



Efficient data storage on the CECI clusters

Ariel Lozano

CÉCI HPC Training 27 Nov 2024



DISCLOSURE



WARNING: No data on the CECI clusters has backups

You are responsible of copying over your useful data you need to store long term somewhere else

Some of the CECI universities provide solutions see:

https://support.ceci-hpc.be/doc/_contents/ManagingFiles/LongtermStorage.html



Some context

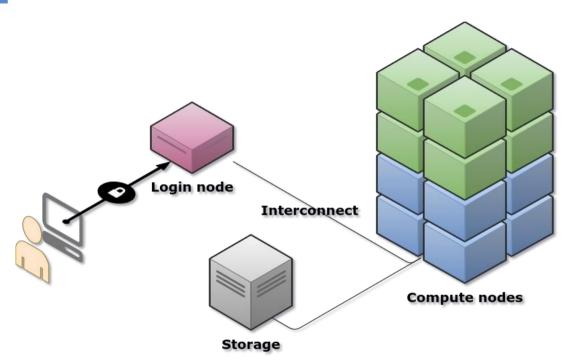
- Nowadays the best performant units of long term storage provides ~2 GB/s of sequential read/write. This can go down to about ~400MB/s for random read/write of many small files.
- Basic sequential write test on a laptop with a consumer NVMe SSD: 2TB Intel SSD 660P Series

```
$ dd if=/dev/zero of=test2GBdump bs=1M count=2048; sync
2048+0 records in
2048+0 records out
2147483648 bytes (2.1 GB, 2.0 GiB) copied, 0.842955 s, 2.5 GB/s
```

- Basic test with a single task writing on the storage.
- The CPU access the SSD directly via PCI express lanes.



Previous: HPC cluster



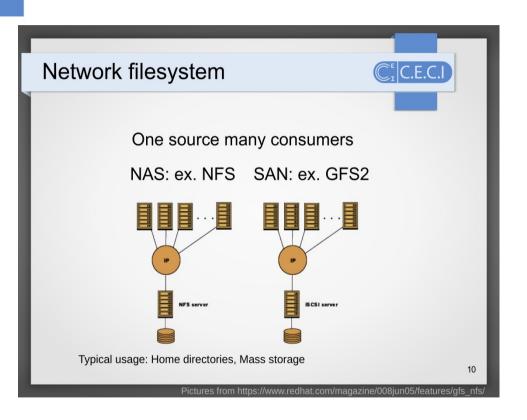
"Introduction to high-performance computing" (Frédéric Wautelet)

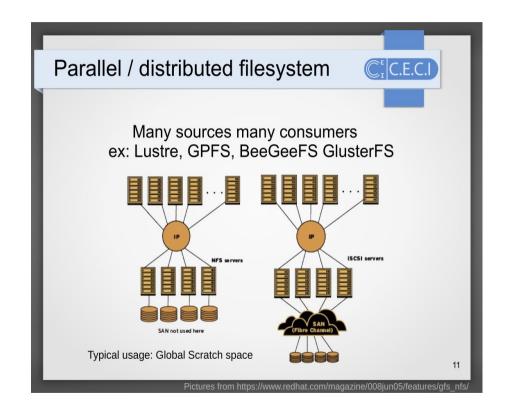
 A computer 'cluster' is a group of linked computers working together closely, so that in many respects they form a single computer

 Corollary: Access to most of the different storage solutions happens via the network



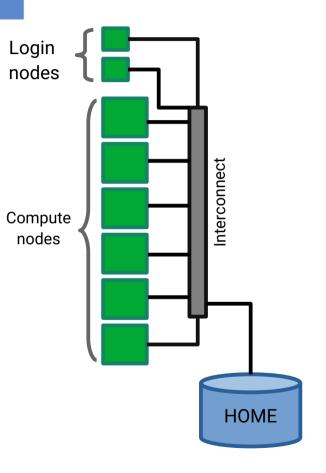
Previous: Network storage solutions





Damien François, "Introduction to data storage and access"

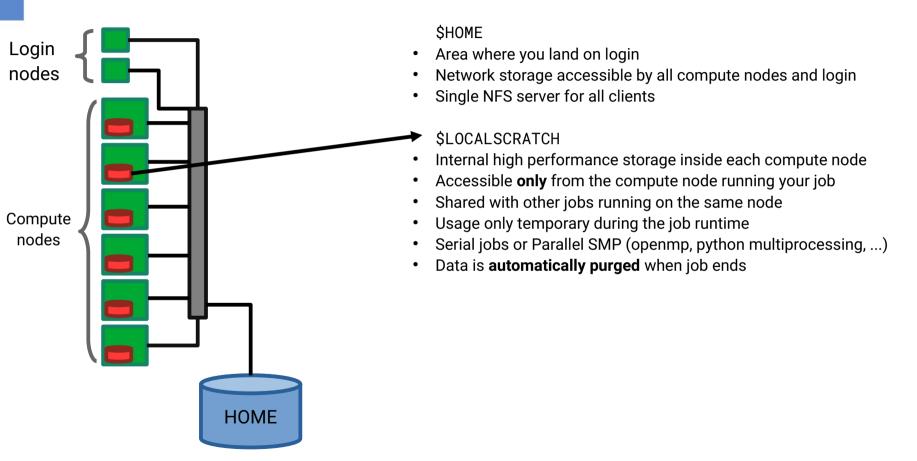




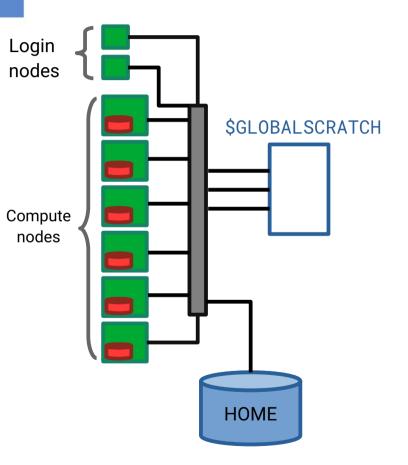
\$HOME

- Area where you land on login
- Network storage accessible by all compute nodes and login
- Single NFS server for all clients









\$HOME

- Area where you land on login
- Network storage accessible by all compute nodes and login
- Single NFS server for all clients

SLOCALSCRATCH

- Internal high performance storage inside each compute node
- Accessible only from the compute node running your job
- Shared with other jobs running on the same node
- Usage only temporary during the job runtime
- Serial jobs or Parallel SMP (openmp, python multiprocessing, ...)
- Data is **automatically purged** when job ends

\$GLOBALSCRATCH

- Implemented via different setups but usually a parallel filesystem
- Network storage accessible by all compute nodes and login
- Can be composed of a single or multiple storage sources
- All jobs but only option for multinode-parallel jobs (big MPI jobs)
- Data there stays persistently (but all is removed in yearly maintenances)
- Please cleanup from time to time



How much data can we handle on each area? check the ceci-quota command

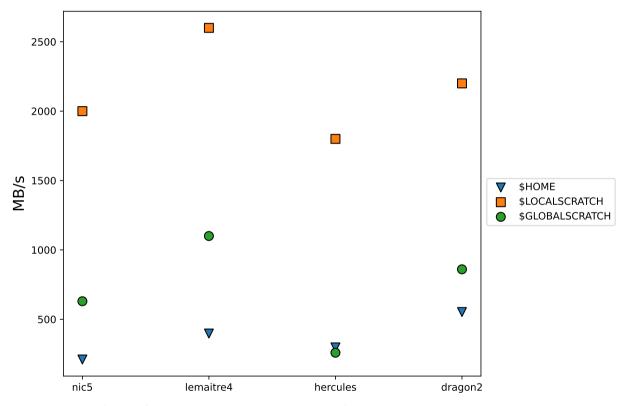
Cluster	\$HOME (nfs server)	\$L0CALSCRATCH (hardware support)	\$GLOBALSCRATCH (fstype)
NIC5	100 GB	370GB (local SSD)	5TB (520TB beegfs)
Lemaitre4	100 GB	180GB (local SSD)	XX ^[1] (320TB beegfs)
Dragon2	40 GB	3TB (HDD RAID0)	XX ^[1] (60TB beegfs)
Hercules	200 GB	her2-w065096: 1TB her2-w099126: 4TB her2-w127128: 8TB (HDD RAID0)	400GB soft / 4TB hard (nfs server)

More info: https://support.ceci-hpc.be/doc/_contents/ManagingFiles/Storage.html#quota-label



^[1] No limits enforced but remember resources are shared among all ~800 CECI users!!

Sequential write speed (dump of a 2GB file)



- This is **NOT** a definitive benchmark of the filesystems. Pattern is of a single core job doing a single write at the end.
- Different I/O patterns on your job will produce diverse results

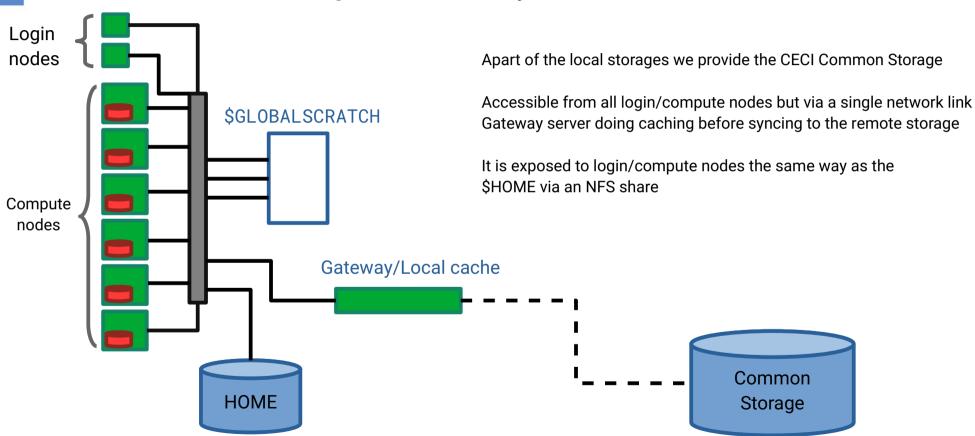


Wrap-up

- \$LOCALSCRATCH will be always the ideal for single core jobs
- If all your input/output data volume for your job fits on \$LOCALSCRATCH use it your code will speed up
 just for doing that
- \$GLOBALSCRATCH is the only choice for parallel multi-node jobs
- \$GLOBALSCRATCH can also be used to store big input data, or recover useful output for a job working on \$LOCALSCRATCH
- There's no reason to use \$HOME for job I/O. Performance is the lowest and the usable space the smallest

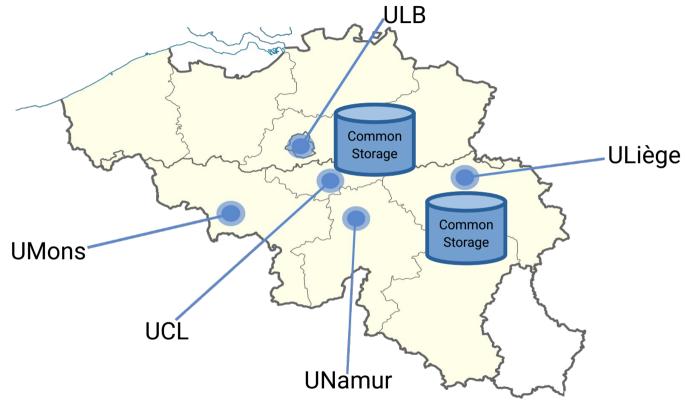


external remote storage accesible by all clusters





external remote storage accesible by all clusters



The main storage servers are in ULiège and UCL
There is a dedicated data interconnect among the 5 sites for this solution



external remote storage accesible by all clusters

/CECI/home

- Personal directory path defined via \$CECIHOME variable
- Quota of 100GB

/CECI/trsf

- Personal directory path defined via \$CECITRSF variable
- Meant only for **temporary** copying from one cluster to another
- Data here is subject to be purged every 6 months
- Ouota of 1TB soft 10TB hard

/CECI/proj

- Area where a team with a project can get a common folder for sharing data
- Must be requested by a PI
- Quota decided according to the project's needs

/CECI/soft

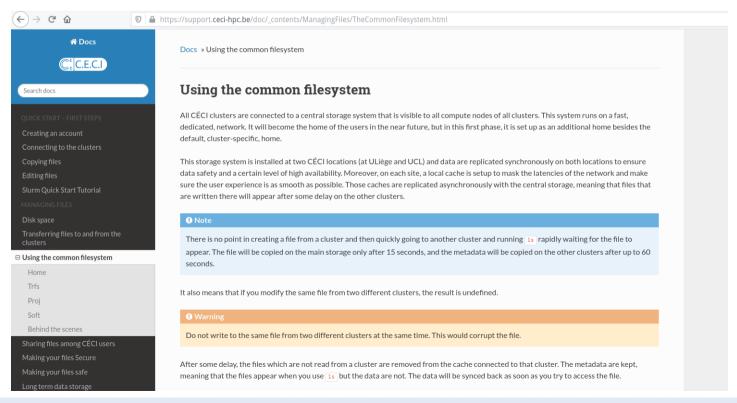
Used only by the sysadmins for software installations



external remote storage accesible by all clusters

For more details check our detailed documentation

https://support.ceci-hpc.be/doc/_contents/ManagingFiles/TheCommonFilesystem.html





Used space and quotas?

Just use the ceci-quota command on any cluster

```
[myuser@dragon2.dragon2-ctrl0: ~]---> $ ceci-quota
Diskquotas for user myuser
Filesystem
                        limit
                                  files
                                            limit
               used
$HOME
                                 205641 unlimited
     7.3 GiB
                   40.0 GiB
$CECIHOME 11.4 GiB 100.0 GiB
                                   4390
                                           100000
$CECITRSF
           64.0 kiB
                                      8 unlimited
                   1.0 TiB
```

```
[myuser@lm4-f001: ~]---> $ ceci-quota
Diskquotas for user myuser
Filesystem
               used
                                  files
                                            limit
                        limit
$HOME 4.14G
                    100G
                                  3.82K
/scratch 4.3 GB unlimited
                                        unlimited
SCECIHOME 11.4 GiB
                   100.0 GiB
                                   4390
                                           100000
$CECITRSF
           64.0 kiB
                   1.0 TiB
                                        unlimited
```



How do we control the data location from a Slurm job?

Making use of the pre-defined environment variables:

\$HOME

\$LOCALSCRATCH

\$GLOBALSCRATCH

\$CECIHOME

Extra useful variables defined on-the-fly when submitting a job:

\$SLURM_JOB_ID the Job ID value \$SLURM_SUBMIT_DIR directory where the job was submitted from



LOCALSCRATCH example

```
#!/bin/bash
#SBATCH -- job-name=stest1
#SBATCH --time=00:15:00
#SBATCH --ntasks=1
#SBATCH --mem-per-cpu=1000
#SBATCH --partition=batch
module load releases/2021b
module load SciPy-bundle/2021.10-foss-2021b
# define some useful directory names
RUNDIR="${LOCALSCRATCH}"
SUBMITDIR="${SLURM_SUBMIT_DIR}"
# on this example we assume our input files are on the
# same directory where we run sbatch myjob.sh
cp -r ${SUBMITDIR}/input_1000.in ${RUNDIR}/input.in
# change to the run directory on the compute node
cd ${RUNDIR}
# execute your code
python ${HOME}/project1/mycode/mycode1.py
# recover your useful output
cp -r long.out ${SUBMITDIR}/
```

- Python code that requires just an input file "input.in"
- The code is located on a folder inside my \$HOME
- The only useful output it will produce is "long.out"



GLOBALSCRATCH example

```
$ mkdir -p $GLOBALSCRATCH/mviob1000
$ cp -r input_1000.in $GLOBALSCRATCH/myjob1000/input.in
$ cd $GLOBALSCRATCH/myjob1000
> i create my submission script myjob.sh as e.g. below
#!/bin/bash
#SBATCH -- job-name=gtest1
#SBATCH --time=00:15:00
#SBATCH --ntasks=1
#SBATCH --mem-per-cpu=1000
#SBATCH --partition=batch
module load releases/2021b
module load SciPy-bundle/2021.10-foss-2021b
python ${HOME}/project1/mycode/mycode1.py
> and we can submit it directly from here
$ sbatch myjob.sh
```

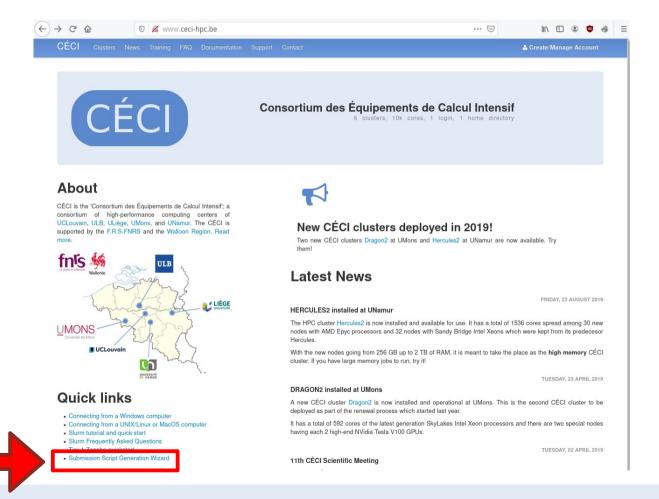
We can prepare everything before inside \$GLOBALSCRATCH, input and submission script, then submit from there without extra data movements.

This is just an illustrative example!

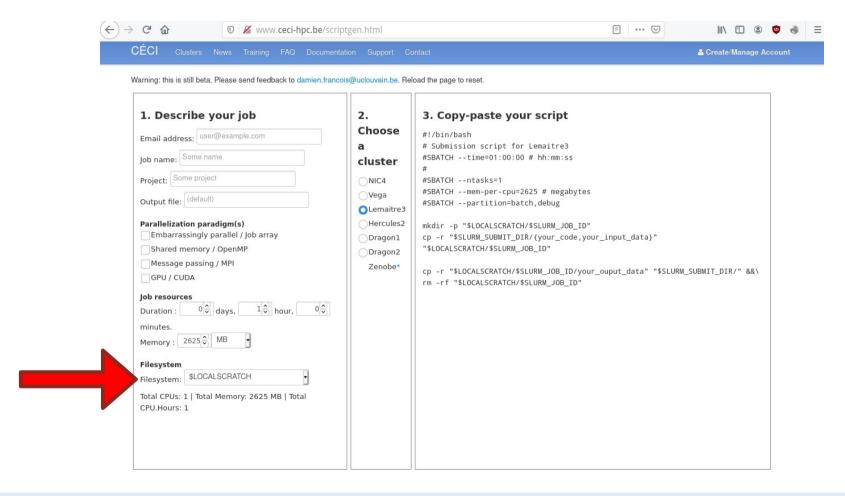
For single node jobs where all input/output fits on LOCALSCRATCH use the previous approach

Or also **consider a mix** if the input data is too big, but the produced output fits on LOCALSCRATCH











Examples

We are going to check the examples available on the clusters at:

cat /CECI/proj/training/ceci_storages/README.md



To wrap up

For all clusters

Never do direct I/O on your \$HOME

Prioritize the usage of \$LOCALSCRATCH if your jobs allow it (e.g. jobs running on a single node) Remember this area is shared with other users of the node and there's no quota!!

Never redirect outputs to -> /tmp use always \$LOCALSCRATCH instead

Lemaitre4 and NIC5

For your multi-node parallel jobs **always** use \$GLOBALSCRATCH **never** your \$HOME



Remember to backup your useful data somewhere else outside the clusters

