



UCL Université catholique de Louvain

INSTITUT DE CALCUL INTENSIF ET DE STOCKAGE DE MASSE

CÉCI/CISM HPC training sessions



Consortium des Equipements de Calcul Intensif en Fédération Wallonie-Bruxelles

<http://www.cec-hpc.be> &
<http://www.cism.ucl.ac.be> (meanly the FAQ)

log on lemaitre4:

```
[localuser@localmachine]$  
ssh -X -i ~/.ssh/id_rsa.cec  
ceciloginname@lemaitre4.cism.ucl.ac.be  
Enter passphrase for key 'id_rsa.cec':
```

Welcome to

```
 /  ( - / / ) ( / / / / ( - / /
```

Massively parallel CISM-CECI cluster

40 nodes: 2 x AMD EPYC 9534 64-Core processors (128 HT) 768GB RAM
non-blocking 100Gbps Infiniband network
318T BeeGFS global scratch

contact, support: egs-cism@listes.uclouvain.be

~~~~~  
1948/10240 CPUs available (load 80%) - 131 jobs running, 9 pending.

\* Job info for user bvr: 0 job running, 0 pending.

\* Diskquotas for user bvr

| Filesystem | used | limit | files | limit |
|------------|------|-------|-------|-------|
|------------|------|-------|-------|-------|

```
$HOME          16.5G      100G      131
$GLOBALSCRATCH 0.0kB unlimited 0 unlimited
$CECIHOME       365.4MB    100.0GB   690    100000
$CECITRSF       0.0kB     1.0TB     1 unlimited
* Account expiration: 2033-05-12
```

Don't know where to start?

--> [http://www.cec-hpc.be/install\\_software.html](http://www.cec-hpc.be/install_software.html)

--> [http://www.cec-hpc.be/slurm\\_tutorial.html](http://www.cec-hpc.be/slurm_tutorial.html)

```
[bvr@lm4-f001 ~]$
```

alias

env

PATH and MANPATH

**Modules and Software on Lemaitre4 or on Hercules2, Dragon2, nic5...**

-----  
Meta Modules

-----  
SitePackage releases/2021b (S) releases/2023a  
(S,L,D) tis/2018.01 (S,L)  
StdEnv (L) releases/2022b (S) releases/2023b (S)  
use.own

Toolchains

A Toolchain is a collection of compiler and libraries that are often used together and known to interoperate perfectly

intel >< foss

Toolain Independent Software = TIS

module load/avail/list/purge/swap

```
module avail | av          list available software
(module)
```

```
module load | add [module] set up the environment to use the software (ml)
module list                list currently loaded software
module purge               clears the environment
module spider              list all possible modules
module show                 show the commands in the module file
module help                 get help
```

```
module show GCC
```

```
module spider
```

```
user collection : module save | restore
```

Easybuild

```
apt-get install Python-3.7 :-)
yum install ...
rpm -Ivh ...
tar -xvf *.tgz; make; make install
```

<https://easybuild.readthedocs.io/en/latest/>

EasyBuild is a software build and installation framework that allows you to manage (scientific) software on High Performance Computing (HPC) systems in an efficient way.

Toolchains : one or more compilers + librairies (e.g. MPI, BLAS/LAPACK,...)  
foss, intel

```
eb -S WRF
```

(long!)

```
module load use.own
```

----- /home/ucl/pan/bvr/.local/easybuild/modules/all -----

## Software on multi-architecture cluster

example on Manneback

```
# sinfo
```

```
Partitions:
Def* (5days) keira (5days) cp3 (5days) cp3-gpu (5days) gpu (5days)
Nodes:
#Nodes Partition Features Cores/Slots Memory GPUs
16 cp3 CascadeLake,Xeon,4214 48 187G
1 cp3-gpu SandyBridge,Xeon,E5-2640 20 63G TeslaK80:2
15 cp3 IvyBridge,Xeon,E5-2695v2 48 126G
2 cp3 K10,Opteron,6134 16 31G
8 cp3 Rome,EPYC,7452 128 504G
19 cp3 SkyLake,Xeon,4116 48 187G
25 Def* Haswell,Xeon,E5-2630v3 16 63G
8 Def* IvyBridge,Xeon,E5-2650v2 16 63G
1 Def* Milan,EPYC,7452 128 504G
13 Def* SandyBridge,Xeon,E5-2650 16 63G
1 Def* SandyBridge,Xeon,E5-4620 32 126G
1 Def* SandyBridge,Xeon,E5-4640 32 252G
6 Def* SkyLake,Xeon,5118 24 94G
1 Def* Xeon,E5649 12 47G
2 Def* Xeon,E5649 24 47G
1 Def* Zen,EPYC,7551 128 504G
1 gpu CascadeLake,Xeon,5217,Tesla,TeslaV100 16 377G TeslaV100:2
1 gpu CascadeLake,Xeon,5217,Tesla,TeslaV100 32 377G TeslaV100:2
1 gpu CascadeLake,Xeon,6244,GeForce,GeForceRTX2080T 32 376G GeForceRTX2080Ti:6
1 gpu Milan,EPYC,7313,TeslaMIG,1g.10gb 64 252G 1g.10gb:14
1 gpu Milan,EPYC,7313,Tesla,TeslaA100 64 252G TeslaA100:2
1 gpu Milan,EPYC,7313,Tesla,TeslaA100_80 64 252G TeslaA100_80:2
2 gpu Rome,EPYC,7302,Tesla,TeslaA100 64 504G TeslaA100:2
1 gpu Rome,EPYC,7352,GeForce,GeForceRTX3090 96 504G GeForceRTX3090:4
2 keira Rome,EPYC,7742 256 252G
4 keira Rome,EPYC,7742 256 504G
Filesystems:
Filesystem quota
$CECIHOME 100.0GiB
$CECITRSF 1.0TiB
$HOME 50G
$GLOBALSCRATCH unlimited
```

```
[bvr@mbackml ~]$ ls /mb-stor/soft/localsoft/
```

```
build RedHat-6_6-45-7_None RedHat-7_23-49-0_None RedHat-7_6-26-5_None RedHat-7_6-
62-4_None RedHat-7_6-85-7_None
cecisw RedHat-7_16-9-1_None RedHat-7_25-1-1_None RedHat-7_6-44-2_Infiniband RedHat-7_6-
63-2_None tmpdir
licenses RedHat-7_21-1-2_None RedHat-7_6-23-6_None RedHat-7_6-44-2_None RedHat-7_6-
79-1_None
noarch RedHat-7_23-1-2_None RedHat-7_6-26-5_Infiniband RedHat-7_6-45-7_None RedHat-7_6-
85-4_None
```

on e.g. mb-zen001

module load OpenBLAS

```
[bvr@mb-zen001 ~]$ df -h /opt/sw/arch
```

| Filesystem                                          | Used | Avail | Use% | Mounted on   | Size |
|-----------------------------------------------------|------|-------|------|--------------|------|
| mbackm:/mb-stor/soft/localsoft/RedHat-7_23-1-2_None | 2.4T | 2.7T  | 47%  | /opt/sw/arch | 5.0T |

exercice 1 :

```
cp /tmp/flops.c ~
```

```
nano compilescript
```

with a GCC 4.x.x

then a GCC 8.3.0

then the last GCC available

then with the intel compiler icc

exercice 2 :

```
eb --search Hello
```

```
eb /usr/easybuild/easyconfigs/h/Hello/Hello-2.10-GCCcore-8.2.0.eb
```

```
building Bison-3.0.5.eb (stop, I don't want to ^C)
```

```
eb --extended-dry-run (or -x)
```

```
module load GCCcore/8.2.0 ... releases ?
```