

The background of the slide is a photograph of a large, modern building with a complex facade of glass and metal panels, likely the LRZ building. The image is overlaid with a semi-transparent blue filter. A dark blue horizontal bar is positioned across the middle of the image, containing the title and date text.

Introduction to Multiuser Cluster Systems at LRZ

October, 10th 2023

- **Aim:** provide an introduction to multiuser cluster systems in general and to those operated at the Leibniz Supercomputing Centre (LRZ), specifically
- You will probably benefit the most if you're not yet familiar with the LRZ HPC/HPDA/HPAI infrastructure, but plan to work with these systems in the future
- A majority of systems will be covered in more detail in dedicated sessions later this week

By the end of today's workshop, you should have a general understanding of multiuser HPC/HPDA/HPAI cluster systems and the basic skills to successfully interact remotely with such systems at LRZ

User perspective

User Perspective: System Access



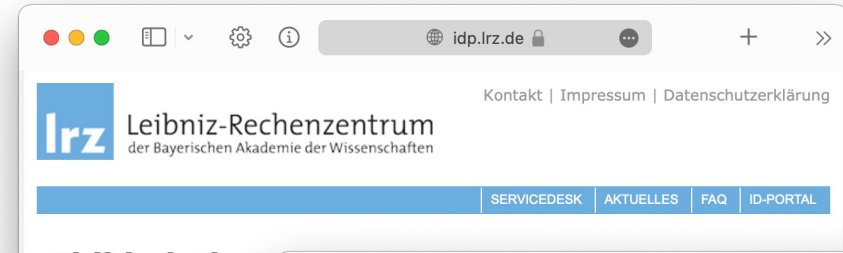
```
ssh lxlogin1.lrz.de ~
~ $ ssh lxlogin1.lrz.de
(di67pif@lxlogin1.lrz.de) Password:
(di67pif@lxlogin1.lrz.de) !!! 2FA !!! 2FA !!! 2FA !!! 2FA !!! 2FA !!! 2FA !!! 2FA !!! 2FA !!! 2FA !!!
All LRZ cluster login nodes require now a second factor for authentication!
Please refer to https://doku.lrz.de/x/EgDxBw
Note for using push tokens:
Without PIN directly press enter upon the 2FA prompt to receive the push token
Token_Response:
Last Login: Mon Oct 9 18:27:41 2023 from i59f7e60d.versanet.de

Welcome to the CoolMUC-2 Infiniband Cluster, one of the linux cluster systems
operated by Leibniz Supercomputing Centre (LRZ).

Please submit SLURM batch scripts with a VALID email address for production
jobs. Short-running programs and testing are most suited for being carried
out within SLURM interactive shells.
DO NOT run any extensive computational programs on login nodes!
Misuse of the interactive resources will lead to violating accounts being
blocked from access to the cluster.

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Documentation:
https://doku.lrz.de/display/PUBLIC/Linux+Cluster
Messages/System Status:
https://doku.lrz.de/display/PUBLIC/High+Performance+Computing
Slurm Usage Instructions:
https://doku.lrz.de/display/PUBLIC/Available+SLURM+clusters+and+features

intel-mpi: using intel wrappers for mpicc, mpif77, etc
di67pif@cm2login1:~>
```



Log in

Domain: ADS

User Name:

Password:

Shibboleth W

Token-based Login

Token code (di67pif):

Perform login for this service only

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User Perspective: Environment & Workspace



- These are systems shared by many users, i.e. other people will be working on the same (login) node at the same time.
- Be aware of your surroundings and considerate of your fellow colleagues!

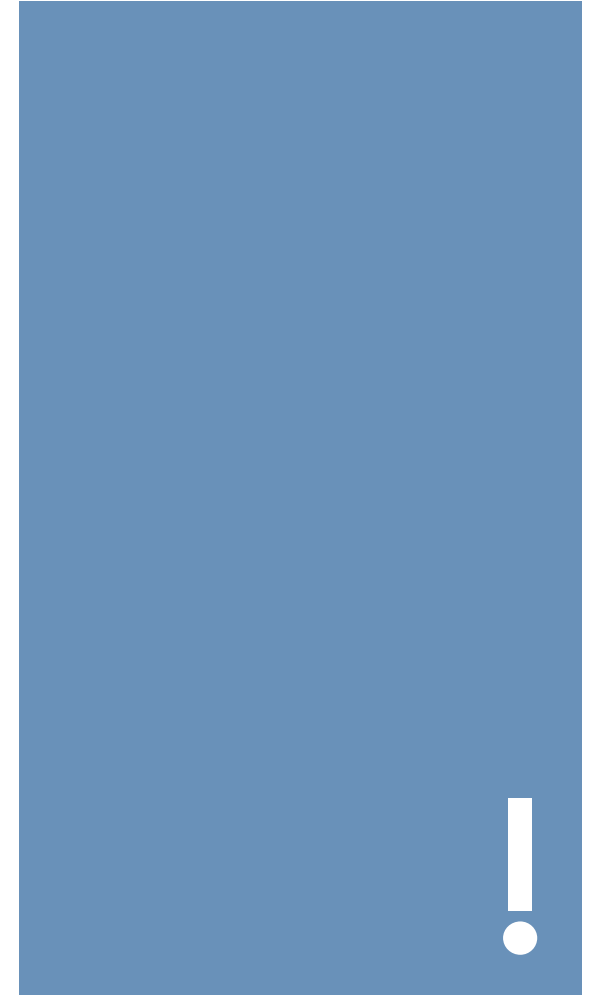
```
ssh lxlogin1.lrz.de ~
ssh -fish
09.10., 6:50 PM
di67pif@cm2login1:/dss/dsshhome1/lxc00> w
18:50:22 up 27 days, 8:55, 46 users, load average: 4.51, 5.31, 5.81
USER      TTY      FROM          LOGIN@      IDLE   JCPU   PCPU   WHAT
ra35fud   pts/6    th-ws-7010m59.th Thu15  10:38m  2:00m  23:23 /dss/ds
ra35fud   pts/13   th-ws-7010m59.th Thu15  10:40m  1:45m  21:15 /dss/ds
di57ril   pts/14   dynamic-002-215- Sun10  51:02   5.90s  5.90s  -bash
ra78wan2  pts/19   244-152-163-10.l Sat23  43:46m  0.27s  0.27s  -bash
ra35fud   pts/28   th-ws-7010m59.th 020ct23  4days  1:41m  0.36s  /dss/ds
ga26kes2  pts/33   10.152.188.171 26Sep23  3days  60.96s  2.35s  -tcsh
t388110   pts/36   f166.tum.vpn.lrz 18:22   59.00s  0.11s  0.11s  -bash
ge72xes2  pts/38   10.162.92.110   Fri17   2:45m  1.38s  0.26s  bash
t388110   pts/41   f166.tum.vpn.lrz 18:22   14:24   0.32s  0.32s  -bash
ge49hid2  pts/42   onat.frm2.tum.de 18Sep23 20days 0.14s  0.14s  -bash
ra68mop   pts/44   10.163.213.247  Sun11   4:02m  1.04s  1.04s  -bash
ga38qon3  pts/47   129.187.45.149  Fri12   2:48m  42:20  42:03 /dss/ds
ge52wid2  pts/58   ip139188.forst.w 26Sep23 25:24m  2.15s  2.15s  -bash
ga92ziv3  pts/17   hirusako.aer.ed. Wed14   1:30m  0.31s  0.31s  -bash
di68miy   pts/8    pd9fe2ea2.dip0.t 28Sep23 4:49m  0.85s  0.85s  -bash
ga84qec2  pts/10   10.162.204.183  22Sep23 6:23m  1.24s  1.24s  -bash
ga26kes2  pts/54   10.152.188.171  020ct23 7days  0.66s  0.66s  -tcsh
di98mug2  pts/66   p4fca8d79.dip0.t 18:24   19:34   0.16s  0.16s  -bash
di67kah   pts/68   10.153.163.46   09:07   9:20m  0.14s  0.14s  -bash
di67pif   pts/73   i59f7e60d.versan 18:35   3.00s  0.13s  0.02s  w
ga38qon3  pts/74   129.187.45.149  Fri13   2:44m  44:27  44:26 /dss/ds
di93xej   pts/75   10.156.37.219   13:48   5:01m  4.56s  4.43s  /usr/bi
ga26kes2  pts/80   10.152.188.171  26Sep23 3days  8.30s  1.94s  -tcsh
ga38qon3  pts/82   129.187.45.149  Fri13   2:47m  39:39  39:39 /dss/ds
ra57dut   pts/84   lmb1dp1-wxrob08. 25Sep23 9:17m  0.18s  0.18s  -bash
ra98fif   pts/77   10.153.191.141  16:38   3:50   0.30s  0.30s  -bash
di67kah   pts/88   10.153.163.46   09:07   4:33m  0.79s  0.79s  -bash
ka641ot   pts/89   gw-acgd1.net.fh- 22Sep23 12days 0.51s  0.51s  -bash
di39dux   pts/90   10.153.163.218  09:09   6:01m  2.80s  2.80s  -bash
di67kah   pts/92   10.153.163.46   09:19   7:08m  0.58s  0.58s  -bash
```

```
ssh lxlogin1.lrz.de ~
ssh -fish
09.10., 6:50 PM
di67pif@cm2login1:/dss/dsshhome1/lxc00> ls
a2832ba di39yol di82zos ga84coc2 gu92dot2 ra43cob ru47qah
atlas001 di46jof di82tun ga84coc3 gu92vih2 ra46jim ru48fak2
atlas051 di46puy di98tap ga84wug2 gu95lun2 ra52fef2 ru54vax2
atlas055 di46sap dteam007 ga86ket2 h039uaa ra52hen ru57maj
atlas066 di46taf ga26buq2 ga92wes2 h039uac ra52mer ru58guj2
atlas096 di49jat ga27rug2 ga92wof2 h039y36 ra52wos ru62guf
atlas034 di49mir ga34hed2 ga92yuh2 h039y45 ra56dut ru64nib
atlas104 di49qap ga34kat2 ga95nik2 ka85bup ra56yol ru64waf2
atlas107 di49suf ga34nox2 ga95xaf2 ka97kuk ra57biv ru67ban
atlas115 di49tom ga35hiw2 ga98dig2 lmu29425 ra57laj2 ru67yuf
atlas130 di52doh ga35piw2 ge23jiq2 lu26mur2 ra57lon ru68qum
atlas135 di52doz2 ga38coq2 ge24por2 lu28fam ra75kuw ru73jac
atlas137 di52mit ga38lix2 ge25don2 lu28tej ra75pan ru74jac
atlas139 di52qaw ga39dig2 ge29xac2 lu43fup2 ra78wuh ru74mou
atlas175 di67hal ga42jol2 ge29yig2 lu57gup9 ra96bui ru76qiq
atlas192 di67pif ga46luh2 ge34ket3 lu65cug ra98cit ru76tap
atlasprd di68tek ga48zoj2 ge35pom2 lu79hip3 ri32bet ru78zob
biokurs102 di68vad ga49cen2 ge37tiq2 lu79hun2 ri32bor ru83pey2
biokurs110 di69heg ga53vuj2 ge38aqx2 lu96mah6 ri35xob ru84xox
biokurs125 di69pun ga54ger2 ge39dum2 nmmda009 ri42bof2 ru85kil2
biokurs157 di72mer ga58qes2 ge45cix2 nmmda012 ri47pih ru86wed
biokurs197 di72run ga58roj3 ge45set2 nmqc011 ri58huc ru87cir4
biokurs220 di72zuy2 ga58sur2 ge46tov2 ne53qez2 ri58mey ru94puk
biokurs257 di73gov ga58yec2 ge47wus2 ne65nib2 ri65cal ru95mof
biokurs283 di73wor3 ga58zer2 ge69sid2 ne85lif2 ri83xep t388110
di25mlp2 di73wux ga59mer2 ge73woy2 ngscourse03 ri85voq t5112ae
di25seqa di73yux ga62kuy2 ge86gis2 ngscourse12 ri96kit t5431ad
di25wuw di75gem ga62sed2 ge89sih2 ngscourse14 ru23qir2 t7846ac
di29wad di75nef ga62tan2 ge98bej2 ngscourse15 ru27qod uh101ai
di29waj di75dan ga63yep2 ge98hun2 ngscourse26 ru32kel2 uh341ae
di34god di76dax ga67dij2 ge98sig2 ra35pim ru32yiv uh351bp
di34jag di76ral ga68jov6 genomics06 ra36jip ru36mij uj311ci
```

```
ssh lxlogin1.lrz.de ~
ssh -fish
8%
9.4 GB
root 27591 0.0 0.0 0 0 ? S Sep28 0:00 [kworker/10:0]
di93qiz 27648 0.0 0.0 22688 2436 ? Ss Oct06 0:00 tmux
root 52566 0.0 0.0 0 0 ? S Oct07 0:03 [kworker/23:0]
di93sig 52918 0.0 0.0 23116 672 ? Ss Sep12 0:00 tmux
di93sig 52919 0.0 0.0 30908 8 pts/39 Ss+ Sep12 0:00 -bash
root 53091 0.0 0.0 127464 8332 ? Ss 18:35 0:00 sshd: di67pif [priv]
di67pif 53105 0.0 0.0 127464 5124 ? R 18:35 0:00 sshd: di67pif@pts/73
di67pif 53107 0.0 0.0 31844 10812 pts/73 Ss 18:35 0:00 -bash
root 53656 0.0 0.0 0 0 ? S 18:37 0:00 [kworker/29:0]
di93xej 53747 0.0 0.0 68700 3592 ? S 11:24 0:00 dbus-daemon --nofork --print-address 4 --session
root 53995 0.0 0.0 0 0 ? S Sep14 0:00 [kworker/19:2]
ga26kes2 53997 0.0 0.0 59296 0 pts/80 S Sep27 0:00 dbus-launch --autolaunch 473632f0f9e04159814ae522ae309b5
ga26kes2 53998 0.0 0.0 68712 80 ? Ss Sep27 0:00 /usr/bin/dbus-daemon --syslog-only --fork --print-pid 6
di93qiz 54001 0.0 0.0 8340 4 pts/70 T Sep27 0:00 less run_norm.slurm
root 54254 0.0 0.0 0 0 ? S 11:26 0:00 [mmkproc]
di39tel 54554 0.0 0.0 31952 8 ? Ss Sep20 0:00 SCREEN -S Tim
di39tel 54555 0.0 0.0 32100 8 pts/46 Ss+ Sep20 0:00 /bin/bash
ga26kes2 54650 0.0 0.0 298400 13048 pts/99 S+ Oct06 0:00 emacs -nw PPP.PCF
root 54765 0.0 0.0 127472 0 ? Ss Sep26 0:00 sshd: ge52wid2 [priv]
root 54944 0.0 0.0 127472 3508 ? Ss Oct06 0:00 sshd: ga38qon3 [priv]
ga38qon3 54951 0.0 0.0 129296 3508 ? S Oct06 0:00 sshd: ga38qon3@notty
ga38qon3 54952 0.0 0.0 35220 2020 ? S Oct06 0:00 /usr/lib/ssh/sftp-server
ge52wid2 54955 0.0 0.0 128784 1912 ? S Sep26 0:20 sshd: ge52wid2@pts/58
ge52wid2 54956 0.0 0.0 34212 2760 pts/58 Ss+ Sep26 0:02 -bash
di93sig 55169 0.0 0.0 15912 0 ? Ss Sep12 0:00 ssh-agent
di93xej 55253 0.0 0.0 68700 0 ? S Oct04 0:00 dbus-daemon --nofork --print-address 4 --session
di93qiz 55305 0.0 0.0 8340 4 pts/70 T Sep27 0:00 less run_norm.slurm
di93qiz 55512 0.0 0.0 102064 0 pts/69 TL Sep27 0:00 salloc --clusters=serial --partition=serial_std --mem=55
root 55602 0.0 0.0 0 0 ? S Sep21 0:20 [kworker/54:2]
root 56155 0.0 0.0 0 0 ? S Oct02 0:43 [mmkproc]
root 56536 0.0 0.0 0 0 ? S Sep29 0:14 [kworker/20:1]
root 56585 0.0 0.0 0 0 ? S Sep28 3:07 [mmkproc]
di93xej 57065 0.0 0.0 68700 3536 ? S 15:05 0:00 dbus-daemon --nofork --print-address 4 --session
```

User Perspective: Environment & Workspace

- You don't have administrative rights on these systems, i.e. no root access.
- This may be in contrast to your local machine and certain usage patterns and/or expectations may therefore not apply, e.g.,
 - you will not be able to use the `sudo` command
 - you're prohibited from making system-wide modifications
 - disk access is restricted to your home directory (and possibly other storage areas accessible to your account, e.g., your DSS containers)
- That said, your home (directory) is your castle – there, anything goes!

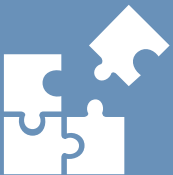


- If available on the system, modules allow for the dynamic modification of environment variables, e.g., they provide a flexible way to access various applications and libraries available on the system
- List the currently active modules (loaded by default):
`$ module list`
- Search for available modules:
`$ module available <module>` or
`$ module av <module>`
- Get more information about a specific module:
`$ module show <module>`
- Use `$ module load <module>` to apply the changes of a module to the environment

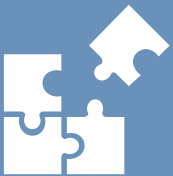
- **Conda** (<https://conda.io>) is “a package, dependency and environment management for any language – Python, R, Ruby, Lua, Scala, Java, JavaScript, C/ C++, FORTRAN, and more”.
- **pip** (<https://pip.pypa.io>) is “the package installer for Python. You can use it to install packages from the Python Package Index and other indexes”.

Make sure to install packages to the home directory instead of the system-wide default location:

```
$ pip install --user <package>
```



- `wget` a binary from the internet
 - `wget http://free-software.ru/download/get-rich.bin`
- **Compile** yourself
 - `git clone https://github.com/ggerganov/whisper.cpp`
 - `cd whisper.cpp`
 - `make`



User Perspective: OS-level Virtualization, Containers

- Isolated **user space** instances, called containers, allow programs running inside to only see the container's contents and devices assigned to the container.
- Thus, the environment inside a container can essentially be modified freely, typically **providing (encapsulated) root privileges**
- The most prominent container runtime, Docker, is typically not available on multiuser systems, but you will encounter alternatives
 - Charliecloud (<https://hpc.github.io/charliecloud/>)
 - Enroot (<https://github.com/NVIDIA/enroot>)
- Containers imposes no noticeable overhead, i.e. there should be no performance impact and parallelization, GPU access, etc. should – if set up correctly – work as expected
- Containers are UDSS: User Defined Software Stacks: you're basically independent from the environment created by system administrators, but you will only receive limited support for the environment created instead (inside the container).

