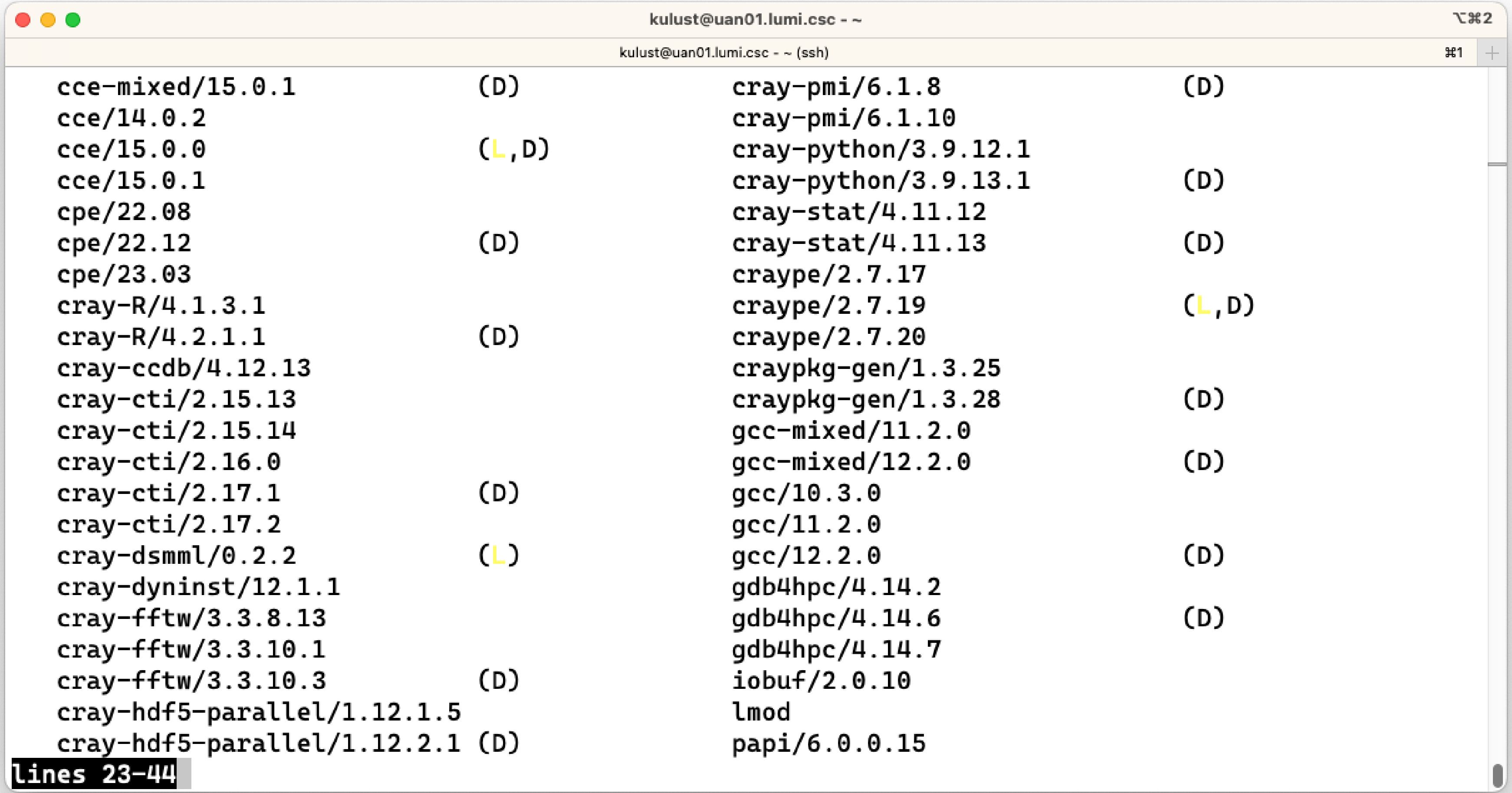
module av


kulust@uan01.lumi.csc - ~

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

```
---------------- EasyBuild managed software for software stack unknown on LUMI-X -----------------
   ARMForge/22.0.1         lumi-tools/23.03  (S)        lumi-workspaces/0.1
   Vampir/10.0.0           lumi-tools/23.04  (S,L,D)    lumio-ext-tools/1.0.0
   Vampir/10.2.1   (D)     lumi-vnc/20230110            lumio/1.0.0

-------------------------------------- HPE-Cray PE modules ---------------------------------------
   PrgEnv-amd/8.3.3                                 cray-mpixlate/1.0.0.6
   PrgEnv-aocc/8.3.3                                cray-mpixlate/1.0.1.10         (D)
   PrgEnv-cray-amd/8.3.3                            cray-mrnet/5.0.4
   PrgEnv-cray/8.3.3             (L)                cray-openshmemx/11.5.6
   PrgEnv-gnu-amd/8.3.3                             cray-openshmemx/11.5.7         (D)
   PrgEnv-gnu/8.3.3                                 cray-openshmemx/11.5.8
   amd-mixed/5.2.3                                  cray-pals/1.2.0
   amd/5.2.3                     (5.0.2:5.2.0)      cray-pals/1.2.5                (D)
   aocc-mixed/3.2.0                                 cray-pals/1.2.11
   aocc/3.2.0                                       cray-parallel-netcdf/1.12.2.5
   atp/3.14.13                                      cray-parallel-netcdf/1.12.3.1 (D)
   atp/3.14.16                   (D)                cray-parallel-netcdf/1.12.3.3
   atp/3.14.18                                      cray-pmi-lib/6.0.17
   cce-mixed/14.0.2                                 cray-pmi/6.0.17
   cce-mixed/15.0.0                                 cray-pmi/6.1.3
lines 1-22
```

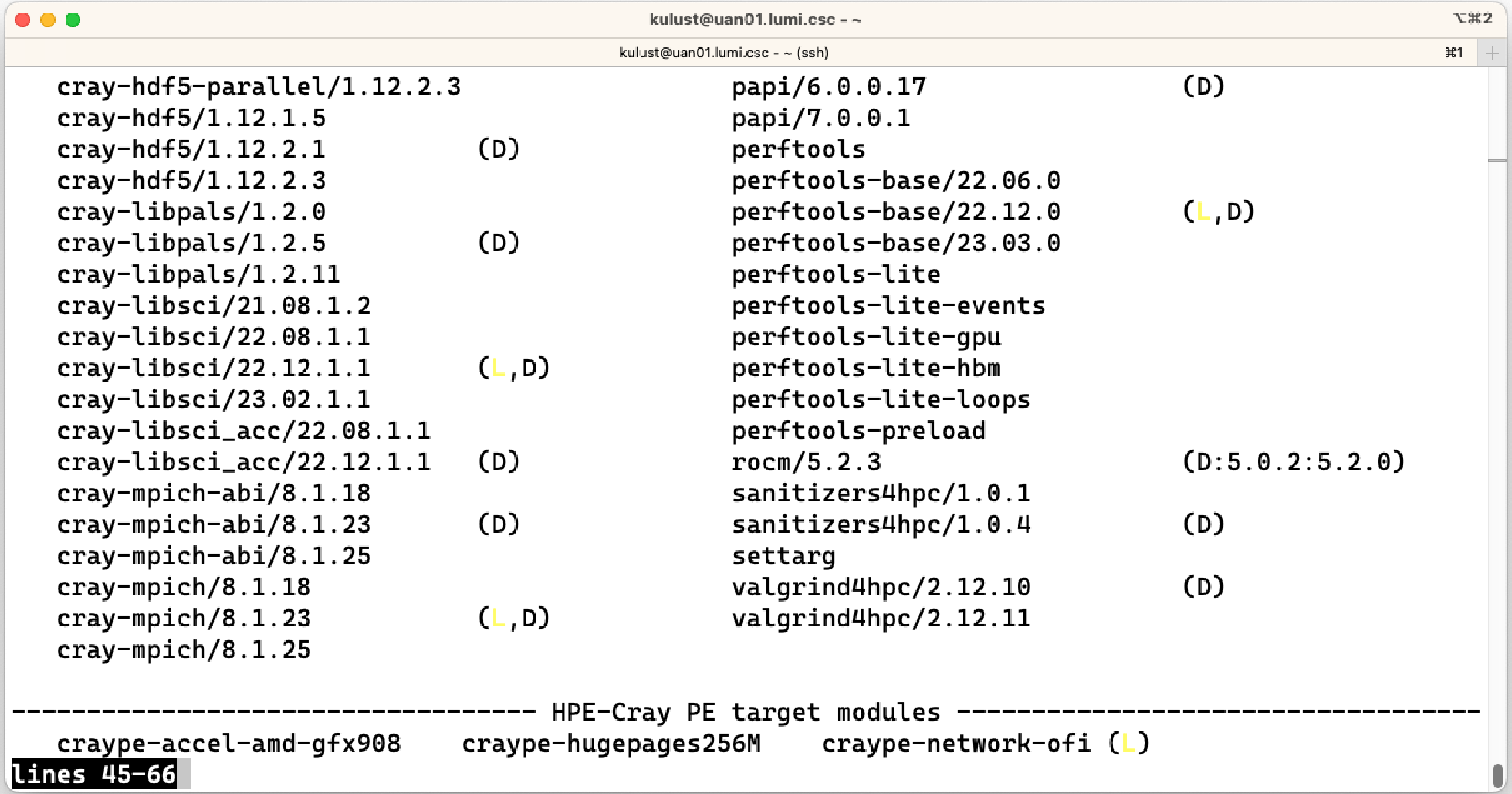
module av (2)


kulust@uan01.lumi.csc - ~

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

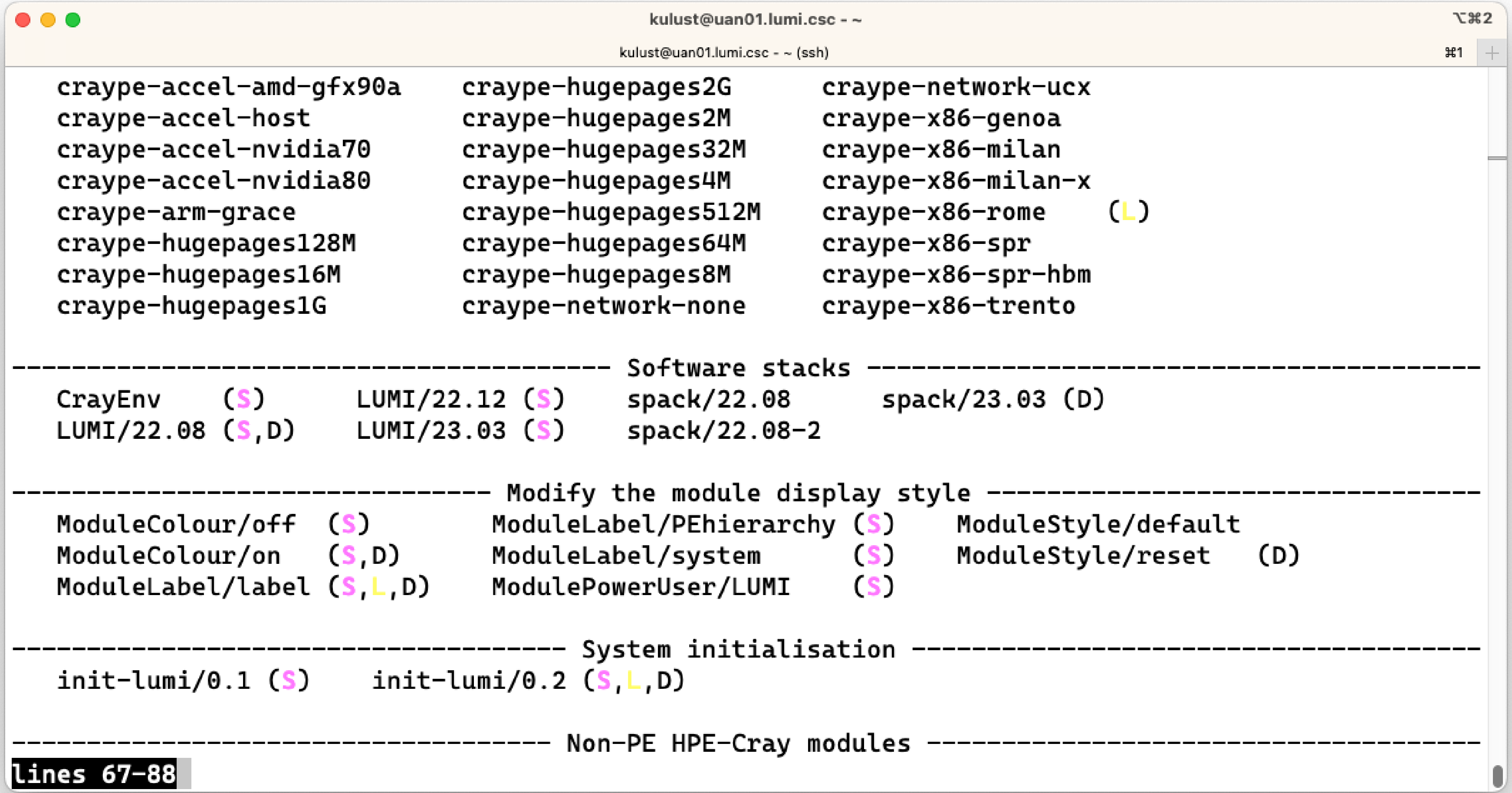
```
   cce-mixed/15.0.1            (D)        cray-pmi/6.1.8             (D)
   cce/14.0.2                             cray-pmi/6.1.10
   cce/15.0.0                  (L,D)      cray-python/3.9.12.1
   cce/15.0.1                             cray-python/3.9.13.1       (D)
   cpe/22.08                              cray-stat/4.11.12
   cpe/22.12                   (D)        cray-stat/4.11.13          (D)
   cpe/23.03                              craype/2.7.17
   cray-R/4.1.3.1                         craype/2.7.19              (L,D)
   cray-R/4.2.1.1              (D)        craype/2.7.20
   cray-ccdb/4.12.13                      craypkg-gen/1.3.25
   cray-cti/2.15.13                       craypkg-gen/1.3.28         (D)
   cray-cti/2.15.14                       gcc-mixed/11.2.0
   cray-cti/2.16.0                        gcc-mixed/12.2.0           (D)
   cray-cti/2.17.1             (D)        gcc/10.3.0
   cray-cti/2.17.2                        gcc/11.2.0
   cray-dsmml/0.2.2            (L)        gcc/12.2.0                 (D)
   cray-dyninst/12.1.1                    gdb4hpc/4.14.2
   cray-fftw/3.3.8.13                     gdb4hpc/4.14.6             (D)
   cray-fftw/3.3.10.1                     gdb4hpc/4.14.7
   cray-fftw/3.3.10.3          (D)        iobuf/2.0.10
   cray-hdf5-parallel/1.12.1.5            lmod
   cray-hdf5-parallel/1.12.2.1 (D)        papi/6.0.0.15
lines 23-44
```

module av (3)


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

```
   cray-hdf5-parallel/1.12.2.3                  papi/6.0.0.17               (D)
   cray-hdf5/1.12.1.5                           papi/7.0.0.1
   cray-hdf5/1.12.2.1          (D)              perftools
   cray-hdf5/1.12.2.3                           perftools-base/22.06.0
   cray-libpals/1.2.0                           perftools-base/22.12.0      (L,D)
   cray-libpals/1.2.5          (D)              perftools-base/23.03.0
   cray-libpals/1.2.11                          perftools-lite
   cray-libsci/21.08.1.2                        perftools-lite-events
   cray-libsci/22.08.1.1                        perftools-lite-gpu
   cray-libsci/22.12.1.1       (L,D)            perftools-lite-hbm
   cray-libsci/23.02.1.1                        perftools-lite-loops
   cray-libsci_acc/22.08.1.1                    perftools-preload
   cray-libsci_acc/22.12.1.1   (D)              rocm/5.2.3                  (D:5.0.2:5.2.0)
   cray-mpich-abi/8.1.18                        sanitizers4hpc/1.0.1
   cray-mpich-abi/8.1.23       (D)              sanitizers4hpc/1.0.4        (D)
   cray-mpich-abi/8.1.25                        settarg
   cray-mpich/8.1.18                            valgrind4hpc/2.12.10        (D)
   cray-mpich/8.1.23           (L,D)            valgrind4hpc/2.12.11
   cray-mpich/8.1.25

----------------------------------- HPE-Cray PE target modules ----------------------------------------
   craype-accel-amd-gfx908    craype-hugepages256M    craype-network-ofi (L)
lines 45-66
```

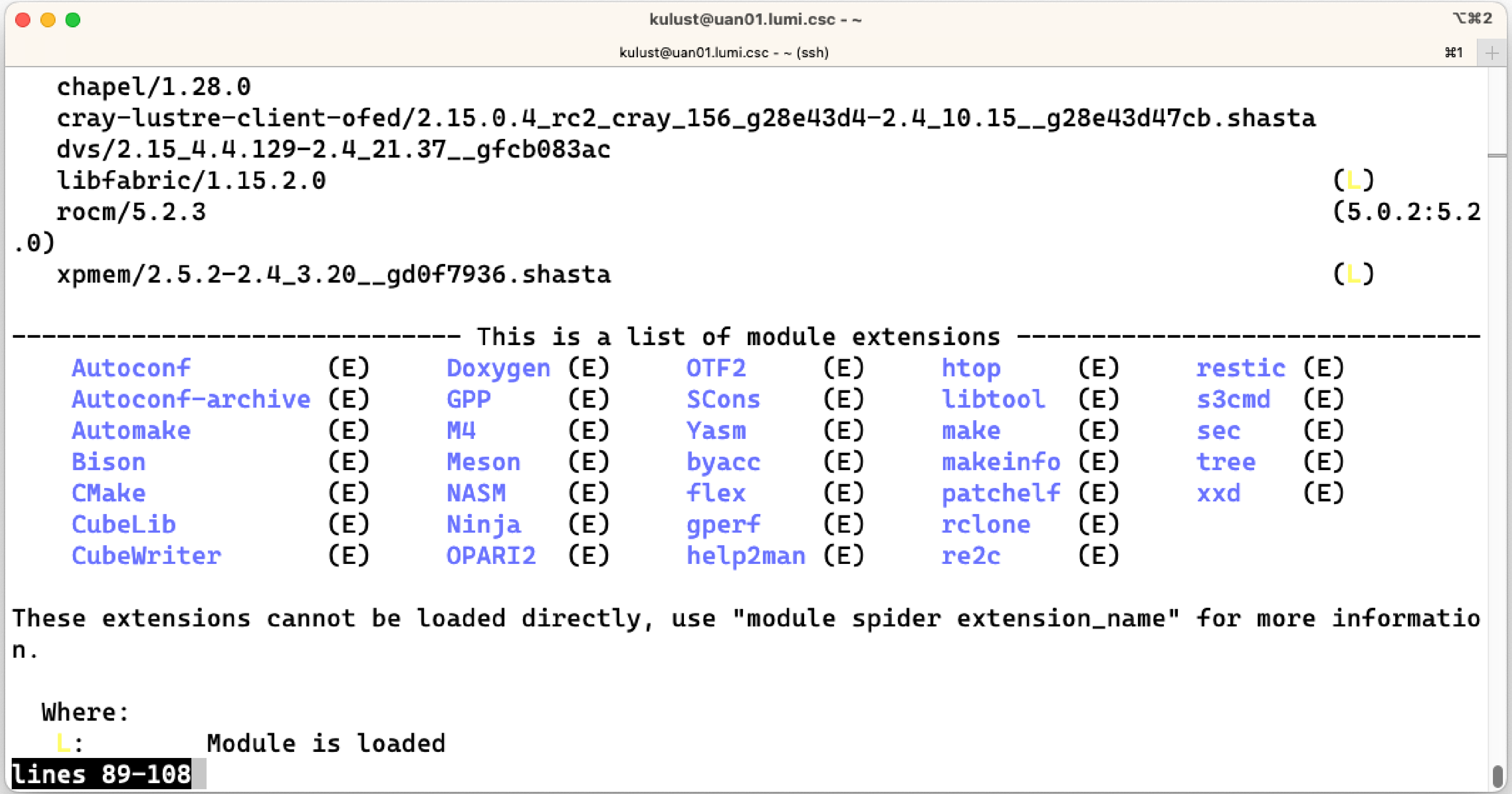
module av (4)


kulust@uan01.lumi.csc - ~

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

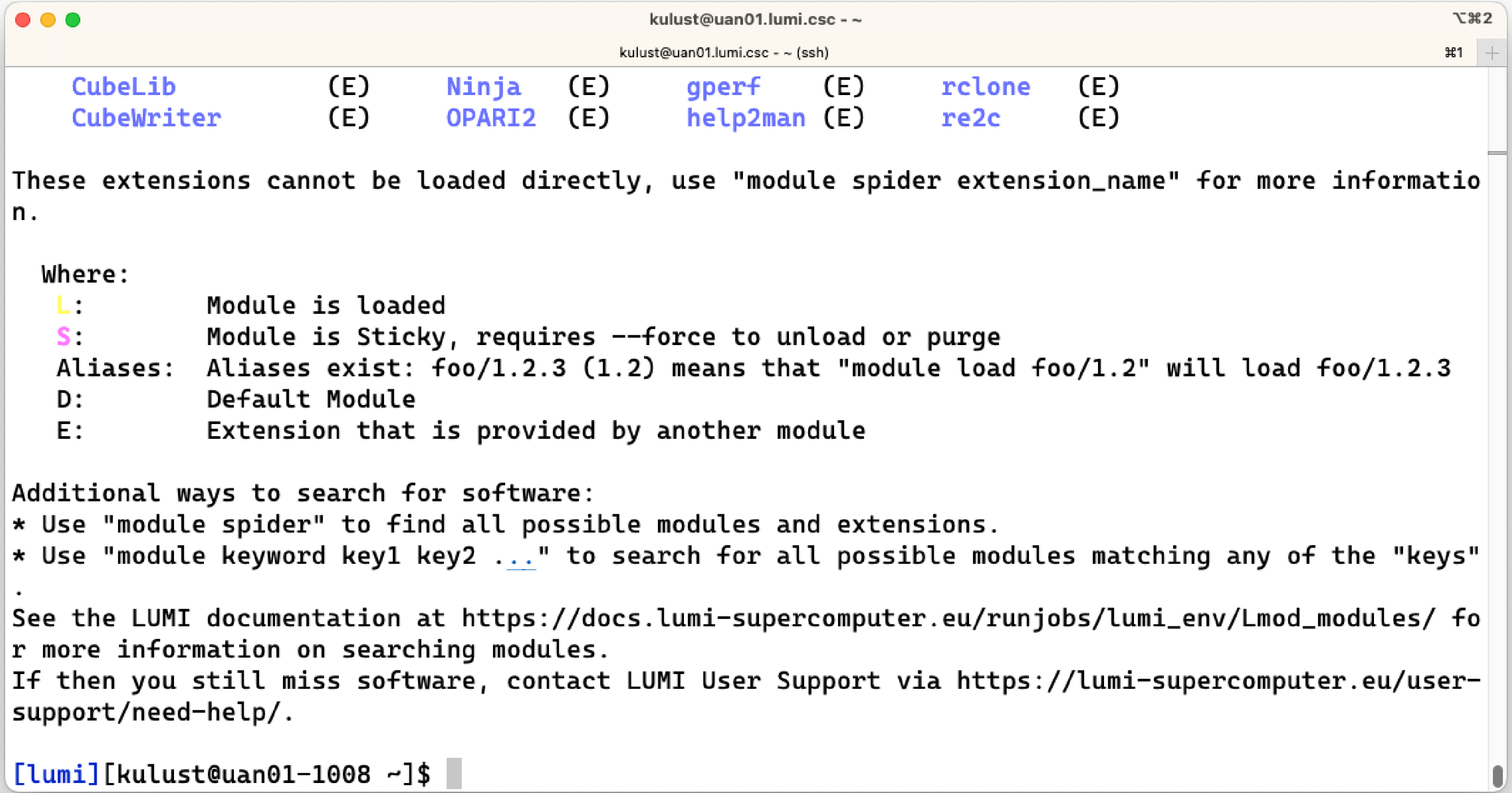
```
   craype-accel-amd-gfx90a    craype-hugepages2G      craype-network-ucx
   craype-accel-host          craype-hugepages2M      craype-x86-genoa
   craype-accel-nvidia70      craype-hugepages32M     craype-x86-milan
   craype-accel-nvidia80      craype-hugepages4M      craype-x86-milan-x
   craype-arm-grace           craype-hugepages512M    craype-x86-rome    (L)
   craype-hugepages128M       craype-hugepages64M     craype-x86-spr
   craype-hugepages16M        craype-hugepages8M      craype-x86-spr-hbm
   craype-hugepages1G         craype-network-none     craype-x86-trento

---------------------------------------- Software stacks ------------------------------------------
   CrayEnv     (S)      LUMI/22.12 (S)    spack/22.08       spack/23.03 (D)
   LUMI/22.08 (S,D)     LUMI/23.03 (S)    spack/22.08-2

-------------------------------- 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)    init-lumi/0.2 (S,L,D)

----------------------------------- Non-PE HPE-Cray modules --------------------------------------
lines 67-88
```

module av (5)



```
   chapel/1.28.0
   cray-lustre-client-ofed/2.15.0.4_rc2_cray_156_g28e43d4-2.4_10.15__g28e43d47cb.shasta
   dvs/2.15_4.4.129-2.4_21.37__gfcb083ac
   libfabric/1.15.2.0                                                               (L)
   rocm/5.2.3                                                                       (5.0.2:5.2
.0)
   xpmem/2.5.2-2.4_3.20__gd0f7936.shasta                                            (L)

------------------------------ This is a list of module extensions ------------------------------
    Autoconf         (E)     Doxygen (E)     OTF2     (E)     htop      (E)     restic (E)
    Autoconf-archive (E)     GPP     (E)     SCons    (E)     libtool   (E)     s3cmd  (E)
    Automake         (E)     M4      (E)     Yasm     (E)     make      (E)     sec    (E)
    Bison            (E)     Meson   (E)     byacc    (E)     makeinfo  (E)     tree   (E)
    CMake            (E)     NASM    (E)     flex     (E)     patchelf  (E)     xxd    (E)
    CubeLib          (E)     Ninja   (E)     gperf    (E)     rclone    (E)
    CubeWriter       (E)     OPARI2  (E)     help2man (E)     re2c      (E)

These extensions cannot be loaded directly, use "module spider extension_name" for more informatio
n.

  Where:
   L:         Module is loaded
lines 89-108
```

module av (6)


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

```
    CubeLib          (E)      Ninja    (E)      gperf    (E)      rclone   (E)
    CubeWriter       (E)      OPARI2   (E)      help2man (E)      re2c     (E)

These extensions cannot be loaded directly, use "module spider extension_name" for more informatio
n.

  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 the "keys"
.
See the LUMI documentation at https://docs.lumi-supercomputer.eu/runjobs/lumi_env/Lmod_modules/ fo
r 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@uan01-1008 ~]$
```

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 and unfolded PE hierarchy
  - `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!
- More customisation possible via LMOD environment variables

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 = module
  - 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

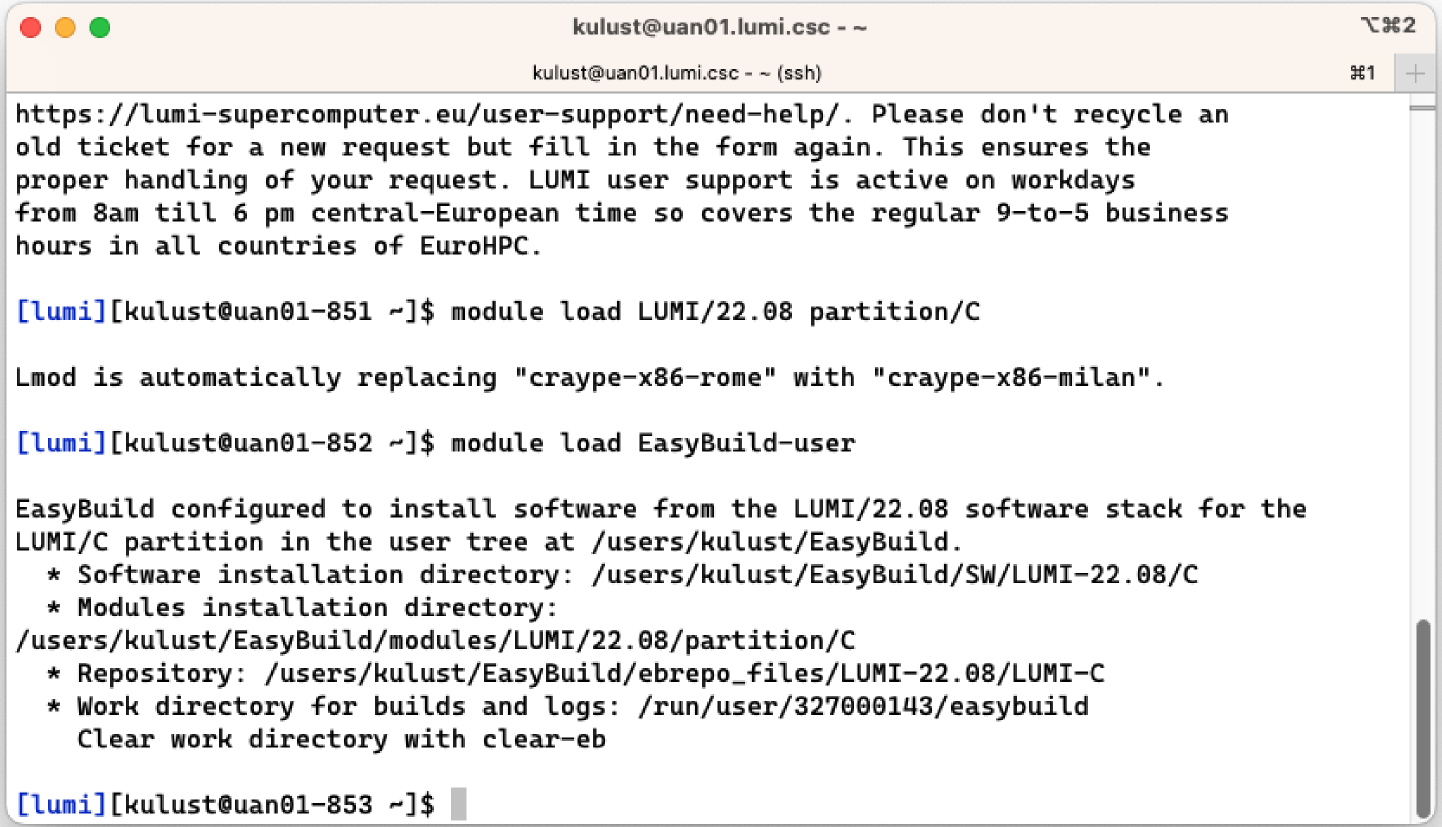
Installing
Step 1: Where to install

- 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`
- 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`
- 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

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



kulust@uan01.lumi.csc - ~

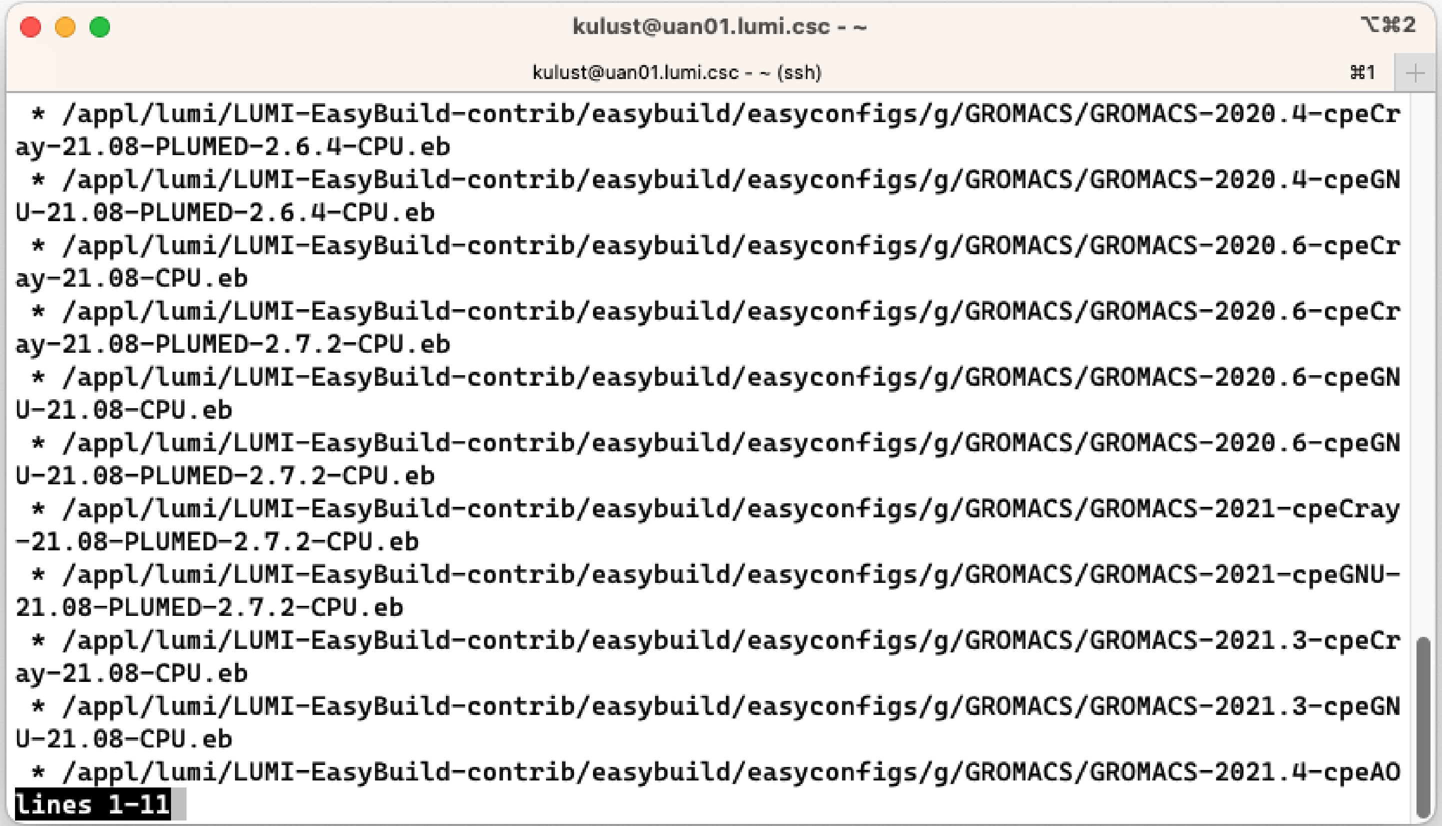
kulust@uan01.lumi.csc - ~ (ssh)

```
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`

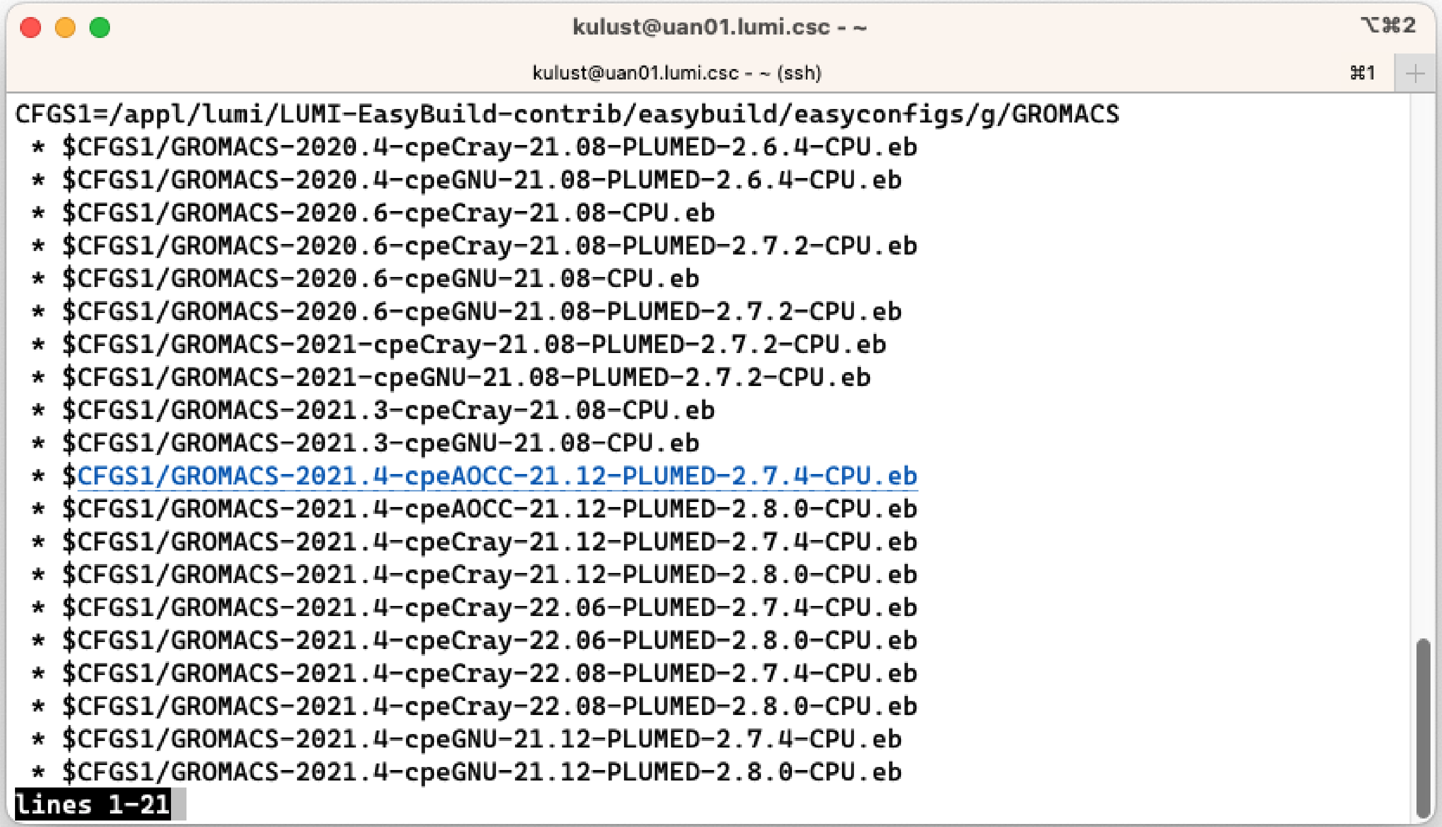


kulust@uan01.lumi.csc - ~ ⌥⌘2

kulust@uan01.lumi.csc - ~ (ssh) ⌘1

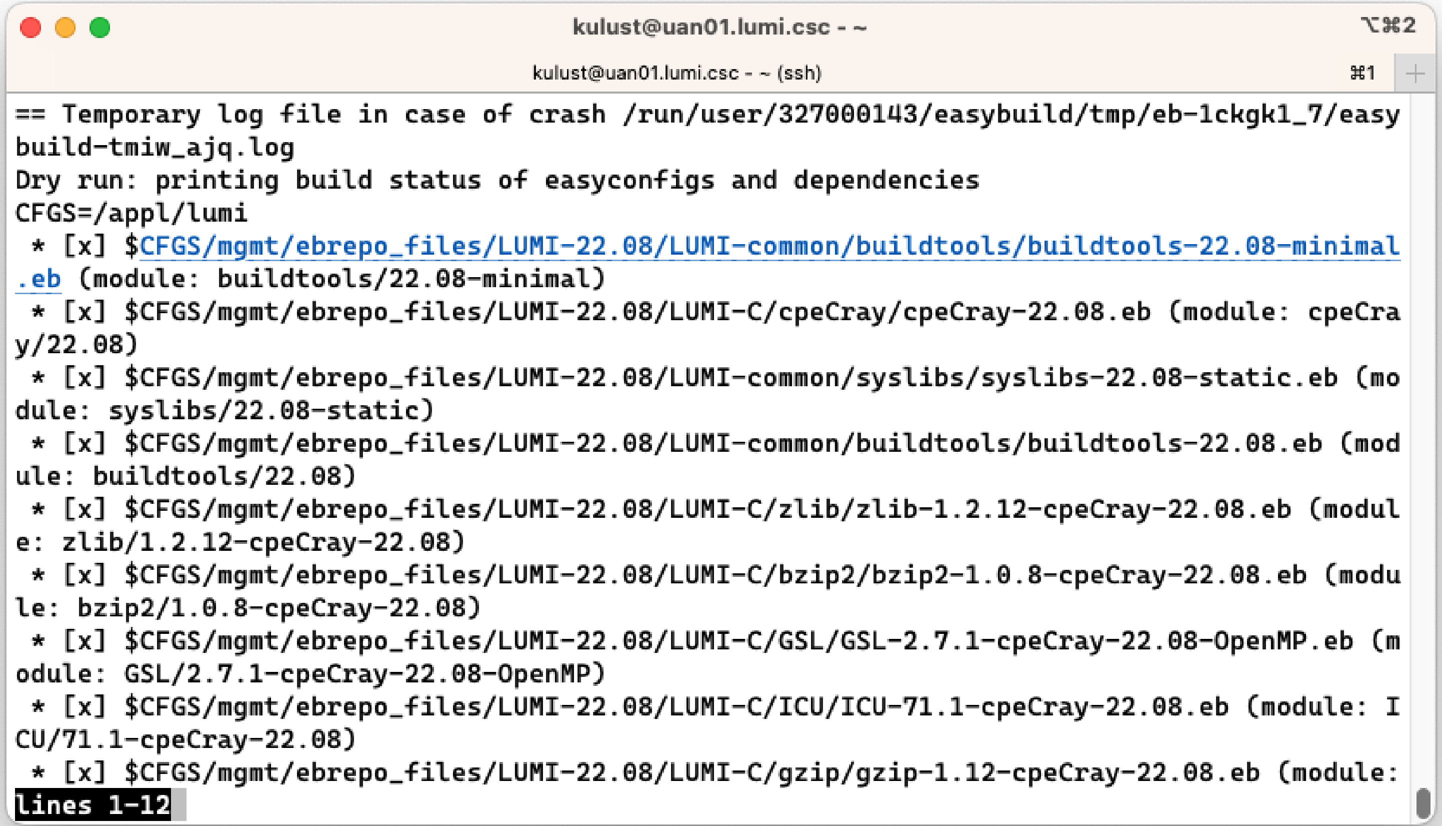
```
 * /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS/GROMACS-2020.4-cpeCr
ay-21.08-PLUMED-2.6.4-CPU.eb
 * /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS/GROMACS-2020.4-cpeGN
U-21.08-PLUMED-2.6.4-CPU.eb
 * /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS/GROMACS-2020.6-cpeCr
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


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

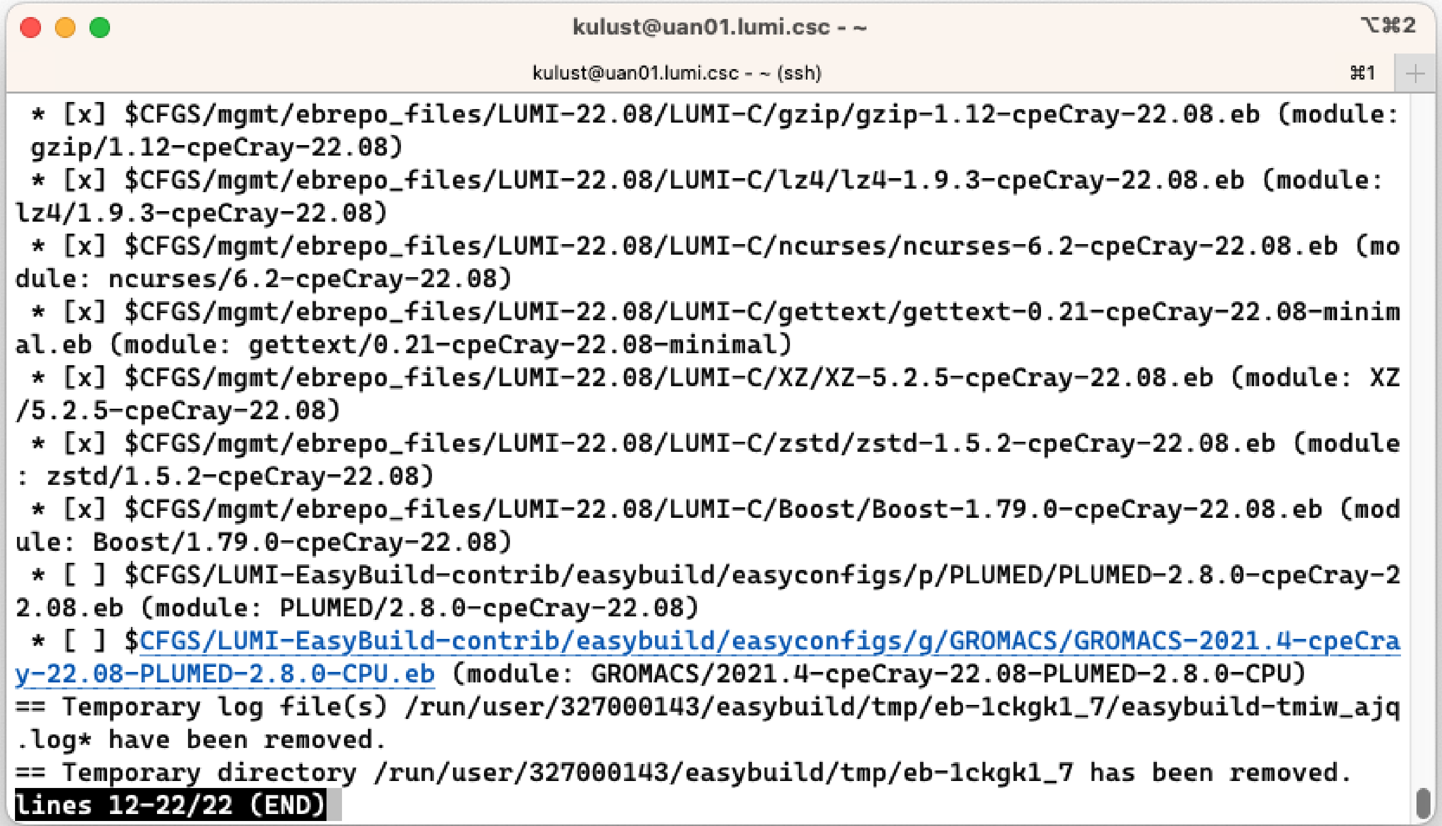
```
CFGS1=/appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS
 * $CFGS1/GROMACS-2020.4-cpeCray-21.08-PLUMED-2.6.4-CPU.eb
 * $CFGS1/GROMACS-2020.4-cpeGNU-21.08-PLUMED-2.6.4-CPU.eb
 * $CFGS1/GROMACS-2020.6-cpeCray-21.08-CPU.eb
 * $CFGS1/GROMACS-2020.6-cpeCray-21.08-PLUMED-2.7.2-CPU.eb
 * $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



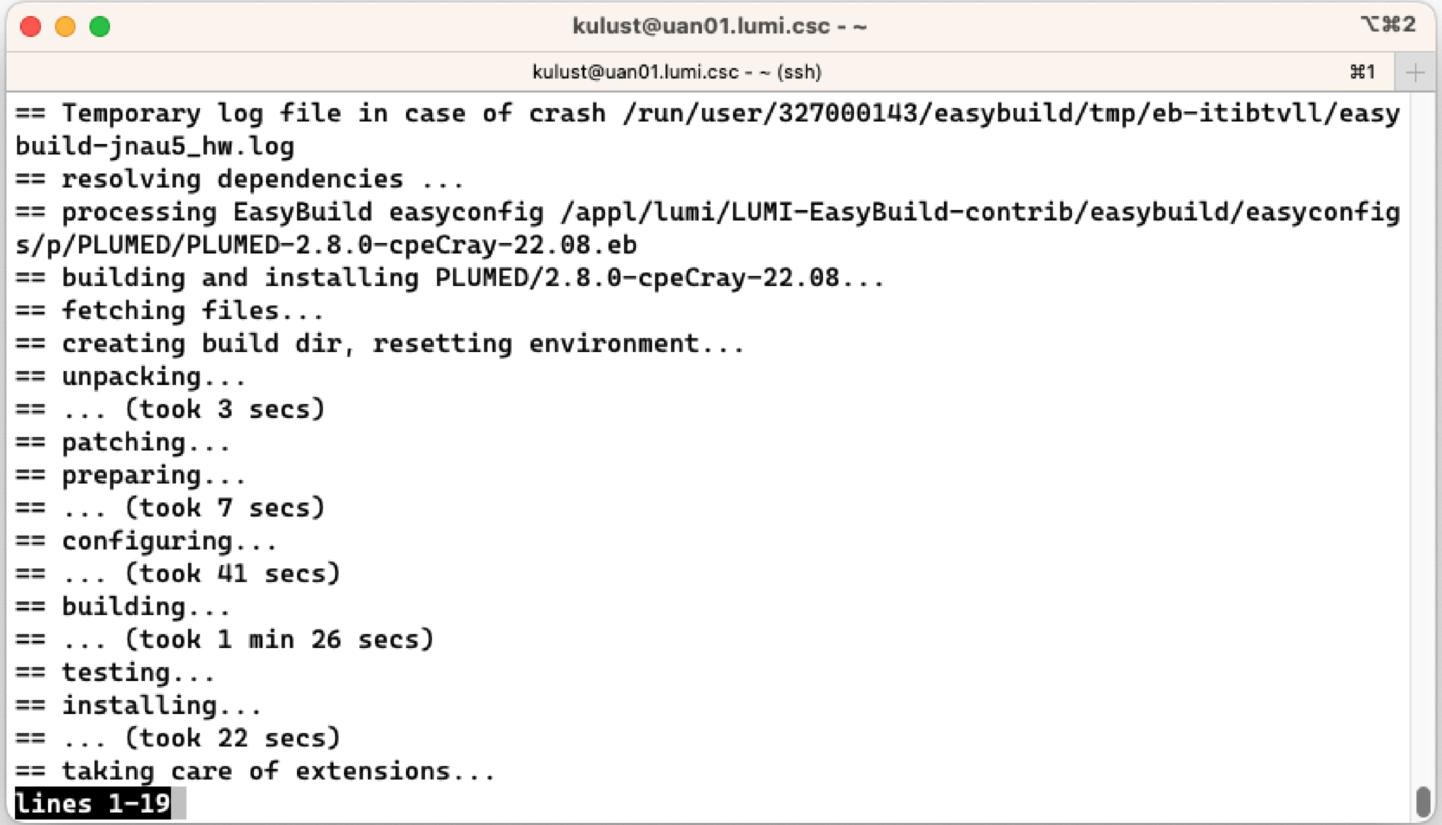
```
== Temporary log file in case of crash /run/user/327000143/easybuild/tmp/eb-1ckgk1_7/easy
build-tmiw_ajq.log
Dry run: printing build status of easyconfigs and dependencies
CFGS=/appl/lumi
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-22.08/LUMI-common/buildtools/buildtools-22.08-minimal
.eb (module: buildtools/22.08-minimal)
 * [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 (2)


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

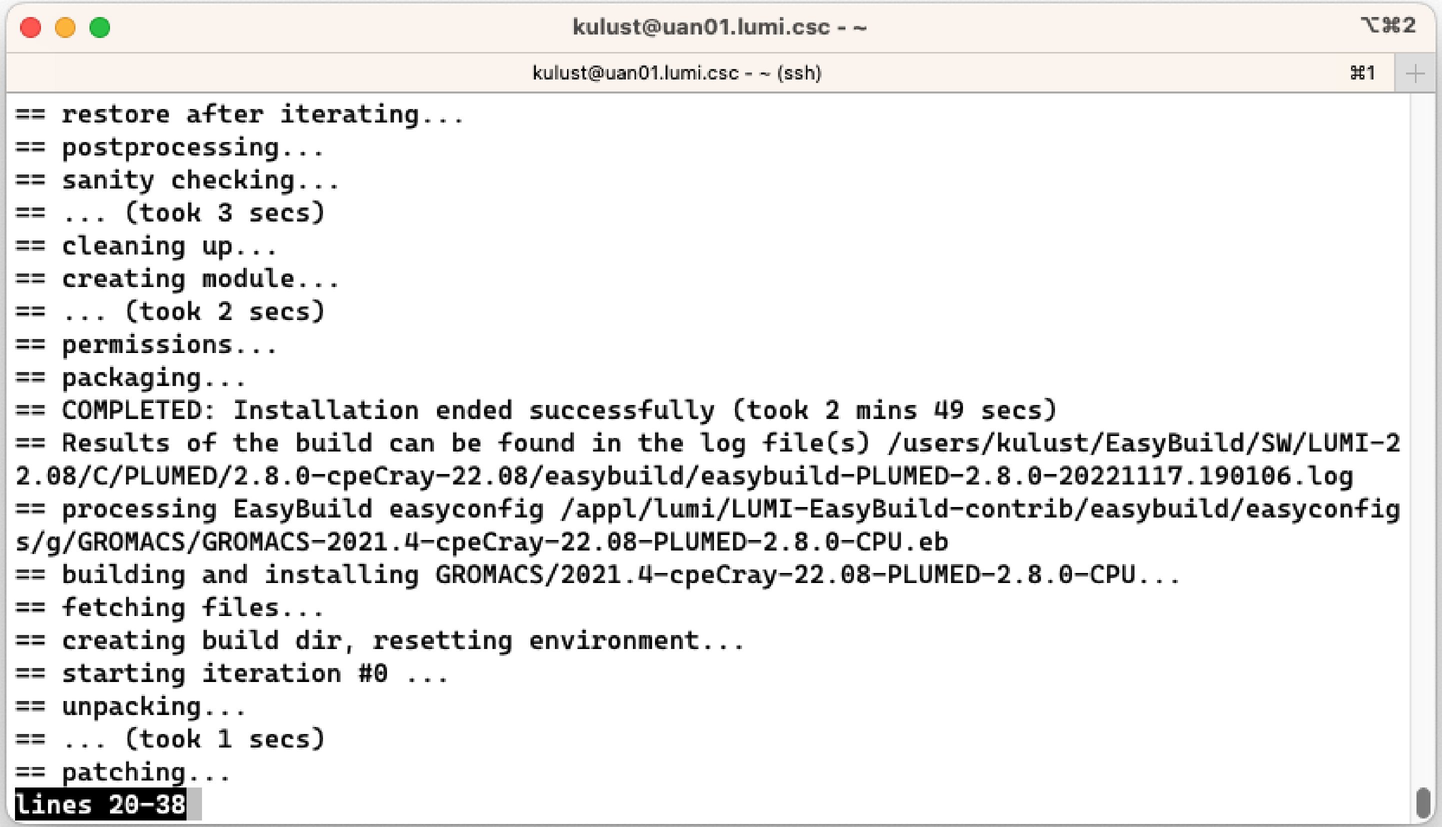


kulust@uan01.lumi.csc - ~

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

```
== 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
```

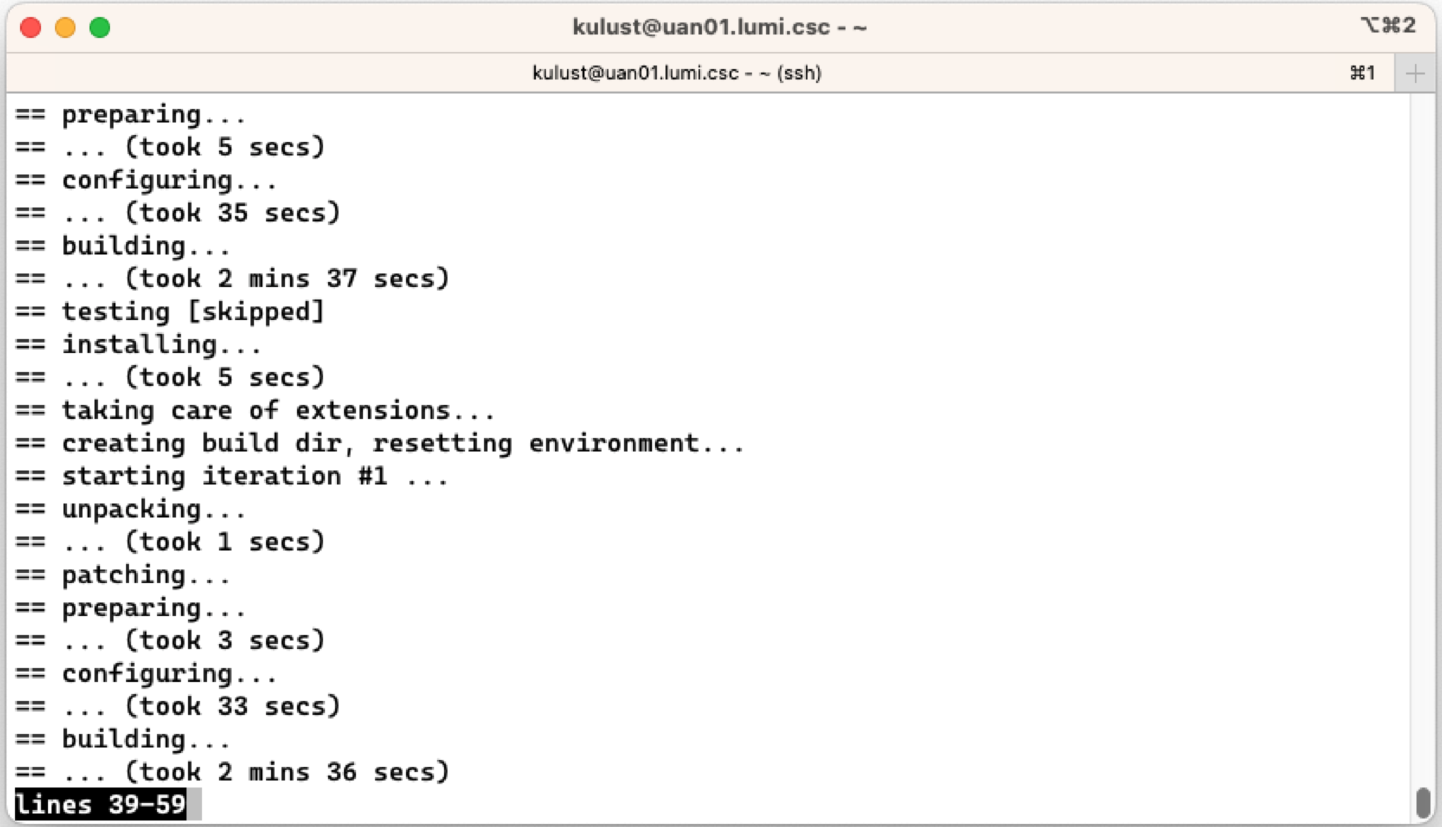
eb GROMACS-2021.4-cpeCray-22.08-PLUMED-2.8.0-CPU.eb -r (2)


kulust@uan01.lumi.csc - ~

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

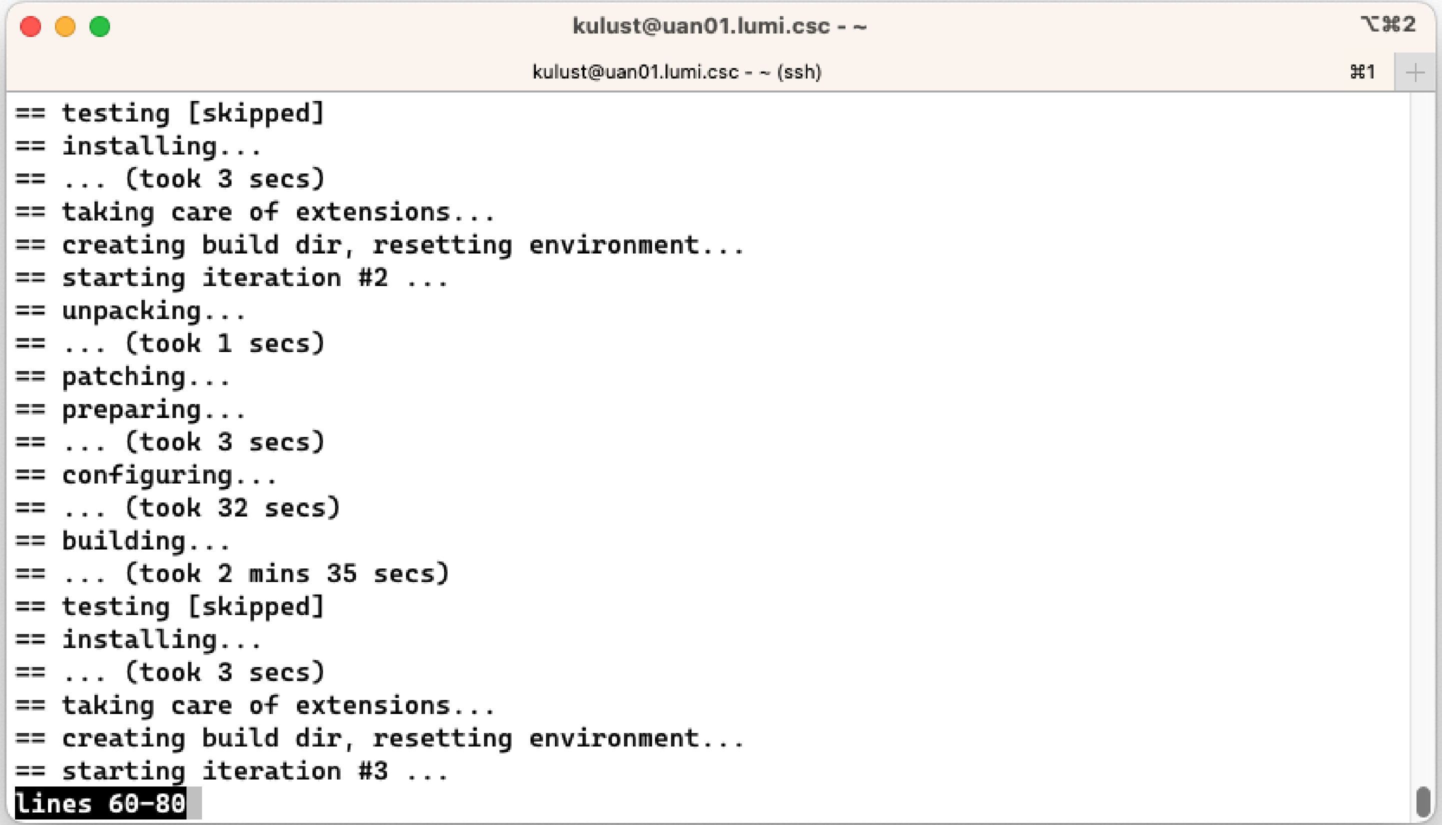
```
== restore after iterating...
== postprocessing...
== sanity checking...
== ... (took 3 secs)
== cleaning up...
== creating module...
== ... (took 2 secs)
== permissions...
== packaging...
== COMPLETED: Installation ended successfully (took 2 mins 49 secs)
== Results of the build can be found in 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 (3)



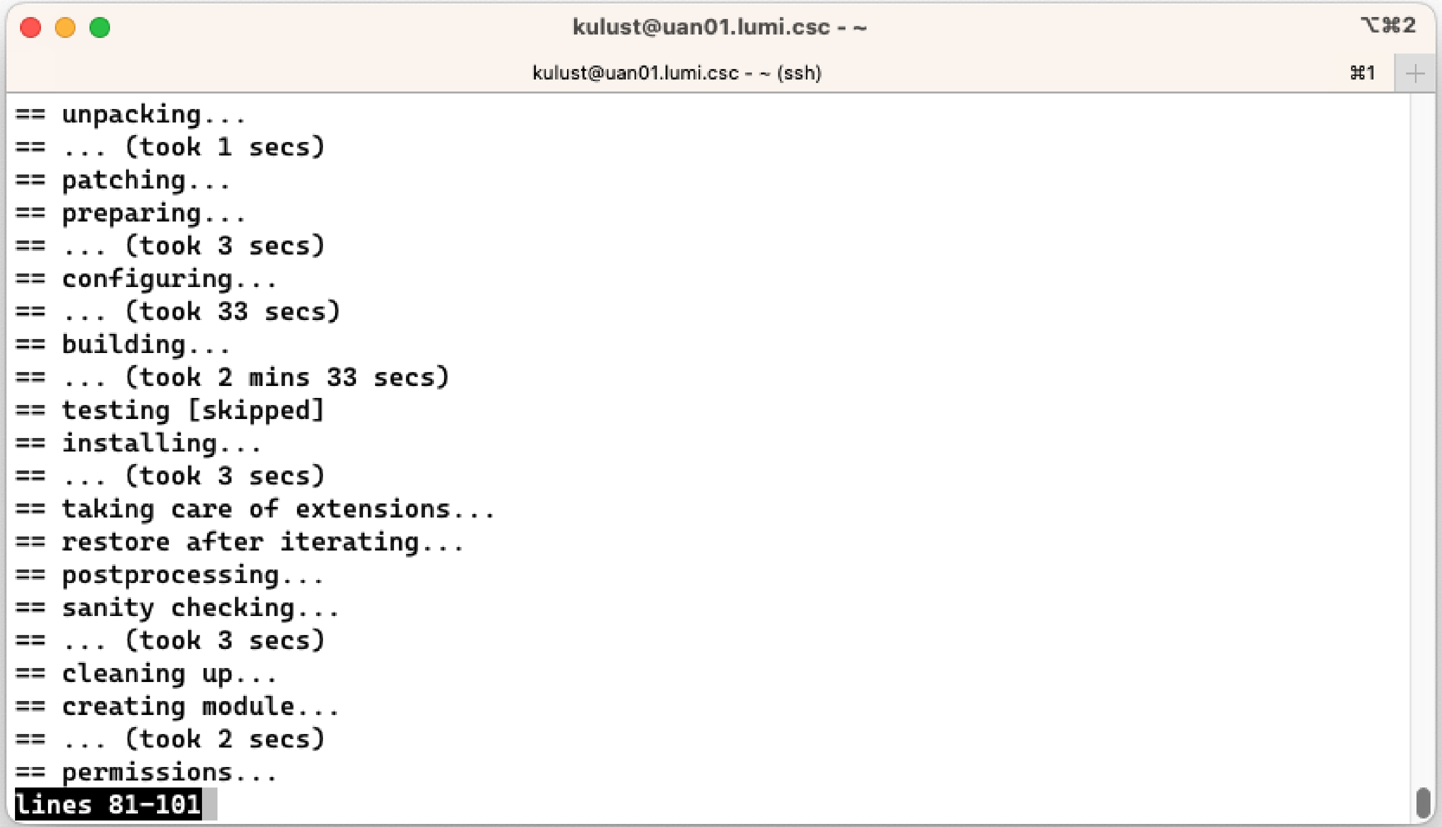
```
== preparing...
== ... (took 5 secs)
== configuring...
== ... (took 35 secs)
== building...
== ... (took 2 mins 37 secs)
== testing [skipped]
== installing...
== ... (took 5 secs)
== taking care of extensions...
== creating build dir, resetting environment...
== starting iteration #1 ...
== unpacking...
== ... (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 (4)



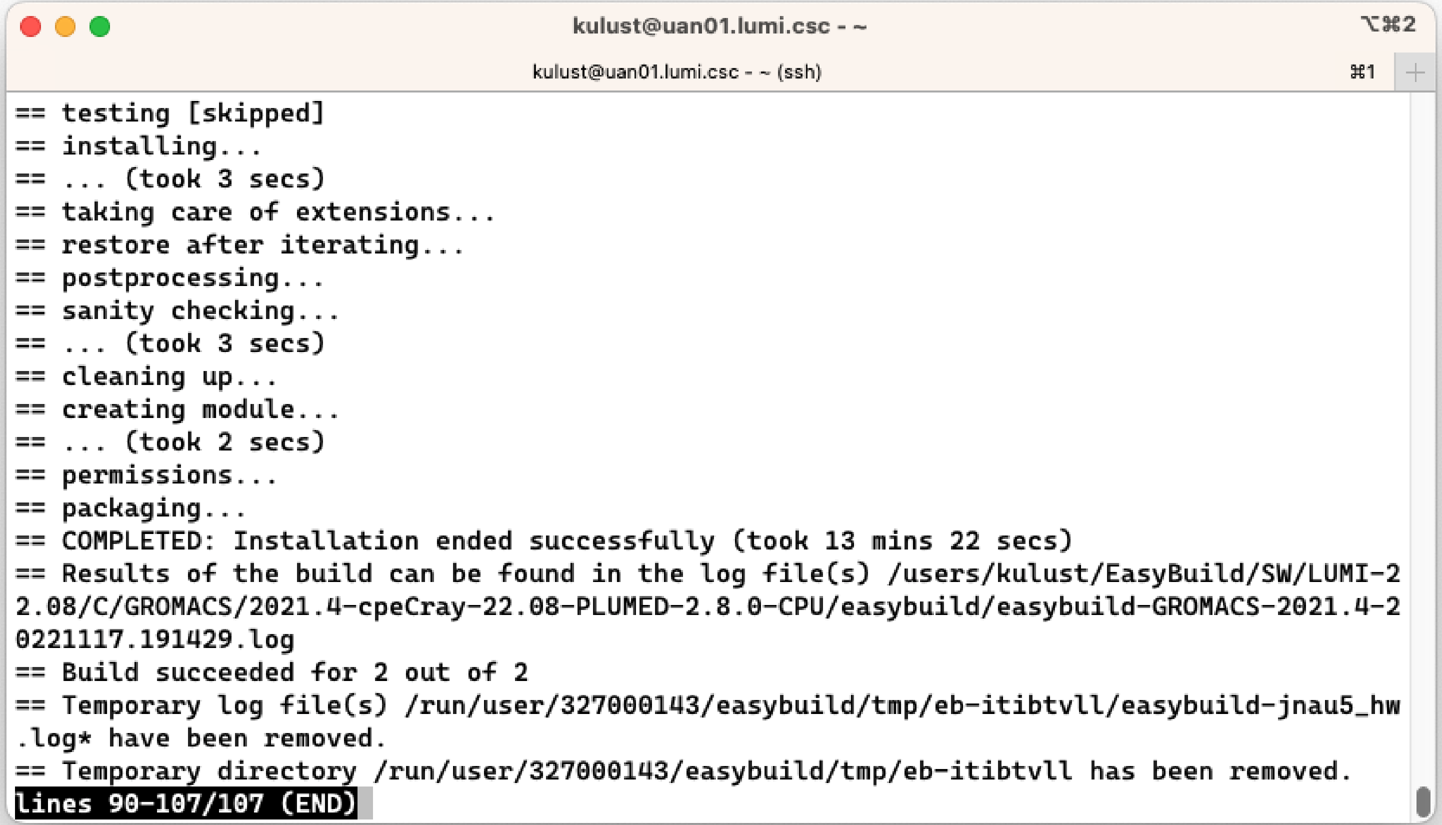
```
== testing [skipped]
== installing...
== ... (took 3 secs)
== taking care of extensions...
== creating build dir, resetting environment...
== starting iteration #2 ...
== unpacking...
== ... (took 1 secs)
== patching...
== preparing...
== ... (took 3 secs)
== configuring...
== ... (took 32 secs)
== 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 (5)



```
== 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 (6)


kulust@uan01.lumi.csc - ~

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

```
== 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

EasyBuild 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 lumi-supercomputer.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

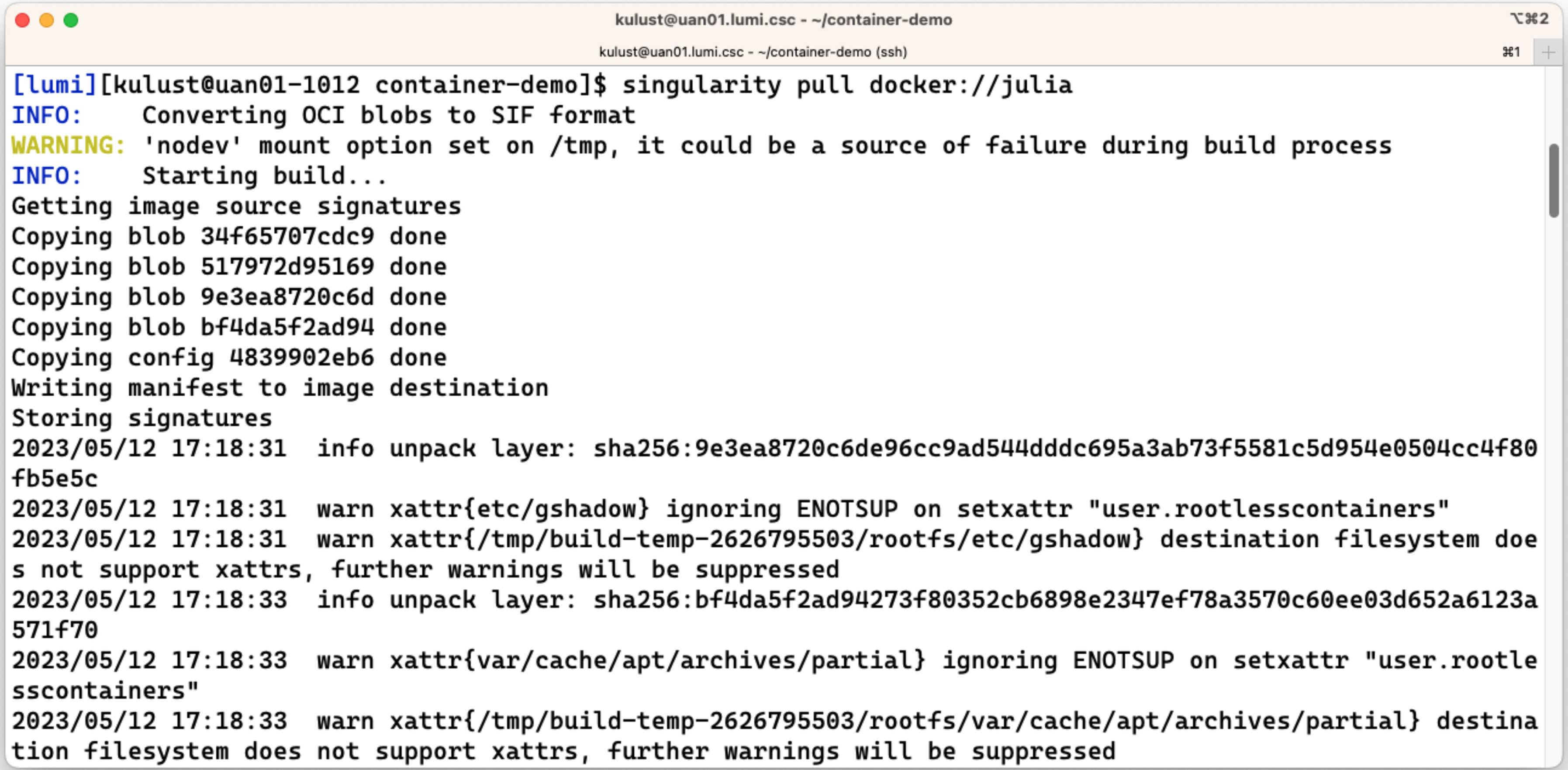
But what can they then do on LUMI?

- **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



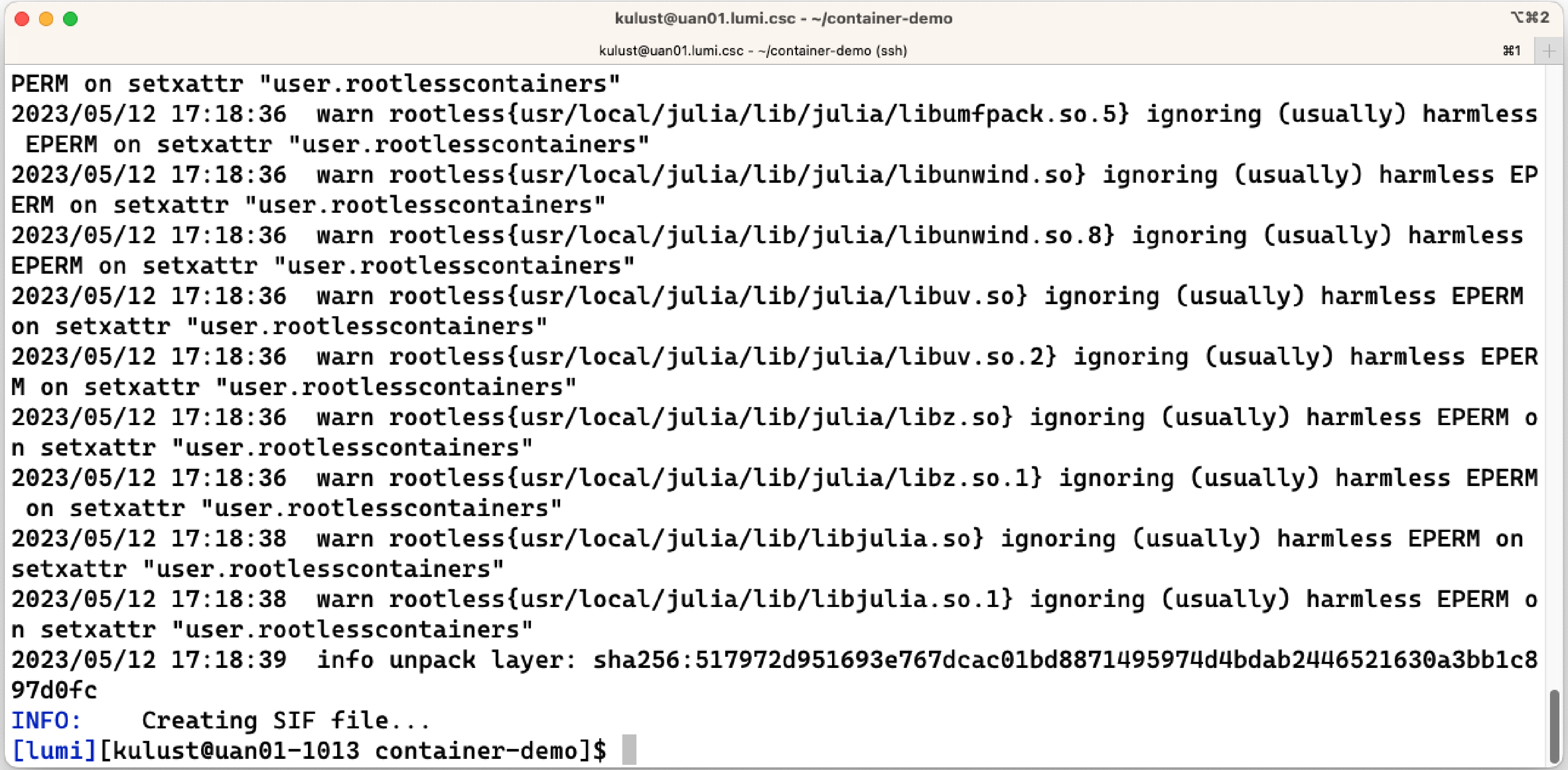
kulust@uan01.lumi.csc - ~/container-demo

kulust@uan01.lumi.csc - ~/container-demo (ssh)

```
[lumi][kulust@uan01-1012 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 34f65707cdc9 done
Copying blob 517972d95169 done
Copying blob 9e3ea8720c6d done
Copying blob bf4da5f2ad94 done
Copying config 4839902eb6 done
Writing manifest to image destination
Storing signatures
2023/05/12 17:18:31  info unpack layer: sha256:9e3ea8720c6de96cc9ad544dddc695a3ab73f5581c5d954e0504cc4f80
fb5e5c
2023/05/12 17:18:31  warn xattr{etc/gshadow} ignoring ENOTSUP on setxattr "user.rootlesscontainers"
2023/05/12 17:18:31  warn xattr{/tmp/build-temp-2626795503/rootfs/etc/gshadow} destination filesystem doe
s not support xattrs, further warnings will be suppressed
2023/05/12 17:18:33  info unpack layer: sha256:bf4da5f2ad94273f80352cb6898e2347ef78a3570c60ee03d652a6123a
571f70
2023/05/12 17:18:33  warn xattr{var/cache/apt/archives/partial} ignoring ENOTSUP on setxattr "user.rootle
sscontainers"
2023/05/12 17:18:33  warn xattr{/tmp/build-temp-2626795503/rootfs/var/cache/apt/archives/partial} destina
tion filesystem does not support xattrs, further warnings will be suppressed
```

singularity pull docker://julia

LUMI

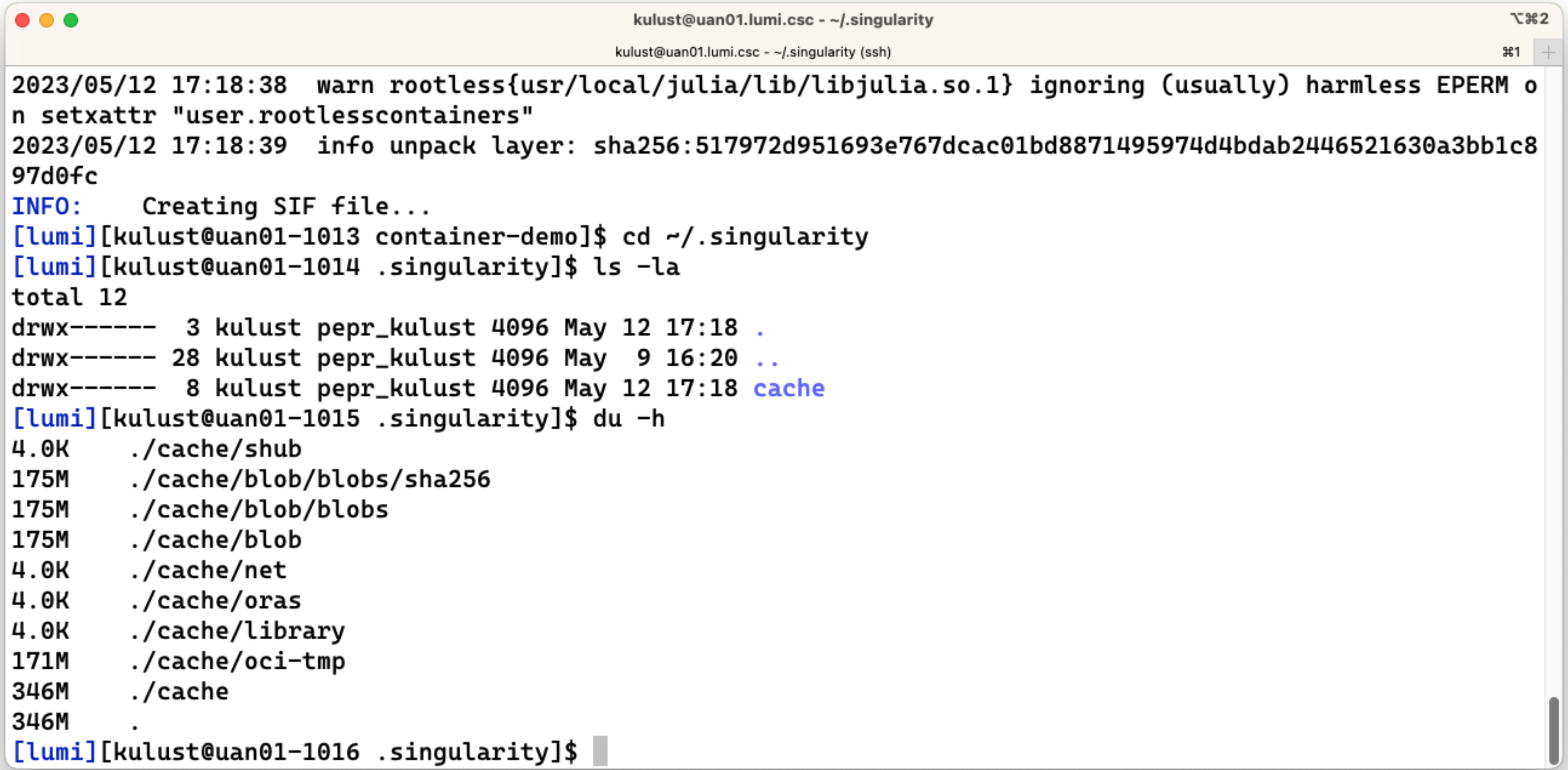


kulust@uan01.lumi.csc - ~/container-demo

kulust@uan01.lumi.csc - ~/container-demo (ssh)

```
PERM on setxattr "user.rootlesscontainers"
2023/05/12 17:18:36  warn rootless{usr/local/julia/lib/julia/libumfpack.so.5} ignoring (usually) harmless
 EPERM on setxattr "user.rootlesscontainers"
2023/05/12 17:18:36  warn rootless{usr/local/julia/lib/julia/libunwind.so} ignoring (usually) harmless EP
ERM on setxattr "user.rootlesscontainers"
2023/05/12 17:18:36  warn rootless{usr/local/julia/lib/julia/libunwind.so.8} ignoring (usually) harmless
EPERM on setxattr "user.rootlesscontainers"
2023/05/12 17:18:36  warn rootless{usr/local/julia/lib/julia/libuv.so} ignoring (usually) harmless EPERM
on setxattr "user.rootlesscontainers"
2023/05/12 17:18:36  warn rootless{usr/local/julia/lib/julia/libuv.so.2} ignoring (usually) harmless EPER
M on setxattr "user.rootlesscontainers"
2023/05/12 17:18:36  warn rootless{usr/local/julia/lib/julia/libz.so} ignoring (usually) harmless EPERM o
n setxattr "user.rootlesscontainers"
2023/05/12 17:18:36  warn rootless{usr/local/julia/lib/julia/libz.so.1} ignoring (usually) harmless EPERM
 on setxattr "user.rootlesscontainers"
2023/05/12 17:18:38  warn rootless{usr/local/julia/lib/libjulia.so} ignoring (usually) harmless EPERM on
setxattr "user.rootlesscontainers"
2023/05/12 17:18:38  warn rootless{usr/local/julia/lib/libjulia.so.1} ignoring (usually) harmless EPERM o
n setxattr "user.rootlesscontainers"
2023/05/12 17:18:39  info unpack layer: sha256:517972d951693e767dcac01bd887149597 4d4bdab244521630a3bb1c8
97d0fc
INFO:    Creating SIF file...
[lumi][kulust@uan01-1013 container-demo]$
```

singularity pull docker://julia


kulust@uan01.lumi.csc - ~/.singularity
⌥⌘2
kulust@uan01.lumi.csc - ~/.singularity (ssh)
⌘1

```
2023/05/12 17:18:38  warn rootless{usr/local/julia/lib/libjulia.so.1} ignoring (usually) harmless EPERM o
n setxattr "user.rootlesscontainers"
2023/05/12 17:18:39  info unpack layer: sha256:517972d951693e767dcac01bd887149597 4d4bdab244652163 0a3bb1c8
97d0fc
INFO:    Creating SIF file...
[lumi][kulust@uan01-1013 container-demo]$ cd ~/.singularity
[lumi][kulust@uan01-1014 .singularity]$ ls -la
total 12
drwx------  3 kulust pepr_kulust 4096 May 12 17:18 .
drwx------ 28 kulust pepr_kulust 4096 May  9 16:20 ..
drwx------  8 kulust pepr_kulust 4096 May 12 17:18 cache
[lumi][kulust@uan01-1015 .singularity]$ du -h
4.0K    ./cache/shub
175M    ./cache/blob/blobs/sha256
175M    ./cache/blob/blobs
175M    ./cache/blob
4.0K    ./cache/net
4.0K    ./cache/oras
4.0K    ./cache/library
171M    ./cache/oci-tmp
346M    ./cache
346M    .
[lumi][kulust@uan01-1016 .singularity]$
```

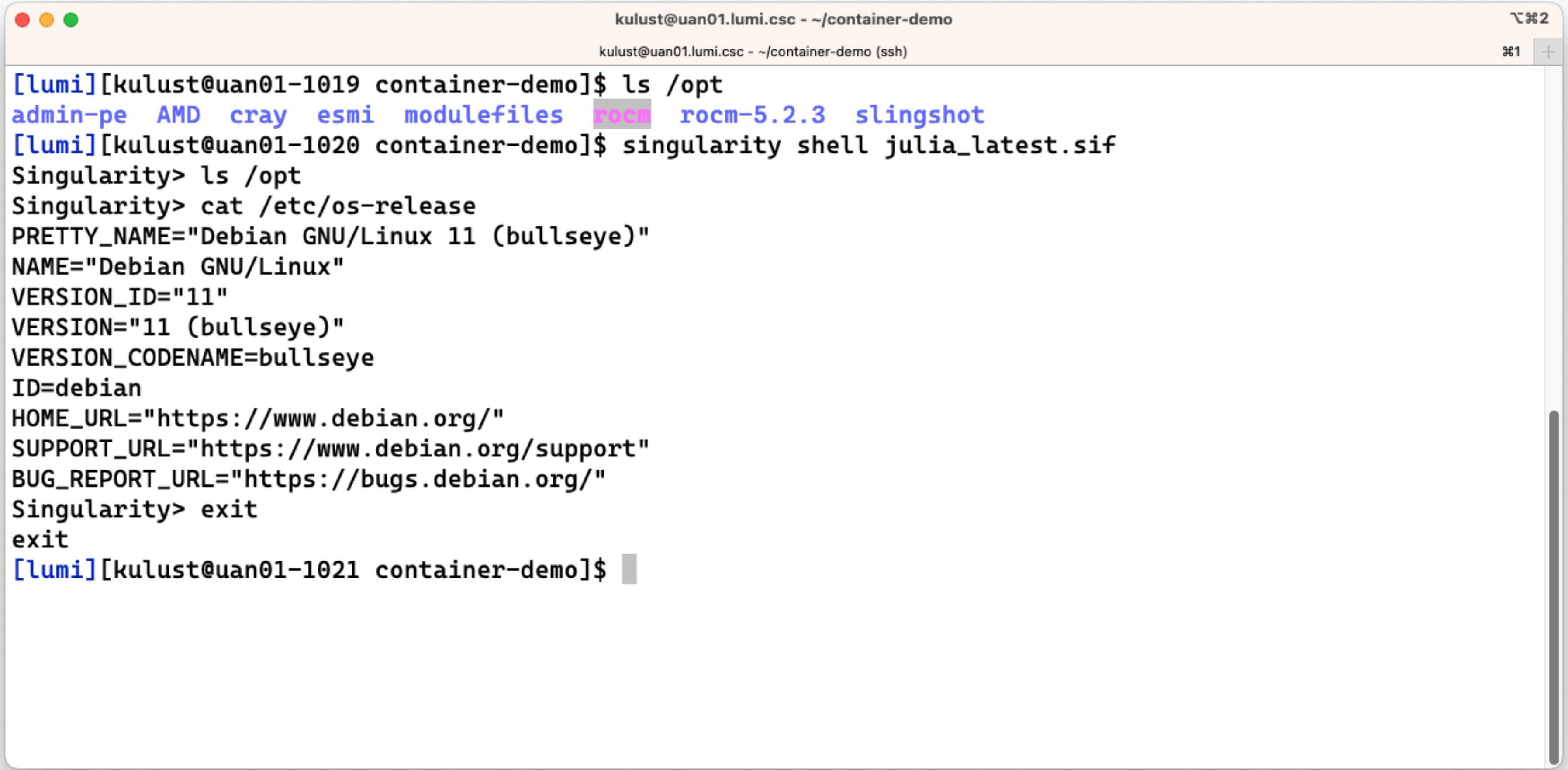
Managing containers (2)

- Building containers
  - Support for building containers is very limited on LUMI: no elevated privileges but also no fakeroot.
  - 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

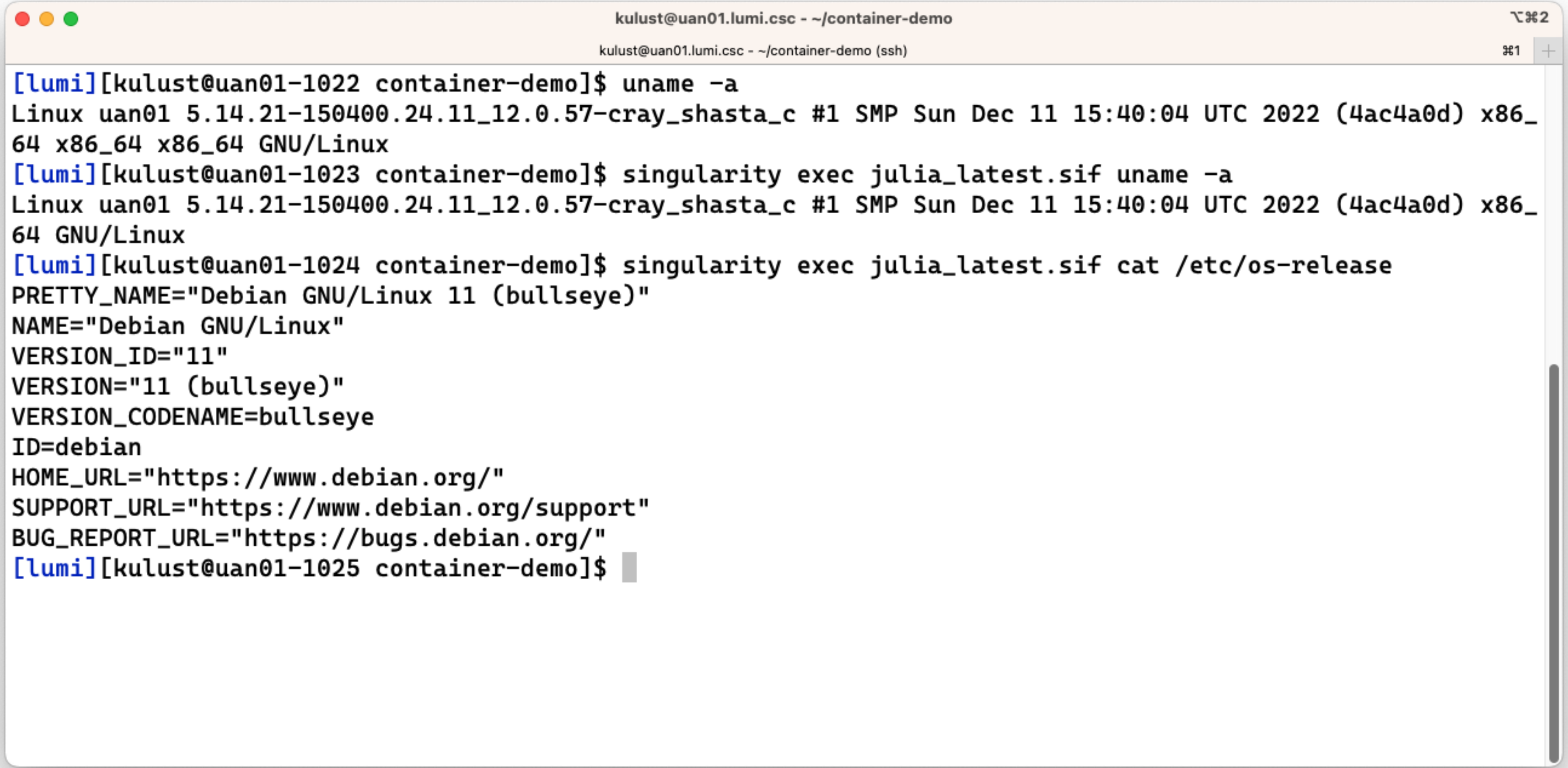


kulust@uan01.lumi.csc - ~/container-demo ⌥⌘2

kulust@uan01.lumi.csc - ~/container-demo (ssh) ⌘1

```
[lumi][kulust@uan01-1019 container-demo]$ ls /opt
admin-pe  AMD  cray  esmi  modulefiles  rocm  rocm-5.2.3  slingshot
[lumi][kulust@uan01-1020 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@uan01-1021 container-demo]$
```

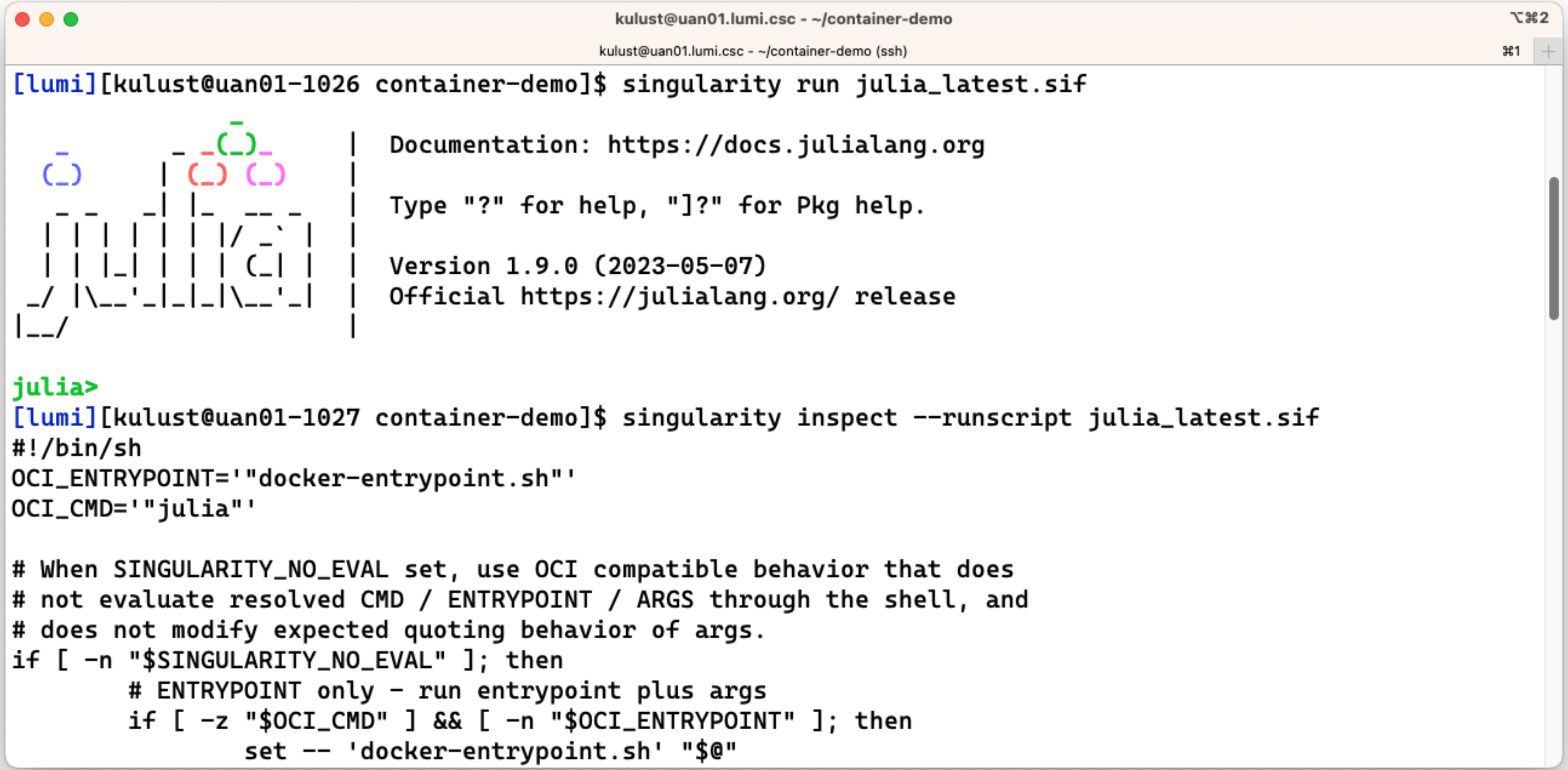
singularity exec julia_latest.sif uname -a


kulust@uan01.lumi.csc - ~/container-demo

kulust@uan01.lumi.csc - ~/container-demo (ssh)

```
[lumi][kulust@uan01-1022 container-demo]$ uname -a
Linux uan01 5.14.21-150400.24.11_12.0.57-cray_shasta_c #1 SMP Sun Dec 11 15:40:04 UTC 2022 (4ac4a0d) x86_
64 x86_64 x86_64 GNU/Linux
[lumi][kulust@uan01-1023 container-demo]$ singularity exec julia_latest.sif uname -a
Linux uan01 5.14.21-150400.24.11_12.0.57-cray_shasta_c #1 SMP Sun Dec 11 15:40:04 UTC 2022 (4ac4a0d) x86_
64 GNU/Linux
[lumi][kulust@uan01-1024 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@uan01-1025 container-demo]$
```

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



```
kulust@uan01.lumi.csc - ~/container-demo
kulust@uan01.lumi.csc - ~/container-demo (ssh)
[lumi][kulust@uan01-1026 container-demo]$ singularity run julia_latest.sif
               _
   _       _ _(_)_     |  Documentation: https://docs.julialang.org
  (_)     | (_) (_)    |
   _ _   _| |_  __ _   |  Type "?" for help, "]?" for Pkg help.
  | | | | | | |/ _` |  |
  | | |_| | | | (_| |  |  Version 1.9.0 (2023-05-07)
 _/ |\__'_|_|_|\__'_|  |  Official https://julialang.org/ release
|__/                   |

julia>
[lumi][kulust@uan01-1027 container-demo]$ singularity inspect --runscript julia_latest.sif
#!/bin/sh
OCI_ENTRYPOINT='"docker-entrypoint.sh"'
OCI_CMD='"julia"'

# When SINGULARITY_NO_EVAL set, use OCI compatible behavior that does
# not evaluate resolved CMD / ENTRYPOINT / ARGS through the shell, and
# does not modify expected quoting behavior of args.
if [ -n "$SINGULARITY_NO_EVAL" ]; then
        # ENTRYPOINT only - run entrypoint plus args
        if [ -z "$OCI_CMD" ] && [ -n "$OCI_ENTRYPOINT" ]; then
                set -- 'docker-entrypoint.sh' "$@"
```

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)

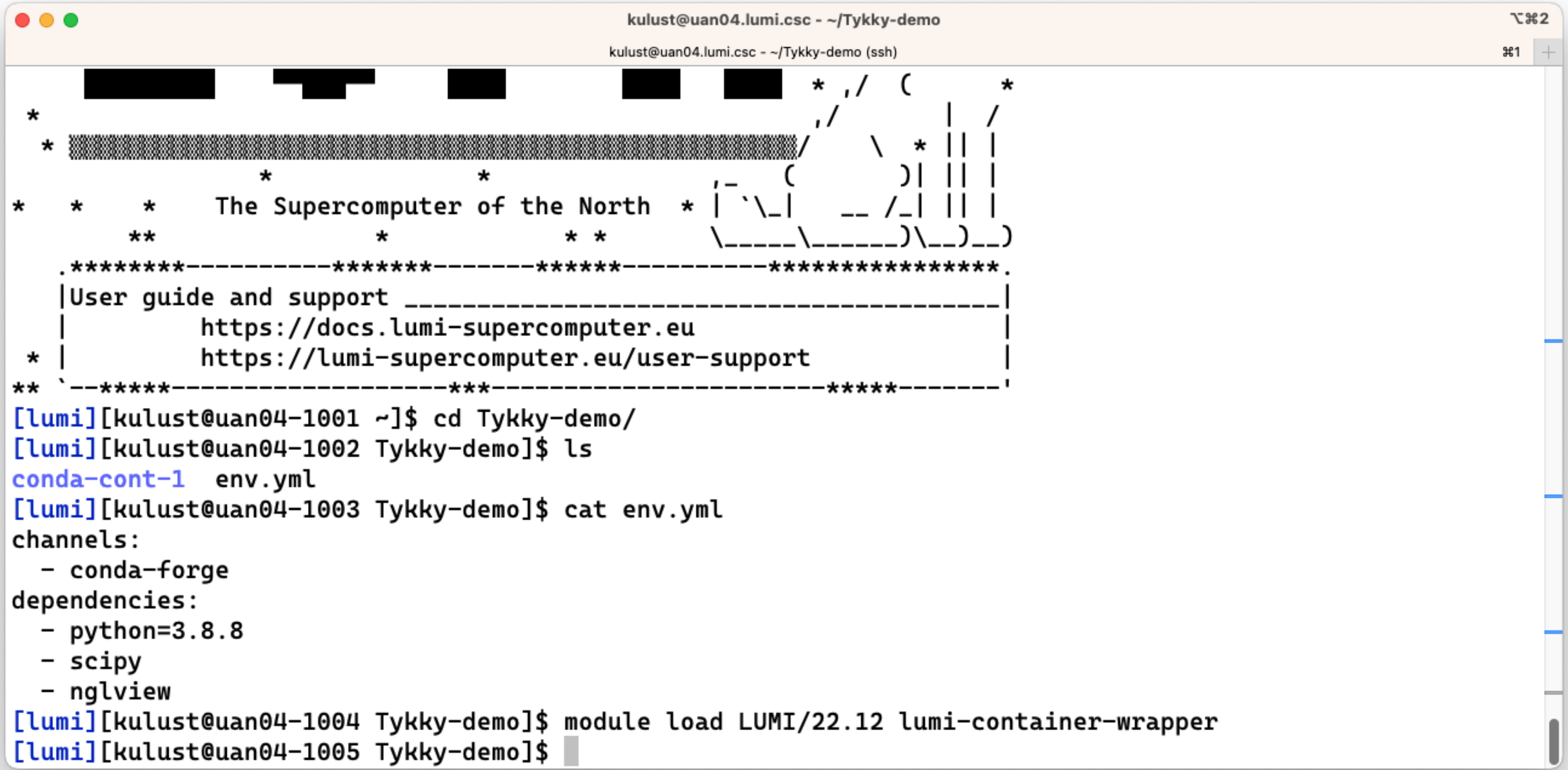
Environment enhancements

- 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)

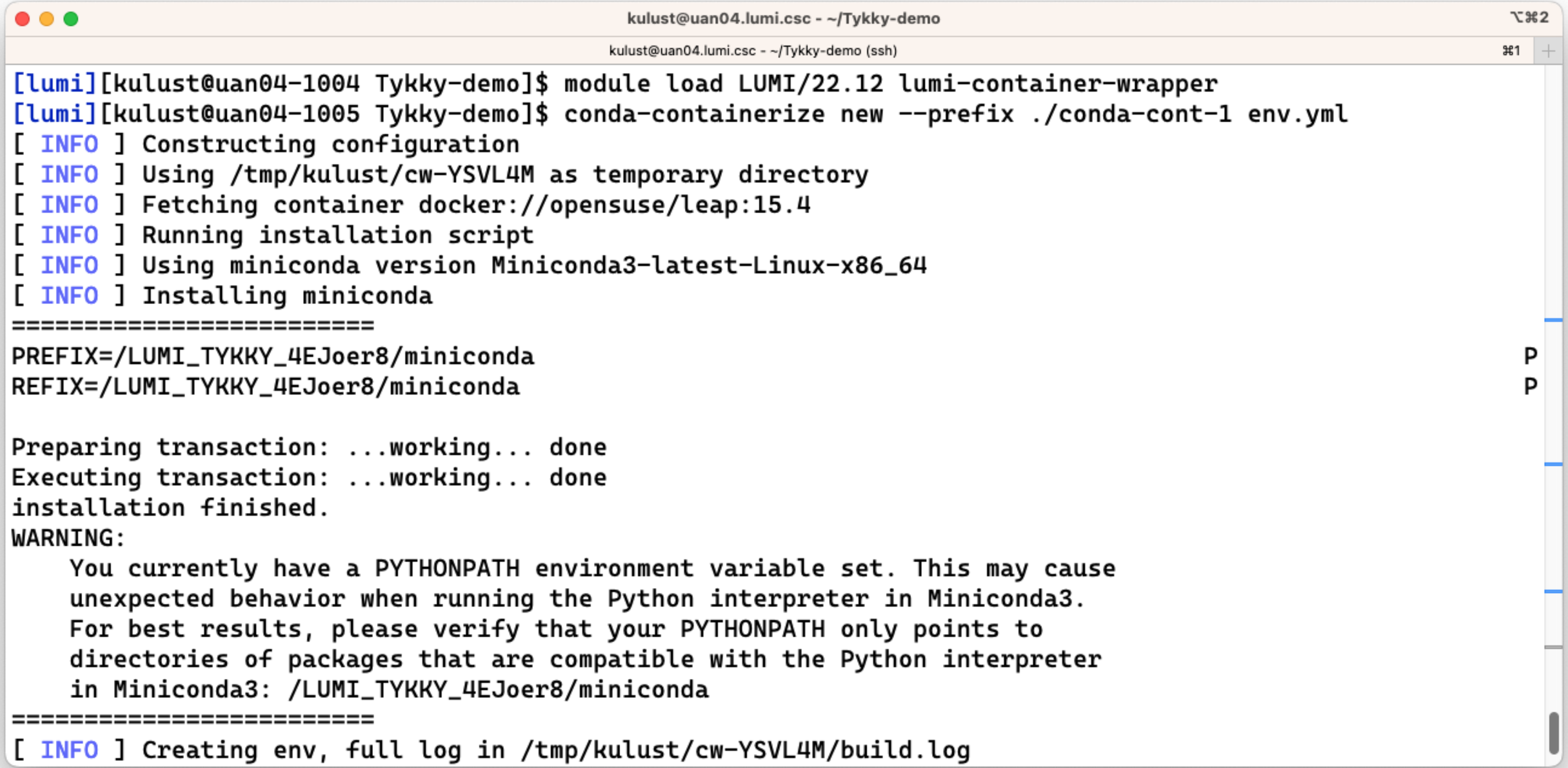


kulust@uan04.lumi.csc - ~/Tykky-demo

kulust@uan04.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@uan04-1001 ~]$ cd Tykky-demo/
[lumi][kulust@uan04-1002 Tykky-demo]$ ls
conda-cont-1  env.yml
[lumi][kulust@uan04-1003 Tykky-demo]$ cat env.yml
channels:
  - conda-forge
dependencies:
  - python=3.8.8
  - scipy
  - nglview
[lumi][kulust@uan04-1004 Tykky-demo]$ module load LUMI/22.12 lumi-container-wrapper
[lumi][kulust@uan04-1005 Tykky-demo]$
```

lumi-container-wrapper (2)

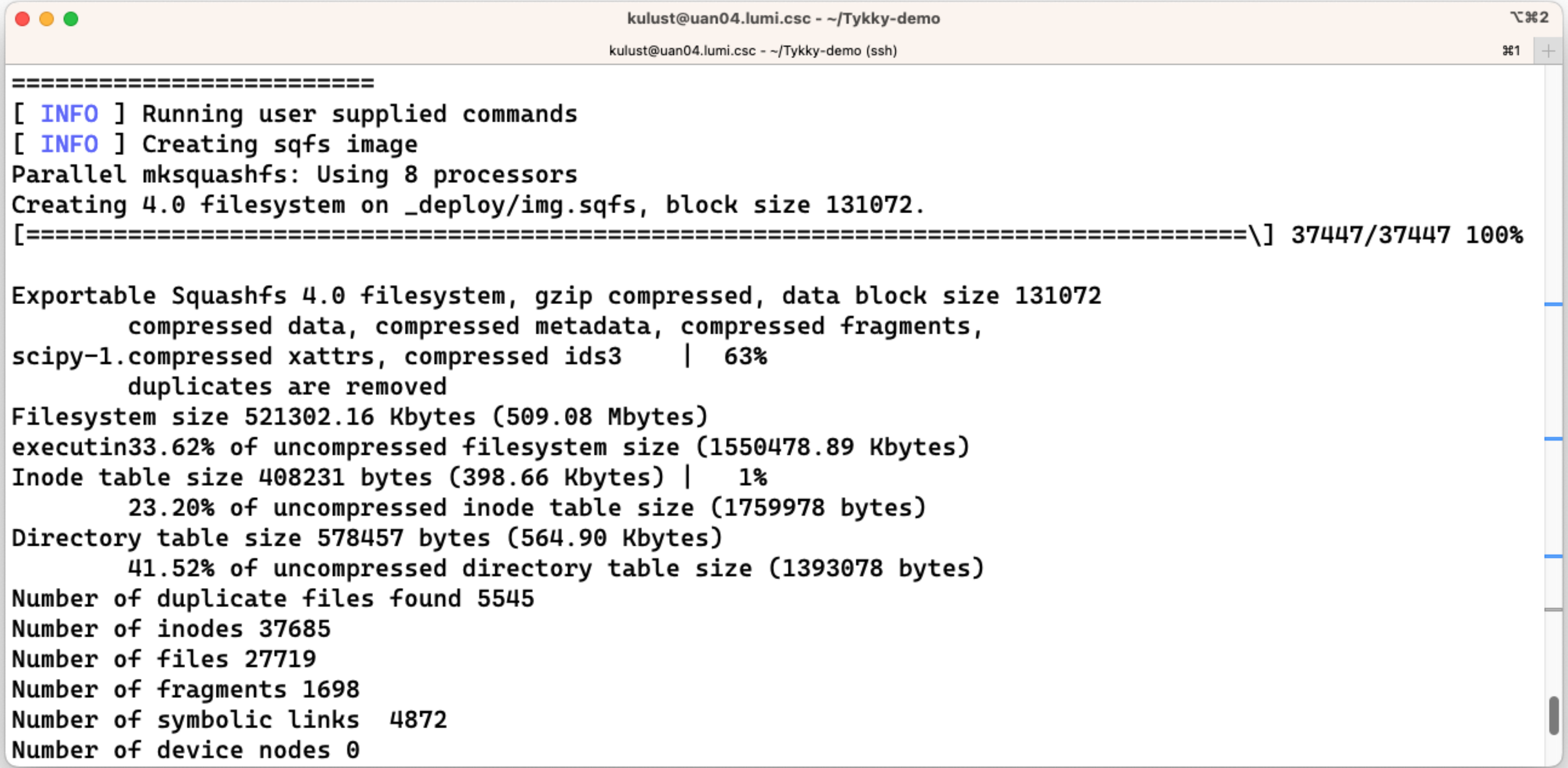

kulust@uan04.lumi.csc - ~/Tykky-demo

kulust@uan04.lumi.csc - ~/Tykky-demo (ssh)

```
[lumi][kulust@uan04-1004 Tykky-demo]$ module load LUMI/22.12 lumi-container-wrapper
[lumi][kulust@uan04-1005 Tykky-demo]$ conda-containerize new --prefix ./conda-cont-1 env.yml
[ INFO ] Constructing configuration
[ INFO ] Using /tmp/kulust/cw-YSVL4M as temporary directory
[ INFO ] Fetching container docker://opensuse/leap:15.4
[ INFO ] Running installation script
[ INFO ] Using miniconda version Miniconda3-latest-Linux-x86_64
[ INFO ] Installing miniconda
=========================
PREFIX=/LUMI_TYKKY_4EJoer8/miniconda                                                                        P
REFIX=/LUMI_TYKKY_4EJoer8/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_TYKKY_4EJoer8/miniconda
=========================
[ INFO ] Creating env, full log in /tmp/kulust/cw-YSVL4M/build.log
```

lumi-container-wrapper (3)

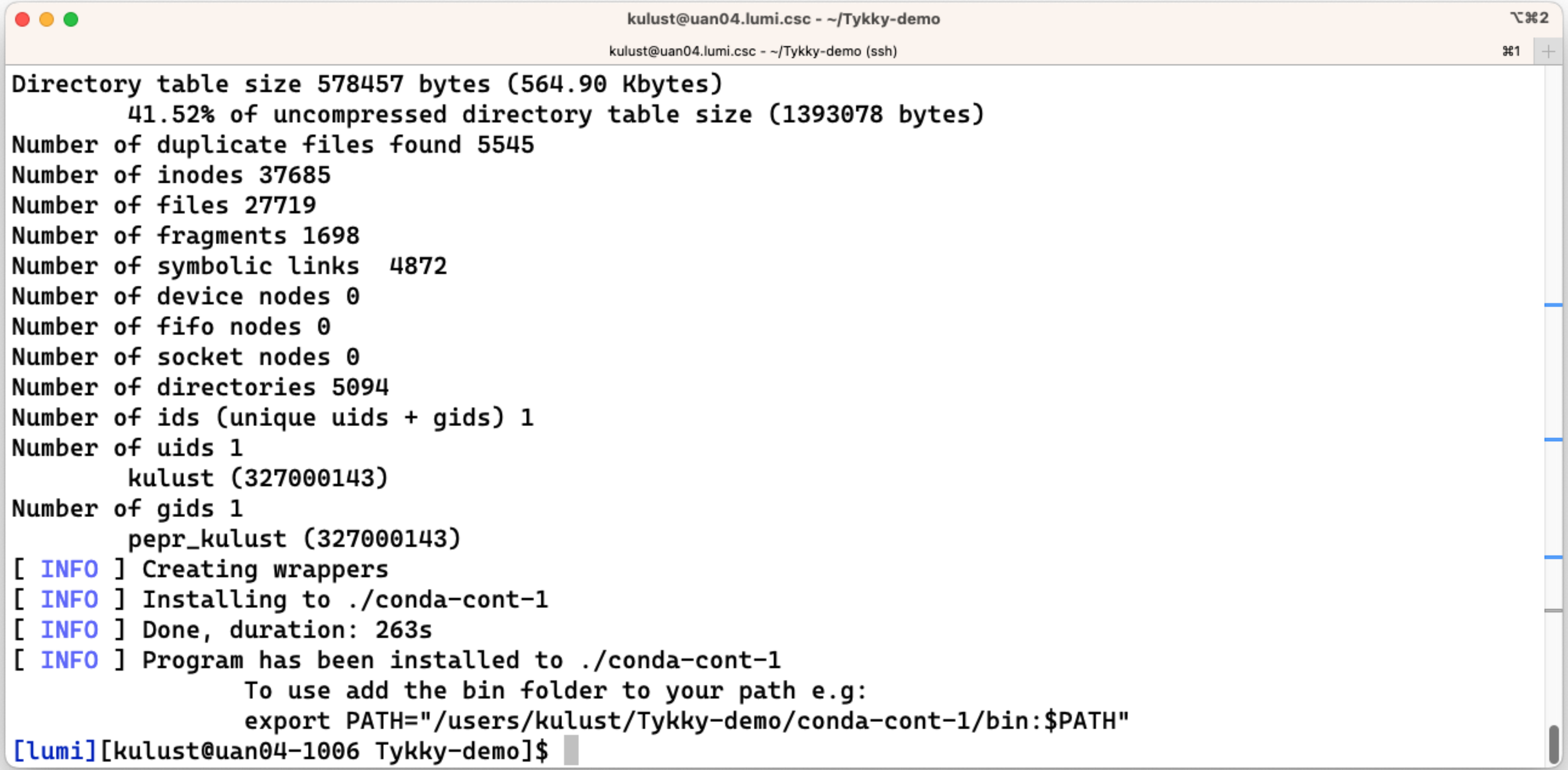
LUMI


kulust@uan04.lumi.csc - ~/Tykky-demo
kulust@uan04.lumi.csc - ~/Tykky-demo (ssh)

```
=========================
[ 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.
[==========================================================================\] 37447/37447 100%

Exportable Squashfs 4.0 filesystem, gzip compressed, data block size 131072
        compressed data, compressed metadata, compressed fragments,
scipy-1.compressed xattrs, compressed ids3    |  63%
        duplicates are removed
Filesystem size 521302.16 Kbytes (509.08 Mbytes)
executin33.62% of uncompressed filesystem size (1550478.89 Kbytes)
Inode table size 408231 bytes (398.66 Kbytes) |   1%
        23.20% of uncompressed inode table size (1759978 bytes)
Directory table size 578457 bytes (564.90 Kbytes)
        41.52% of uncompressed directory table size (1393078 bytes)
Number of duplicate files found 5545
Number of inodes 37685
Number of files 27719
Number of fragments 1698
Number of symbolic links  4872
Number of device nodes 0
```

lumi-container-wrapper (4)

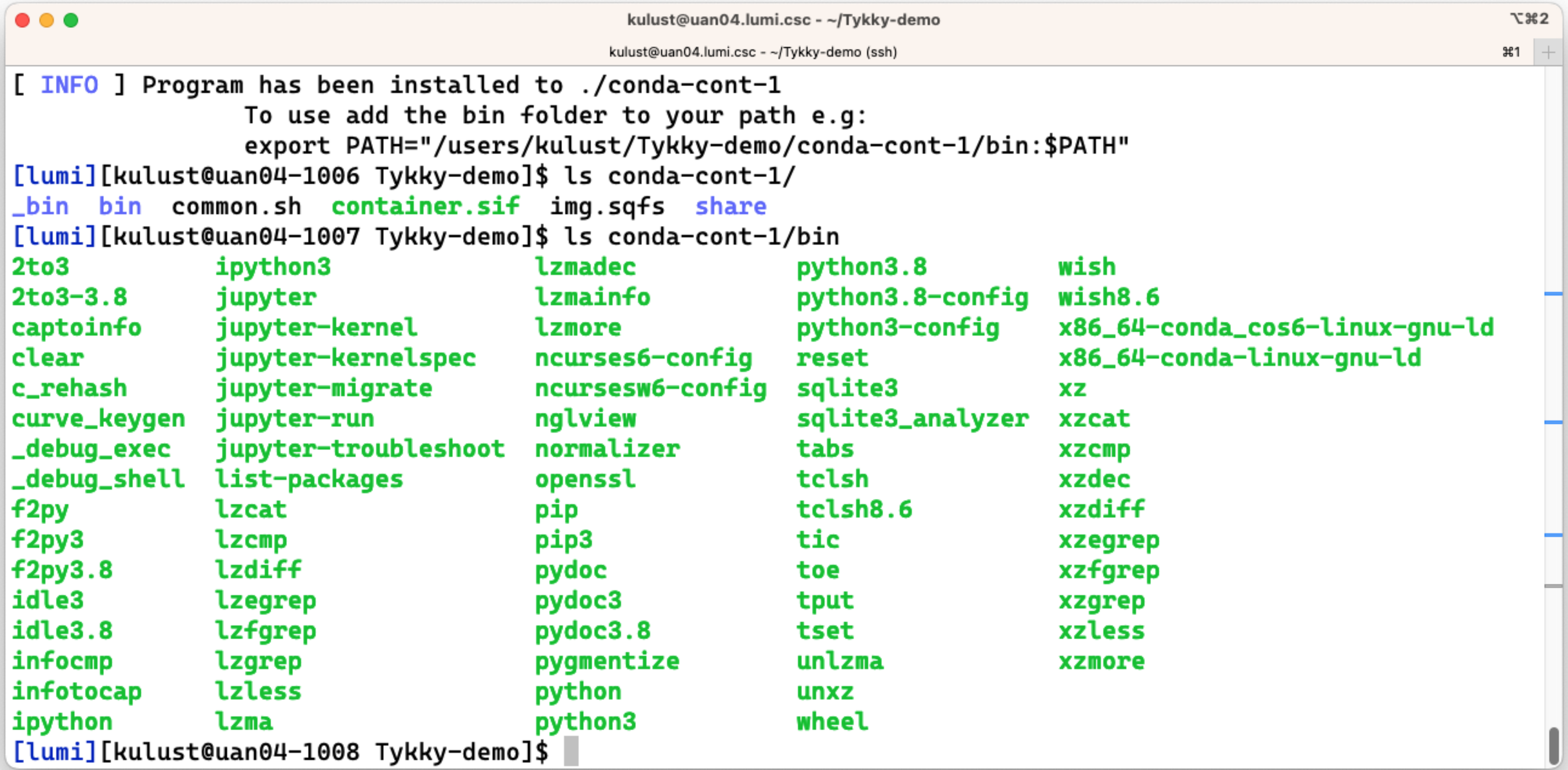
L U M I


kulust@uan04.lumi.csc - ~/Tykky-demo

kulust@uan04.lumi.csc - ~/Tykky-demo (ssh)

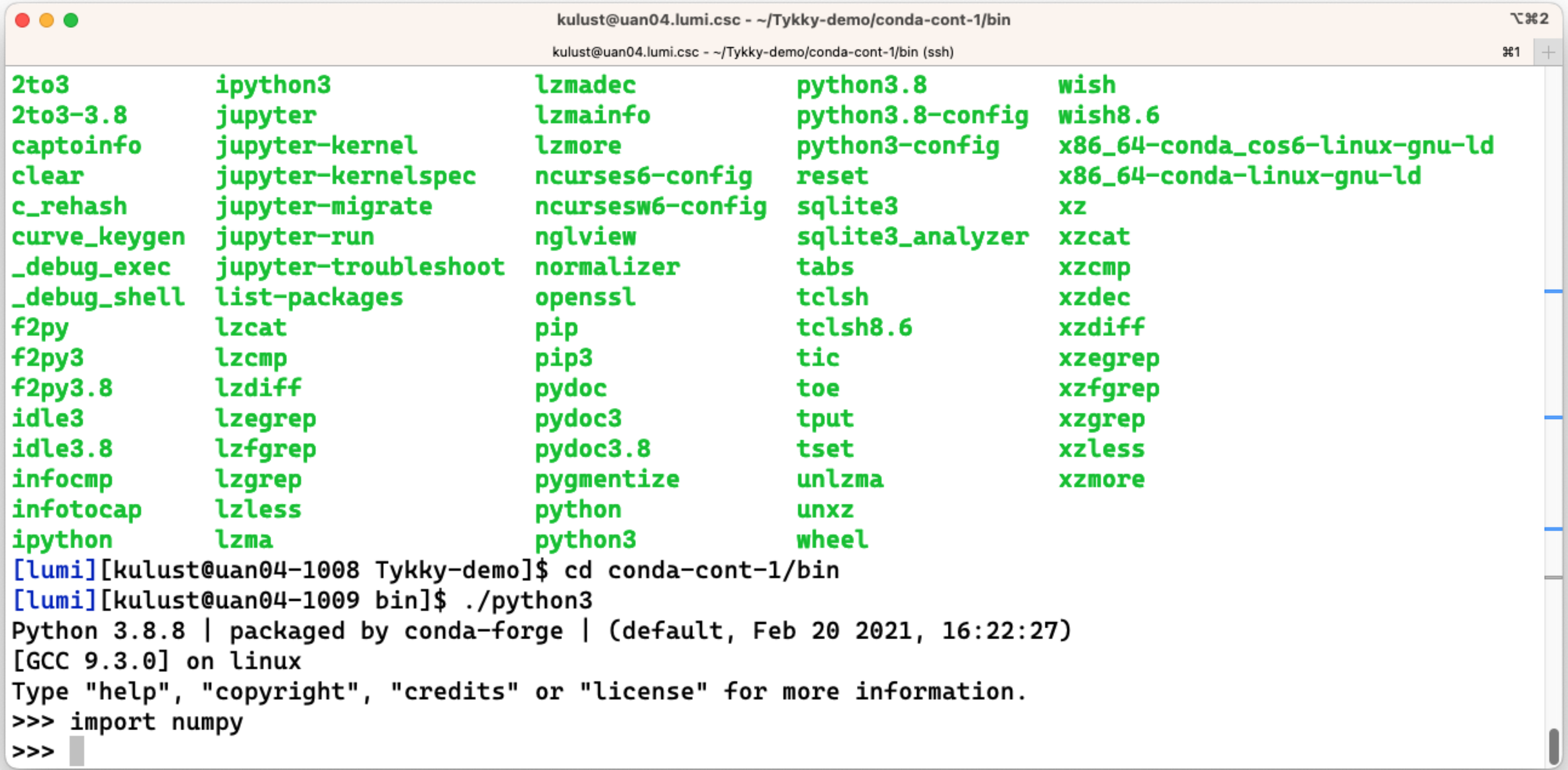
```
Directory table size 578457 bytes (564.90 Kbytes)
        41.52% of uncompressed directory table size (1393078 bytes)
Number of duplicate files found 5545
Number of inodes 37685
Number of files 27719
Number of fragments 1698
Number of symbolic links  4872
Number of device nodes 0
Number of fifo nodes 0
Number of socket nodes 0
Number of directories 5094
Number of ids (unique uids + gids) 1
Number of uids 1
        kulust (327000143)
Number of gids 1
        pepr_kulust (327000143)
[ INFO ] Creating wrappers
[ INFO ] Installing to ./conda-cont-1
[ INFO ] Done, duration: 263s
[ INFO ] Program has been installed to ./conda-cont-1
                To use add the bin folder to your path e.g:
                export PATH="/users/kulust/Tykky-demo/conda-cont-1/bin:$PATH"
[lumi][kulust@uan04-1006 Tykky-demo]$
```

lumi-container-wrapper (5)


kulust@uan04.lumi.csc - ~/Tykky-demo
kulust@uan04.lumi.csc - ~/Tykky-demo (ssh)

```
[ INFO ] Program has been installed to ./conda-cont-1
              To use add the bin folder to your path e.g:
              export PATH="/users/kulust/Tykky-demo/conda-cont-1/bin:$PATH"
[lumi][kulust@uan04-1006 Tykky-demo]$ ls conda-cont-1/
_bin  bin  common.sh  container.sif  img.sqfs  share
[lumi][kulust@uan04-1007 Tykky-demo]$ ls conda-cont-1/bin
2to3          ipython3             lzmadec           python3.8          wish
2to3-3.8      jupyter              lzmainfo          python3.8-config   wish8.6
captoinfo     jupyter-kernel       lzmore            python3-config     x86_64-conda_cos6-linux-gnu-ld
clear         jupyter-kernelspec   ncurses6-config   reset              x86_64-conda-linux-gnu-ld
c_rehash      jupyter-migrate      ncursesw6-config  sqlite3            xz
curve_keygen  jupyter-run          nglview           sqlite3_analyzer   xzcat
_debug_exec   jupyter-troubleshoot normalizer        tabs               xzcmp
_debug_shell  list-packages        openssl           tclsh              xzdec
f2py          lzcat                pip               tclsh8.6           xzdiff
f2py3         lzcmp                pip3              tic                xzegrep
f2py3.8       lzdiff               pydoc             toe                xzfgrep
idle3         lzegrep              pydoc3            tput               xzgrep
idle3.8       lzfgrep              pydoc3.8          tset               xzless
infocmp       lzgrep               pygmentize        unlzma             xzmore
infotocap     lzless               python            unxz
ipython       lzma                 python3           wheel
[lumi][kulust@uan04-1008 Tykky-demo]$
```

lumi-container-wrapper (6)


kulust@uan04.lumi.csc - ~/Tykky-demo/conda-cont-1/bin
kulust@uan04.lumi.csc - ~/Tykky-demo/conda-cont-1/bin (ssh)

```
2to3           ipython3             lzmadec            python3.8          wish
2to3-3.8       jupyter              lzmainfo           python3.8-config   wish8.6
captoinfo      jupyter-kernel       lzmore             python3-config     x86_64-conda_cos6-linux-gnu-ld
clear          jupyter-kernelspec   ncurses6-config    reset              x86_64-conda-linux-gnu-ld
c_rehash       jupyter-migrate      ncursesw6-config   sqlite3            xz
curve_keygen   jupyter-run          nglview            sqlite3_analyzer   xzcat
_debug_exec    jupyter-troubleshoot normalizer         tabs               xzcmp
_debug_shell   list-packages        openssl            tclsh              xzdec
f2py           lzcat                pip                tclsh8.6           xzdiff
f2py3          lzcmp                pip3               tic                xzegrep
f2py3.8        lzdiff               pydoc              toe                xzfgrep
idle3          lzegrep              pydoc3             tput               xzgrep
idle3.8        lzfgrep              pydoc3.8           tset               xzless
infocmp        lzgrep               pygmentize         unlzma             xzmore
infotocap      lzless               python             unxz
ipython        lzma                 python3            wheel
[lumi][kulust@uan04-1008 Tykky-demo]$ cd conda-cont-1/bin
[lumi][kulust@uan04-1009 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.
- Only very limited support to build containers on LUMI due to security concerns.