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Introduction to HPC-UGent

Oct 16th 2019 - PRETREF workshop

https://www.ugent.be/hpc/en/training/2019/pretref

hpc@ugent.be

https://ugent.be/hpc

Vlaanderen
is computing

HPC-UGent

hpc@ugent.be

Part of ICT Department of Ghent University

Our mission

HPC-UGent provides centralised scientific computing services, training, and support for researchers from Ghent University, industry, and other knowledge institutes.

Our core values

Empowerment - Centralisation - Automation - Collaboration

HPC-UGent: staff

Stijn De Weirdt
technical lead

Kenneth Hoste
user support & training

Andy Georges
sysadmin, tools

Balázs Hajgató
sysadmin, tools

Ewald Pauwels
team lead

Wouter Depypere
sysadmin, hardware

Kenneth Waegeman
sysadmin, storage

Álvaro Simón García
cloud, user support

Bart Verheyde
sysadmin, hardware

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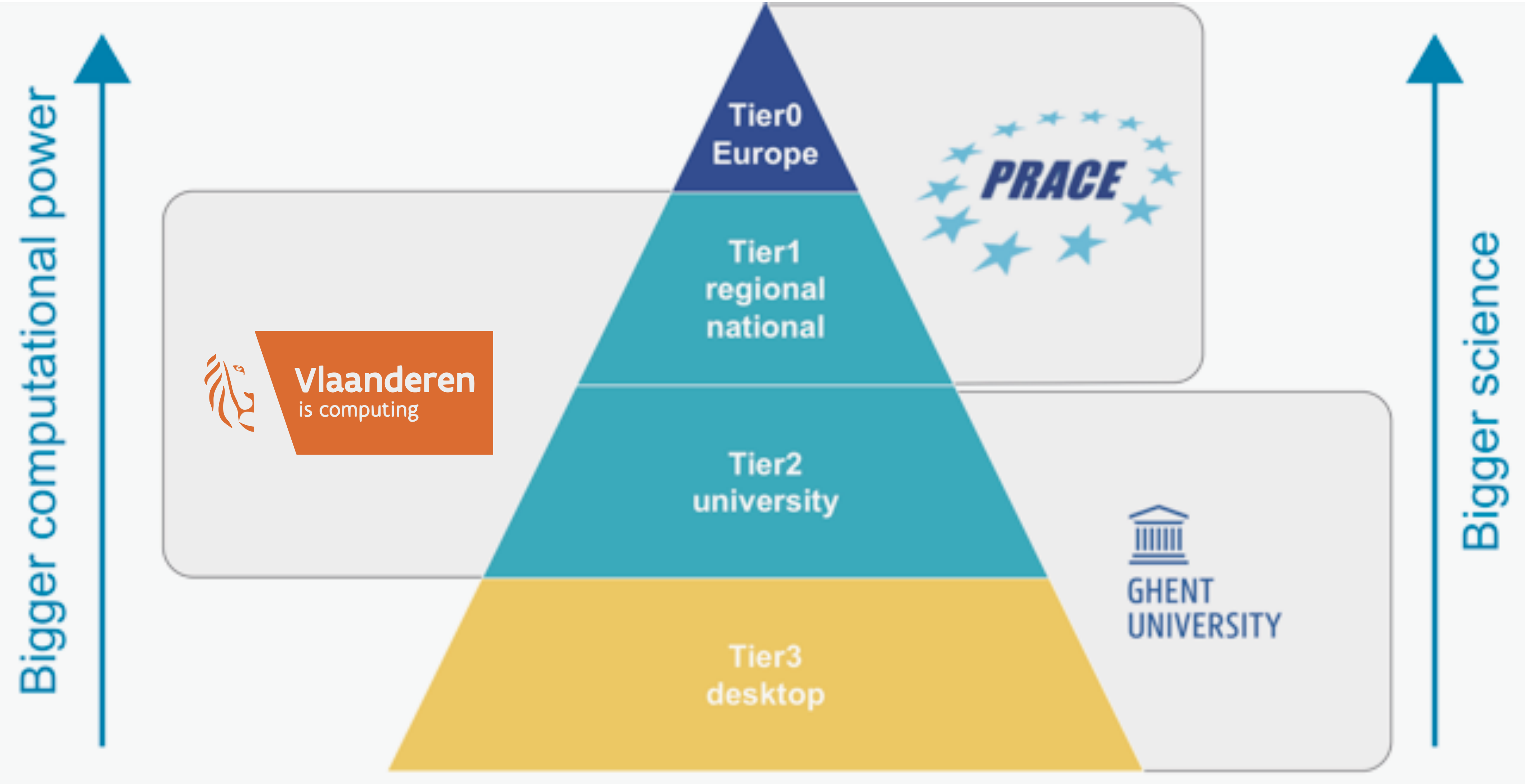
Centralised hardware
in the UGent datacenter
at campus Sterre (building S10)

Centralised hardware



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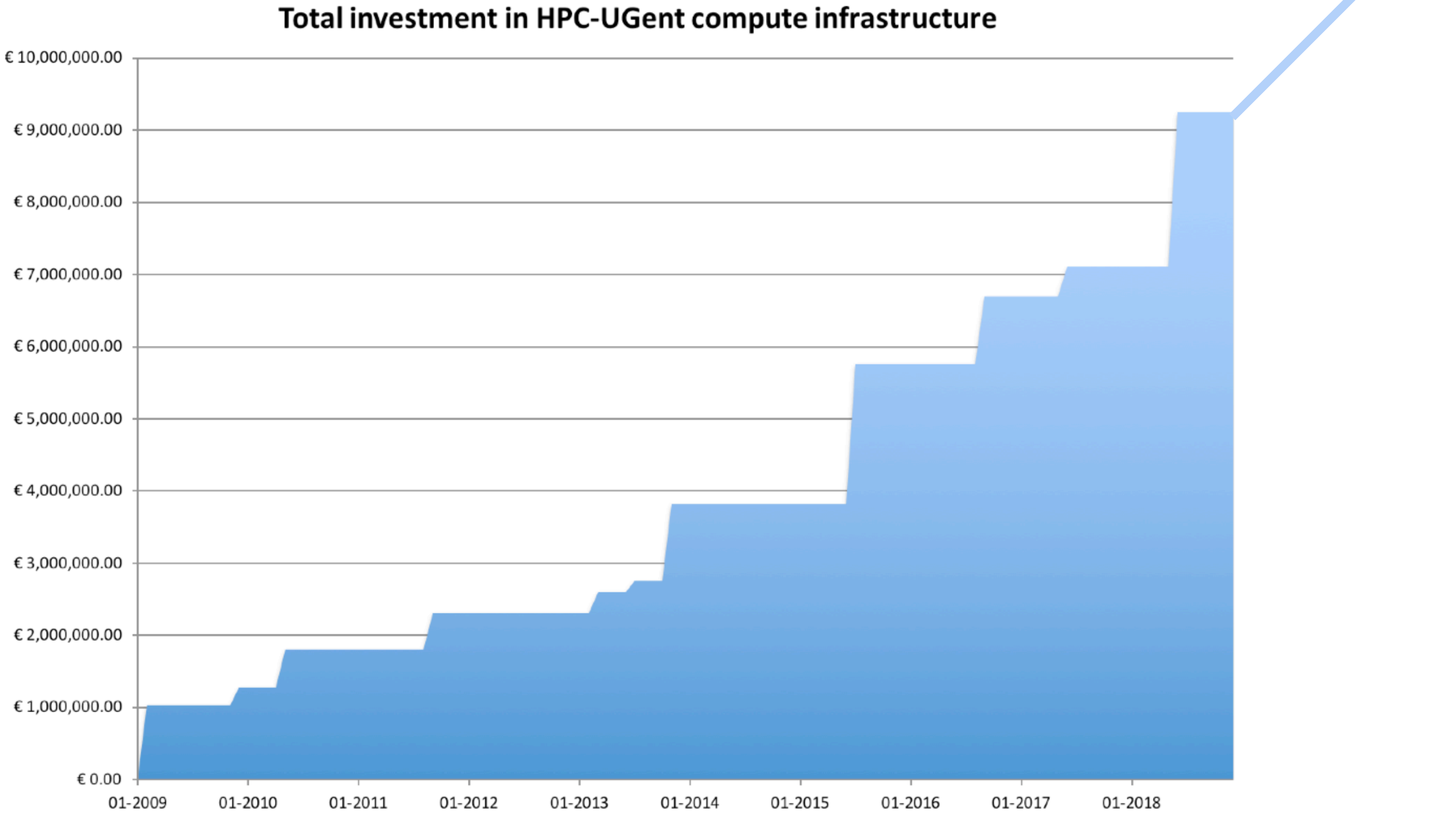
HPC-UGent Tier-2 (STEVIN): central investments

1548 - 1620
°Bruges

STEVIN
HPC
infrastructure



Financing by:

Vlaanderen
is computing

HPC-UGent
users

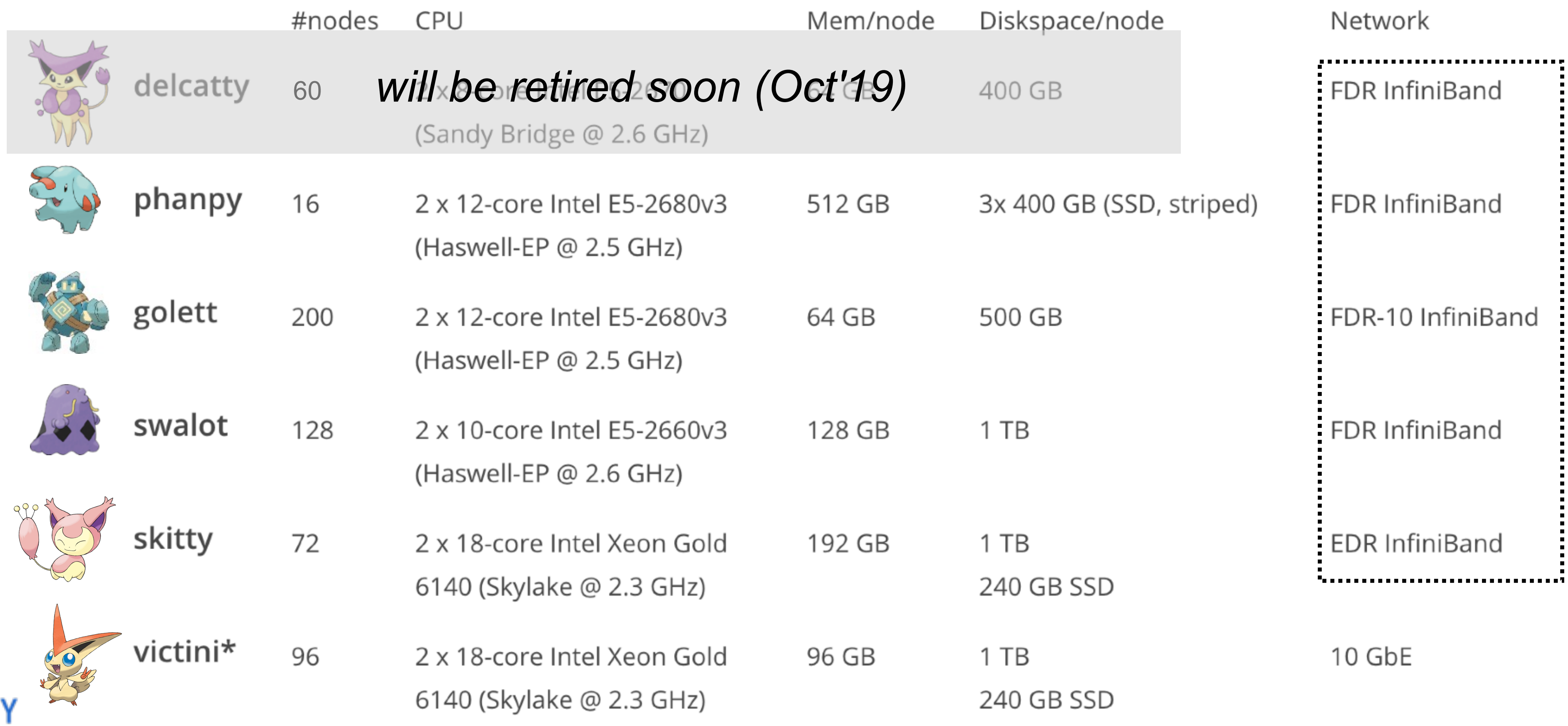
HPC-UGent Tier-2 (STEVIN)

https://www.ugent.be/hpc/en/infrastructure

6 Tier-2 clusters

~600 workernodes, ~15,000 cores

Compute clusters



	#nodes	CPU	Mem/node	Diskspace/node	Network
delcatty	60	2 x 8-core Intel E5-2670 (Sandy Bridge @ 2.6 GHz)	64 GB	400 GB	FDR InfiniBand
phanpy	16	2 x 12-core Intel E5-2680v3 (Haswell-EP @ 2.5 GHz)	512 GB	3x 400 GB (SSD, striped)	FDR InfiniBand
golett	200	2 x 12-core Intel E5-2680v3 (Haswell-EP @ 2.5 GHz)	64 GB	500 GB	FDR-10 InfiniBand
swalot	128	2 x 10-core Intel E5-2660v3 (Haswell-EP @ 2.6 GHz)	128 GB	1 TB	FDR InfiniBand
skitty	72	2 x 18-core Intel Xeon Gold 6140 (Skylake @ 2.3 GHz)	192 GB	1 TB 240 GB SSD	EDR InfiniBand
victini*	96	2 x 18-core Intel Xeon Gold 6140 (Skylake @ 2.3 GHz)	96 GB	1 TB 240 GB SSD	10 GbE

will be retired soon (Oct'19)

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HPC-UGent Tier-2 (STEVIN)

Network connections between nodes ('interconnect')

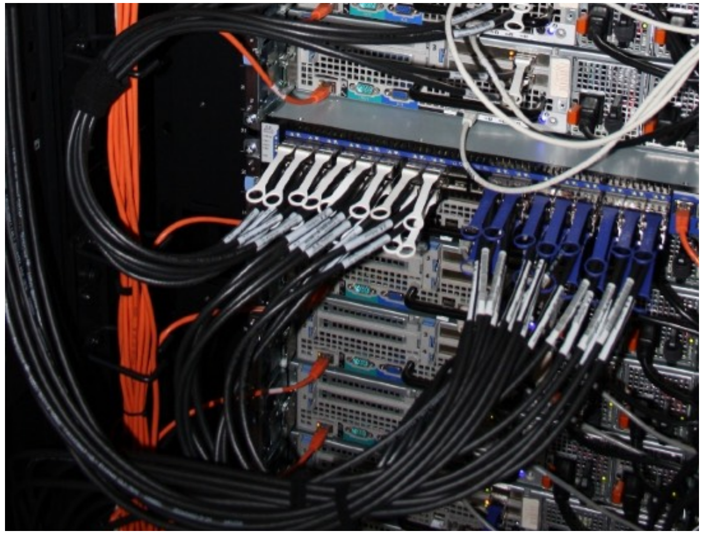
Ethernet: 1-10 Gbit/s

€

for single core/node jobs

(too slow for fast inter-node communication)

Infiniband: 50 - 100 Gbit/s



€€(€)

required for MPI jobs

HPC-UGent Tier-2 (STEVIN)

https://www.ugent.be/hpc/en/infrastructure

"joltik": new GPU cluster (currently in pilot)

- *10 workernodes, each with:*
  - *2x 16-core Intel Xeon Gold 6242 2.8GHz (Cascade Lake)*
  - *230GB (usable) RAM memory in total*
  - *4 NIVIDIA Volta V100 GPUs (32GB GPU memory)*
- *Infiniband interconnect (double EDR)*
- *available software: TensorFlow, PyTorch, GROMACS, ...*

ETA for general availability: early 2020

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VSC Tier-2 infrastructure

Vlaams Supercomputer Centrum

(Flemish Supercomputer Center)

https://www.vscentrum.be/offer

Antwerp University association
Brussels University association
Ghent University association
KU Leuven association Limburg association University-Colleges

auha

universitaire associatie BRUSSEL

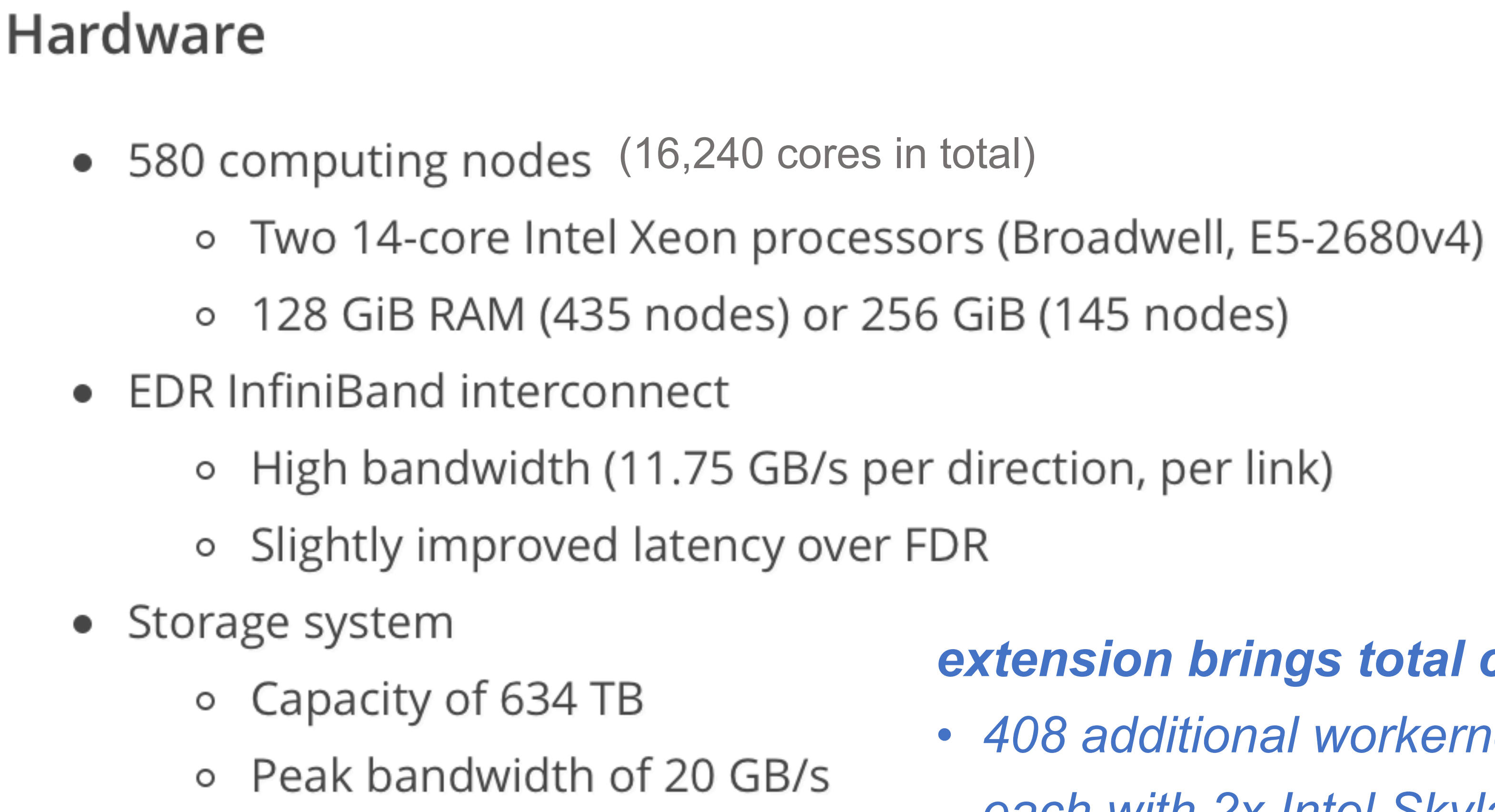
ASSOCIATIE UNIVERSITEIT GENT

ASSOCIATIE KU LEUVEN

ASSOCIATIE UNIVERSITEIT-HOGESCHOLEN LIMBURG

VSC Tier-1 – BrENIAC (@ KUL)

For up to date information, see:
https://www.vscentrum.be/tier1



Hardware

- 580 computing nodes (16,240 cores in total)
  - Two 14-core Intel Xeon processors (Broadwell, E5-2680v4)
  - 128 GiB RAM (435 nodes) or 256 GiB (145 nodes)
- EDR InfiniBand interconnect
  - High bandwidth (11.75 GB/s per direction, per link)
  - Slightly improved latency over FDR
- Storage system
  - Capacity of 634 TB
  - Peak bandwidth of 20 GB/s

extension brings total compute power to ~1.5 PFlops

- *408 additional workernodes, each with 2x Intel Skylake 14-core processors*
- *+ double the scratch storage volume*

VSC Tier-1 – BrENIAC (@ KUL)

For academics (all Flemish research centers):

- *Free of charge*
- Starting Grant (500 node days)
  - Fill in application form (https://www.vscentrum.be/tier1), send it to hpcinfo@kuleuven.be (cc hpc@ugent.be)
- Project access (500 to 5000+ nodedays)
  - 3 evaluation moments per year
  - Application form: see https://www.vscentrum.be/tier1
- **Don't hesitate to contact hpc@ugent.be for help!**

VSC Tier-1 – BrENIAC (@ KUL)

For industry:

- Exploratory access (500 node days)
  - *Free of charge*
  - Contact hpc@ugent.be
- Contract access
  - FWO/UGent/company contract
  - Payed usage (~13 euro / *node* / day)
  - Contact hpc@ugent.be
- More information: https://www.vscentrum.be/tier1

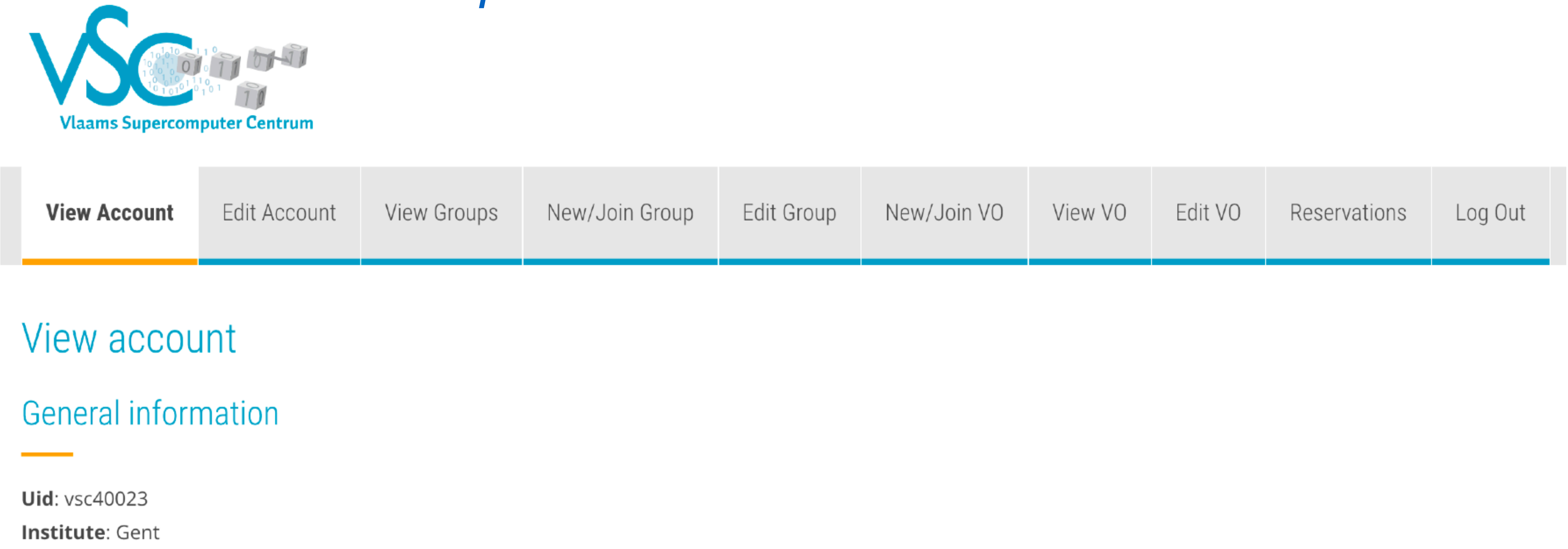
Getting a VSC account

- **See Chapter 2 in HPC-UGent tutorial**
- https://www.ugent.be/hpc/en/access/faq/access
- All users of AUGent can request a VSC account
    - Researchers & staff
    - Master/Bachelor students (after motivation of ZAP)
- **VSC account can be used to access HPC infrastructure on all VSC sites**
- Subscribed to hpc-announce and hpc-users mailing lists
- Beware of using HPC for teaching/exam purposes!
    - No guarantee on HPC availability (power outage/maintenance)
    - Have a backup plan at hand
    - Advisable teaching/exam formula: project work

Managing your VSC account

- You can manage your VSC account via the VSC account page:

https://account.vscentrum.be



View account

General information

Uid: vsc40023

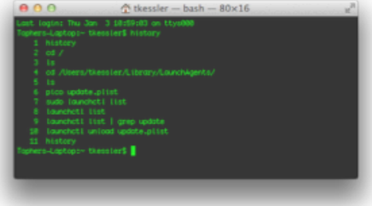
Institute: Gent

Workflow on HPC infrastructure

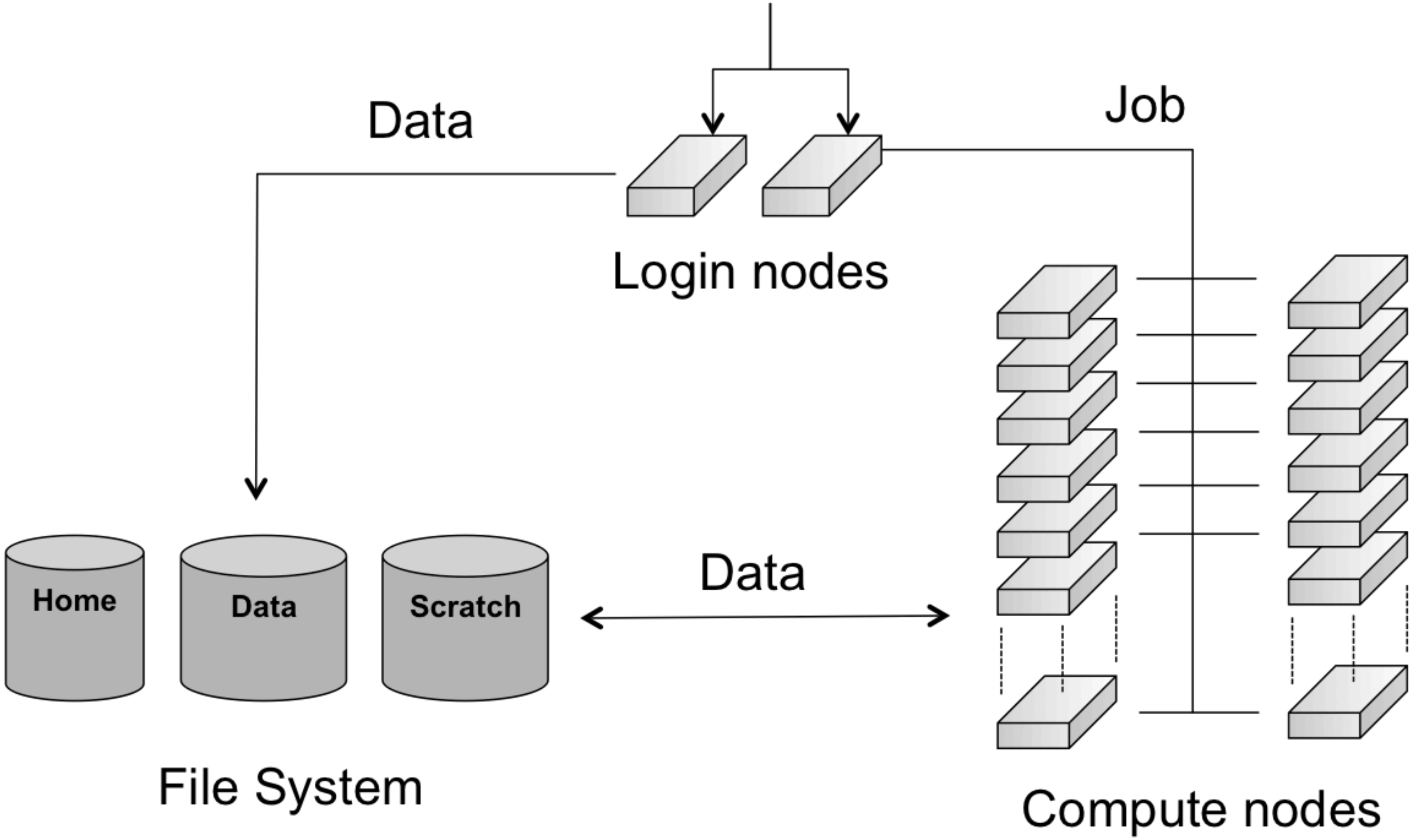
1. Connect to login nodes
2. Transfer your files
3. (Compile your code and test it)
4. Create a job script
5. Submit your job
6. Be patient
   - Your job gets into the queue
   - Your job gets executed
   - Your job finishes
7. Move your results

High-level overview of HPC-UGent infrastructure

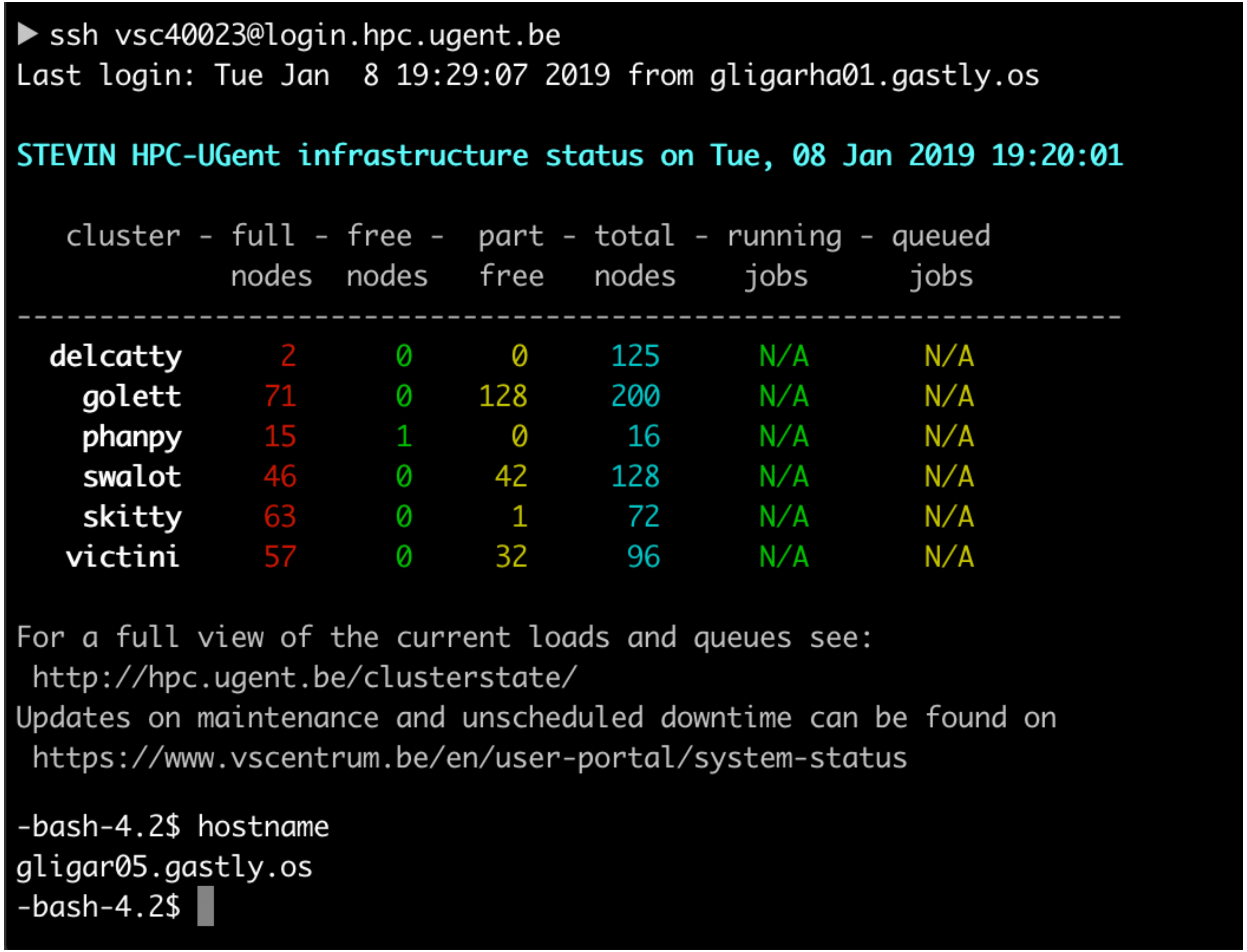
Terminal



```
Last login: Thu Jan  3 10:59:03 on ttys000
Tophers-Laptop:~ tkessler$ history
    1  history
    2  cd /
    3  ls
    4  cd /Users/tkessler/Library/LaunchAgents/
    5  ls
    6  pico update.plist
    7  sudo launchctl list
    8  launchctl list
    9  launchctl list | grep update
   10  launchctl unload update.plist
   11  history
Tophers-Laptop:~ tkessler$ 
```



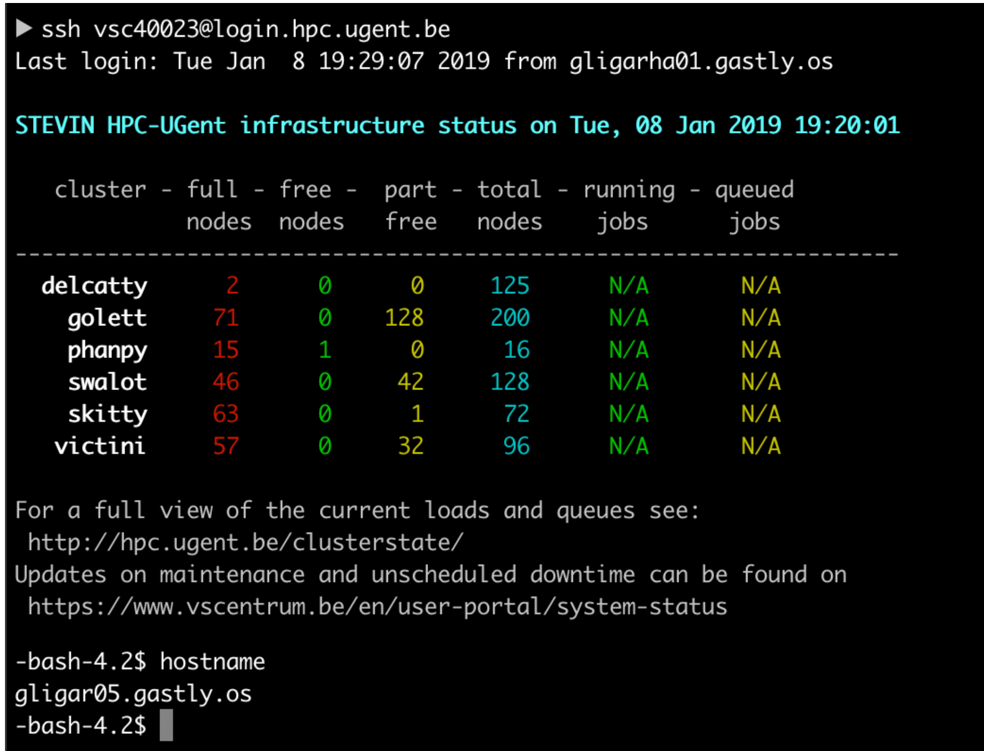
Connected to an HPC-UGent login node



```
▶ ssh vsc40023@login.hpc.ugent.be
Last login: Tue Jan  8 19:29:07 2019 from gligarha01.gastly.os

STEVIN HPC-UGent infrastructure status on Tue, 08 Jan 2019 19:20:01

   cluster - full - free -  part - total - running - queued
             nodes  nodes   free   nodes    jobs      jobs
-------------------------------------------------------------------
  delcatty      2      0      0     125      N/A       N/A
    golett     71      0    128     200      N/A       N/A
    phanpy     15      1      0      16      N/A       N/A
    swalot     46      0     42     128      N/A       N/A
    skitty     63      0      1      72      N/A       N/A
   victini     57      0     32      96      N/A       N/A

For a full view of the current loads and queues see:
 http://hpc.ugent.be/clusterstate/
Updates on maintenance and unscheduled downtime can be found on
 https://www.vscentrum.be/en/user-portal/system-status

-bash-4.2$ hostname
gligar05.gastly.os
-bash-4.2$
```

Basic Linux tutorial

- **a basic Linux tutorial is available in the HPC-UGent documentation**, available at https://www.ugent.be/hpc/en/support/documentation.htm
- covers basic usage of the shell environment
- explains commonly used commands
- focus on HPC context & job scripts
- includes a couple of basic exercises
- for questions or problems, don't hesitate to contact `hpc@ugent.be` !



```
▶ ssh vsc40023@login.hpc.ugent.be
Last login: Tue Jan  8 19:29:07 2019 from gligarha01.gastly.os

STEVIN HPC-UGent infrastructure status on Tue, 08 Jan 2019 19:20:01

   cluster - full - free -  part - total - running - queued
             nodes  nodes   free   nodes     jobs      jobs
---------------------------------------------------------------------
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    golett     71      0    128     200      N/A       N/A
    phanpy     15      1      0      16      N/A       N/A
    swalot     46      0     42     128      N/A       N/A
    skitty     63      0      1      72      N/A       N/A
   victini     57      0     32      96      N/A       N/A

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-bash-4.2$ hostname
gligar05.gastly.os
-bash-4.2$ █
```

Workflow on HPC infrastructure

1. **Connect to login nodes**
2. **Transfer your files**
3. (Compile your code and test it)

See Chapter 3 in HPC-UGent tutorial

- Users interact with the HPC infrastructure via the login nodes
- No direct access to the workernodes
  (except when a job is running on it)

- Your job gets executed
- Your job finishes

7. **Move your results**

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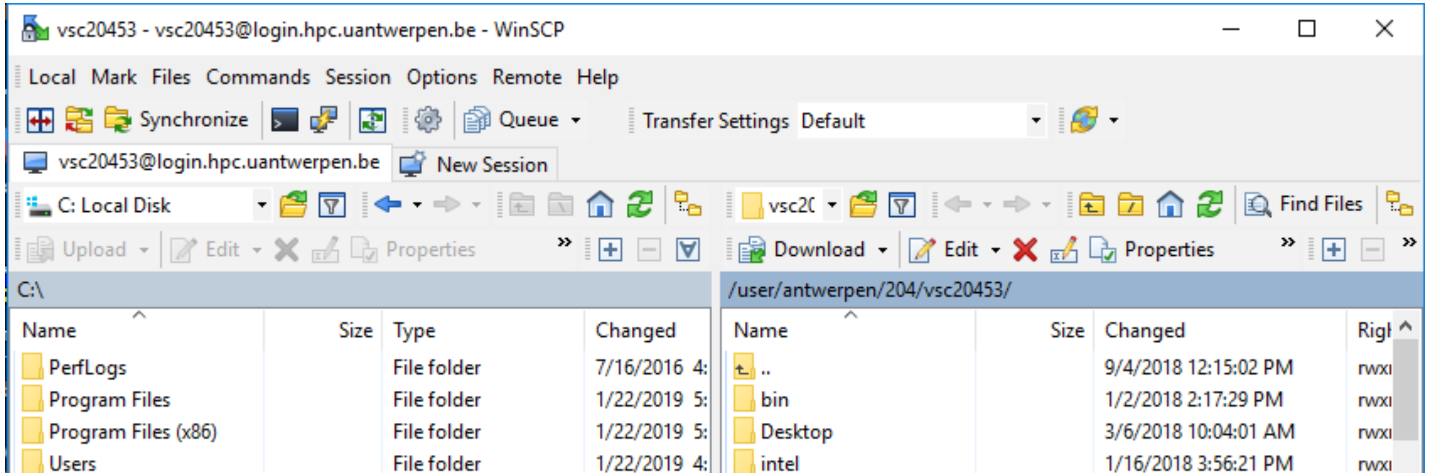
Transferring files to/from the HPC-UGent infrastructure

- **see section 3.2 in HPC-UGent tutorial for detailed information**
- via login nodes
- on Linux or macOS:
  - using '`scp`' in terminal window (use '`scp -r`' for directories)
    - or '`rsync`' for large transfers (can be restarted)
  - or graphical tool like built-in file manager or Cyberduck
- on Windows: WinSCP tool (left: own system; right: HPC; drag 'n drop)


vsc20453 - vsc20453@login.hpc.uantwerpen.be - WinSCP
Local Mark Files Commands Session Options Remote Help
Synchronize
Queue
Transfer Settings Default
vsc20453@login.hpc.uantwerpen.be
New Session
C: Local Disk
vsc2(
Find Files
Upload
Edit
Properties
Download
Edit
Properties

C:\

Name	Size	Type	Changed
PerfLogs		File folder	7/16/2016 4:
Program Files		File folder	1/22/2019 5:
Program Files (x86)		File folder	1/22/2019 5:
Users		File folder	1/22/2019 4:

/user/antwerpen/204/vsc20453/

Name	Size	Changed	Rigl
..		9/4/2018 12:15:02 PM	rwxi
bin		1/2/2018 2:17:29 PM	rwxi
Desktop		3/6/2018 10:04:01 AM	rwxi
intel		1/16/2018 3:56:21 PM	rwxi

Workflow on HPC infrastructure

1. Connect to login nodes
2. Transfer your files
3. (Compile your code and test it)
4. **Create a job script**
5. Submit your job

- Choose correct PBS directives (Chapter 4, 11)
- Load software modules (Chapter 4)
- Useful environment variables (Chapter 4)
- Access files on shared filesystems (Chapter 6)

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What is a job script?

```
#!/bin/bash
echo "hello world"
```

A job (shell) script is a **text file** that specifies:

- the ***resources*** that are required by the calculation

  (number of nodes/cores, amount of memory, how much time, ...)
- the ***software*** that is used for the calculation

  (via `module load` commands)
- the steps that should be done to execute the calculation

  (starting from `$HOME`), specified as **shell *commands***, typically:

  1) staging in of input files

  2) running the calculation

  3) staging out of results

Job scripts: required resources via #PBS directives

```
#!/bin/bash
#PBS -N solving_42                ## job name
#PBS -l nodes=1:ppn=4             ## single-node job, 4 cores
#PBS -l walltime=10:00:00         ## max. 10h of wall time
#PBS -l vmem=50gb                 ## max. 50GB virtual memory
<rest of job script>
```

- required resources can be specified via `#PBS` lines in job script (or via qsub)
- **maximum walltime: 72 hours**
- for longer jobs, use *checkpointing*
  - preferably internal/application checkpointing
  - external checkpointing by submitting jobs via *csub*
    - see Chapter 14 in HPC-UGent tutorial

Job scripts: software modules

- All user-end software is made available via *modules*
- Modules prepare the environment for using the software
- Module naming scheme: `<name>/<version>-<toolchain>[-<suffix>]`

Load a module to use the software:

```
$ module load Python/3.6.6-intel-2018b
```

See currently loaded modules using:

`$ module list` or `$ ml`

Get overview of available modules using:

`$ module avail` or `$ ml av`

- Only mix modules built with the same (version of) compiler toolchain.
  e.g., `intel` (Intel compilers, Intel MPI, Intel MKL (BLAS, LAPACK))
- **See also section 4.1 in HPC-UGent tutorial**

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Job scripts: useful environment variables

(most of these are only defined in the context of jobs!)

- **`$PBS_JOBID`**
  - job id of running job
- **`$PBS_O_WORKDIR`**
  - directory from which job was submitted on login node
  - common to use '`cd $PBS_O_WORKDIR`' at beginning of job script
- **`$PBS_ARRAYID`**
  - array id of running job; only relevant when submitting array jobs (`qsub -t`)
- **`$TMPDIR`**
  - Local directory specific to running job
  - **Cleaned up automatically when job is done!**
- **`$EBROOTFOO, $EBVERSIONFOO`**
  - root directory/version for software package Foo
  - only available when module for Foo is loaded

Job scripts: input data & filesystems

- See Section 6.2 in HPC-UGent tutorial
- Think about input/output:
  - How will you *stage in* your data and input files?
  - How will you *stage out* your output files?
- Manually (on login nodes) vs automatically (as a part of job script)

- **Home filesystem**: only for limited number of small files & scripts
- **Data filesystem (`$VSC_DATA*`)**: ‘long-term’ storage, large files
- **Scratch filesystems (`$VSC_SCRATCH*`)**: for ‘live’ input/output data in jobs

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Storage quota

- home directory (`$VSC_HOME`): 3GB (fixed)
- personal data directory (`$VSC_DATA`): 25GB (fixed)
- personal scratch directory (`$VSC_SCRATCH`): 25GB (fixed)
- current quota usage can be consulted on VSC accountpage

  https://account.vscentrum.be
- **more storage quota (GBs, TBs) available for virtual organisations (VOs)**

  see Section 6.7 in HPC-UGent tutorial
- additional quota can be requested via https://account.vscentrum.be/django/vo/edit
- shared directories with VO members: `$VSC_DATA_VO`, `$VSC_SCRATCH_VO`
- personal VO subdirectories: `$VSC_DATA_VO_USER`, `$VSC_SCRATCH_VO_USER`

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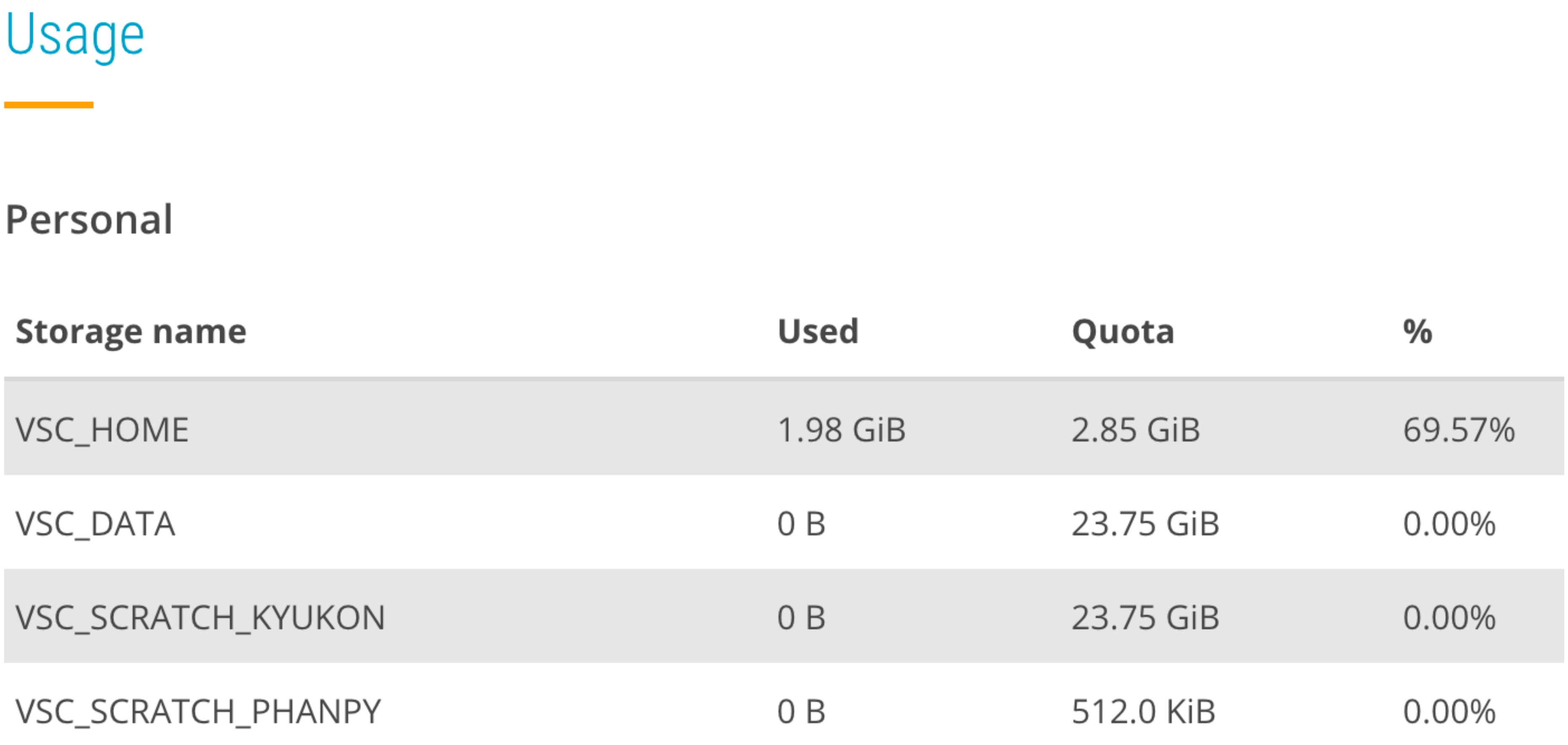
Current storage usage - personal directories

- consult VSC accountpage - *https://account.vscentrum.be* ("**View Account**" tab) *(for now, only data volumes, not number of files (inode quota))*



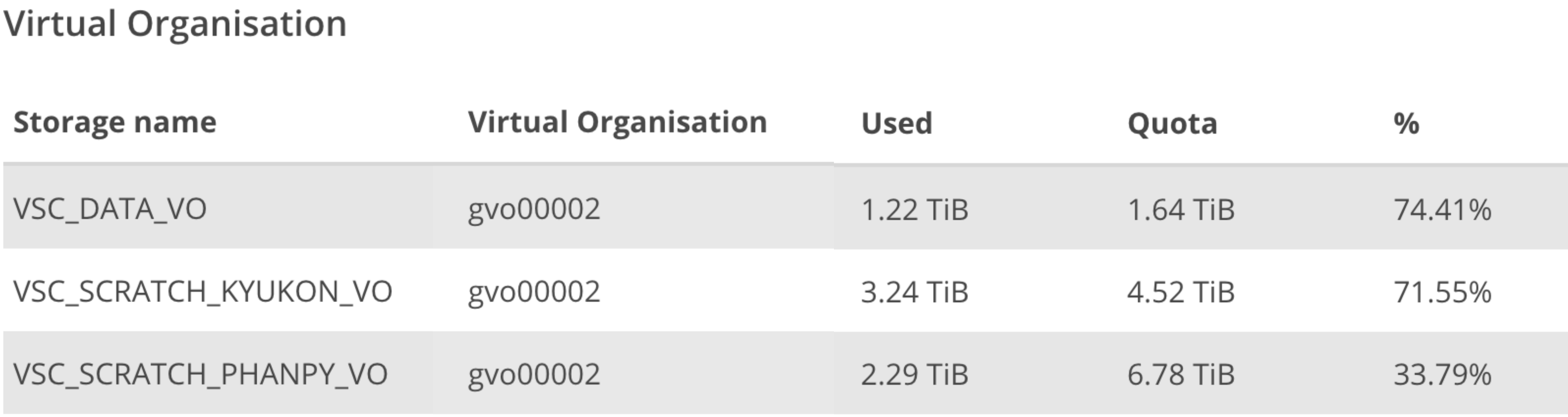
Usage

Personal

Storage name	Used	Quota	%
VSC_HOME	1.98 GiB	2.85 GiB	69.57%
VSC_DATA	0 B	23.75 GiB	0.00%
VSC_SCRATCH_KYUKON	0 B	23.75 GiB	0.00%
VSC_SCRATCH_PHANPY	0 B	512.0 KiB	0.00%

Current storage usage - own VO directories

- consult VSC accountpage - *https://account.vscentrum.be* ("**View Account**" tab) *(for now, only data volumes, not number of files (inode quota))*

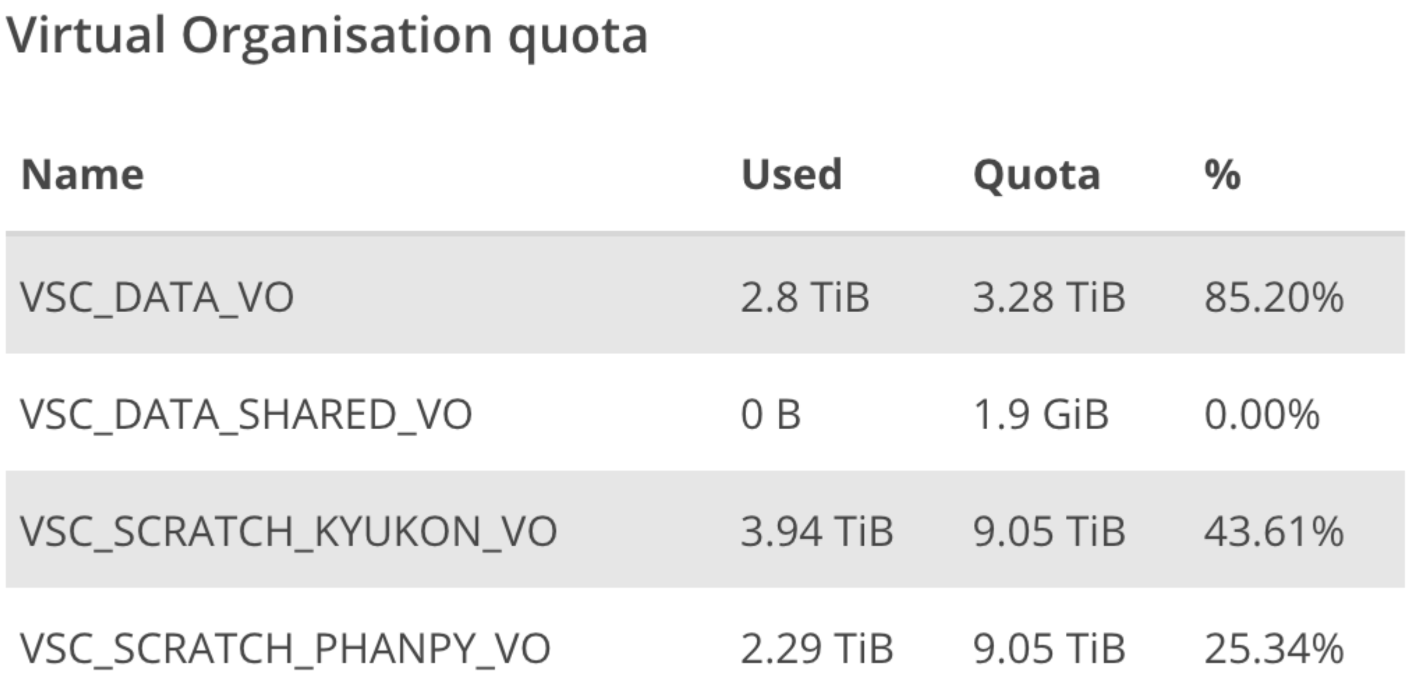


Virtual Organisation

Storage name	Virtual Organisation	Used	Quota	%
VSC_DATA_VO	gvo00002	1.22 TiB	1.64 TiB	74.41%
VSC_SCRATCH_KYUKON_VO	gvo00002	3.24 TiB	4.52 TiB	71.55%
VSC_SCRATCH_PHANPY_VO	gvo00002	2.29 TiB	6.78 TiB	33.79%

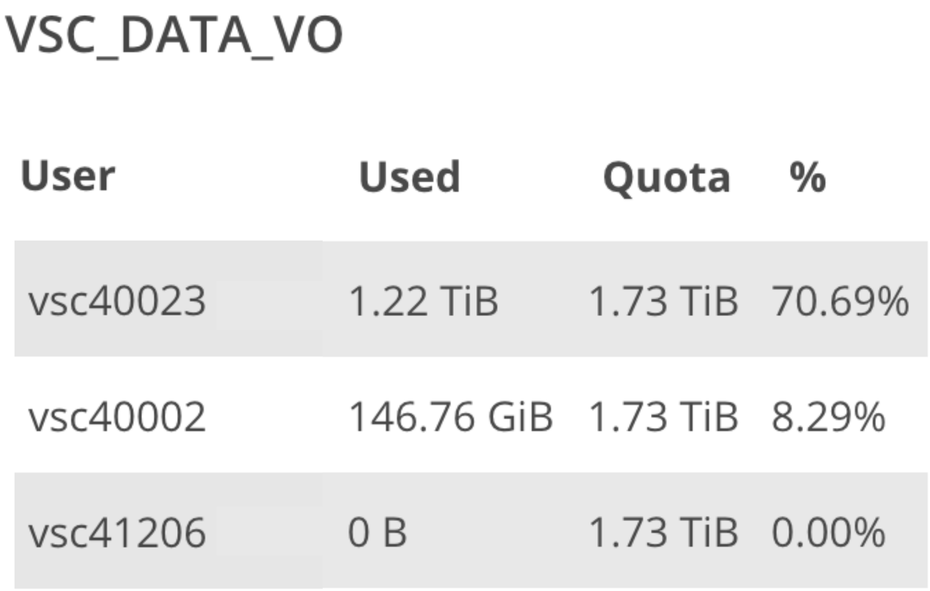
Current storage usage - total VO usage

- consult VSC accountpage - *https://account.vscentrum.be* (**"View VO"** tab) *(for now, only data volumes, not number of files (inode quota))*
- **detailed info per VO member can only be consulted by VO administrators!**



Virtual Organisation quota

Name	Used	Quota	%
VSC_DATA_VO	2.8 TiB	3.28 TiB	85.20%
VSC_DATA_SHARED_VO	0 B	1.9 GiB	0.00%
VSC_SCRATCH_KYUKON_VO	3.94 TiB	9.05 TiB	43.61%
VSC_SCRATCH_PHANPY_VO	2.29 TiB	9.05 TiB	25.34%



VSC_DATA_VO

User	Used	Quota	%
vsc40023	1.22 TiB	1.73 TiB	70.69%
vsc40002	146.76 GiB	1.73 TiB	8.29%
vsc41206	0 B	1.73 TiB	0.00%

Job scripts: full example (single-core job)

```
#!/bin/bash
#PBS -N count_example         ## job name
#PBS -l nodes=1:ppn=1         ## single-node job, single core
#PBS -l walltime=2:00:00      ## max. 2h of wall time

module load Python/3.6.6-intel-2018b
# copy input data from location where job was submitted from
cp $PBS_O_WORKDIR/input.txt $TMPDIR
# go to temporary working directory (on local disk) & run
cd $TMPDIR
python -c "print(len(open('input.txt').read()))" > output.txt
# copy back output data, ensure unique filename using $PBS_JOBID
cp output.txt $VSC_DATA/output_${PBS_JOBID}.txt
```

Job scripts: full example (multi-node job)

```
#!/bin/bash
#PBS -N mpi_hello             ## job name
#PBS -l nodes=2:ppn=all       ## 2 nodes, all cores per node
#PBS -l walltime=2:00:00      ## max. 2h of wall time

module load intel/2018b
module load vsc-mympirun

# go to working directory, compile and run MPI hello world
cd $PBS_O_WORKDIR
mpicc mpi_hello.c -o mpi_hello
mympirun ./mpi_hello
```

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Jobs scripts: generated output files

- **Your job script may produce informative/warning/error messages.**
  - Two output files are created for each job: stdout (*.o) + stderr (*.e)
  - Located in directory where job was submitted from (by default)
  - Messages produced by a particular command in the job script can be "caught" and redirected to a particular file instead.

    ```
    example > out.log 2> err.log
    ```

    (see section 5.1 of our Linux tutorial for more details)
- In addition, the software used for the calculation may have generated additional output files (very software-specific).

Workflow on HPC infrastructure

1. Connect to login nodes

- Chapter 4 in course notes
- Demo: qsub, qstat, qdel
- Job scheduling

4. Create a job script
5. Submit your job
6. Be patient
   - Your job gets into the queue
   - Your job gets executed
   - Your job finishes
7. Move your results

Demo: qsub, qstat, qdel

- Submit job scripts from a login node to a cluster for execution using **qsub**:

```
$ module swap cluster/golett
$ qsub example.sh
12345.master19.golett.gent.vsc
```

- An overview of the active jobs is available via **qstat**:

```
$ qstat
Job id           Name     User     Time Use      S  Queue
--------------   ------   ----------   --------  -  -----
12345.master19   example  vsc40000    07:39:30  R  long
```

- To remove a job that is no longer necessary, use **qdel**:

```
$ qdel 12345
```

Job scheduling

- All our clusters use a *fair-share* scheduling policy.
- No guarantees on when job will start, so **plan ahead**!
- Job priority is determined by:
  - *historical usage*
    - aim is to balance usage over users
    - infrequent/frequent users => higher/lower priority
  - *requested resources* (# nodes/cores, walltime, memory, ...)
    - larger resource request => lower priority
  - *time waiting in queue*
    - queued jobs get higher priority over time
  - *user limits*
    - avoid that a single user fills up an entire cluster

Embarrassingly parallel jobs

- Use case: lots of ((very) short) single-core tasks
- Submitting lots of tiny jobs (minutes of walltime) is not a good idea
  - overhead for each job (node health checks), lots of bookkeeping (job scripts, failed jobs, output files)
- Better approach:
  - Array jobs
    - Single job script, but still lots of submitted jobs
    - Each job is assigned a unique id (`$PBS_ARRAYID`); can be used to select input file, parameters, …
  - GNU parallel (https://www.gnu.org/software/parallel/parallel_tutorial.html)
    - General-purpose tool to easily running shell commands in parallel with different inputs
    - Use '`parallel`' command in your job script
  - **Worker** (see Chapter 12 in HPC-UGent tutorial *https://www.ugent.be/hpc/en/support/documentation.htm*)
    - One single job that processes a bunch of tasks (multi-core or even multi-node)
    - Job script is parameterized, submit with '`wsub`' rather than '`qsub`'

Software installations

To submit a request for software installation:

https://www.ugent.be/hpc/en/support/software-installation-request

Always include:

- software name and website
- location to download source files
  - or make install files available in your account
- build instructions (if you have them)
- a simple test case with expected output
  - including instructions on how to run it

Requests may take a while to process; make the request sooner rather than later!

http://easybuilders.github.io/easybuild

Questions, problems, getting help

Don't hesitate to contact HPC-UGent support: hpc@ugent.be

Always include:

- VSC login id
- clear description of problem (or question)
- location of job script and output/error files in your account
    - don’t send them in attachment, we prefer to look at it ‘in context’
- job IDs, which cluster

Preferably use your UGent email address.

Alternatives:

- short meeting (for complex problems, big projects)
- hpc-users mailing list