Introduction to HPC-UGent

18 Nov 2022

GHENT UNIVERSITY

https://ugent.be/hpc

hpc@ugent.be

VLAAMS SUPERCOMPUTER CENTRUM

Vlaanderen is supercomputing

Documentation

- An HPC-UGent tutorial is available on the HPC-UGent website
- Download it here: https://www.ugent.be/hpc/en/support/documentation.htm
- We will specifically use information from these chapters:

1) Introduction to HPC

2) Getting an HPC account

3) Connecting to the HPC infrastructure

4) Running batch jobs

6) Running jobs with input/output data

8) Using the HPC-UGent web portal

11) Fine-tuning job specifications

22) HPC-UGent interactive and debug cluster

HPC-UGent in a nutshell

- Part of ICT Department of Ghent University (DICT)
- 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

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The HPC-UGent team

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Team lead

Stijn De Weirdt
Technical lead

Wouter Depypere
System administration

Kenneth Hoste
User support & training

Kenneth Waegeman
System administration (storage)

Andy Georges
System administration

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System administration (cloud)

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User support

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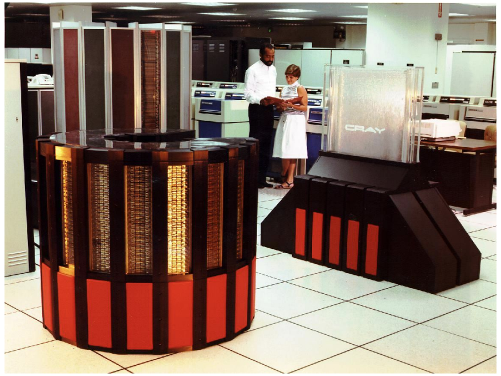
System administration

What is High-Performance Computing (HPC)?

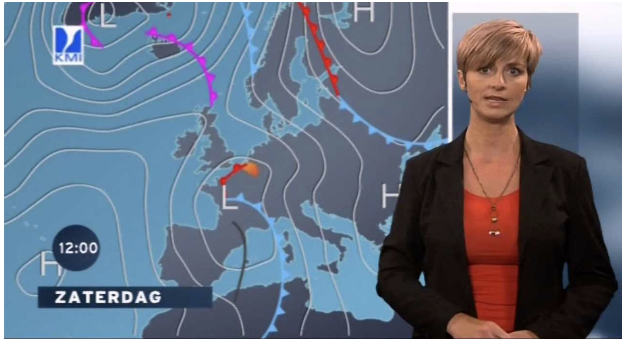
- **High Performance Computing (HPC)** is running computations on a supercomputer, a system at the frontline of contemporary processing capacity – particularly in terms of size, supported degree of ***parallelism***, network interconnect, and (total) available memory & disk space.
- A **computer cluster** consists of a set of loosely or tightly connected computers (also called (worker)nodes) that work together so that in many respects they can be viewed as a single system.
- HPC is also known as “supercomputing”, or more broadly “scientific computing”

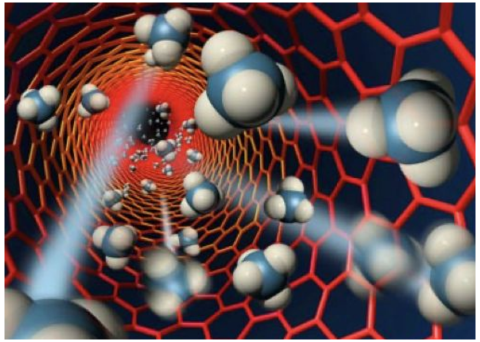
What is High-Performance Computing (HPC)?

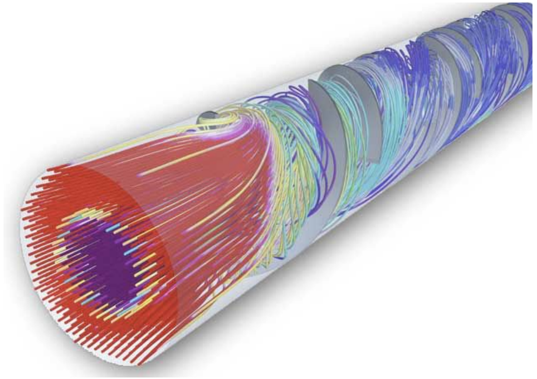
harness power of multiple interconnected cores/nodes/processing units



What are supercomputers used for?



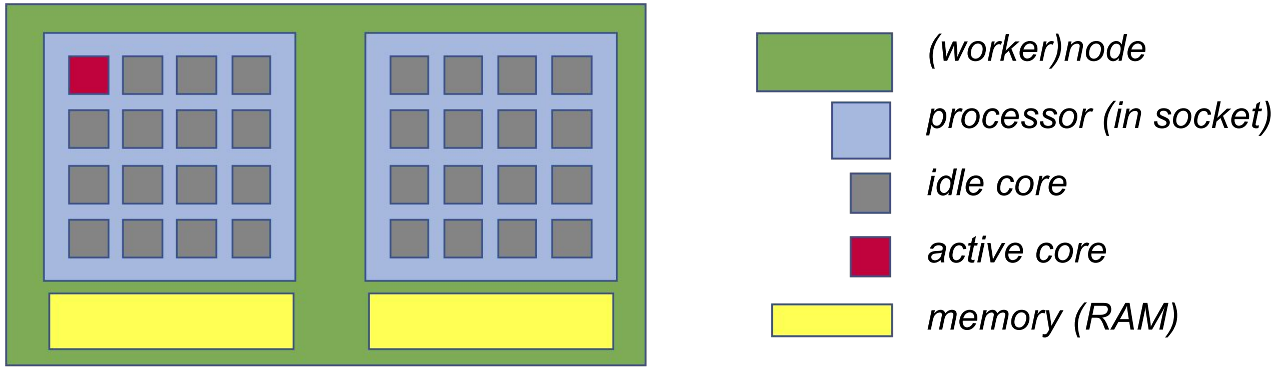




Terminology: cores, CPUs, processors, (worker)nodes

Modern servers, also referred to as **(worker)nodes** in the context of HPC, include one or more *sockets*, each housing a **multi-core processor** (next to memory, disk(s), network cards, …). A modern (micro)processor consists of **multiple cores** that are used to execute computations.

Example:
a single workernode with two 16-core processors running a single core job



Not shown here: local disk, network cards, GPUs, …

Parallel vs sequential software (single-node or multi-node)

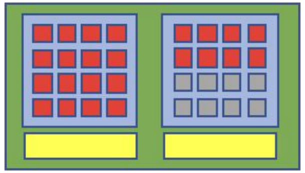
In **parallel** software, many calculations are carried out simultaneously. This is based on the principle that large problems can often be divided into smaller tasks, which are then solved concurrently ("in parallel").

Example: OpenFOAM can easily use 160 cores at the same time to solve a CFD problem.

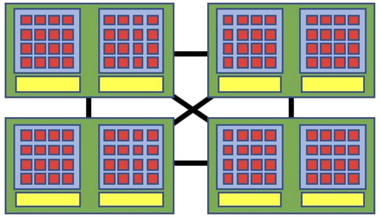
There are two common parallel programming paradigms (among others):

- **OpenMP** for shared memory systems (multi-threading) → on cores of a *single* node
- **MPI** for distributed memory systems (multi-processing) → on cores of multiple nodes

OpenMP software can use multiple or all cores in a single node



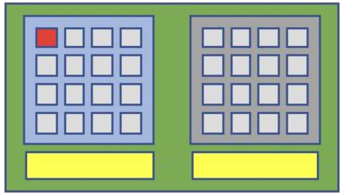
MPI software can use (all) cores in multiple nodes



Parallel vs **sequential** software (single-core)

Sequential (a.k.a. serial) software does not do calculations in parallel,

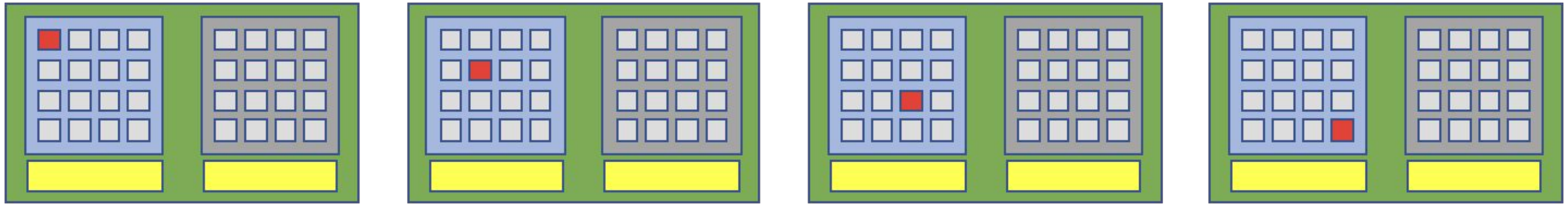
i.e. it only uses one **single core** of a single workernode.



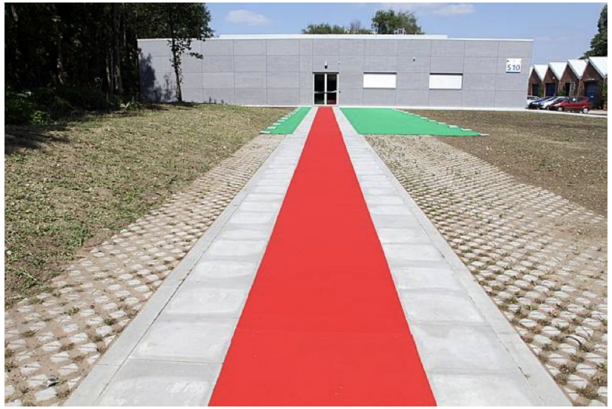
This type of software does not run faster by just throwing cores (or nodes) at it...

But, you can run multiple instances at the same time!

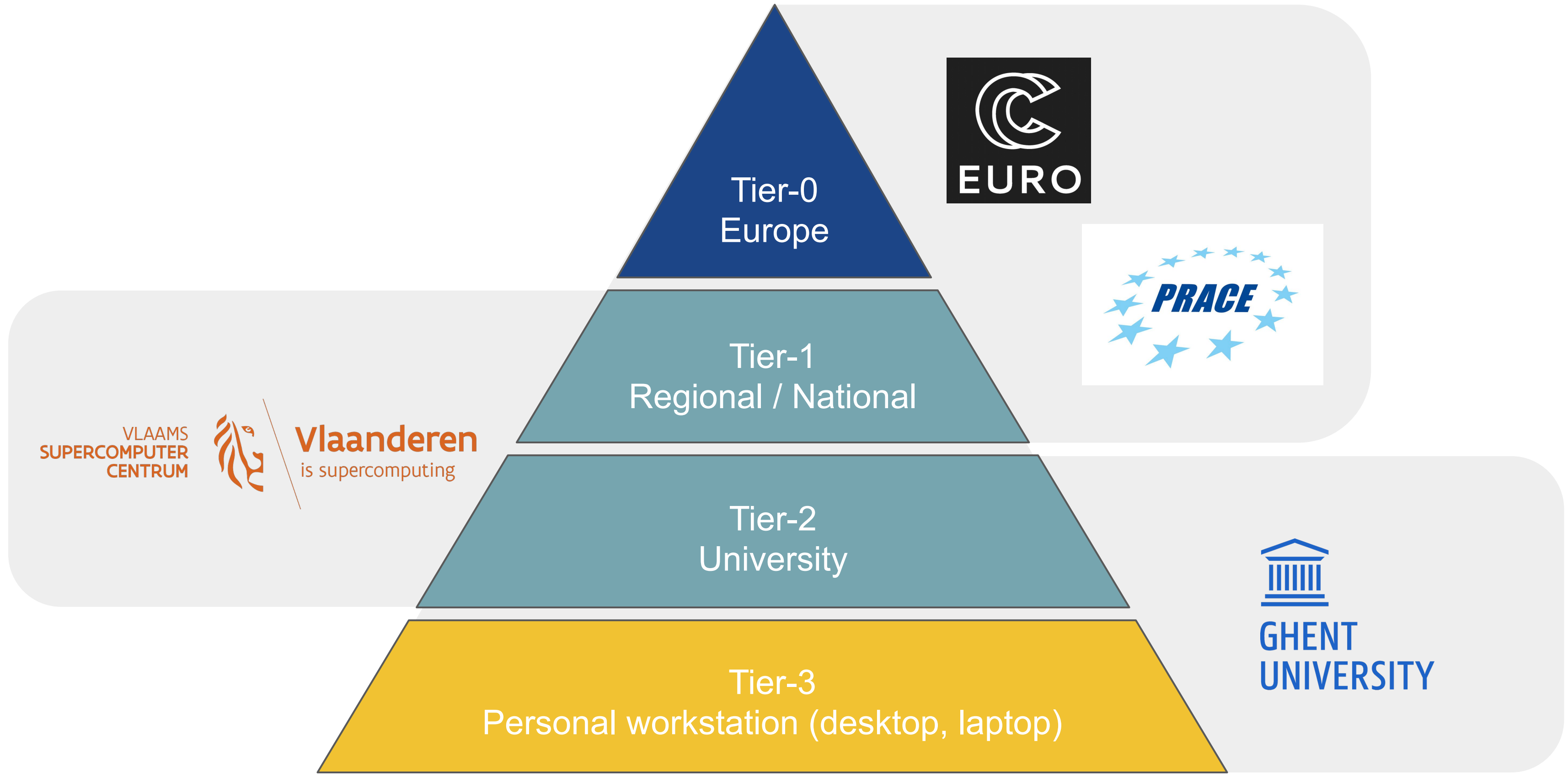
Example: running a Python script 100 times on 100 cores to quickly analyse 100 datasets



Centralised hardware in UGent datacenter (S10 @ Sterre)



Different "tiers" of computational science


Tier-0
Europe
Tier-1
Regional / National
Tier-2
University
Tier-3
Personal workstation (desktop, laptop)
EURO
PRACE
VLAAMS SUPERCOMPUTER CENTRUM
Vlaanderen is supercomputing
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HPC-UGent Tier-2 infrastructure

- HPC-UGent Tier-2 infrastructure consists of **8 clusters** (+ login nodes, shared storage, …)
- Different types of clusters:
  - CPU-only batch cluster (no high-speed network, no fast access to shared storage)
  - CPU-only compute clusters
  - GPU clusters
  - CPU-only interactive + debug cluster
- **Available for academic researchers free of charge**, funding through FWO; usage by industry via a pay-as-you-use contract (after free exploratory period)
- All running **Red Hat Enterprise Linux 8** (RHEL8) as operating system

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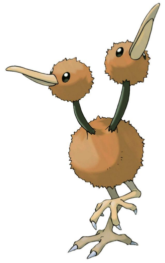
https://www.ugent.be/hpc/en/infrastructure

HPC-UGent Tier-2 batch cluster: victini

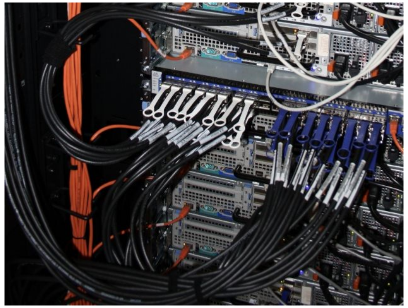
- 96 workernodes, each with 36 cores (Intel Skylake) + ~88GB of memory + local disk
- **No high-speed network** between workernodes (10-Gbit Ethernet)
- **No fast connection to shared filesystems** (only via NFS)
- **Default cluster** (at least currently, will change to *doduo* cluster soon!)
- Only recommended for **single-core / single-node jobs that are *not* I/O-intensive**

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

HPC-UGent Tier-2 compute clusters

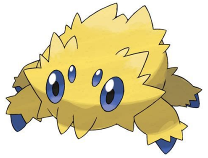


- `swalot`: 128 nodes, each with 20 cores (Intel Haswell) + ~125GB of memory
- `skitty`: 72 nodes, each with 36 cores (Intel Skylake) + ~180GB of memory
- `kirlia`: 16 nodes, each with 36 cores (Intel Cascade Lake) + **~740GB** of memory
- `doduo`: 128 nodes, each with **96 cores (AMD Rome)** + 250GB of memory
  (soon to be the default cluster!)
- All with:
  - high-speed Infiniband network between nodes
  - fast access to shared filesystems
  - local disk



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

HPC-UGent Tier-2 GPU clusters



- `joltik`: 10 nodes,
  each with 32 CPU cores (Intel Cascade Lake),
  4 NVIDIA V100 GPUs (32GB of GPU memory),
  ~250GB of system memory

- `accelgor`: 9 nodes,
  each with 48 CPU cores (AMD Milan),
  4 NVIDIA A100 GPUs (80GB of GPU memory),
  ~500GB of system memory

- Both with high-speed network, fast access to shared filesystems, local disk

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

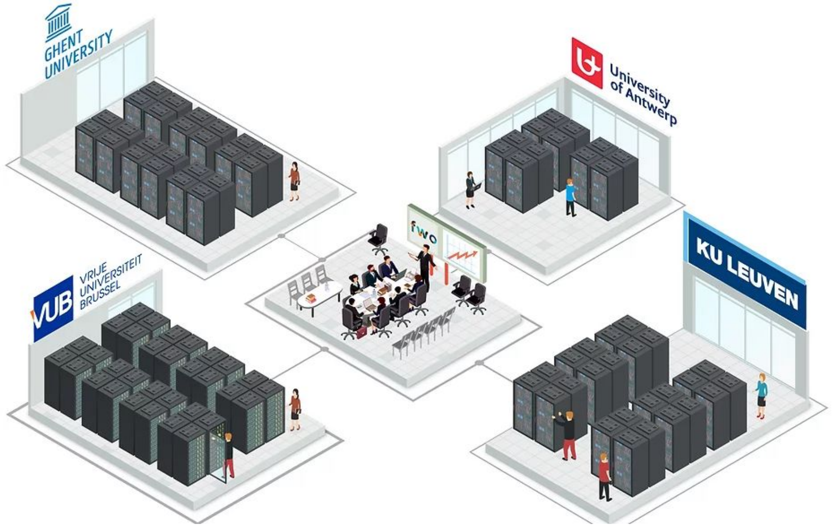
HPC-UGent Tier-2 interactive + debug cluster: slaking

- 10 nodes, each with 24 cores (Intel Haswell) + ~500GB of memory
- Incl. high-speed network, fast access to shared storage, local disk
- Recycled hardware from old `phanpy` cluster (retired in March 2021)
- **Heavily oversubscribed!** More running jobs => all jobs run slower (due to CPU sharing)
- **Strict user limits:**
  - Max. 3 jobs running, 5 jobs in queue
  - 8 cores + 27GB of memory in use (in total)
- ⇒ **No waiting time for jobs to start**! Perfect for debug jobs, or interactive use (web portal)
- See also dedicated Chapter 22 in HPC-UGent tutorial

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

VSC Tier-2 infrastructure

- You can use your VSC account to access HPC infrastructure provided by other VSC hubs
- Your `$VSC_HOME` and `$VSC_DATA` directories are available on each of these systems



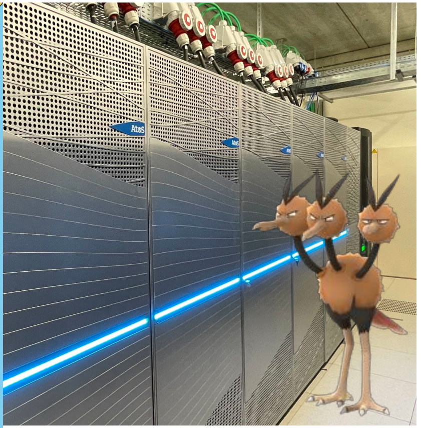
https://docs.vscentrum.be/en/latest/hardware.html

VSC Tier-1 compute cluster "Hortense"

phase I: `dodrio`

compute@vscentrum.be

- **Hosted, operated, and supported by HPC-UGent team**
- 336 CPU-only nodes, each with 128 AMD Rome cores + 256/512GB of memory
- 20 GPU nodes, each with 48 AMD Rome cores + 4x NVIDIA A100 (40GB) + 256GB mem.
- High-speed Infiniband network (HDR-100) + 3PB of dedicated scratch storage



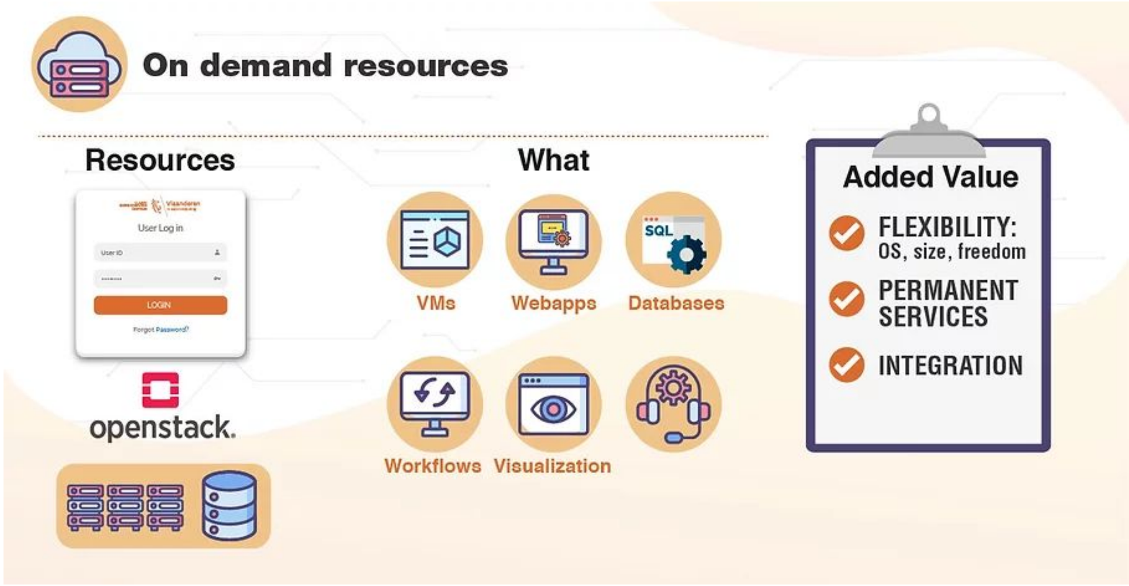
- **Project-based access** (free of charge, funded by FWO)
- 3 cut-off dates per year for submitting project proposals
- Project duration is typically 8 months
- 500k - 5M core hours (CPU-only) or 1k - 25k GPU hours

https://www.vscentrum.be/compute

https://docs.vscentrum.be/en/latest/gent/tier1_hortense.html

VSC Tier-1 cloud

- **Project-based access**
- Free of charge
- **Self-managed virtual machines**
- For use cases that are not a good fit for compute clusters
- More info: https://www.vscentrum.be/cloud
- Contact: cloud@vscentrum.be



Getting a VSC account

- All members of UGent association can request a VSC account
  - Researchers & staff
  - Master/Bachelor students
- **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 (due unexpected power outage, maintenance, …)
  - Have a backup plan at hand
  - Advisable teaching/exam formula: project work
- See also Chapter 2 in HPC-UGent tutorial

https://www.ugent.be/hpc/en/access/faq/access

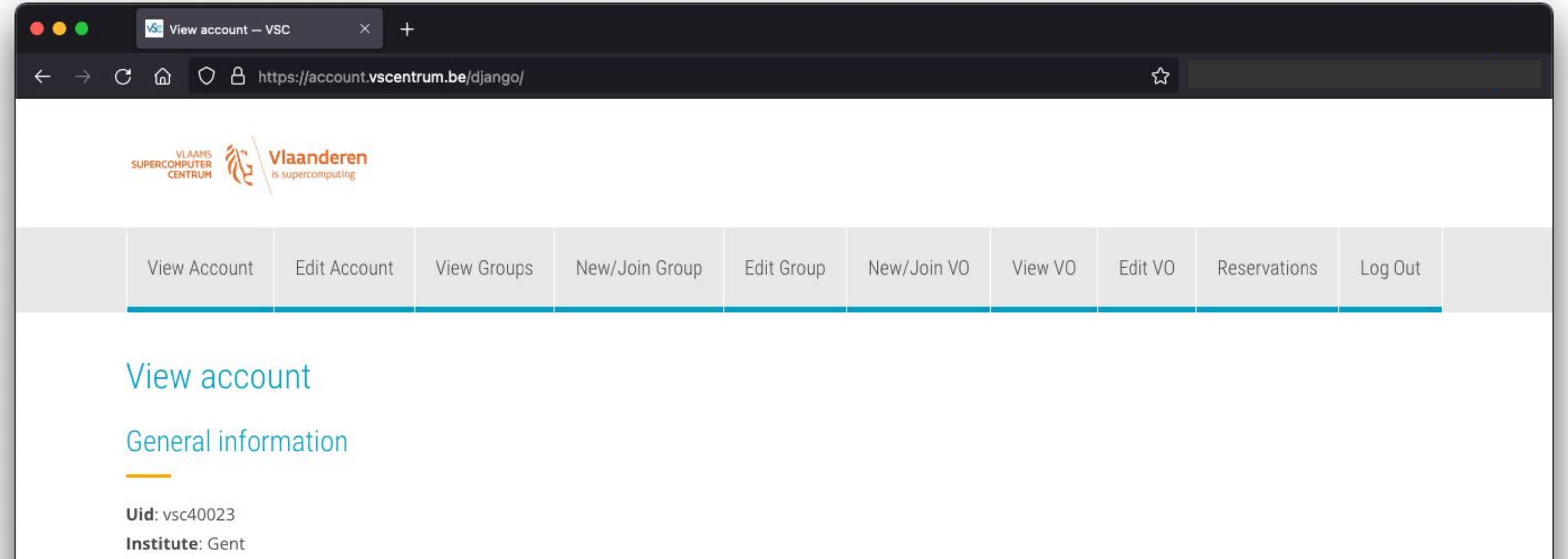
Managing your VSC account

You can manage your VSC account via the VSC account page

https://account.vscentrum.be

Can be used to join/leave user groups, consult storage usage, request more storage quota, …

nanage your Virtual Organisation (VO), …



View account

General information

Uid: vsc40023

Institute: Gent

Workflow on HPC-UGent infrastructure

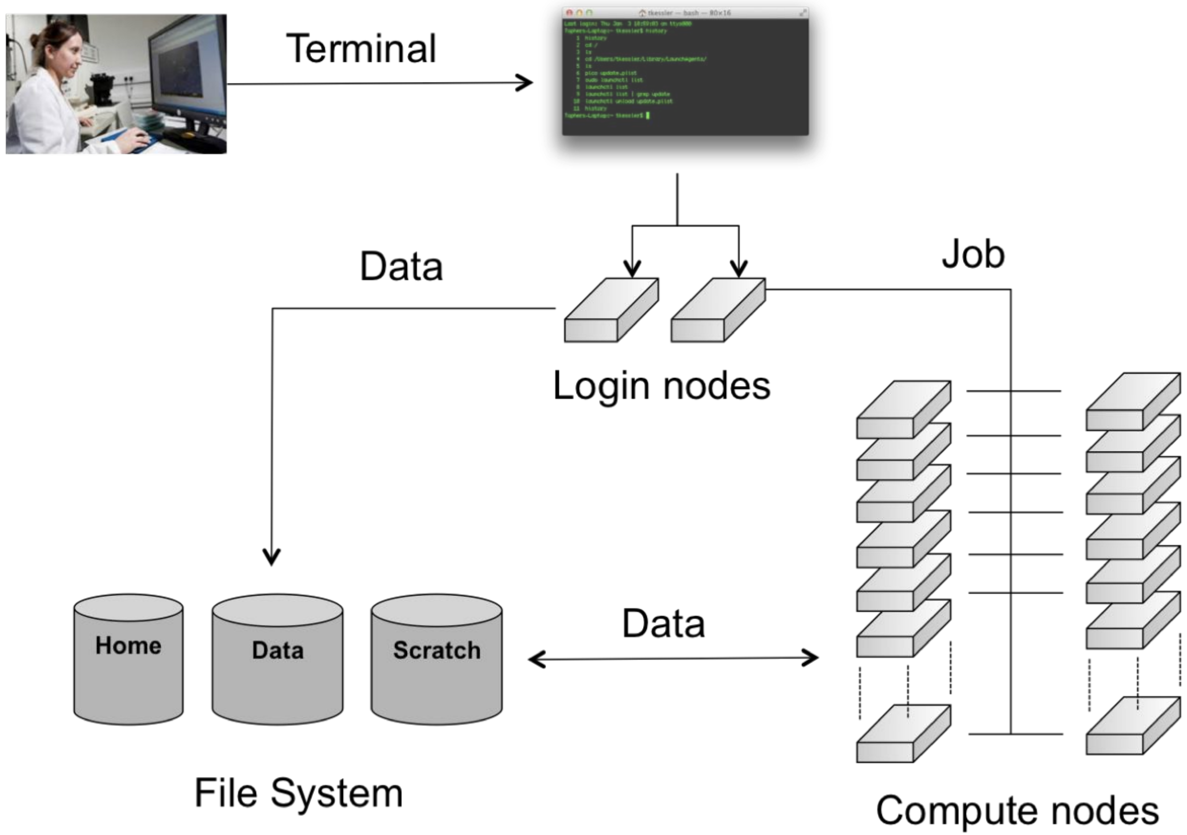
1. Connect to login nodes
2. Transfer your files
3. (Compile your code and test it)
4. Create a job script
5. Submit your job
6. Be patient

   - Your job gets into the queue

   - Your job gets executed

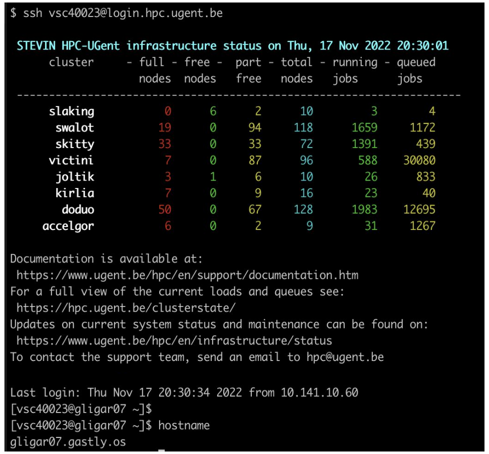
   - Your job finishes
7. Inspect and/or move your results

High-level overview of HPC-UGent infrastructure



```
tkessler — bash — 80×16
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$ 
```

Connecting to the HPC-UGent login nodes

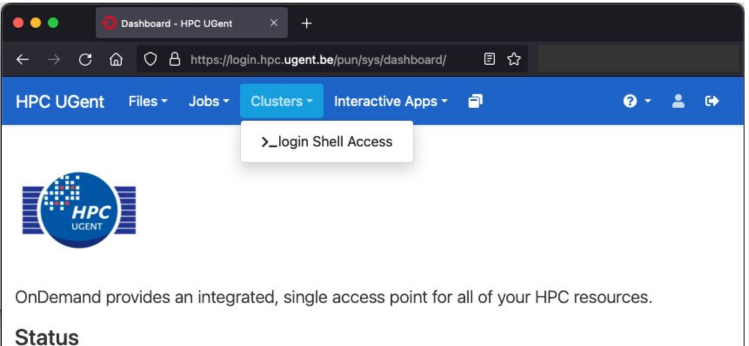


```
$ ssh vsc40023@login.hpc.ugent.be

 STEVIN HPC-UGent infrastructure status on Thu, 17 Nov 2022 20:30:01
      cluster     - full - free -  part - total - running - queued
                    nodes  nodes   free   nodes   jobs      jobs
 ----------------------------------------------------------------------
      slaking           0      6      2      10         3        4
       swalot          19      0     94     118      1659     1172
       skitty          33      0     33      72      1391      439
      victini           7      0     87      96       588    30080
       joltik           3      1      6      10        26      833
       kirlia           7      0      9      16        23       40
        doduo          50      0     67     128      1983    12695
     accelgor           6      0      2       9        31     1267

Documentation is available at:
 https://www.ugent.be/hpc/en/support/documentation.htm
For a full view of the current loads and queues see:
 https://hpc.ugent.be/clusterstate/
Updates on current system status and maintenance can be found on:
 https://www.ugent.be/hpc/en/infrastructure/status
To contact the support team, send an email to hpc@ugent.be

Last login: Thu Nov 17 20:30:34 2022 from 10.141.10.60
[vsc40023@gligar07 ~]$
[vsc40023@gligar07 ~]$ hostname
gligar07.gastly.os
```

Option 1: using SSH (classic way): `login.hpc.ugent.be`

- Requires SSH client + SSH private key
- Windows: PuTTy - macOS/Linux: `ssh` command
- See Chapter 3 of the [HPC-UGent documentation]()
- For transferring files: `scp` or `rsync` command, WinSCP, Cyberduck, …

Option 2: using the HPC-UGent web portal: https://login.hpc.ugent.be



OnDemand provides an integrated, single access point for all of your HPC resources.

Status

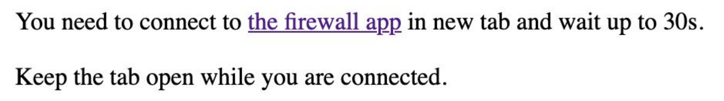
- ○ Powered by [Open OnDemand]()
- ○ Works with a standard internet browser (Firefox, Chrome, …)
- ○ Does not require SSH private key (only login via UGent account)
- ○ Provides file browser, shell session, desktop environment, …
- ○ See Chapter 8 of the [HPC-UGent documentation]()

Connection restrictions

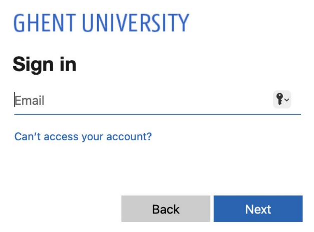
For security reasons, some connection restrictions have been put in place.

Connecting to the HPC-UGent login nodes is only possible when if one of the following applies:

- Using a university network (WiFi in UGent building, or UGent VPN)
- Using a Belgian commercial internet provider (take this into account when you're travelling!)
- Your IP address has been whitelisted
  - Automatically (and temporary) via the VSC firewall app: https://firewall.vscentrum.be
  - By exception (for example for corporate networks)


You need to connect to the firewall app in new tab and wait up to 30s.

Keep the tab open while you are connected.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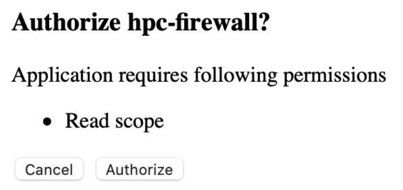
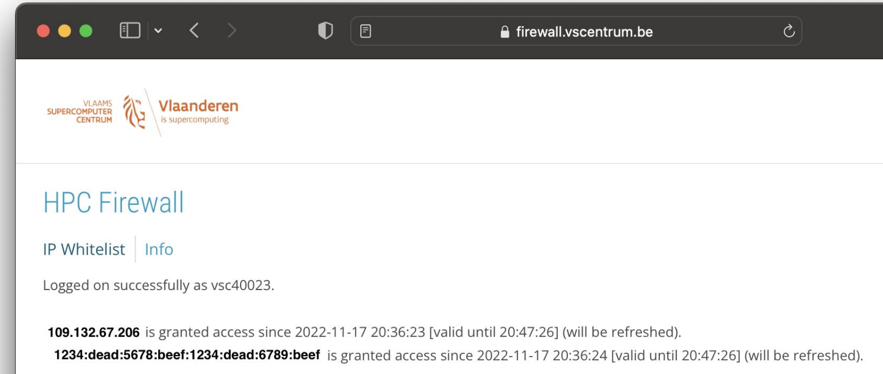
Sign in


Authorize hpc-firewall?

Application requires following permissions

- Read scope

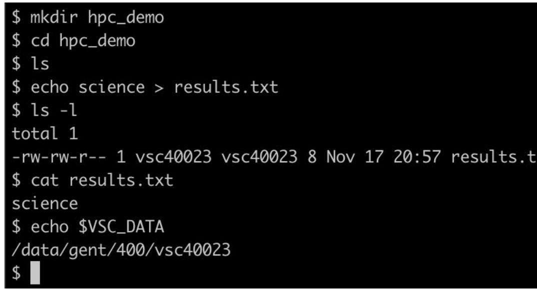


HPC Firewall

Logged on successfully as vsc40023.

109.132.67.206 is granted access since 2022-11-17 20:36:23 [valid until 20:47:26] (will be refreshed).
1234:dead:5678:beef:1234:dead:6789:beef is granted access since 2022-11-17 20:36:24 [valid until 20:47:26] (will be refreshed).

Linux command line interface (shell)



```
$ mkdir hpc_demo
$ cd hpc_demo
$ ls
$ echo science > results.txt
$ ls -l
total 1
-rw-rw-r-- 1 vsc40023 vsc40023 8 Nov 17 20:57 results.t
$ cat results.txt
science
$ echo $VSC_DATA
/data/gent/400/vsc40023
$
```

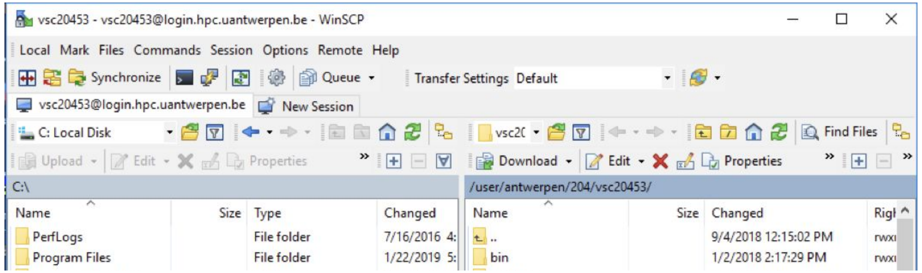
- **Linux shell environment** is standard way of using HPC systems
- Involves typing to run shell commands, or using (bash) scripts
- Example commands: `ls`, `cd`, `mkdir`, `cp`, `mv`, `rm`, `export`, `echo`, ...
- Commands can be “piped” together to do more complex operations
- May feel arhaic, but is actually **very powerful**…
- Same scripting language is used in job scripts
- **Learning the basics of the Linux shell is strongly recommended!**
- See separate basic Linux tutorial at https://www.ugent.be/hpc/en/support/documentation.htm

Transferring files to/from HPC-UGent infrastructure

- Transferring files/to from the HPC-UGent infrastructure is done **via the login nodes**
- Options:
    - Using file browser in HPC-UGent web portal (see “Files” menu item)
    - On Linux or macOS:
        - Using `scp` or `rsync` command in terminal window
        - Using a graphical like the built-in file manager or [Cyberduck]
    - On Windows: using [WinSCP] (left: own system, right: HPC; drag-and-drop)

See also section 3.2 of

HPC-UGent documentation


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
Upload
Edit
Properties
vsc2(
Find Files
Download
Edit
Properties

C:\

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

/user/antwerpen/204/vsc20453/

Name	Size	Changed	Rigl
..		9/4/2018 12:15:02 PM	rwxı
bin		1/2/2018 2:17:29 PM	rwxı

Submitting and managing jobs on HPC-UGent clusters

- HPC-UGent clusters run Slurm as resource manager + job scheduler
- **Torque (PBS) frontend is (still) available and recommended** (via *jobcli* project)
  - `qsub` command to submit jobs, `qdel` command to delete jobs
  - `qstat` command to list queued + running jobs
  - `qalter` command to change jobs (before they start running)
  - `qhold` command to put jobs on hold, qrls to release them again
- Use `--help` option to get list of available options for each command
- Use `--debug` option to get more information about what's going on behind the scenes
- Use `--dryrun` option to inspect what will be done (without actually doing it)

What is a job script?

```
#!/bin/bash

echo "I am a minimal job script"
```

A job script is shell script (a text file that includes shell commands) which specifies:

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

  (number of nodes/cores, amount of memory, how much time is required, …)

- The **software** that is used for the calculation (usually via `module load` commands)

- The steps that should be done to execute the calculation (starting from home dir.), specified as **shell commands**, typically:
  - 1) staging in of input files
  - 2) running the calculation
  - 3) staging out of results

Required resources are specified 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           # 50GB of (virtual) memory required
# rest of job script goes here ...
```

- Required resources can be specified via `#PBS` lines in job script
- Or via options to job submission command (`qsub -l ...`)
- **Maximum walltime of jobs on HPC-UGent clusters: 72 hours (3 days)**
- For longer calculations: break it up in shorter jobs, use a different (faster) cluster, use more cores (if software scales), use some form of “checkpointing”, …

Central software stack via modules [1/2]

- **Scientific software is made available via *environment modules***
- A module prepares the environment for using a particular software application
- Module naming scheme: `<name>/<version>-<toolchain>[-<suffix>]`
- Interacting with module files is done via the `module` command (Lmod)
- Load a module to update the session or job environment for using the software:

```
module load SciPy-bundle/2021.10-intel-2021b
```

- Modules that are required as dependencies will be loaded automatically
- To see list of currently loaded modules, run `module list` (or `ml`)

Central software stack via modules [2/2]

- To get an overview of *all* available modules, run `module avail` (or `ml av`)
- To see available versions for specific software, run `module avail soft_name/`
- To unload all currently loaded modules, run `module purge`
- Modules are installed using a particular toolchain (`foss`, `intel`, ...), which includes C/C++/Fortran compilers, MPI library, BLAS/LAPACK/FFT libraries
- You should only combine modules that were installed with the same toolchain, or a subtoolchain thereof (for example `foss/2021b` + `GCC/11.2.0`)
- See also section 4.1 in HPC-UGent documentation

Useful environment variables for job scripts

(these are only defined in the context of a running job!)

- `$PBS_JOBID`: job id of running job
- `$PBS_O_WORKDIR`: directory from which job was submitted on login node
  - It is common to use `cd $PBS_O_WORKDIR` at beginning of a job script
- `$PBS_ARRAYID`: array id of running job
  - Only relevant when submitting array jobs (`qsub -t`)
- `$TMPDIR`: local unique directory specific to running job
  - Cleaned up automatically when job is done, so make sure to copy result files!
- `$EBROOTXYZ`, `$EBVERSIONXYZ`: root directory/version for software package XYZ
  - Only available when module for XYZ is loaded

Input/output data and shared filesystems

- See Section 6.2 in [HPC-UGent documentation]
- Think about input/output:
  - How and where will you *stage in* your data and input files?
  - How and where will you *stage out* your output and result files?
- Manually (on login nodes) vs automatically (as a part of job script)
- **Home filesystem** (`$VSC_HOME`): only for limited number of small files & scripts
- **Data filesystem** (`$VSC_DATA*`): ‘long-term’ storage, large files
- **Scratch filesystems** (`$VSC_SCRATCH*`): for ‘live’ input/output data in jobs

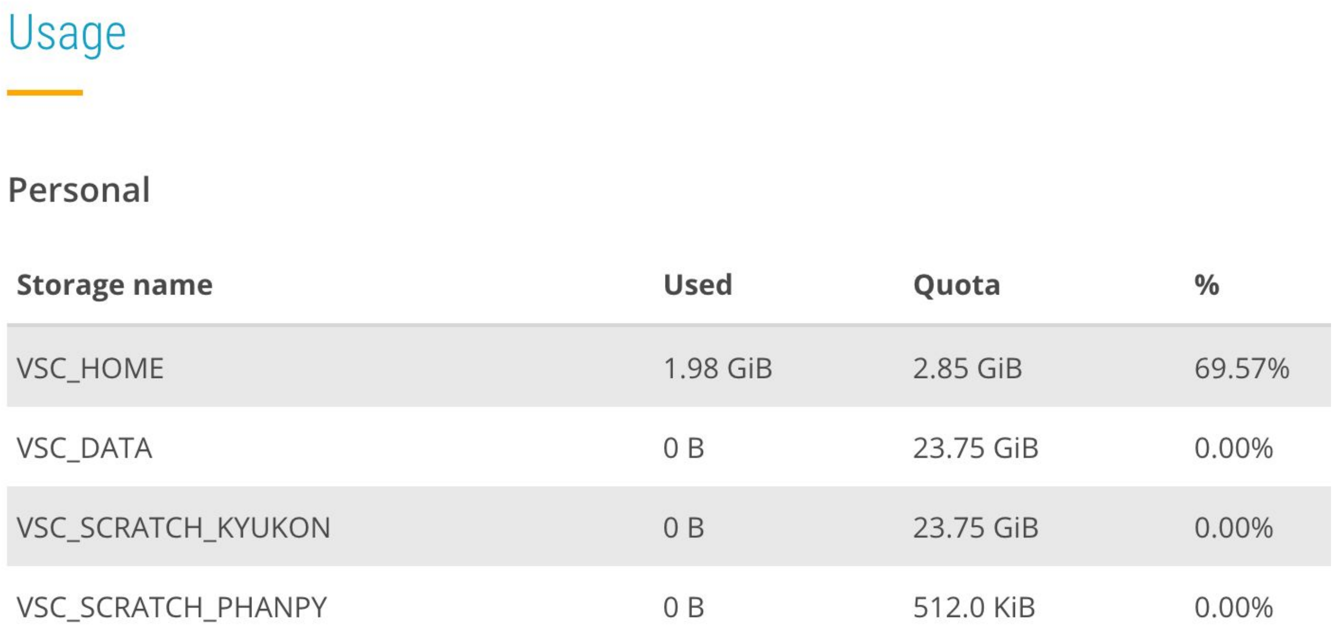
Storage quota

- Home directory (`$VSC_HOME`): 3GB (fixed!)
- Personal data directory (`$VSC_DATA`): 25GB (fixed!)
- Personal scratch directory (`$VSC_SCRATCH`): 25GB (fixed!)
- Current quota usage can be consulted on VSC accountpage
- **More storage quota (100s of GBs, TBs) available for *virtual organisations (VOs)*;** see Section 6.7 in HPC-UGent documentation
- Additional quota can be requested via VSC accountpage ("Edit" tab)
- Shared directories with VO members: `$VSC_DATA_VO`, `$VSC_SCRATCH_VO`
- Personal VO subdirectories: `$VSC_DATA_VO_USER`, `$VSC_SCRATCH_VO_USER`

Current storage usage - personal directories

See *“View Account”* tab on VSC accountpage (https://account.vscentrum.be)

(for now, only data volumes, not number of files (inode quota))



Usage

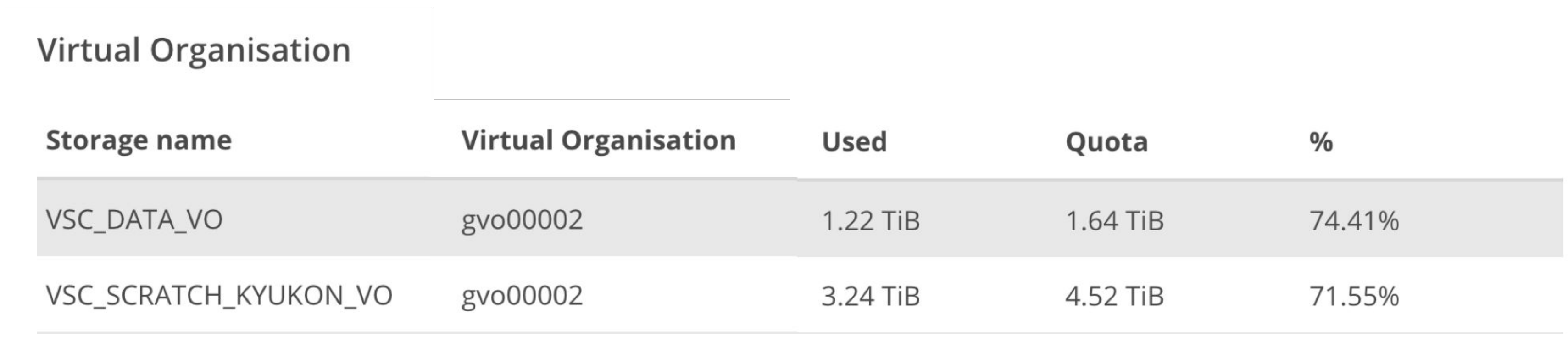
Personal

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

See *"View Account"* tab on VSC accountpage (https://account.vscentrum.be)

(for now, only data volumes, not number of files (inode quota))



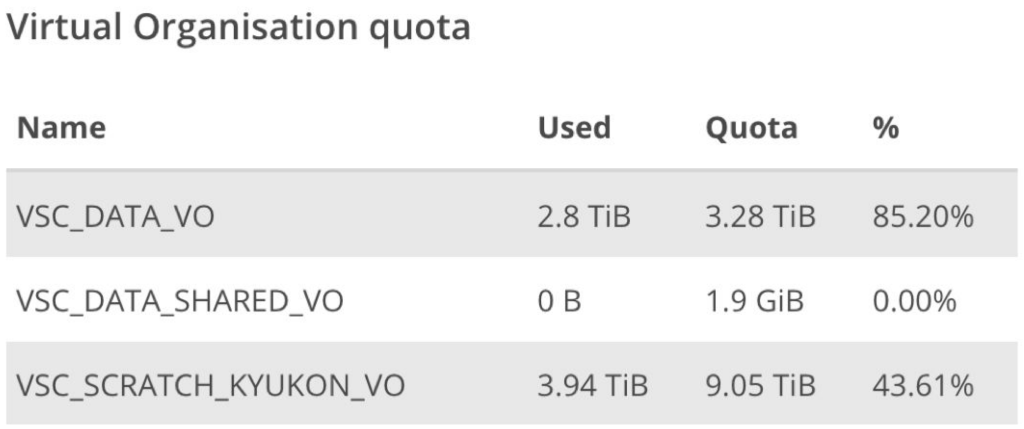
Virtual Organisation

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%

Current storage usage - total usage in VO directories

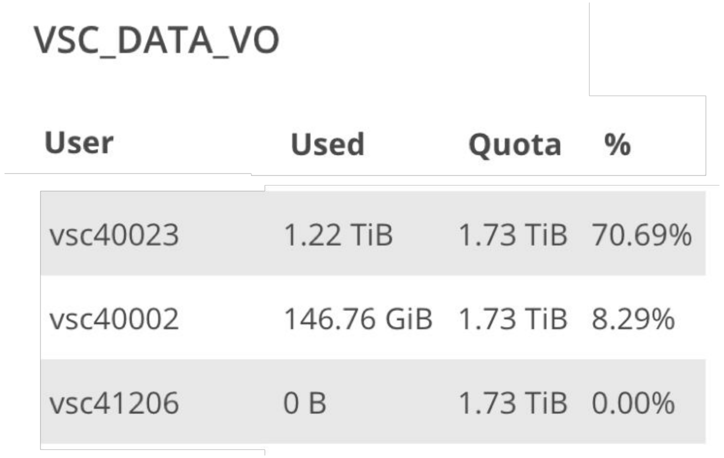
- See [*“View VO”* tab on VSC accountpage]()

  (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_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%

Full example job script (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/3.10.4-GCCcore-11.3.0
# 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 Python code
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
```

Full example job script (multi-node MPI 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/2021b
module load vsc-mympirun

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

Job 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 or result files (very software-specific).

Job submission and management workflow

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

```
$ module swap cluster/slaking

$ qsub example.sh

12345
```

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

```
$ qstat

Job ID    Name        User              Time Use S Queue

------- ----------- -------------- -------- - -------

12345   example       vsc40023         1:32:57  R slaking
```

- To remove a job that is no longer necessary, use the `qdel` command: `qdel 12345`

Job scheduling

- All HPC-UGent clusters use a **fair-share scheduling** policy.
- No guarantees on when job will start (and impossible to predict), so **plan ahead**!
- Job priority is determined by various factors:
  - 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 (output files, etc.)
- Better options:
  - Array jobs
    - Single job script, each (sub)job is assigned a unique id (via `$PBS_ARRAYID`)
  - GNU parallel
    - General-purpose tool to easily run commands in parallel with different inputs
  - Worker tool (see Chapter 12 in HPC-UGent documentation)
    - 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, use the request form:

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

- Requests may take a while to process (especially for new software), so be patient…
- Make the request sooner rather than later!

- All software installations are done using EasyBuild
- Originally developed by HPC-UGent,

  now a worldwide community of experts!
- See also https://easybuild.io

EASYBUILD.io
building software with ease

Questions, problems, getting help

Don't hesitate to contact the HPC-UGent support team via hpc@ugent.be

- Help us help you, always include:
  - VSC login id
  - Clear description of the problem or question, include error messages, …
  - Location of job script and output/error files in your account
  - Preferably don’t send files in attachment, we prefer to look at it ‘in context’...
  - Also mention job IDs, which cluster was used, …
- Preferably use your UGent email address
- Alternatives:
  - Short (Teams) meeting (for complex problems, big projects)
  - `hpc-users` mailing list