Introduction to Tetralith

Photo: Peter Kjellström

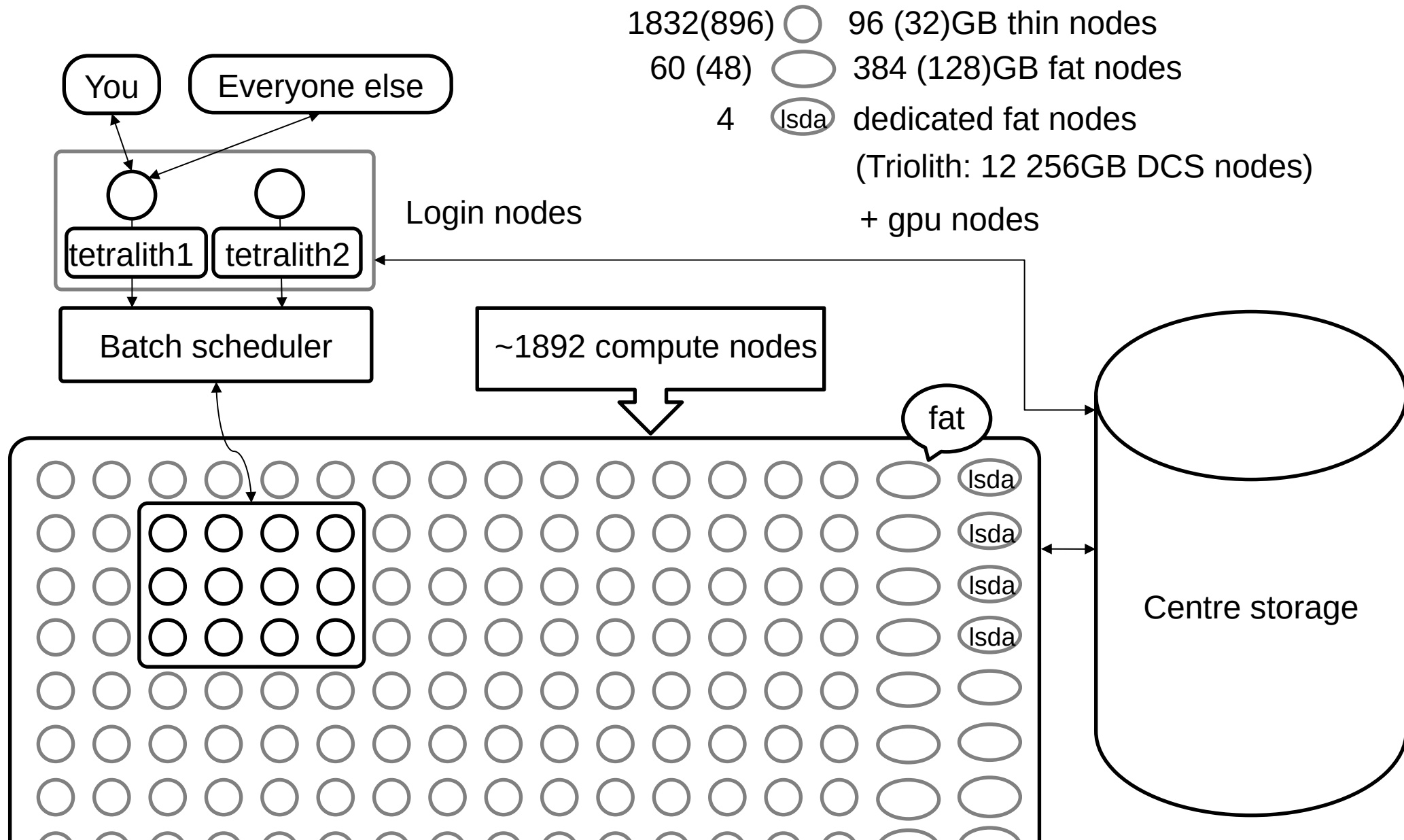Anna Lewinschal, MISU, 2023-03

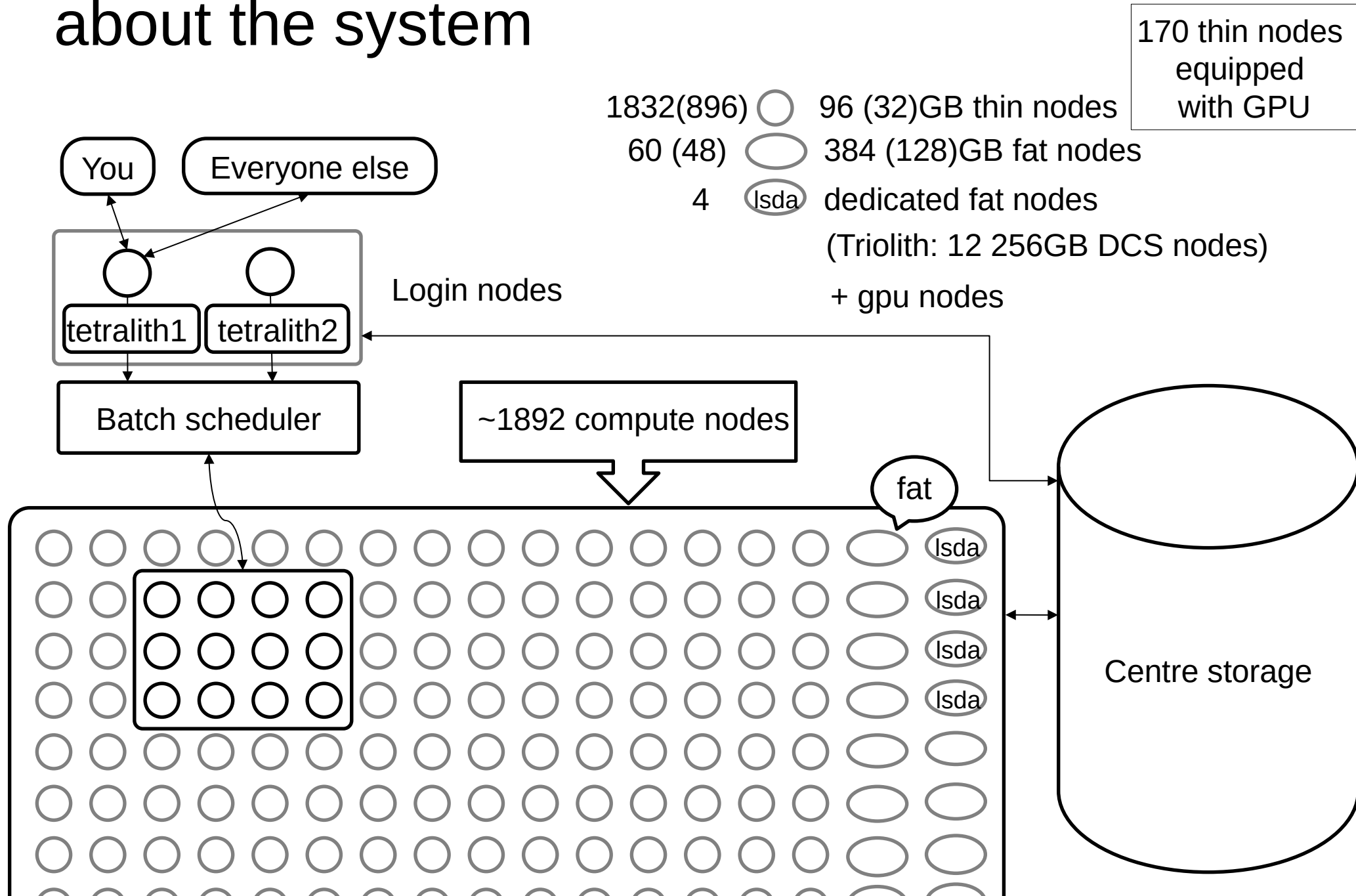# Some numbers and basic information about the system

- National Supercomputer Centre (NSC)

- Two log in nodes: tetralith1/tetralith2

- 1832 thin Intel compute nodes (Triolith: total 1017)

- 32 cores per node (Triolith: 16)

- Slurm queuing system

- CentOS7 Linux operating system (Triolith: CentOS6)

Some numbers and basic information about the system

1832(896) ◯ 96 (32)GB thin nodes

60 (48) ⬭ 384 (128)GB fat nodes

4 (lsda) dedicated fat nodes

(Triolith: 12 256GB DCS nodes)

+ gpu nodes

You

Everyone else

Login nodes

tetralith1 tetralith2

Batch scheduler

~1892 compute nodes

fat

lsda
lsda
lsda
lsda

Centre storage

Some numbers and basic information about the system

170 thin nodes equipped with GPU

1832(896) ◯ 96 (32)GB thin nodes
60 (48) ⬭ 384 (128)GB fat nodes
4 (lsda) dedicated fat nodes
(Triolith: 12 256GB DCS nodes)
+ gpu nodes

You   Everyone else

tetralith1   tetralith2

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Some numbers and basic information about the system

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You   Everyone else

tetralith1   tetralith2

Batch scheduler
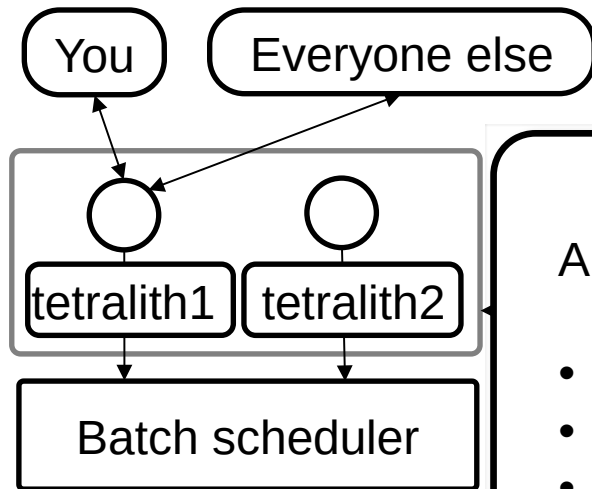
Allowed on the login nodes:

- Run file transfers to and from the system.
- Manage your files (copy, edit, delete files etc).
- Submit batch and interactive jobs (more about that later).
- Run applications that use small amounts of CPU and memory.
- Compile software.

A very simple rule is "don't run things on the login node that will inconvenience other users".

Logging in

- ssh -X x_username@tetralith.nsc.liu.se

   -X X-forwarding to display graphics

- ThinLinc for graphical applications

Working on supercomputers without annoying other users

- NEVER run Matlab on the login node! Or any other heavy application. Use analysis nodes!

- Avoid using resources in a way that blocks other users from using them or prevents them from working efficiently.

Security

- Use different passwords for different systems

- Do not use weak passwords

- Avoid chains of SSH sessions
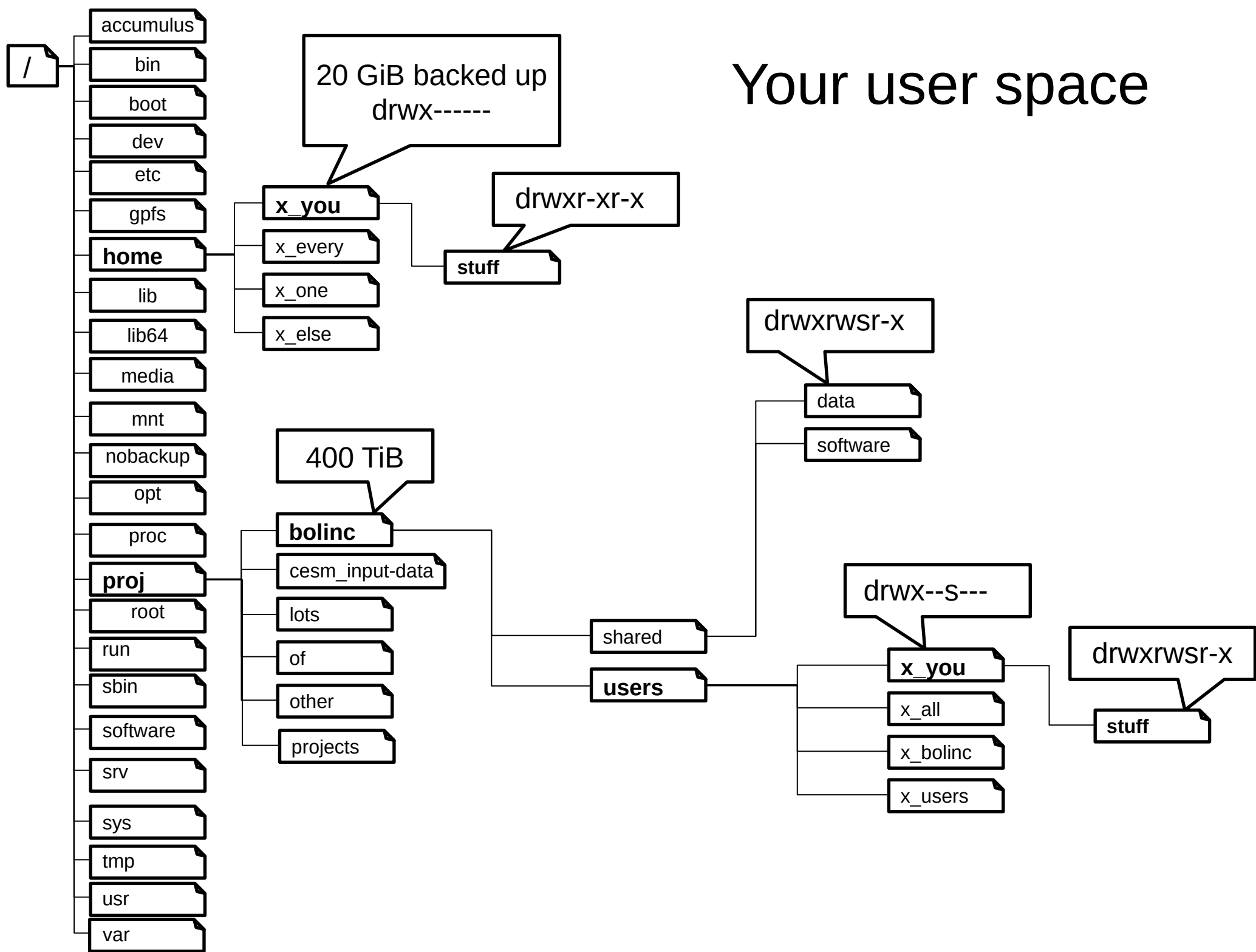
- Check: "Last login: DATE from MACHINE"

Your user space

- Home directory: 20GiB
  Backed up

  /home/x_username

- Centre storage directory: ~400 TiB for bolinc project
  Not backed up

  /proj/bolinc/users/x_username

Your user space

Changing permissions

chmod 755 file/folder

change permissions to
7- rwx for owner
5 - r-x for group and other

1- execute
2 - write
3 - write and execute (2+1)
4 - read
5 - read and execute (4+1)
6 - read and write (4+2)
7 - read write and execute (4+2+1)

chmod –R go-w ./

recursively remove write permission
for group and other from your present
location and down in the file tree

Information about your usage/projects

- projinfo
  displays which projects you are member of and core hour usage statistics

- snicquota
  displays how much space you are using

SUPR portal

- Administrate your projects

- Sign user agreement

- Apply for membership in projects

- Apply for computing hours

- Change email address. Always have a valid email address registered!

- Check resource usage

SUPR - Anna Lewinschal

You are now logged in.

Projects

You belong to the following active projects:

Project	PI	Project Title	Project Type	Centre	Start Date	End Date	Your Role
SNIC 2022/1-1	Qiong Zhang	Climate Modelling at the Bolin Centre fo…	SNIC Large Compute	NSC	2022-07-01	2023-07-01	proxy
SNIC 2022/1-3	Erik Kjellström	S-CMIP: Swedish climate modelling and co…	SNIC Large Compute	(multiple)	2022-07-01	2023-07-01	member
SNIC 2022/2-1	Qiong Zhang	Climate model data storage at the Bolin …	SNIC Large Storage	(multiple)	2022-07-01	2023-07-01	proxy
SNIC 2022/23-411	Erik Kjellström	Data storage for Swedish climate modelli…	SNIC Small Storage	PDC	2022-09-14	2023-07-01	extended member
SNIC 2022/23-4	Hamish Struthers	CESM climate model shared data storage	SNIC Small Storage	NSC	2022-01-07	2023-02-01	proxy
SNIC 2022/23-5	Hamish Struthers	EC-Earth climate model shared data stora…	SNIC Small Storage	NSC	2022-01-07	2023-02-01	member
SNIC 2022/13-17	Thorsten Mauritsen	Next-generation global cloud resolving c…	LUMI XL	LUMI Sweden	2022-07-01	2023-01-01	member

On the projects page you can see all projects you belong to or have belonged to. You can also request membership in new projects.

Go to Projects Page

Accounts

Accounts in this context are the login accounts that you use to login to the resources provided by the centres.

On the accounts page you can see your existing accounts and pending account requests.

Go to Accounts Page

Sidebar

SNIC SUPR

Start
Projects
  SNIC 2022/1-1 (NSC)
  SNIC 2022/1-3 (multicentre)
  SNIC 2022/2-1 (multicentre)
  SNIC 2022/23-411 (PDC)
  SNIC 2022/23-4 (NSC)
  SNIC 2022/23-5 (NSC)
  SNIC 2022/13-17 (LUMI Sweden)
Accounts
Proposals
  SNIC 2022/23-4 (NSC)
  SNIC 2022/23-5 (NSC)
Rounds
Groups
  application-experts
Personal Information
Support
Logout

Logged in as:
Anna Lewinschal
(anna@misu.su.se)

Our projects

- Computing/storage is project based

- Monthly computing hours budget

- Large computing project. Year long project for computing.

- Storage project. Year long project for storage.

- Report usage and results!

- Acknowledgement!

Running a job

- Submitting a batch job. Example:
  sbatch -A projectname -N 2 -t 3-0:00:00 myjob.sh

    N - number of nodes <=> Nx32 cores
    n - number of cores

- Check queue:
  squeue -u x_username

- Cancel a job:
  scancel jobid

- Maximum wall time: 168 h/7 days

SNIC 2022/1-1
Climate Modelling at the
Bolin Centre for Climate Research

Large computing project:

- 2000x1000 core-h/month

- For running GCMs and other computationally expensive applications

- Renewed every year (so far...)

- Report usage and results!

- Acknowledgement!

Acknowledgement

- SNIC - Swedish National Infrastructure for Computing, ended Dec 2022
- SNAC - Swedish National Allocations Committee
- NAISS - National Academic Infrastructure for Supercomputing in Sweden, since Jan 2023

Remember to acknowledge NAISS or SNIC when you publish work where you have used NAISS or SNIC resources!

SNAC has defined the following template for such acknowledgement:

"The computations/simulations/[SIMILAR] were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at [SNIC CENTER] **partially funded by the Swedish Research Council through grant agreement no. 2018-05973**.*"*

"The computations/data handling/[SIMILAR] were/was enabled by resources provided by the National Academic Infrastructure for Supercomputing in Sweden (NAISS) at [NAISS AFFILIATED SITE] partially funded by the Swedish Research Council through **grant agreement no. 2022-06725.**"
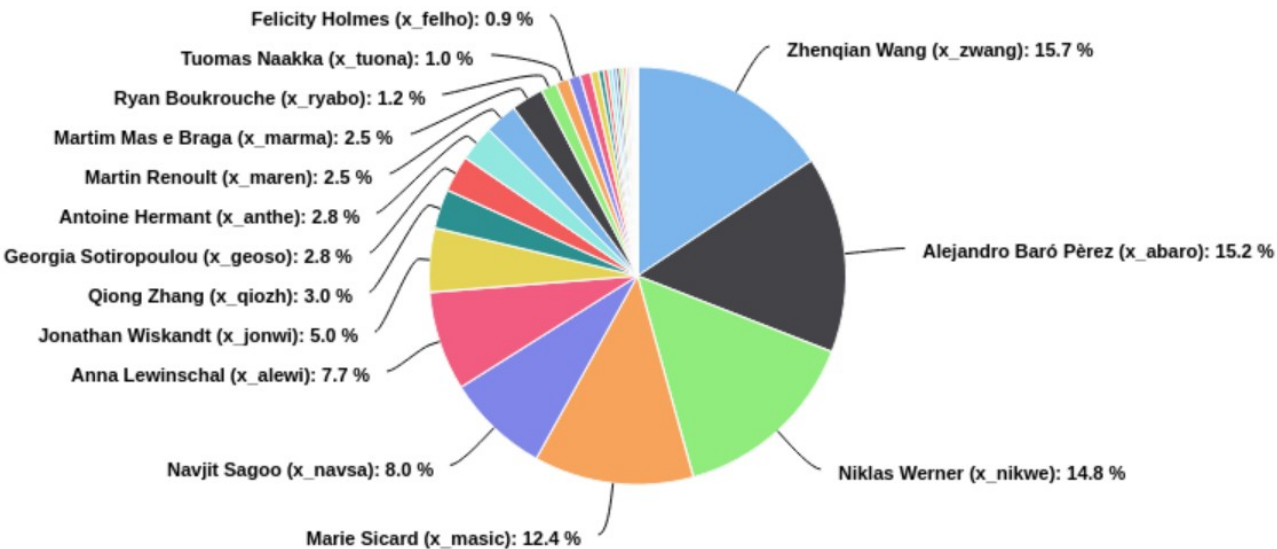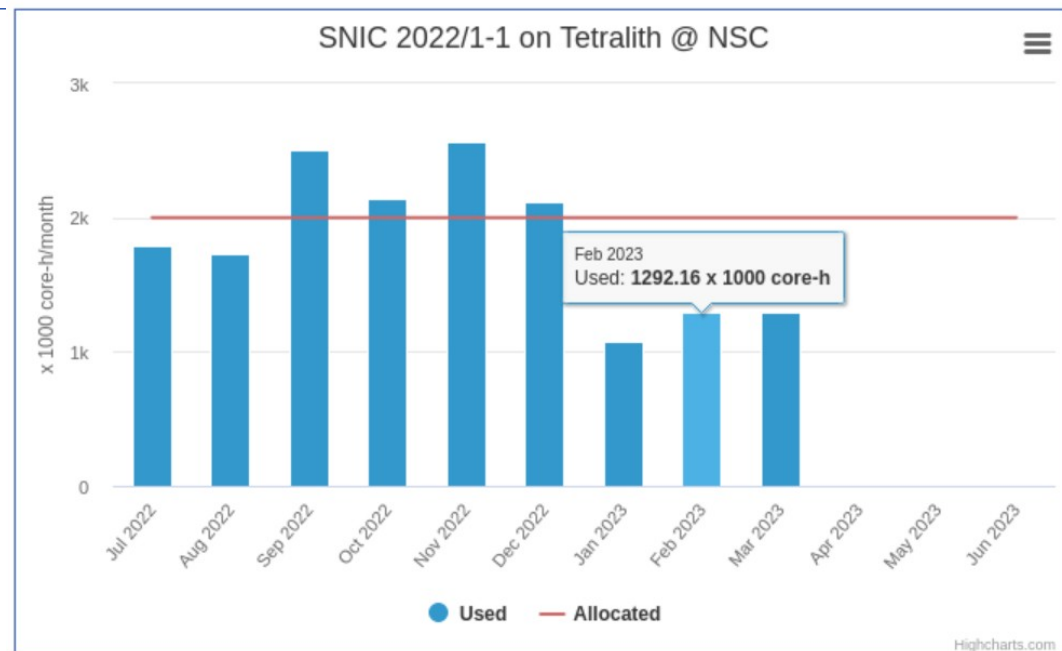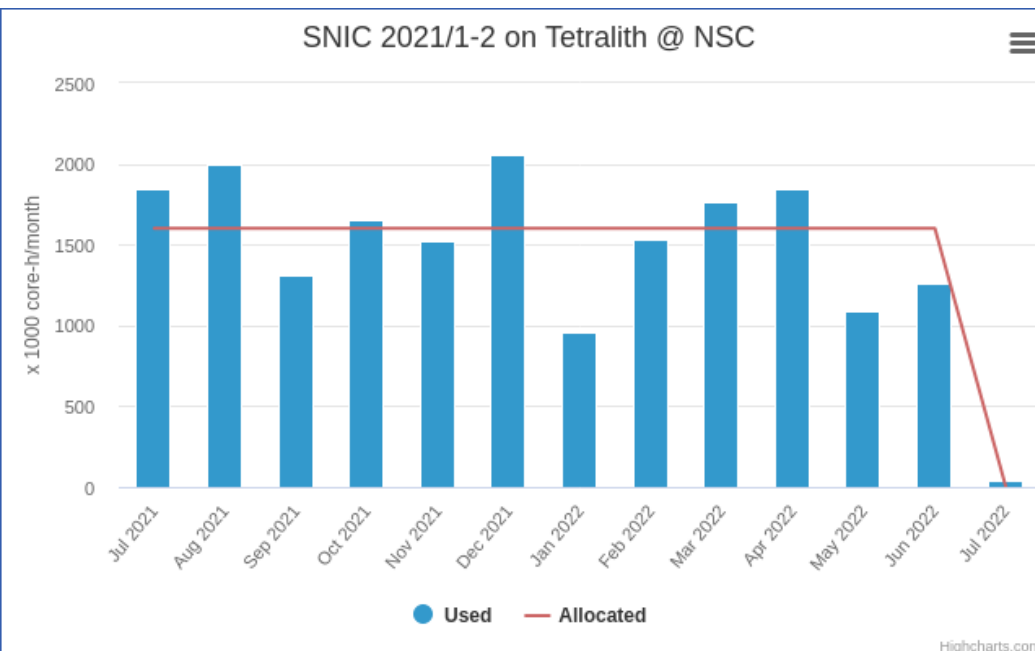
Usage statistics from SUPR for last year's large computing project

Current project

SNIC 2022/2-1

Climate model data storage at the Bolin Centre for Climate Research

Storage project:

- No core hours

- Only for storage

- End date 2023-07-01

- Acknowledgement!

Large scale data analysis
Available for SNIC 2022/1-1 (Compute project)

lsda:

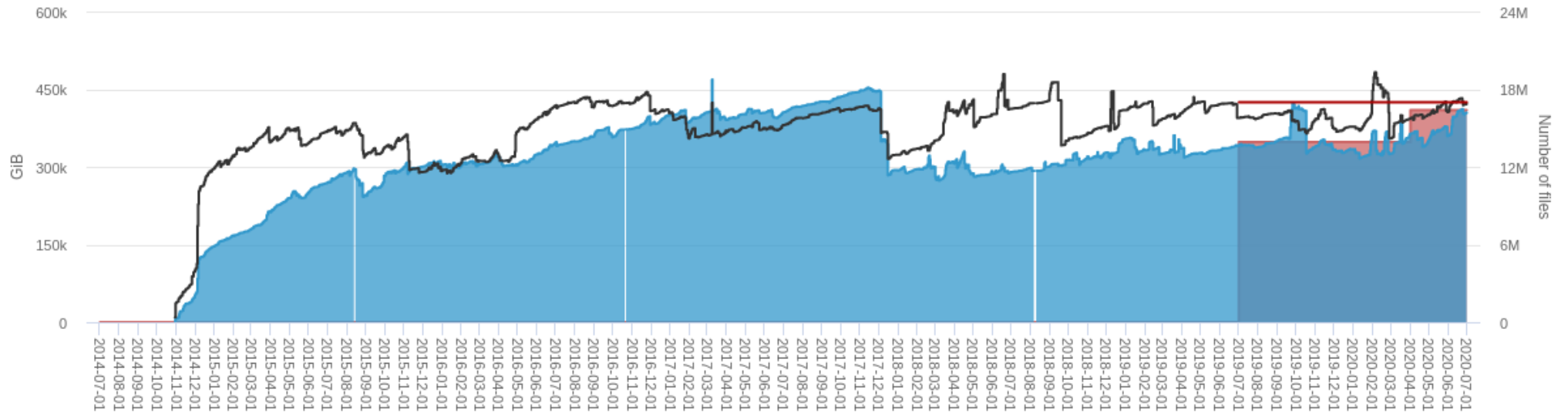Four dedicated fat nodes for interactive use

Running an interactive job. Example:

```
interactive -A snic2022-1-1 --reservation=lsda -t 01:00:00 -n 1
```
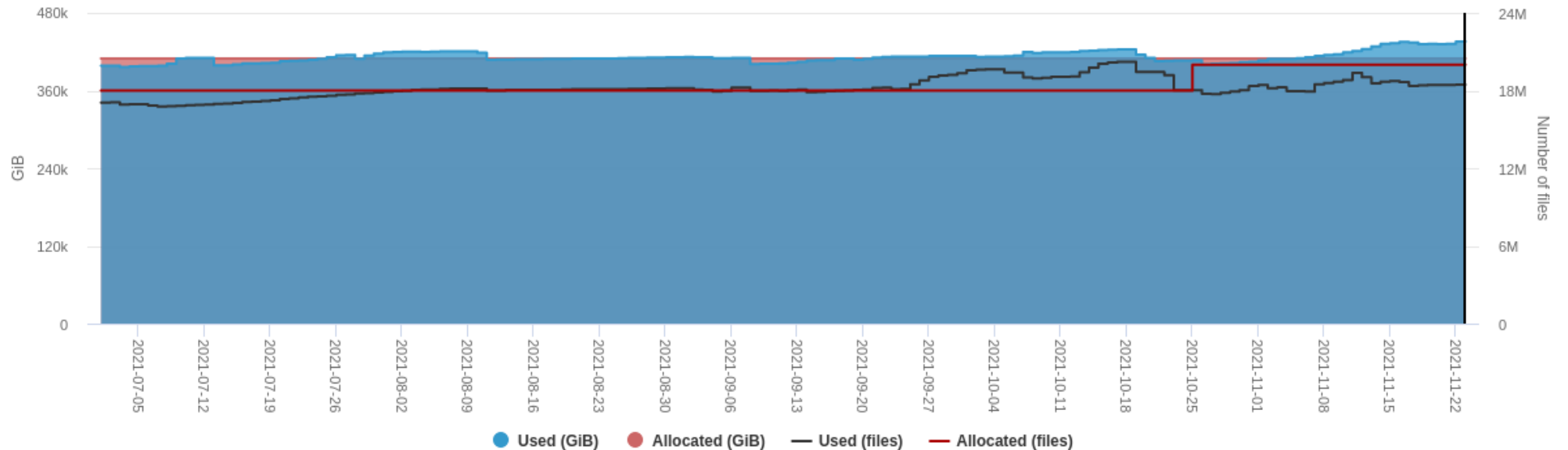
Only 4 nodes! Don't use more cores than you need!

Storage statistics from SUPR
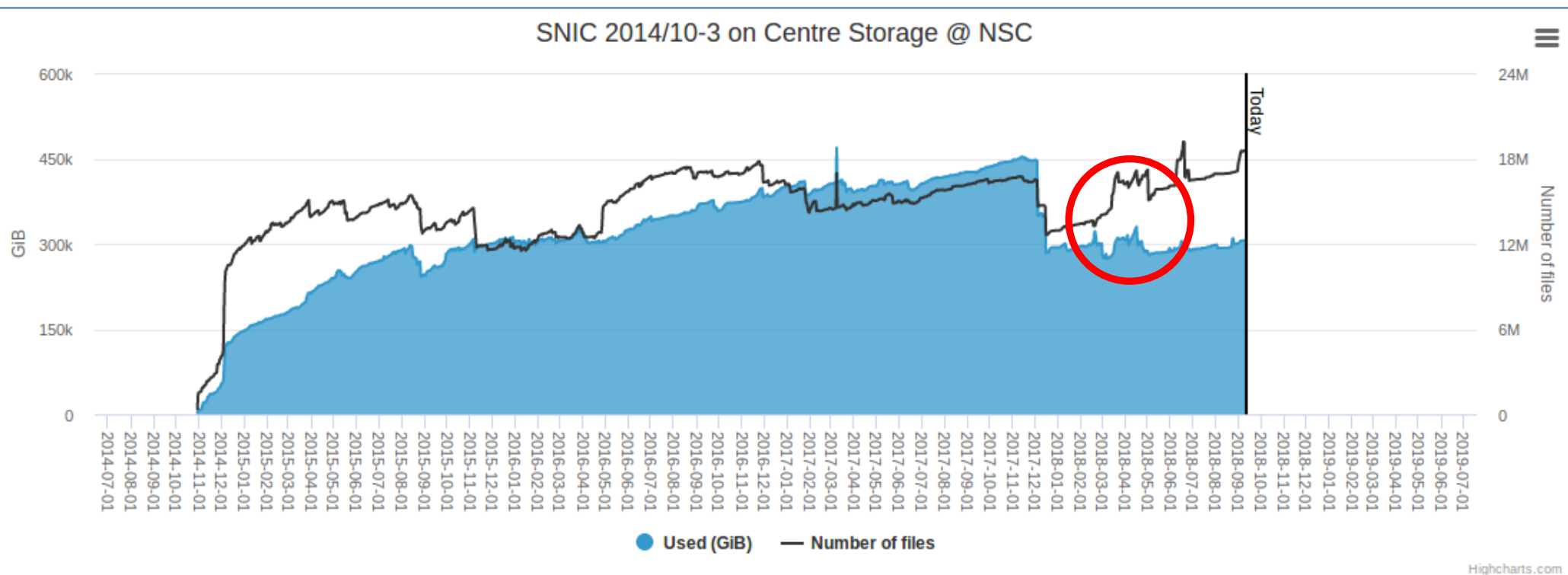

SNIC 2014/10-3 on Centre Storage @ NSC

SNIC 2021/2-1 on Centre Storage @ NSC

● Used (GiB)　● Allocated (GiB)　— Used (files)　— Allocated (files)

Storage statistics from SUPR

Storage statistics from SUPR

Quota exceeded for bolinc on Triolith

Anna Lewinschall
Wed 11/04, 16:38

Francesco Salvatore Rocco Pausata; Sebastian Scher; Henrik Carlson; Srinath Krishnan; Filippa Fransner; Jenny Lindvall; +3 more ⩔

Dear all,

We are currently exceeding our quota for the bolinc (SNIC 2014/10-3) project on Triolith.

Quota for project storage /proj/bolinc (real-time data)
===

Used (GiB)	Quota (GiB)	Hard limit (GiB)	Grace	Used (files)	Quota (files)	Hard limit (files)
313814.1	300000.0	450000.0	25 days	16515535	17000000	25000000

WARNING: The disk usage in /proj/bolinc is above quota!
In 25 days you will not be able to write to /proj/bolinc until enough
of the project's data have been removed from the directory.

If you receive this email you are among the top ten users. Please compress or remove data as soon as possible.

x_frpau   36496.0
x_sebsc   25895.2
x_henca   16700.7

Storage statistics from SUPR

Data security

- Centre storage is not backed up. Data can be lost.

- NSC runs snapshots several times per day. Data can be recovered, but not necessarily most up to date version.

Snapshot

- "Copy" of the file system at a specific time

- Saved ~7 days

/home/.snapshots/2019-10-09T1700+0200/x_username/

/proj/.snapshots/2019-10-09T1701+0200/bolinc/users/x_username/

```
[x_alewi@tetralith1 ~]$ ls /home/.snapshots/
2019-10-09T1700+0200   2019-10-14T1700+0200   2019-10-16T1400+0200   2019-10-17T0900+0200   2019-10-17T1400+0200
2019-10-10T1700+0200   2019-10-15T1700+0200   2019-10-16T1500+0200   2019-10-17T1000+0200   2019-10-17T1500+0200
2019-10-11T1700+0200   2019-10-16T0800+0200   2019-10-16T1600+0200   2019-10-17T1100+0200   2019-10-17T1600+0200
2019-10-12T1700+0200   2019-10-16T1200+0200   2019-10-16T1700+0200   2019-10-17T1200+0200
2019-10-13T1700+0200   2019-10-16T1300+0200   2019-10-17T0800+0200   2019-10-17T1300+0200
```

Storage policy

- Centre storage is not an archiving service

- Inactive/redundant data should be removed

- Compress/zip your data if possible

- Keep down number of files (e.g. use tar)

- Keep track of how much space you use

- Always have a valid email address registered in SUPR

- One day you may have to remove your data

Storage policy

- When you join the project you have to **declare that you understand the user conditions**.

- You will have to **renew your membership on a yearly basis**. If you do not actively join the project, your data will be removed. I.e. **data owned by a user that is no longer a member of the storage project will be removed**.

- The storage project is **intended for members of the Bolin Centre**. If you change affiliation you will have to either:

  1) Remove your data from the Bolin Centre storage project.

  2) Change the ownership of the data to an active user within the Bolin Centre.

  3) Provide a timeline for when the data can be removed.

- **You have to have a valid email address registered in SUPR**. This is the email we will use to contact you regarding your data stored in the storage project. If you fail to reply when contacted, we will remove you from the project. If you do not reapply to become a member of the project, we will delete your data.

- You will have to **report your usage when requested** for continued storage resources.

Application procedure

When you apply for membership, you will be asked to fill in a mandatory message to PI. In this box you **HAVE TO** write:

- That you are aware of the policies regarding data storage in this project outlined below.

- That you are aware of the mandatory SNIC acknowledgement policy for publications derived from the use of this resource.

- Your department and position.

- How long you intend to use the project.

- Secondary contact for your data (e.g. supervisor, PI for project, student etc.)

If your membership application fails to comply with the instructions above, we will deny your membership request. You can then apply again with an amended information specification.

Modules

Software are available through module system

Examples: compilers, netcdf, cdo...

module load modulename

module list

module avail

module help

module show modulename

module purge

Bolin Centre modules

module use /proj/bolinc/shared/software/modules

[x_alewi@tetralith1 ~]$ module avail

------------------------------- /proj/bolinc/shared/software/modules -------------------------------

cdftools/4-intel-2018.u1-bare	mumps/5.1.2-seq-intel-2018b-eb (D)
cmor/3.5.0-intel-2018.u1-bare	netCDF/4.0-gcc-485
ElmerIce/058434f-intel-2018b-eb	OpenIFS/c40r1-intel-2018.u1-bare
h4h5tools/2.2.4-buildenv-intel-2018b-eb	parmetis/4.0.3-intel-2018b-eb
HDFview/3.0.0	ps2eps/1.68
hypre/2.15.1-intel-2018b-eb	RRTM/v3.3-intel-2018.u1-bare
hysplit/rev954-intel-2018a-eb	scotch/6.0.6-intel-2018b-eb
json-c/0.10-intel-2018.u1-bare	uuid/1.6.2-g485
json-c/0.14-intel-2018.u1-bare (D)	uuid/1.6.2-intel-2018.u1-bare (D)
metis/5.1.0-intel-2018b-eb	zlib/1.2.11-gcc-2018a-eb
mumps/5.1.2-par-intel-2018b-eb	

Example: module load netCDF/4.0-gcc-485

softwarename/version-compiler

Bolin Centre modules

Bolin centre conda python environment

Under development...

(Old way:
module load Python/3.7.0-anaconda-5.3.0-extras-nsc1)

module load Anaconda/2022.05-nsc1

conda activate /proj/bolinc/shared/software/Python/3.8.3-extras_BC

Includes cartopy, metpy, pandas, xarray, netcdf4….

Useful things to know

- Accessing local disk "scratch" on a compute node

  /scratch/local

  $SNIC_TMP

  200GiB per thin node, 900GiB per fat node

- Logging in to nodes outside the batch scheduler for e.g. memory monitoring and debugging:

  jobsh -j jobid   nodename

  jobsh -j 374242   n525

- Specific reservations (particular nodes: development nodes, lsda nodes)

  --reservation=devel   8 development nodes (max 2/usr), <1h wall time

  --reservation=lsda   large scale data analysisnodes

Getting help

- Anna Lewinschal (MISU) Scientific programmer
  anna@misu.su.se
  room 670

- Hamish Struthers (NSC) Application expert
  CESM/NorESM/EC-Earth
  struthers@nsc.liu.se
  visits misu every/second month

- www.nsc.liu.se/support/
- NSC staff
  support@nsc.liu.se

Happy computing!