

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

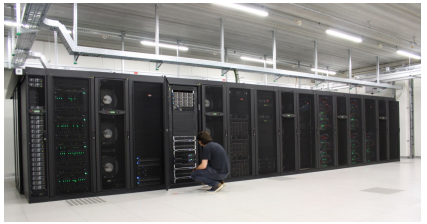
Documentation & support

VLAAMS SUPERCOMPUTER CENTRUM

Vlaanderen is supercomputing

- 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

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Centralised hardware in UGent datacenter (S10 @ Sterre)

Different “tiers” of supercomputers

eurohpc-ju.europa.eu

VSC Tier-1 *Hortense*

Tier-0
Europe

Tier-1
Regional / National

Tier-2
University

Tier-3
Personal workstation (desktop, laptop)

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vscentrum.be

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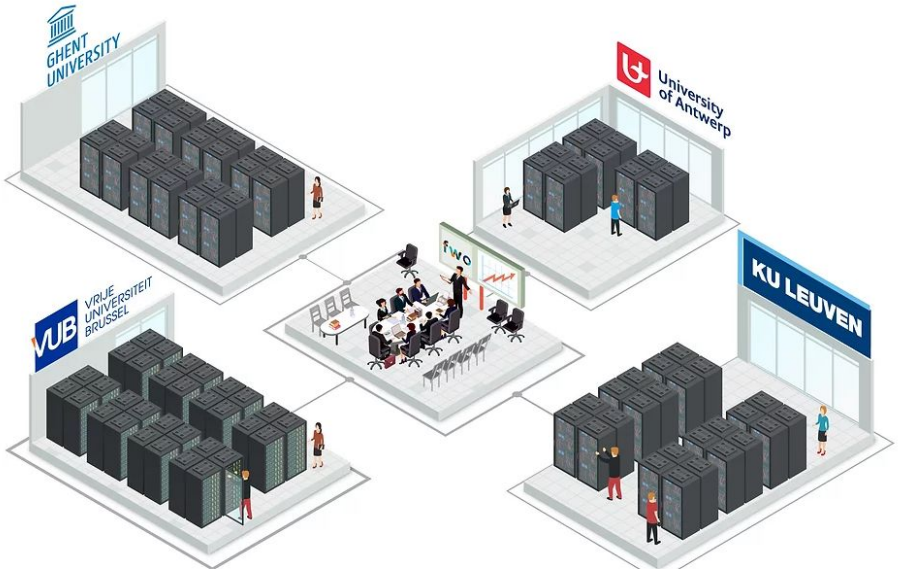
ugent.be/hpc

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



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

VSC Tier-1 compute cluster “Hortense”

(a.k.a. `dodrio`)

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- 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

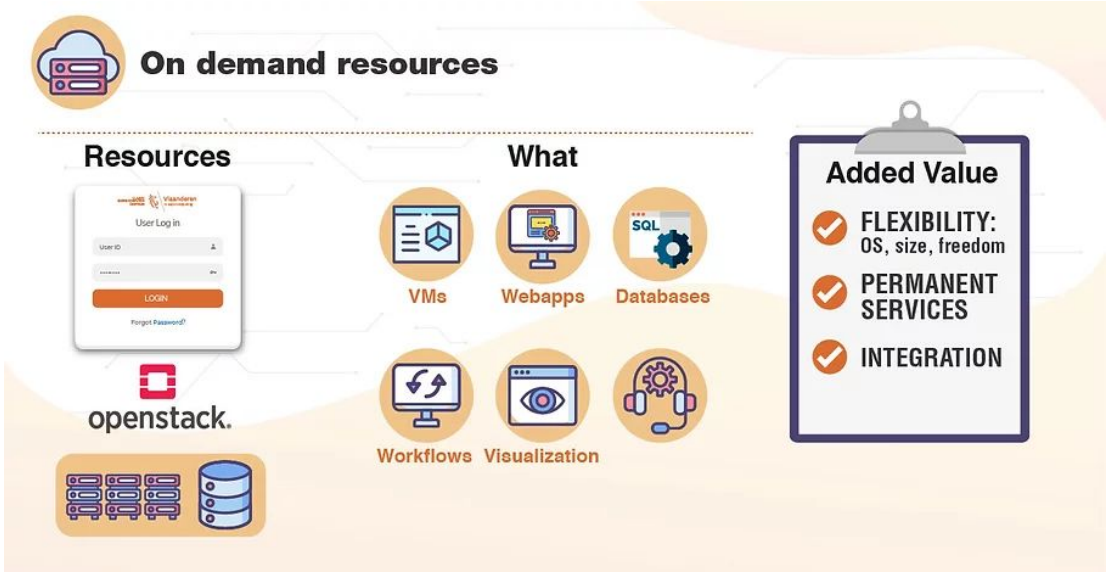
- **Project-based access** (free of charge, funded by FWO)
- 3 cut-off dates per year for submitting project proposals
- Project duration is typically 8 months
- 500k - 5M core hours (CPU-only) or 1k - 25k GPU hours

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



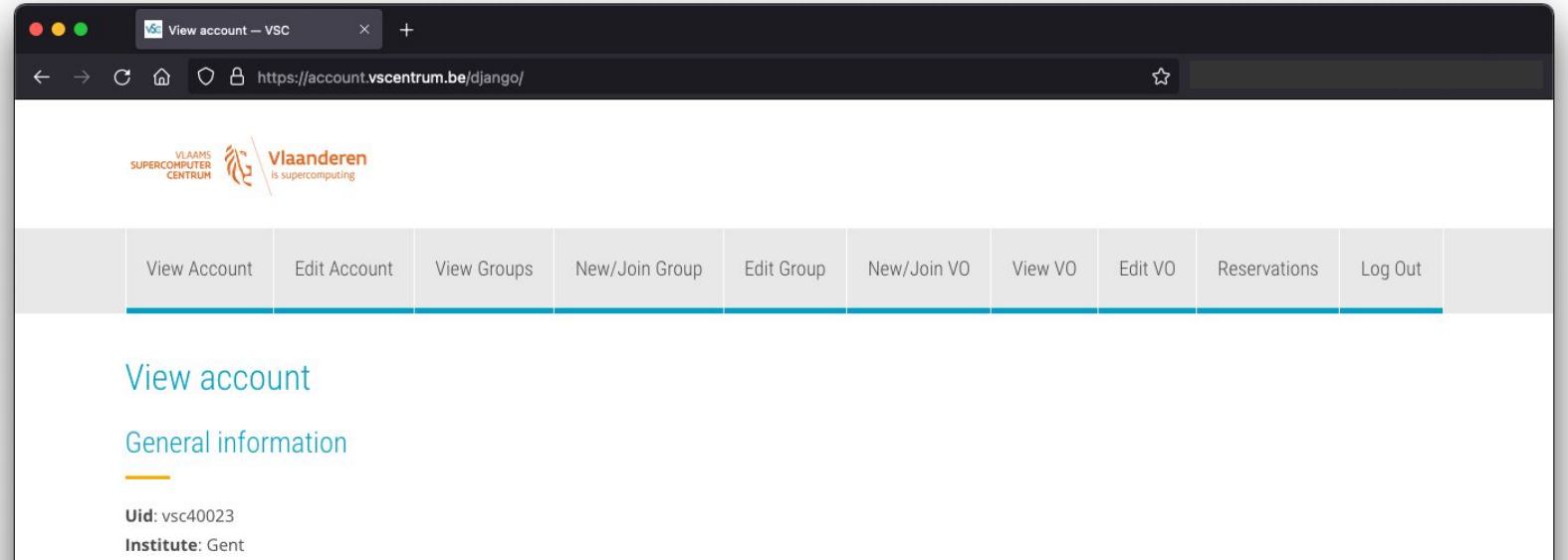
Managing your VSC account

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

Getting access

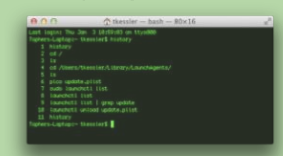
https://login.hpc.ugent.be

Web Portal (No SSH key required)

OR

`ssh tier1.hpc.ugent.be`

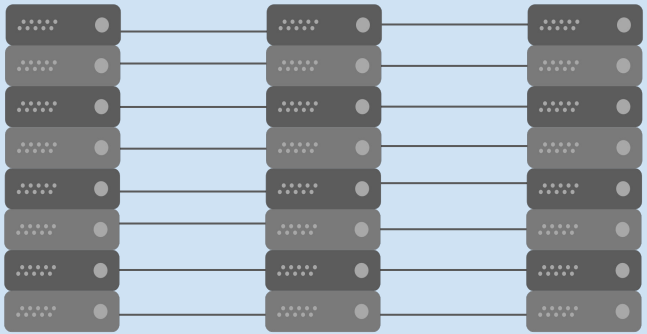
Terminal (requires SSH key)



Login nodes

login55 or *login56*

Compute nodes (where your jobs will run)



Data

File system

Home

Data

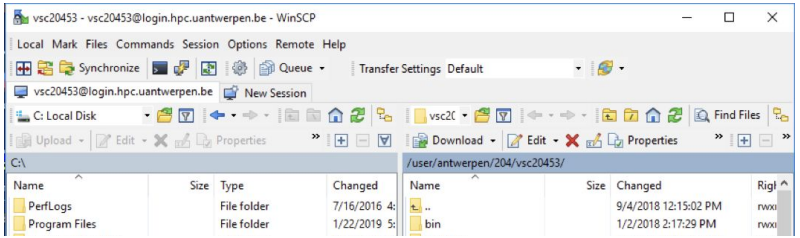
Tier-1 scratch

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      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
```

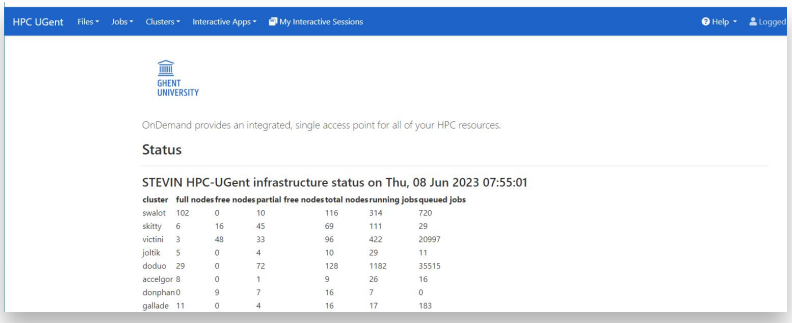
- See dedicated section in HPC-UGent documentation
- `tier1.hpc.ugent.be`
- Requires SSH client + SSH private key
- Windows: PuTTy - macOS/Linux: `ssh` command

- 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!



- See dedicated section of HPC-UGent docs
- https://tier1.hpc.ugent.be
- Powered by Open OnDemand

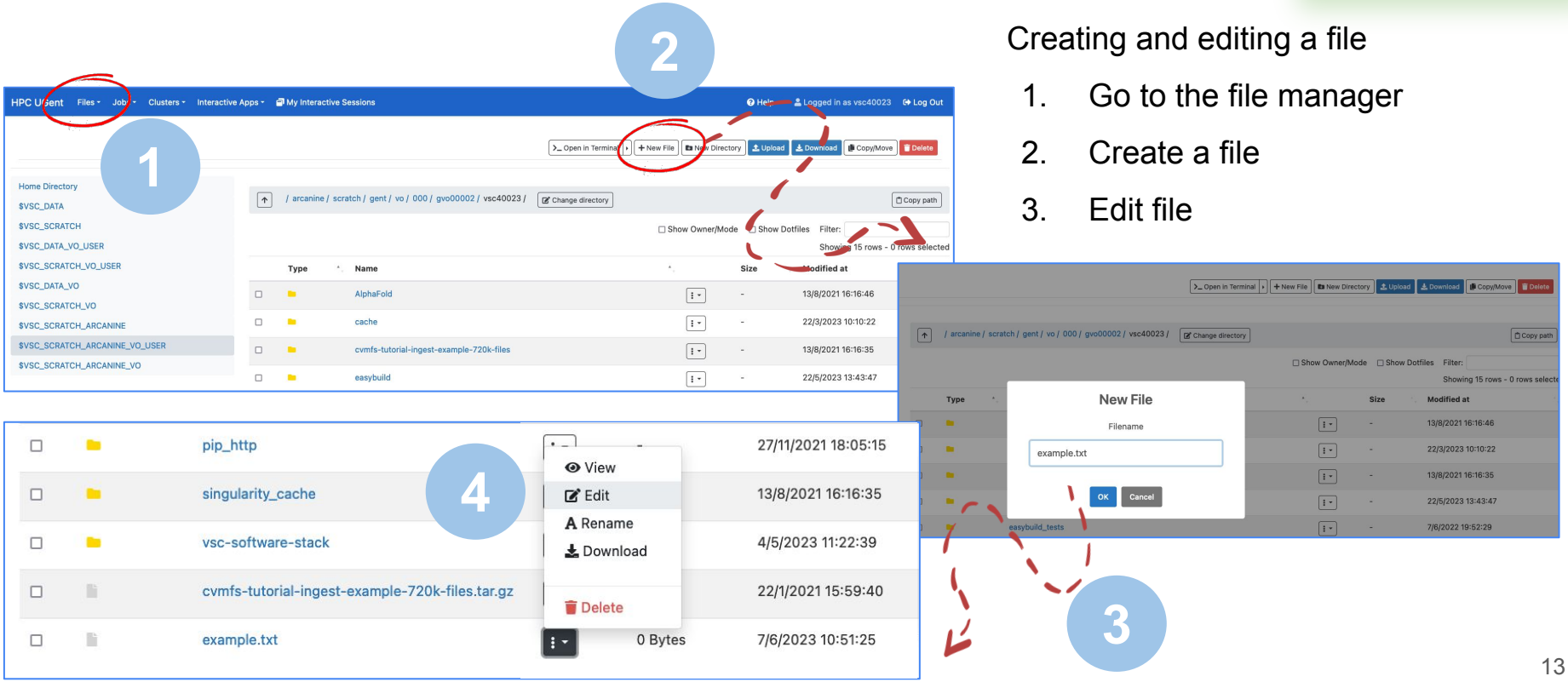
- **Works with a standard internet browser** (Firefox, Chrome, …)
- **Does not require SSH key pair** (only login via university account)
- Provides file browser, shell session, desktop environment, interactive apps, …

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

Recommended!

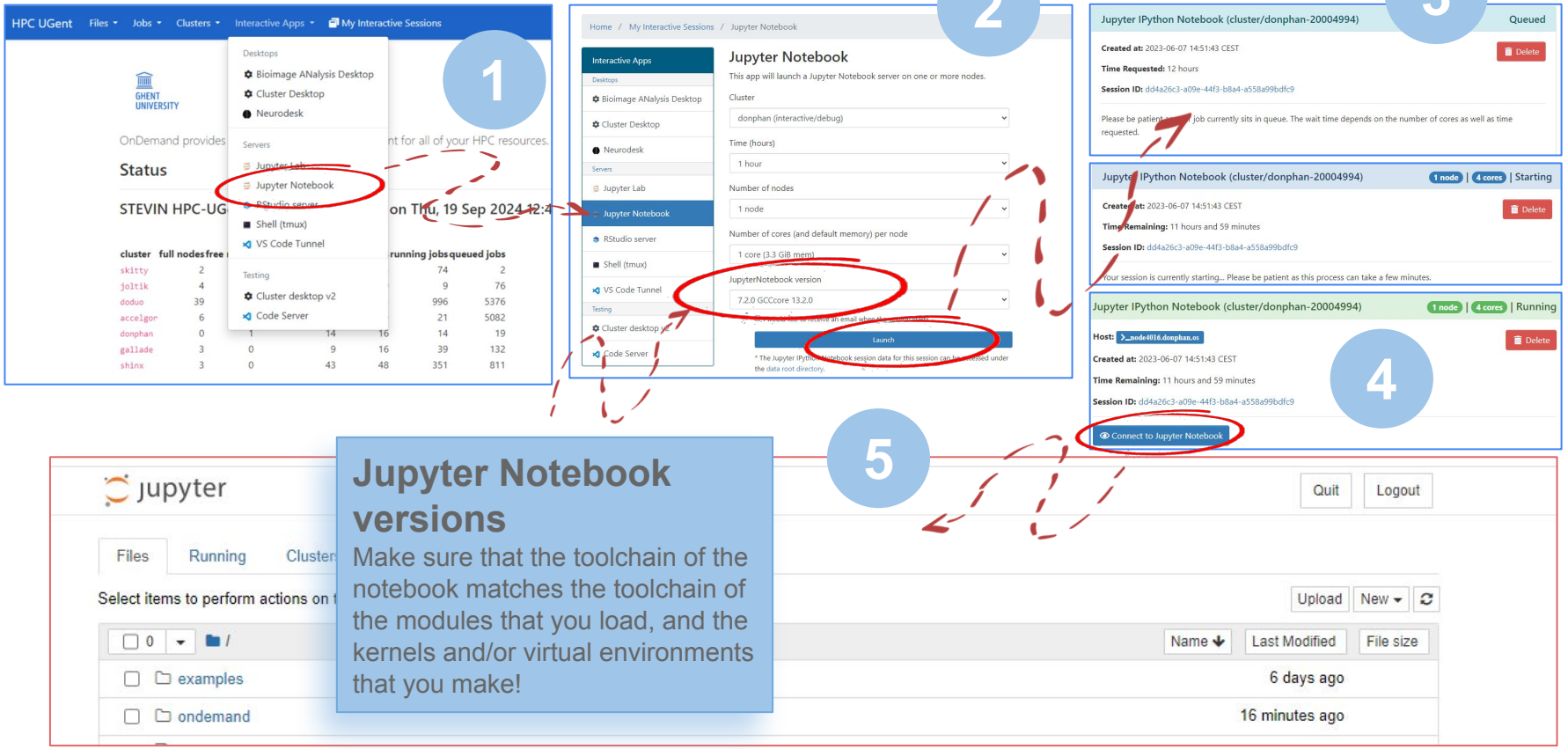
Creating and editing a file

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



UGent web portal: interactive apps (Jupyter notebook)

(Lara)

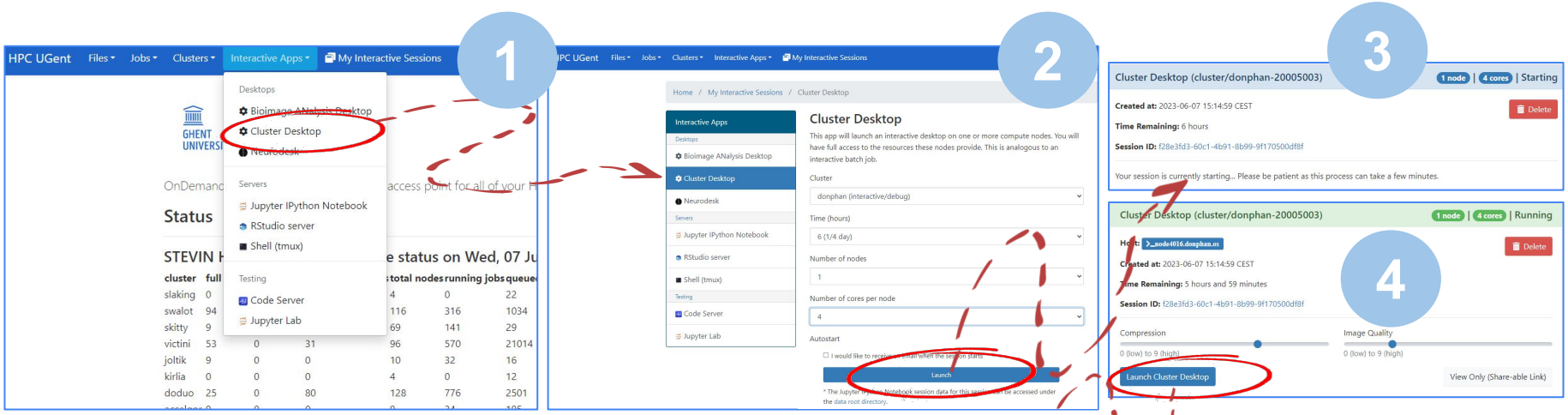


Jupyter Notebook versions

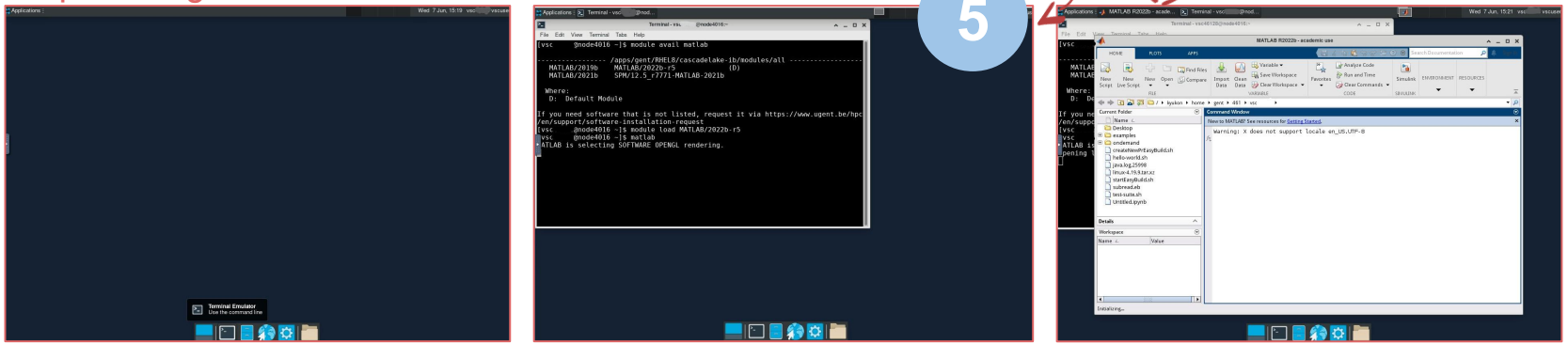
Make sure that the toolchain of the notebook matches the toolchain of the modules that you load, and the kernels and/or virtual environments that you make!

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

(Lara)



Example Using MATLAB



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.

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Sign in

Email

Can't access your account?

Back Next

Authorize hpc-firewall?

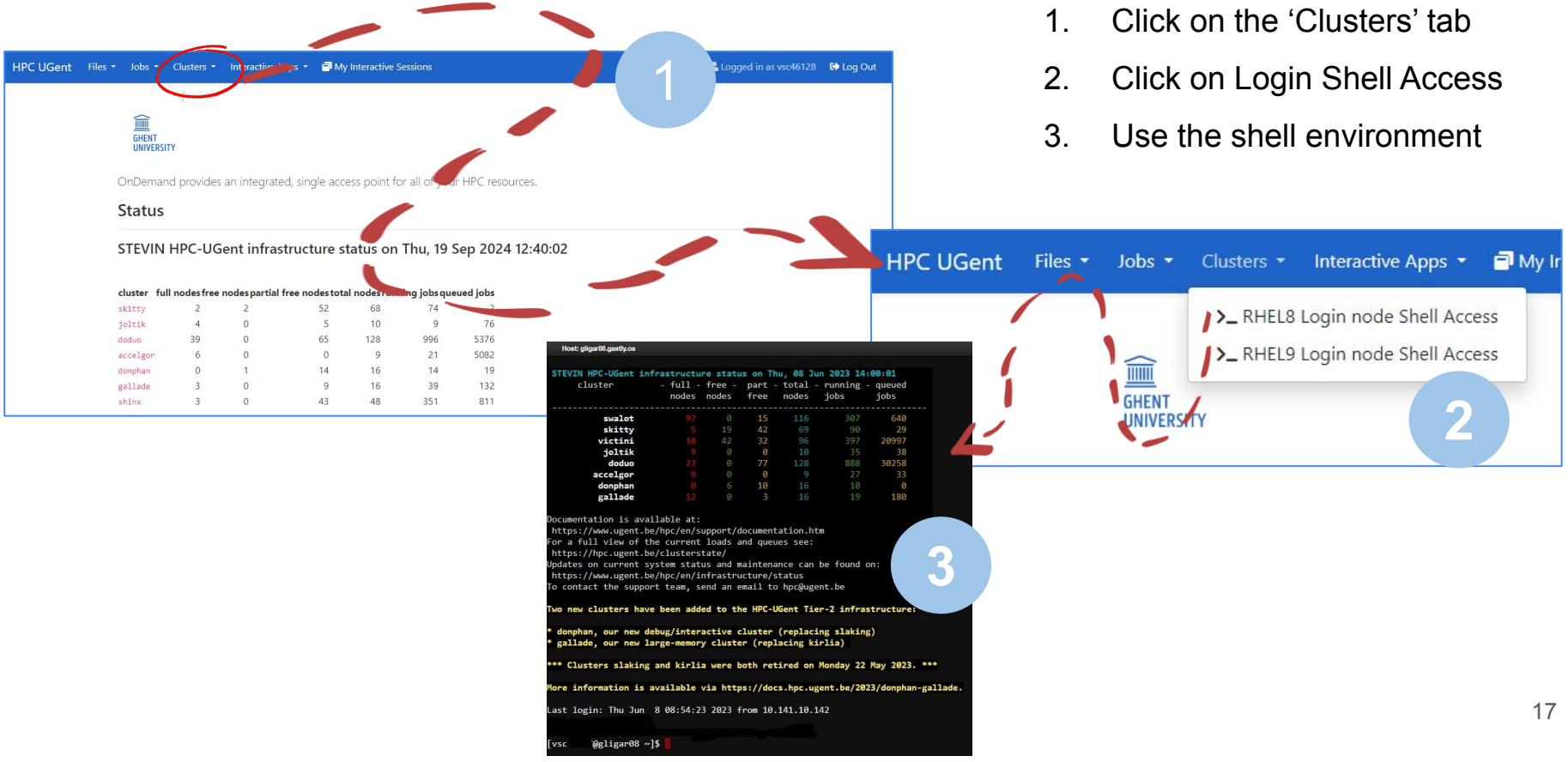
Application requires following permissions

- Read scope

Cancel Authorize

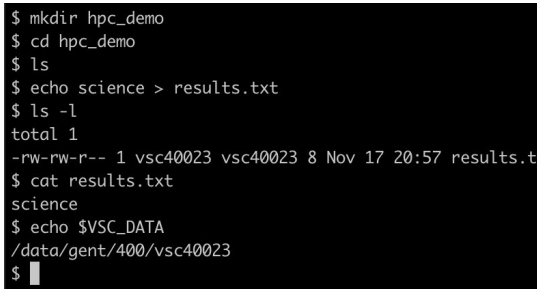
(Lara)

Getting shell access via web portal



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

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

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-mympirun

# 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
mympirun ./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`

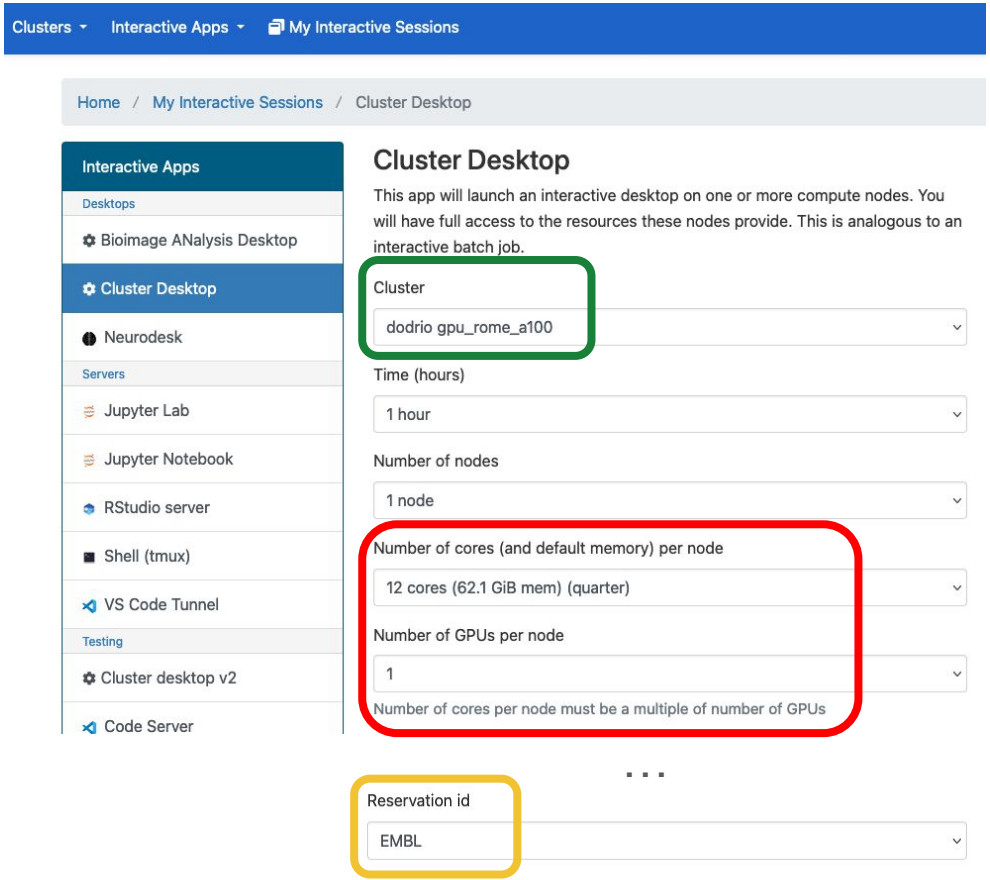
Job submission: GPU reservation for EMBL hackathon

- 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



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

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