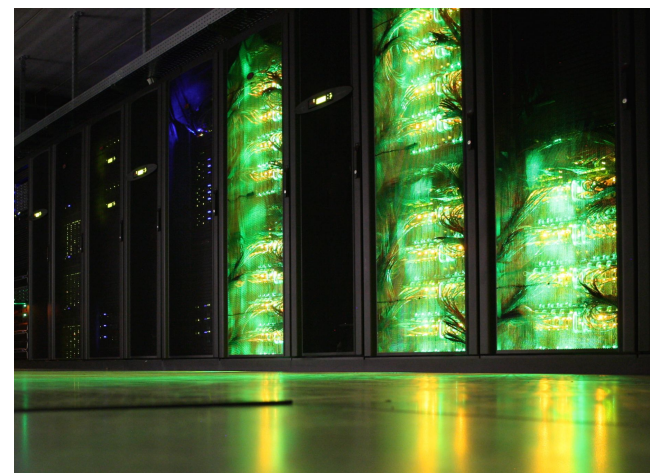




Introduction to VSC Tier-1 Hortense

EMBL hackathon - 2 December 2024



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docs.vscentrum.be/gent/tier1_hortense.html

compute@vscentrum.be

VLAAMS
SUPERCOMPUTER
CENTRUM



Vlaanderen
is supercomputing

Documentation & support



- Extensive documentation available at docs.vscentrum.be/gent/tier1_hortense.html
- Setup and configuration of VSC Tier-1 Hortense is very similar to HPC-UGent Tier-2 infrastructure, so see also docs.hpc.ugent.be
- In case of questions or problems, please contact compute@vscentrum.be

HPC-UGent in a nutshell



- Part of central 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:

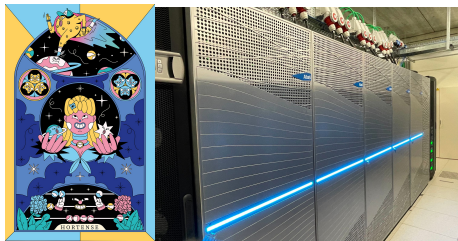
Empowerment - Centralisation - Automation - Collaboration

Centralised hardware in UGent datacenter (S10 @ Sterre)



Different “tiers” of supercomputers

VSC Tier-1 *Hortense*



VLAAMS
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Vlaanderen
is supercomputing

vscentrum.be

Tier-0
Europe

eurohpc-ju.europa.eu



Tier-1
Regional / National



EuroHPC
Joint Undertaking

Tier-2
University



**GHEENT
UNIVERSITY**

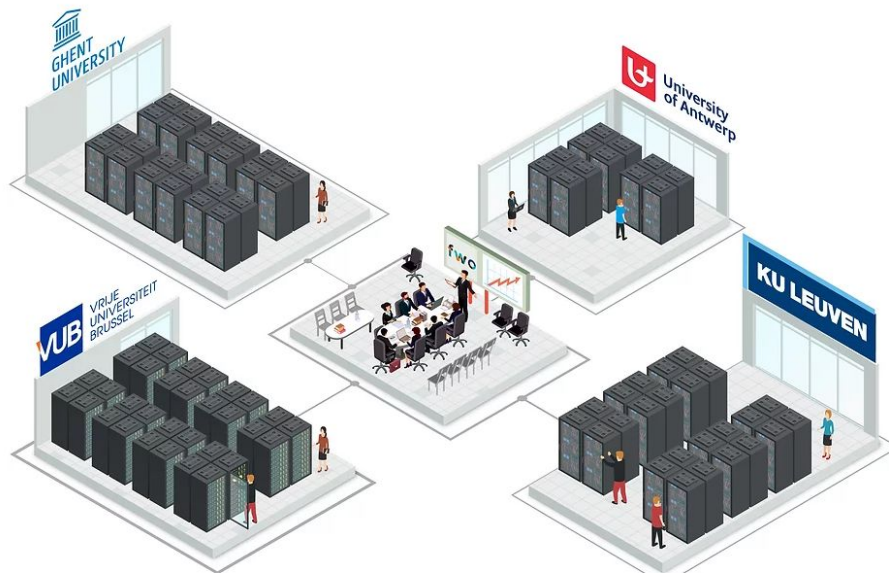


Tier-3
Personal workstation (desktop, laptop)

ugent.be/hpc

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



VSC Tier-1 compute cluster “Hortense”

(a.k.a. dodrio)

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compute@vscentrum.be

- Hosted, operated, and supported by HPC-UGent team since 2021
- 2x 384 CPU-only nodes (128-core AMD Rome or Milan CPUs) + 40 GPU nodes (4x NVIDIA A100)
- **Over 100,000 CPU cores in total!**
- High-speed Infiniband network (HDR-100) + 6PB of dedicated scratch storage



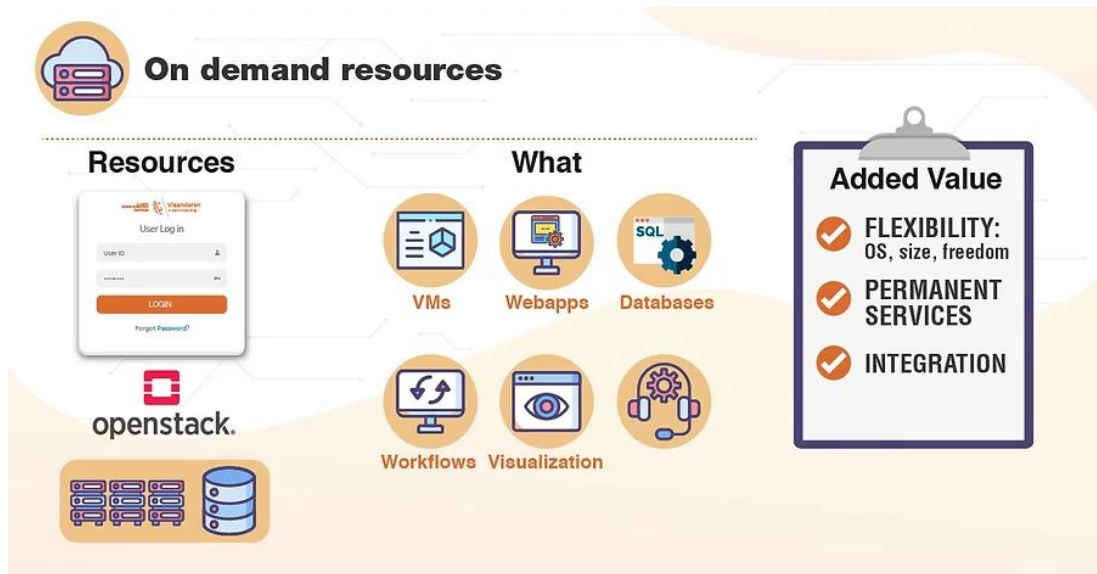
- **Project-based access** (free of charge, funded by FWO)
- 3 cut-off dates per year for submitting project proposals
- Project duration is typically 8 months
- 500k - 5M core hours (CPU-only) or 1k - 25k GPU hours

vscentrum.be/compute

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: vscentrum.be/cloud
- Contact: cloud@vscentrum.be

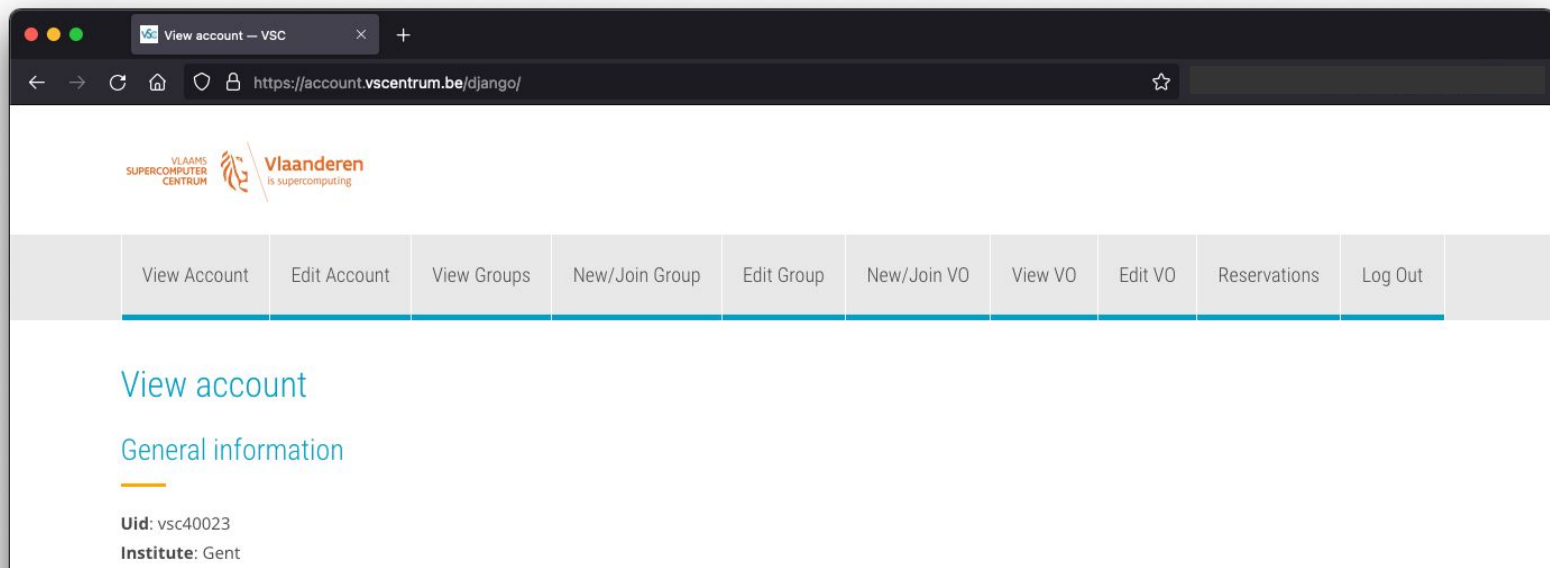


Managing your VSC account

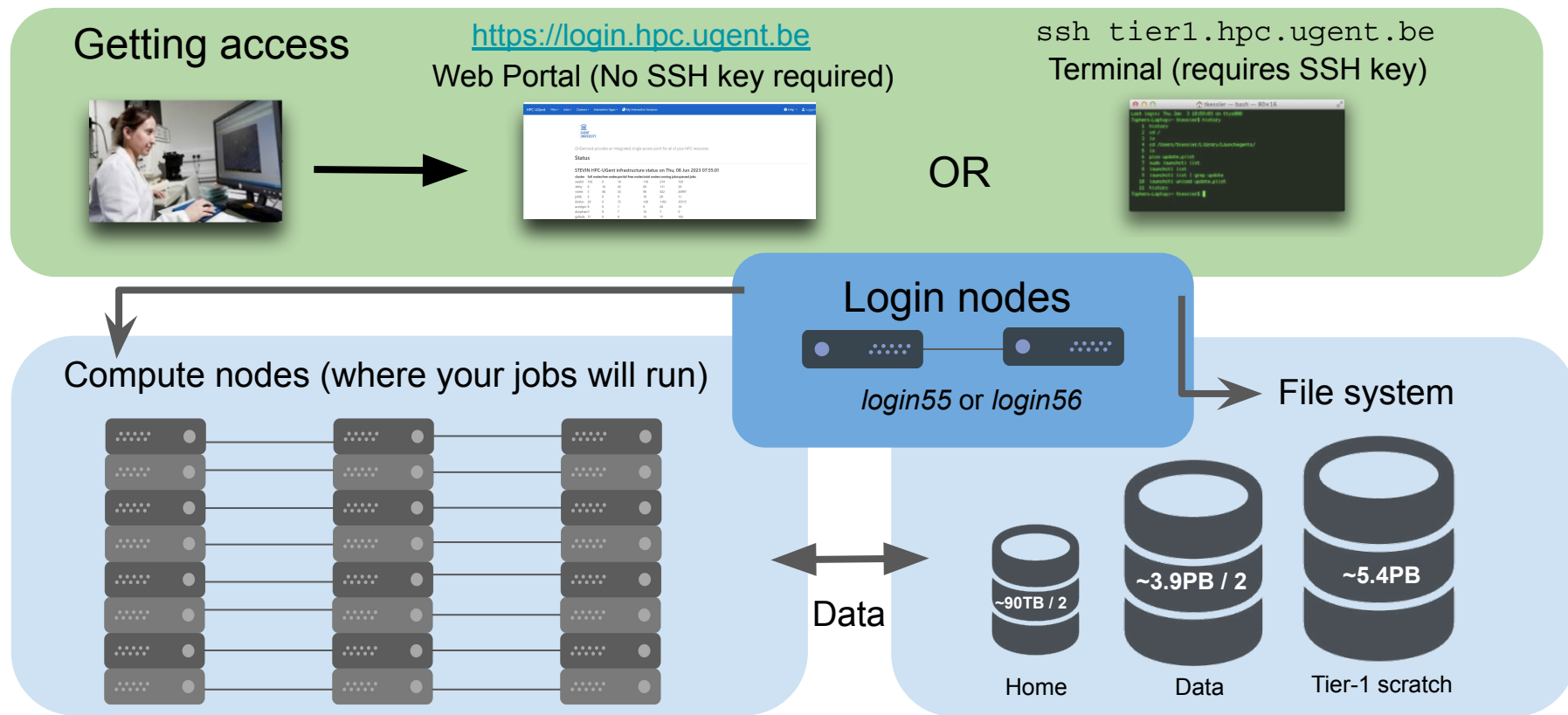
You can manage your VSC account via the VSC account page

account.vscentrum.be

Can be used to join/leave user groups, consult storage usage, request more storage quota, ...
manage your Virtual Organisation (VO), ...



High-level overview of VSC Tier-1 Hortense



Option 1: Connecting to VSC Tier-1 Hortense login nodes with SSH

```
$ 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  18  3  4
swat 19  0  94  118  1659  1172
skitty 33  0  33  72  1391  439
victimi 7  0  87  96  588  39080
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.as
```

- See [dedicated section in HPC-Ugent documentation](#)
- `tier1.hpc.ugent.be`
- Requires SSH client + SSH private key
- Windows: PuTTY - macOS/Linux: `ssh` command

- Transferring files to/from VSC Tier-1 Hortense

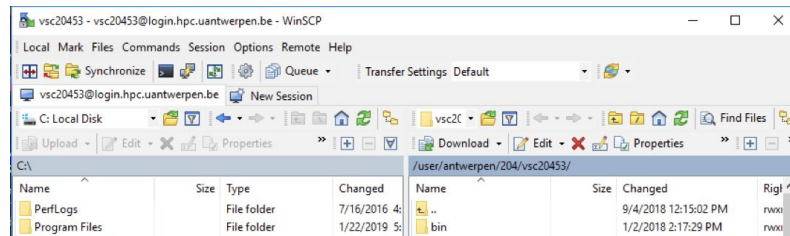
- **Done via the login nodes**

- Options:

- On Linux or macOS:

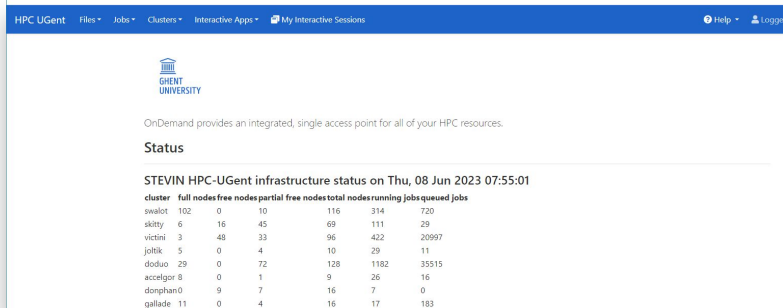
- Using `scp` or `rsync` command in terminal window
 - Using a graphical like the built-in file manager or [Cyberduck](#)

- On Windows: using [WinSCP](#) (left: own system, right: HPC; drag-and-drop)



Option 2: Connecting to VSC Tier-1 Hortense with web portal

Recommended!



The screenshot shows the HPC-Ugent web portal interface. At the top is a navigation bar with links for Files, Jobs, Clusters, Interactive Apps, and My Interactive Sessions. Below the navigation bar is the Ghent University logo and a message stating that OnDemand provides an integrated, single access point for all of your HPC resources. The main section is titled 'Status' and displays the 'STEVIN HPC-Ugent infrastructure status on Thu, 08 Jun 2023 07:55:01'. It contains a table with columns for cluster, full nodes, free nodes, partial free nodes, total nodes, running jobs, queued jobs, and a final column for jobs.

cluster	full nodes	free nodes	partial free nodes	total nodes	running jobs	queued jobs	jobs
swalot	102	0	10	116	314	720	
skitty	6	16	45	69	111	29	
victini	3	48	33	96	422	20997	
joltik	5	0	4	10	29	11	
diodao	29	0	72	128	1182	35515	
accetigor	8	0	1	9	26	16	
donphan0	9	7	16	7	0	0	
gallade	11	0	4	16	17	183	

- See [dedicated section of HPC-Ugent docs](#)
- <https://tier1.hpc.ugent.be>
- Powered by [Open OnDemand](#)

- **Works with a standard internet browser** (Firefox, Chrome, ...)
- **Does not require SSH key pair** (only login via university account)
- Provides file browser, shell session, desktop environment, interactive apps, ...

Option 2: Using the web portal file browser to view, edit, manage files

Recommended!

Creating and editing a file

1. Go to the file manager
2. Create a file
3. Edit file

The screenshots illustrate the process of creating and editing a file in the HPC User web portal:

- Step 1:** The 'Files' tab is selected in the top navigation bar.
- Step 2:** The '+ New File' button is clicked in the top toolbar.
- Step 3:** A 'New File' dialog box appears with 'example.txt' entered in the filename field.
- Step 4:** The file 'example.txt' is listed in the file browser, and a context menu is open over it with 'Edit' selected.

Type	Name	Size	Modified at
Folder	AlphaFold	-	13/8/2021 16:16:46
Folder	cache	-	22/3/2023 10:10:22
Folder	cvmfs-tutorial-ingest-example-720k-files	-	13/8/2021 16:16:35
Folder	easybuild	-	22/5/2023 13:43:47

Type	Name	Size	Modified at
Folder	pip_http	-	27/11/2021 18:05:15
Folder	singularity_cache	-	13/8/2021 16:16:35
Folder	vsc-software-stack	-	4/5/2023 11:22:39
File	cvmfs-tutorial-ingest-example-720k-files.tar.gz	-	22/1/2021 15:59:40
File	example.txt	0 Bytes	7/6/2023 10:51:25

UGent web portal: interactive apps (Jupyter notebook)

1

OnDemand provides...
Status
STEVIN HPC-UGent
cluster full nodes free
skitty 2
joltik 4
doduo 39
acceigon 6
donphan 0
gallade 3
shinx 3

Desktops
Bioimage Analysis Desktop
Cluster Desktop
Neurodesk
Servers
Jupyter Lab
Jupyter Notebook
RStudio server
Shell (tmux)
VS Code Tunnel
Code Server

on Thu, 19 Sep 2024 12:42:42
running jobs queued jobs
Testing 74 2
9 76
996 5376
21 5082
14 19
11 16
39 132
351 811

2

Home / My Interactive Sessions / Jupyter Notebook
Interactive Apps
Desktops
Bioimage Analysis Desktop
Cluster Desktop
Neurodesk
Servers
Jupyter Lab
Jupyter Notebook
RStudio server
Shell (tmux)
VS Code Tunnel
Testing
Cluster desktop v2
Code Server

Jupyter Notebook
This app will launch a Jupyter Notebook server on one or more nodes.
Cluster: donphan (interactive/debug)
Time (hours): 1 hour
Number of nodes: 1 node
Number of cores (and default memory) per node: 1 core (3.3 GiB mem)
Jupyter Notebook version: 7.2.0 GCCore 13.2.0
Launch

3

Jupyter IPython Notebook (cluster/donphan-20004994) Queued
Created at: 2023-06-07 14:51:43 CEST
Time Requested: 12 hours
Session ID: d54a26c3-a09e-44f3-b8a4-a558a99bdcf9
Please be patient... Job currently sits in queue. The wait time depends on the number of cores as well as time requested.

4

Jupyter IPython Notebook (cluster/donphan-20004994) 1 node | 4 cores | Starting
Created at: 2023-06-07 14:51:43 CEST
Time Remaining: 11 hours and 59 minutes
Session ID: d54a26c3-a09e-44f3-b8a4-a558a99bdcf9
Your session is currently starting... Please be patient as this process can take a few minutes.

5

Jupyter IPython Notebook (cluster/donphan-20004994) 1 node | 4 cores | Running
Host: node0116.donphan.nu
Created at: 2023-06-07 14:51:43 CEST
Time Remaining: 11 hours and 59 minutes
Session ID: d54a26c3-a09e-44f3-b8a4-a558a99bdcf9
Connect to Jupyter Notebook

Jupyter Notebook versions
Make sure that the toolchain of the notebook matches the toolchain of the modules that you load, and the kernels and/or virtual environments that you make!

Files Running Clusters
Select items to perform actions on
0 /
examples
ondemand

Quit Logout
Upload New
Name Last Modified File size
6 days ago
16 minutes ago

UGent web portal: interactive apps (desktop for GUI apps)

1. Clicking 'Cluster Desktop' in the Interactive Apps menu.

2. Selecting 'Cluster Desktop' in the Interactive Apps list.

3. Viewing the 'Cluster Desktop' details page.

4. Clicking 'Launch Cluster Desktop' on the details page.

5. Clicking 'Launch' on the 'Cluster Desktop' configuration page.

Example Using MATLAB

5. Clicking 'Launch' on the 'Cluster Desktop' configuration page.

Connection restrictions



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

Connecting to VSC Tier-1 Hortense is only possible when if one of the following applies:

- Using a university network (WiFi in UGent building, 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.

GHENT UNIVERSITY

Sign in

Email

[Can't access your account?](#)

Back

Next

Authorize hpc-firewall?

Application requires following permissions

- Read scope

Cancel

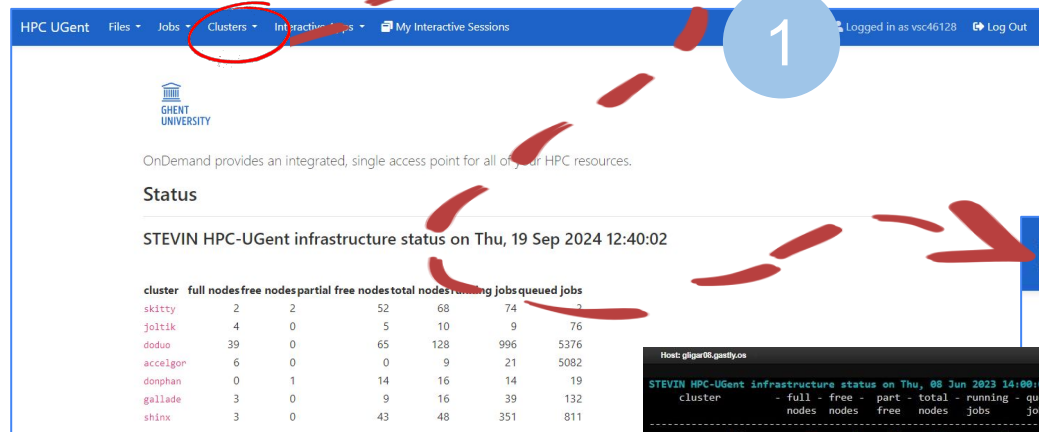
Authorize

(Lara)



Getting shell access via web portal

1. Click on the 'Clusters' tab
2. Click on Login Shell Access
3. Use the shell environment



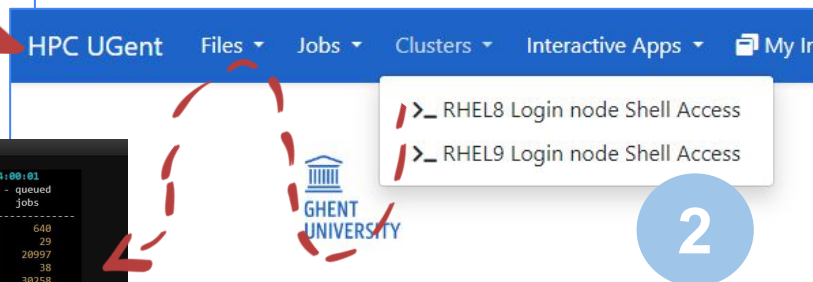
HPC UGent Files Jobs **Clusters** Interactive Apps My Interactive Sessions Logged in as vsc46128 Log Out

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

Status

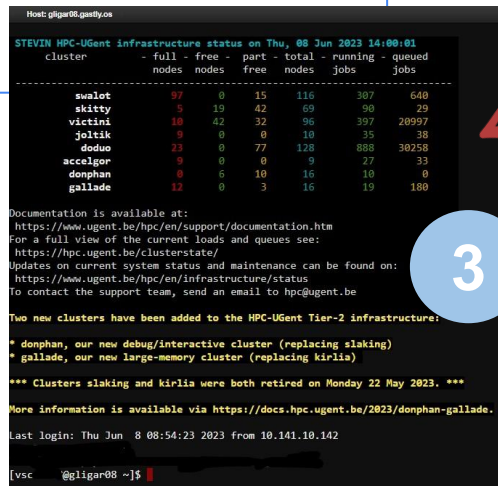
STEVIN HPC-UGent infrastructure status on Thu, 19 Sep 2024 12:40:02

cluster	full nodes	free nodes	partial nodes	total nodes	running jobs	queued jobs
skitty	2	2	52	68	74	2
joltik	4	0	5	10	9	76
doduo	39	0	65	128	996	5376
accelegor	6	0	0	9	21	5082
donphan	0	1	14	16	14	19
gallade	3	0	9	16	39	132
shinx	3	0	43	48	351	811



HPC UGent Files Jobs Clusters Interactive Apps My Interactive Sessions

>_ RHEL8 Login node Shell Access
>_ RHEL9 Login node Shell Access



```
Host: gligar08.guestly.on
STEVIN HPC-UGent infrastructure status on Thu, 08 Jun 2023 14:00:01
cluster - full - free - part - total - running - queued
nodes nodes free nodes jobs jobs jobs
-----
swalot 87 0 15 116 307 640
skitty 5 19 42 69 90 29
victini 10 42 32 96 397 20997
joltik 0 0 0 10 35 38
doduo 23 0 77 128 888 30258
accelegor 0 0 0 9 27 33
donphan 0 6 10 16 10 0
gallade 12 0 3 16 19 180

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

Two new clusters have been added to the HPC-UGent Tier-2 infrastructure:
* donphan, our new debug/interactive cluster (replacing slaking)
* gallade, our new large-memory cluster (replacing kirlia)

*** Clusters slaking and kirlia were both retired on Monday 22 May 2023. ***

More information is available via https://docs.hpc.ugent.be/2023/donphan-gallade.

Last login: Thu Jun 8 08:54:23 2023 from 10.141.10.142

[vsc @gligar08 ~]$
```

Linux command line interface (shell)

- **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 (bash) is used in job scripts
- **Learning the basics of the Linux shell is strongly recommended!**
- See separate basic Linux tutorial at docs.hpc.ugent.be/linux-tutorial

```
$ 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.txt
$ cat results.txt
science
$ echo $VSC_DATA
/data/gent/400/vsc40023
$
```

Submitting and managing jobs on VSC Tier-1 Hortense

- VSC Tier-1 Hortense runs [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)

docs.vscentrum.be/gent/tier1_hortense.html#resource-manager

What is a job script?

```
#!/bin/bash  
echo "I am a minimal job script"
```

A job script is (bash) shell script, a text file that includes shell commands, that 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***
- An env. 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 prepare the session or job environment for using the software:

```
module load SciPy-bundle/2023.07-gfbf-2023a
```
- 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/2023a + GCC/12.3.0`)
- See also [dedicated section in HPC-UGent documentation](#)

Central software stack via modules (example)



```
$ python -V; which python
```

```
Python 3.6.8
```

```
/usr/bin/python
```

```
$ python -c 'import numpy; print(numpy.__version__)'
```

```
Traceback (most recent call last):
```

```
File "<string>", line 1, in <module>
```

```
ModuleNotFoundError: No module named 'numpy'
```

```
$ module load SciPy-bundle/2023.07-gfbf-2023a
```

```
$ python -V; which python
```

```
Python 3.11.3
```

```
/apps/gent/RHEL8/zen2-ib/software/Python/3.11.3-GCCcore-12.3.0/bin/python
```

```
$ python -c 'import numpy; print(numpy.__version__)'
```

```
1.25.1
```

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**: unique *local* 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

Scratch filesystem on VSC Tier-1 Hortense

- See also docs.vscentrum.be/gent/tier1_hortense.html#project-scratch-directories
- Only accessible from VSC Tier-1 Hortense login and worker nodes
- Other shared filesystems (`$VSC_HOME`, `$VSC_DATA`) available, but *should be avoided*
- Use project scratch directory: `$VSC_SCRATCH_PROJECTS_BASE/2024_300`
- Access read-only data (incl. software installations) via `/readonly` mount
See also docs.vscentrum.be/gent/tier1_hortense.html#accessing-data-via-readonly
- Check quota usage via `my_dodrio_quota` command

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

# load Python 3.11, with batteries included (extra PyPI packages)
module load SciPy-bundle/2023.11-gfbf-2023b
# 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 $VSC_SCRATCH_PROJECTS_BASE/2024_300/output_${PBS_JOBID}.txt
```

Full example job script (multi-node MPI job)

```
#!/bin/bash
#PBS -N mpi_hello           # job name
#PBS -l nodes=2:ppn=4       # 2 nodes, 4 cores per node
#PBS -l walltime=2:00:00    # max. 2h of wall time

module load foss/2023a
module load vsc-mypirun

# go to working directory, compile and run MPI hello world program
cd $PBS_O_WORKDIR
# C code for MPI Hello: https://mpitutorial.com/tutorials/mpi-hello-world
mpicc mpi_hello.c -o mpi_hello
mypirun ./mpi_hello
```

Job output files

- **Your job script may produce informative, warning, and/or 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 [dedicated section of our Linux tutorial](#) for more details)

- In addition, the software used for the calculation may have generated additional output or result files (which is 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/dodrio/gpu_rome_a100
```

```
$ 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	vsc40000	1:32:57	R	gpu_rome_a100

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

Job submission: GPU reservation for EMBL hackathon

- Dedicated reservation of 5 GPU nodes (20 A100 GPUs in total) is available
- To submit a job into the reservation:

```
$ module swap cluster/dodrio/gpu_rome_a100
```

```
$ qsub example.sh --pass=reservation=EMBL
```

```
12345
```

- You will only have access to an A100 GPU if you actually request one!
 - `qsub example.sh --pass=reservation=EMBL -l nodes=1:gpus=1`
- See also docs.vscentrum.be/gent/tier1_hortense.html#requesting-gpu-resources

Interactive session via Tier-1 Hortense web portal

Clusters ▾ Interactive Apps ▾ My Interactive Sessions

Home / My Interactive Sessions / Cluster Desktop

Interactive Apps

Desktops

Bioimage AAnalysis Desktop

Cluster Desktop

Neurodesk

Servers

Jupyter Lab

Jupyter Notebook

RStudio server

Shell (tmux)

VS Code Tunnel

Testing

Cluster desktop v2

Code Server

Cluster Desktop

This app will launch an interactive desktop on one or more compute nodes. You will have full access to the resources these nodes provide. This is analogous to an interactive batch job.

Cluster

dodrio gpu_rome_a100

Time (hours)

1 hour

Number of nodes

1 node

Number of cores (and default memory) per node

12 cores (62.1 GiB mem) (quarter)

Number of GPUs per node

1

Number of cores per node must be a multiple of number of GPUs

...

Reservation id

EMBL

Running containers via Apptainer

- Apptainer is available to run (Docker/Singularity/Apptainer) container images
- Quick example with NVIDIA container for TensorFlow:

```
mkdir -p $VSC_SCRATCH_PROJECTS_BASE/2024_300/$USER  
cd $VSC_SCRATCH_PROJECTS_BASE/2024_300/$USER
```

```
unset APPTAINER_TMPDIR  
export APPTAINER_CACHEDIR=/tmp/$USER/apptainer-cache
```

```
apptainer build example.sif docker://nvcr.io/nvidia/tensorflow:24.11-tf2-py3  
apptainer shell --nv /readonly/$PWD/example.sif
```

```
nvidia-smi      # check that GPU is available in container  
python  
>>> from tensorflow.python.client import device_lib  
>>> device_lib.list_local_devices()
```

- See also docs.hpc.ugent.be/apptainer

Documentation & support



- Extensive documentation available at docs.vscentrum.be/gent/tier1_hortense.html
- Setup and configuration of VSC Tier-1 Hortense is very similar to HPC-UGent Tier-2 infrastructure, so see also docs.hpc.ugent.be
- In case of questions or problems, please contact compute@vscentrum.be