



Introduction to HPC-UGent

1 Dec 2023



<https://ugent.be/hpc>

<https://docs.hpc.ugent.be>

hpc@ugent.be

VLAAMS
SUPERCOMPUTER
CENTRUM



Vlaanderen
is supercomputing

Agenda

- [10:00 - 12:00] *Introduction to HPC-UGent* presentation + Q&A
 - Overview of available hardware, getting a VSC account, using the systems, getting support, demos and examples, ...
- [12:00 - 13:00] Sandwich lunch
- [13:00 - 14:00] Guided tour of UGent datacenter 10,
incl. visit to HPC-UGent Tier-2 and VSC Tier-1 cluster
- [14:00 - 17:00] Hands-on session: Getting started with HPC-UGent
 - Login + submitting example jobs
 - Getting started with your own workloads + Q&A

Only for on-site attendees

Documentation

- Extensive documentation on using the HPC-UGent infrastructure is available
- <https://docs.hpc.ugent.be>
- We will specifically use information from these sections:

[Introduction to HPC](#)

[Running jobs with input/output data](#)

[Getting an HPC account](#)

[Using the HPC-UGent web portal](#)

[Connecting to the HPC infrastructure](#)

[Fine-tuning job specifications](#)

[Running batch jobs](#)

[Interactive and debug cluster](#)

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

The HPC-UGent team



Stijn De Weirdt
Technical lead



Kenneth Hoste
User support & training



Andy Georges
System administration



Balázs Hajgató
User support



Ewald Pauwels
Team lead



Wouter Depypere
System administration



Kenneth Waegeman
System administration (storage)



Álvaro Simón García
System administration (cloud)



Lara Peeters
*Project employee
scientific software*

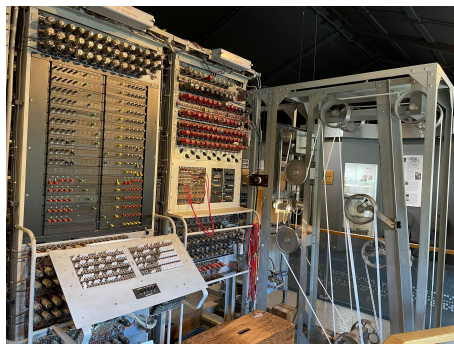
(Kenneth)

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)?

harnessing the power of multiple interconnected cores/nodes/processing units



Colossus - first digital computer (1944)



Cray-2 supercomputer (1985)



"Rack" with desktop PCs in a basement



HPC-UGent Tier-2 infrastructure (2018)



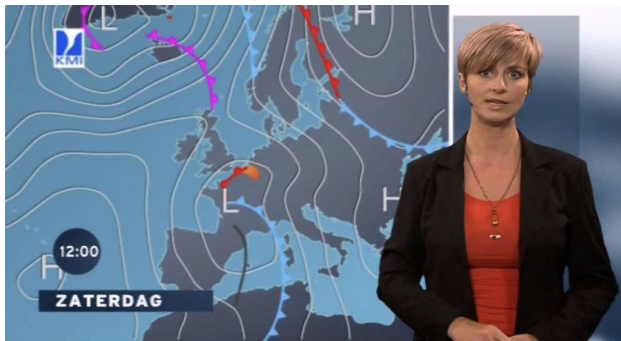
IBM Blue Gene/P in Argonne National Lab (2007)



MareNostrum 4 in Barcelona (2017)

What are supercomputers used for?

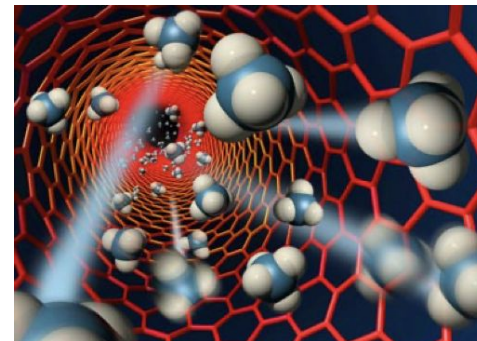
(Lara)



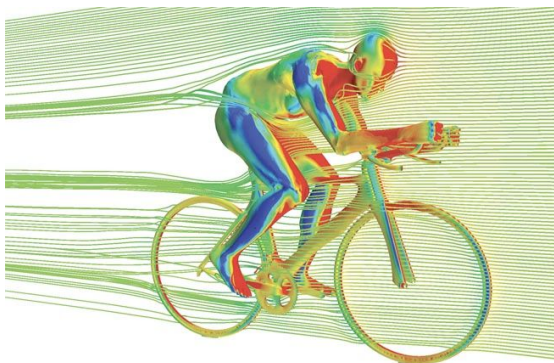
Weather prediction & modelling



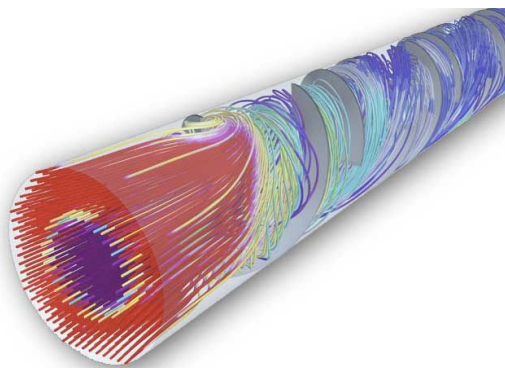
Animation rendering



Molecular modelling, materials research, ...



*Computational Fluid Dynamics (CFD)
Aerodynamics, studying flow of gasses & liquids in volumes, etc.*



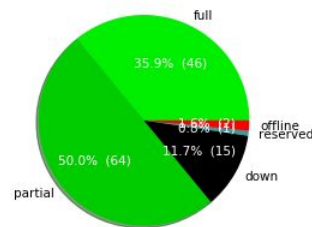
Simulation of atomic weapons, etc.

Terminology: (worker)nodes

- Example cluster from the HPC-UGent
Tier-2 infrastructure: doduo (*default cluster*)
- 128 **(worker)nodes**, also referred to as “servers”
- 1 (worker)node is the equivalent of 1 computer
(but with more cores, memory, ...)
- Check other HPC-UGent Tier-2 clusters

doduo

3501	3502	3503	3504	3505	3506	3507	3508
3509	3510	3511	3512	3513	3514	3515	3516
3517	3518	3519	3520	3521	3522	3523	3524
3525	3526	3527	3528	3529	3530	3531	3532
3533	3534	3535	3536	3537	3538	3539	3540
3541	3542	3543	3544	3545	3546	3547	3548
3549	3550	3551	3552	3553	3554	3555	3556
3557	3558	3559	3560	3561	3562	3563	3564
3565	3566	3567	3568	3569	3570	3571	3572
3573	3574	3575	3576	3577	3578	3579	3580
3581	3582	3583	3584	3585	3586	3587	3588
3589	3590	3591	3592	3593	3594	3595	3596
3597	3598	3599	3600	3601	3602	3603	3604
3605	3606	3607	3608	3609	3610	3611	3612
3613	3614	3615	3616	3617	3618	3619	3620
3621	3622	3623	3624	3625	3626	3627	3628

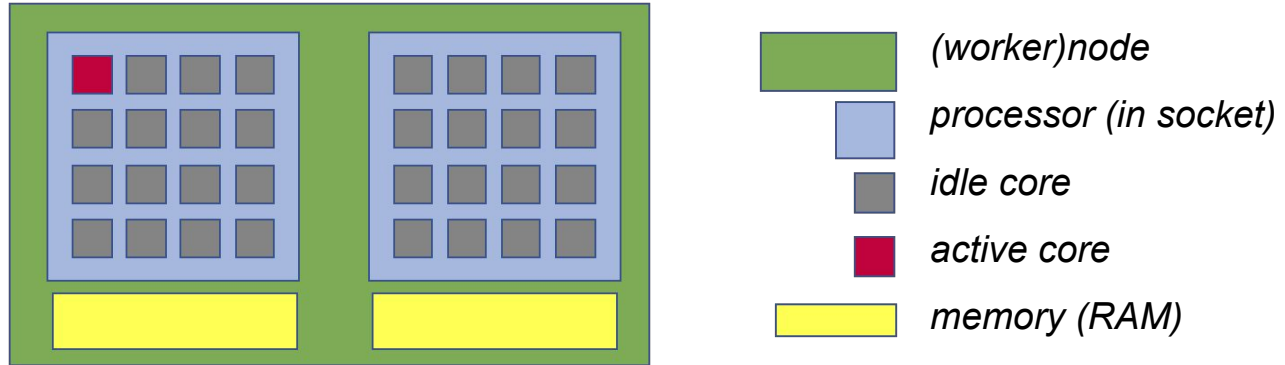


(Lara)

Terminology: cores, CPUs, processors

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, ...

(Lara)

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

In **parallel** software, many calculations are carried out simultaneously.

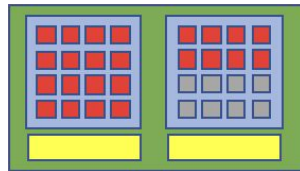
This is based on the principle that large problems can often be divided into smaller tasks, which are then solved concurrently (“in parallel”).

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

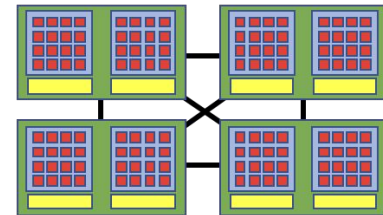
There are two common parallel programming paradigms (among others):

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

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

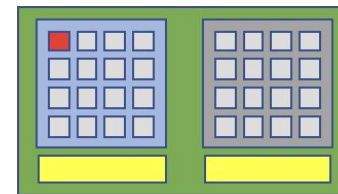


MPI software can use (all) cores in multiple nodes



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

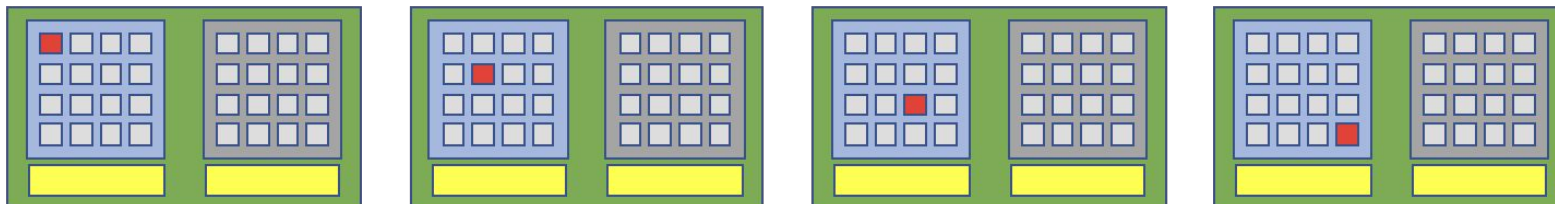
Sequential (a.k.a. serial) software does not do calculations in parallel, it only uses one **single core** of a single workernode.



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

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

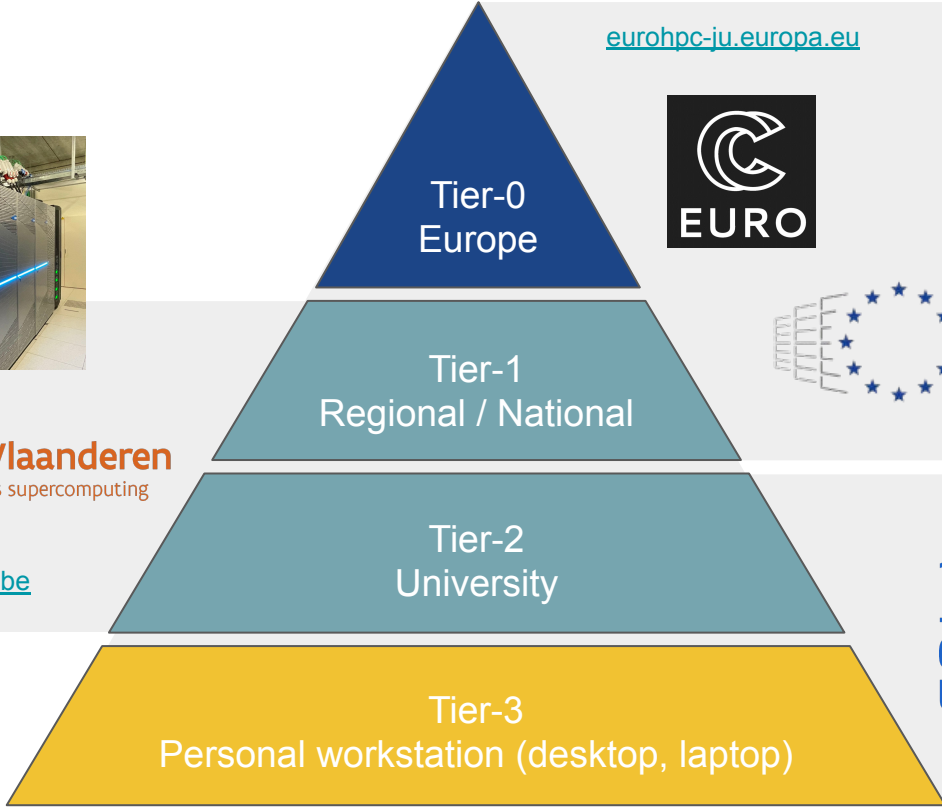
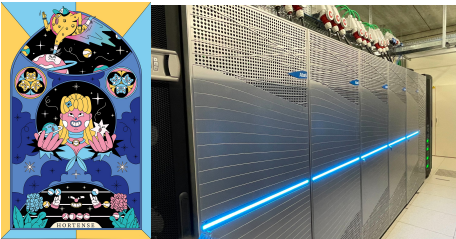
Example: running a Python script 100 times, each on 1 core, to quickly analyse 100 datasets



Centralised hardware in UGent datacenter (S10 @ Sterre)



Different “tiers” of supercomputers



eurohpc-ju.europa.eu



EuroHPC
Joint Undertaking

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HPC-UGent Tier-2 infrastructure

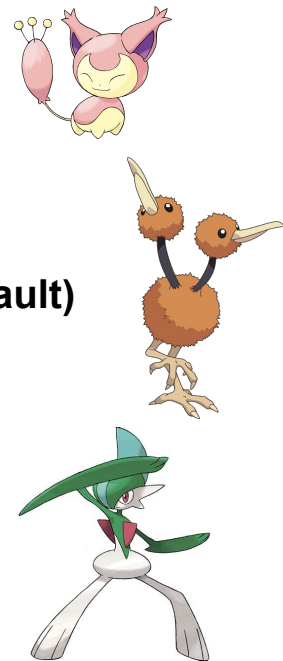
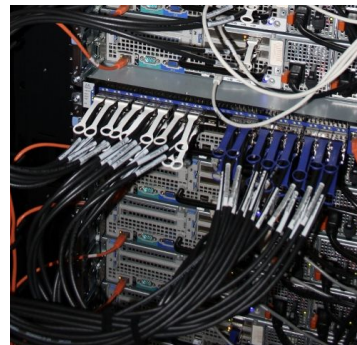


- HPC-UGent Tier-2 infrastructure consists of **7 clusters** (+ login nodes, shared storage, ...)
- Different types of clusters:
 - 3 CPU-only compute clusters (+ 1 pilot cluster)
 - 1 CPU-only batch cluster (no high-speed network, no fast access to shared storage)
 - 2 GPU clusters
 - 1 CPU-only interactive + debug cluster (oversubscribed resources + strict user limits)
- **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



HPC-UGent Tier-2 compute clusters

- `skitty`: 72 nodes, each with 36 cores (Intel Skylake) + ~177GiB of memory
- `doduo`: 128 nodes, each with 96 cores (AMD Rome) + ~250GiB of memory **(default)**
- `gallade`: 16 nodes, each with 128 cores (AMD Milan) + ~940GiB of memory
- All with:
 - High-speed Infiniband network between nodes
 - Fast access to shared file systems
 - Fast local disk (SSD or NVMe)



HPC-UGent Tier-2 batch cluster: victini



- 96 workernodes, each with 36 cores (Intel Skylake) + ~88GiB of memory
- Fast local disk (SSD)
- **No high-speed network** between workernodes (10-Gbit Ethernet)
- **No fast connection to shared filesystems** (only via NFS)
- Only recommended for **single-core / single-node jobs that are *not* I/O-intensive**



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, fast local disk (SSD)



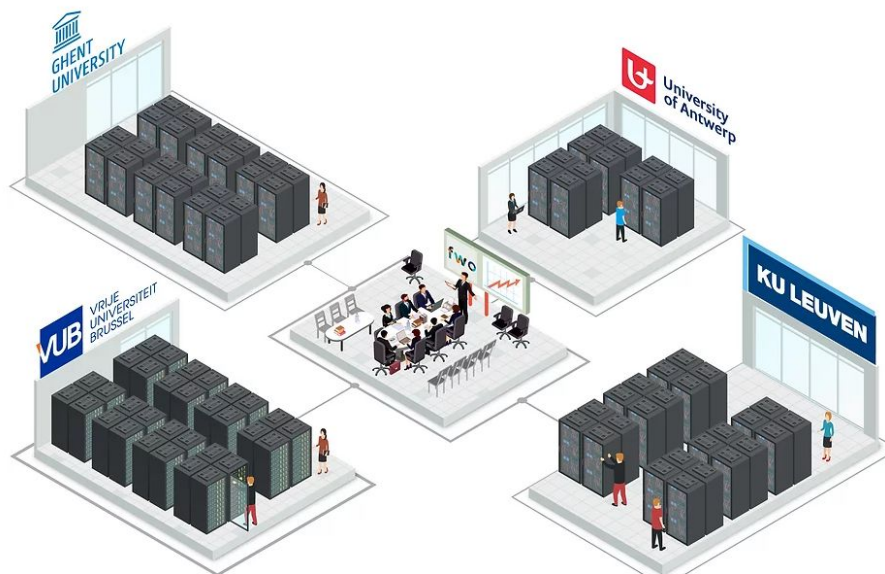
HPC-UGent Tier-2 interactive + debug cluster: donphan

- 16 nodes, each with 36 CPU cores (Intel Cascade Lake) + ~738GB of memory
1 *shared* NVIDIA Ampere A2 GPU (16GB of GPU memory)
- Incl. high-speed network, fast access to shared storage, local disk (NVMe)
- Recycled hardware from old `kirlia` cluster (retired in May 2023)
- **Heavily oversubscribed!** More running jobs => All jobs run slower (due to CPU sharing)
- **Strict user limits:**
 - Max. 3 jobs running, 5 jobs in queue
 - Max. 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 section in HPC-UGent documentation](#)



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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- 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

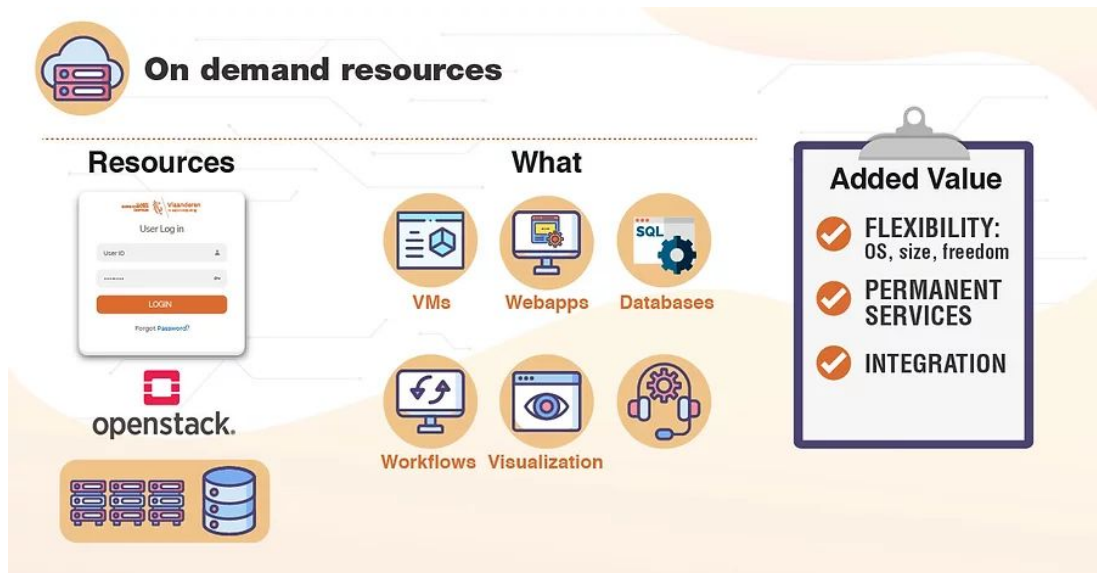
<https://www.vscentrum.be/compute>

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

(Kenneth)

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



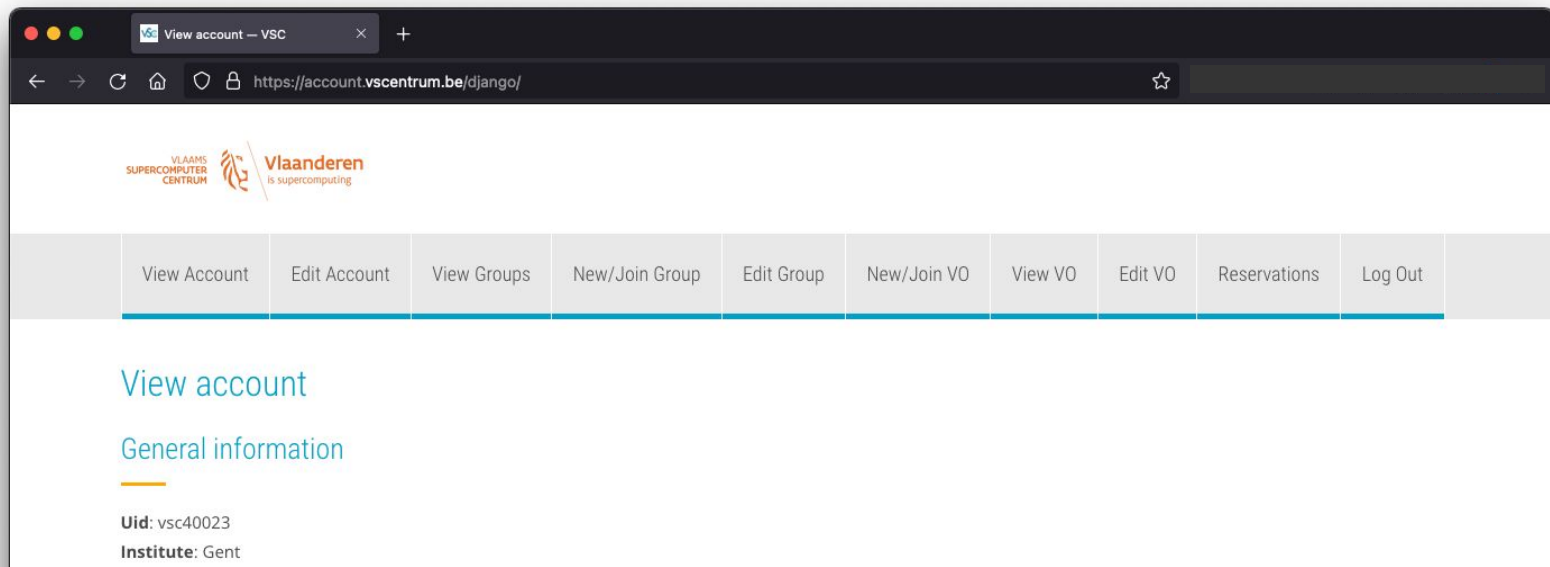
- All members of UGent association can request a VSC account
 - Researchers & staff
 - Master/Bachelor students
- **VSC account can be used to access HPC infrastructure on all VSC sites**
- Subscribed to `hpc-announce` and `hpc-users` mailing lists
- Beware of using HPC for teaching/exam purposes!
 - No guarantee on HPC availability (due unexpected power outage, maintenance, ...)
 - Have a backup plan at hand
 - Advisable teaching/exam formula: project work
- See also [HPC-UGent documentation](#)

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, ...
manage your Virtual Organisation (VO), ...



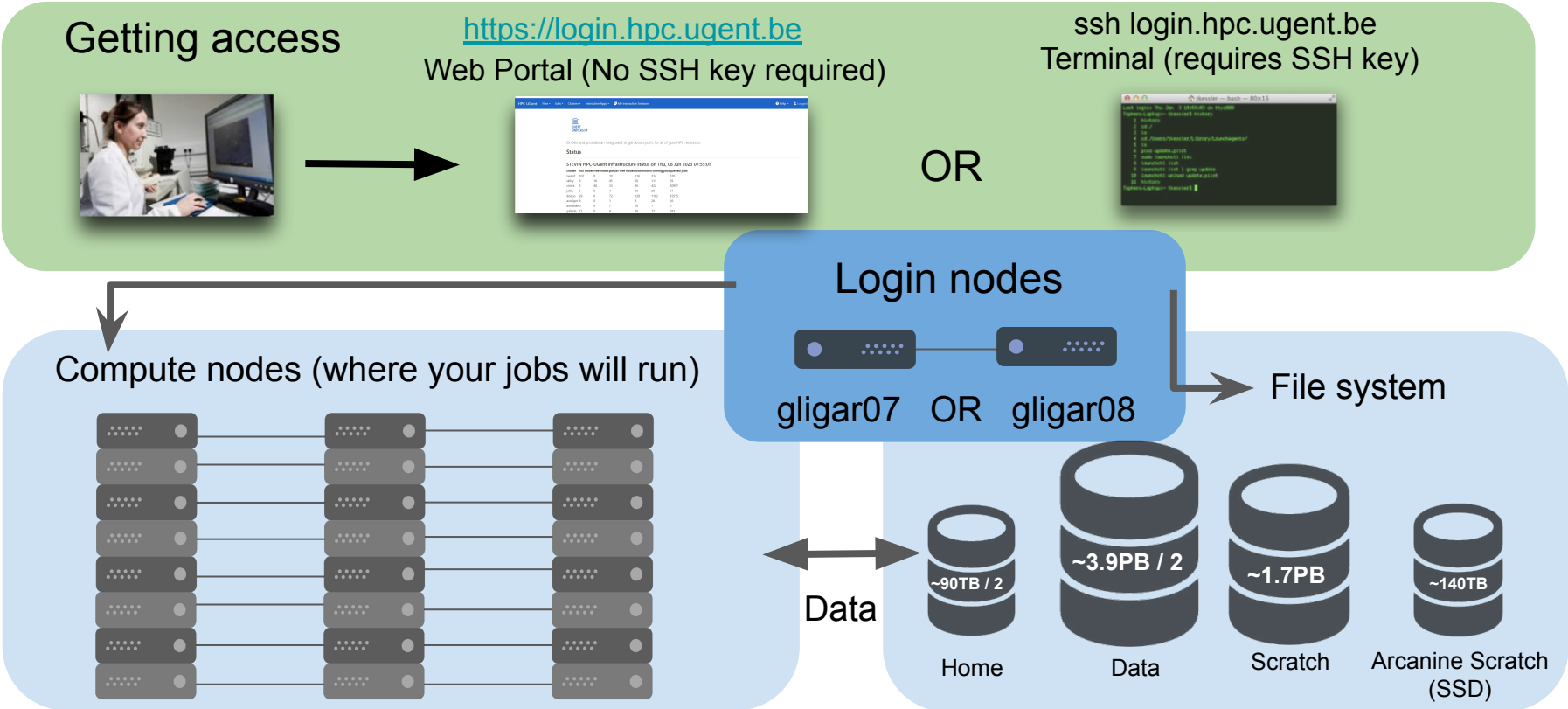
The screenshot shows a web browser window with the URL <https://account.vscentrum.be/django/>. The page header features the VLAAMS SUPERCOMPUTER CENTRUM logo and the Vlaanderen is supercomputing logo. Below the header is a navigation menu with the following items: View Account, Edit Account, View Groups, New/Join Group, Edit Group, New/Join VO, View VO, Edit VO, Reservations, and Log Out. The main content area is titled "View account" and includes a section for "General information" with the following details: Uid: vsc40023 and 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 completes
7. Inspect and/or move your results



High-level overview of HPC-UGent infrastructure



Option 1: Connecting to the HPC-UGent 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
swatbot 19  0  94  118  1659  1172
skitty  33  0  33  72  1391  439
victimi  7  0  87  96  588  30000
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 10.141.110.60
[vsc40023@qligar07 ~]$
[vsc40023@qligar07 ~]$ hostname
qligar07.gastly.os
```

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

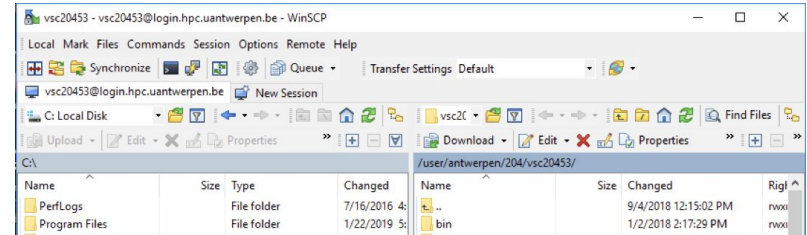
- Transferring files to/from HPC-UGent infrastructure

- Done via the login nodes
- Options:

- On Linux or macOS:

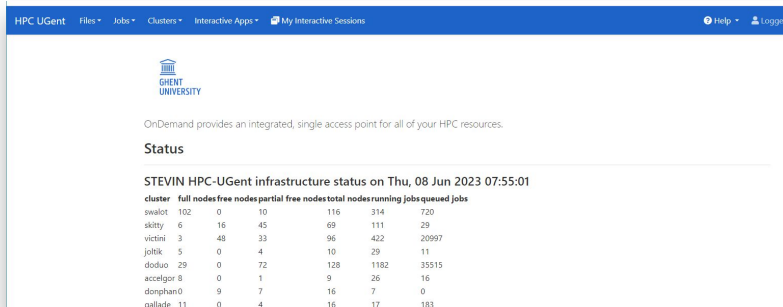
- Using `scp` or `rsync` command in terminal window
- Using a graphical like the built-in file manager or [Cyberduck](#)

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



Option 2: Connecting to the HPC-UGent login nodes with web portal

Recommended!



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

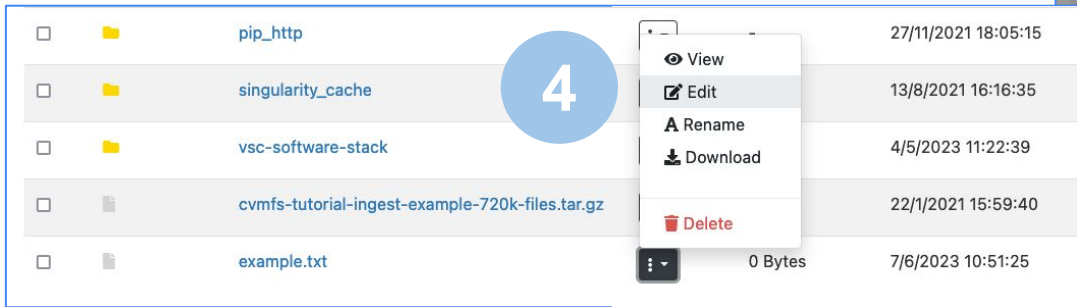
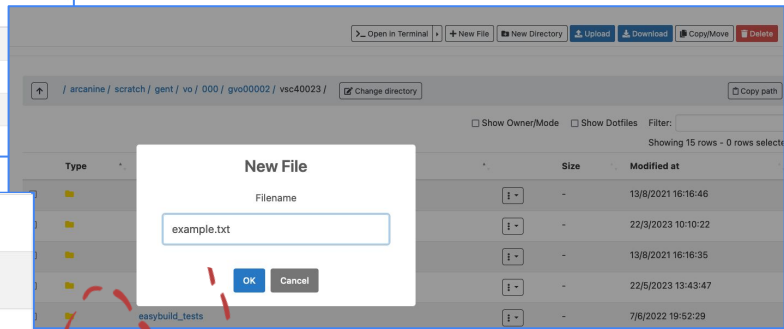
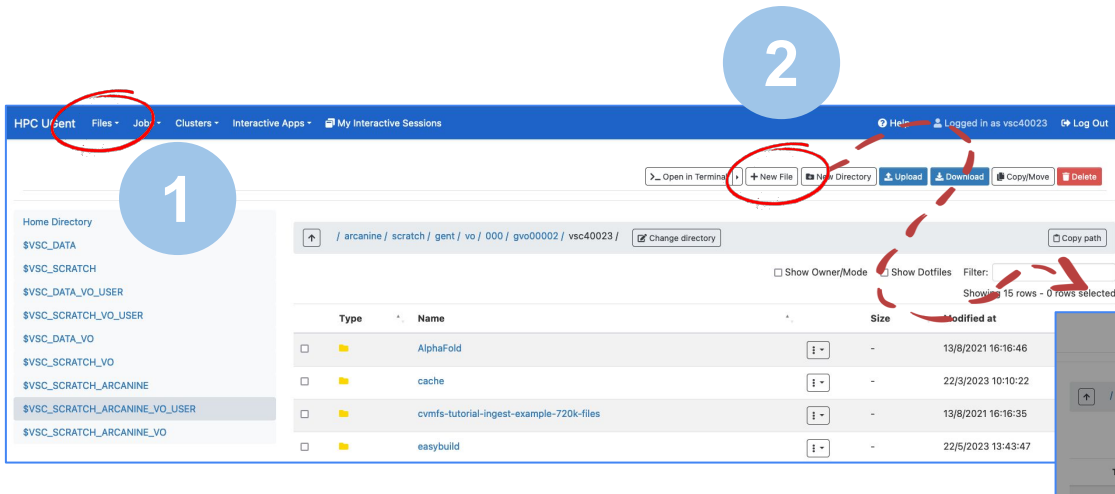
- **Works with a standard internet browser** (Firefox, Chrome, ...)
- **Does not require SSH key pair** (only login via UGent account)
- Provides file browser, shell session, desktop environment, interactive apps, ...

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)

1

The screenshot shows the UGent web portal interface. The 'Interactive Apps' menu is open, and 'Jupyter IPython Notebook' is circled in red. A red dashed arrow points from this menu item to the configuration page in the next screenshot.

2

The screenshot shows the configuration page for the Jupyter IPython Notebook. The 'Launch' button at the bottom is circled in red. A red dashed arrow points from this button to the session status page in the next screenshot.

3

The screenshot shows the session status page for a Jupyter IPython Notebook. The session is in a 'Queued' state. A red dashed arrow points from the 'Launch' button in the previous screenshot to this page.

The screenshot shows the session status page for a Jupyter IPython Notebook. The session is in a 'Starting' state. A red dashed arrow points from the 'Queued' state page to this one.

4

The screenshot shows the session status page for a Jupyter IPython Notebook. The session is in a 'Running' state. The 'Connect to Jupyter Notebook' button is circled in red. A red dashed arrow points from this button to the Jupyter interface in the next screenshot.

5

The screenshot shows the Jupyter web interface. The 'Files' tab is active, showing a file browser with folders like 'examples' and 'ondemand'. The 'Connect to Jupyter Notebook' button from the previous screenshot is circled in red, and a red dashed arrow points to this interface.

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

1

2

3

4

Interactive Apps

- Desktops
 - Bioimage Analysis Desktop
 - Cluster Desktop**
 - Neurodesk
- Servers
 - Jupyter IPython Notebook
 - RStudio server
 - Shell (tmux)
- Testing
 - Code Server
 - Jupyter Lab

Cluster Desktop (cluster/donphan-20005003)

Created at: 2023-06-07 15:14:59 CEST

Time Remaining: 6 hours

Session ID: f28e3f43-60c1-4b91-8b99-9f170500d8f

Your session is currently starting... Please be patient as this process can take a few minutes.

Cluster Desktop (cluster/donphan-20005003)

Created at: 2023-06-07 15:14:59 CEST

Time Remaining: 5 hours and 59 minutes

Session ID: f28e3f43-60c1-4b91-8b99-9f170500d8f

Launch Cluster Desktop

Example Using MATLAB

5

```
matlab
```

```
----- /apps/ugent/BIBL/cascadelake-ib/nodes/all -----  
MATLAB/2019b MATLAB/2022a-r5  
MATLAB/2021b SRV/21.5_77771 MATLAB/2021a  
Where:  
D: Default Node  
If you need software that is not listed, request it via https://www.ugent.be/hpc/  
For supported software installation requests:  
[isc] @node4016 ~$ module load MATLAB/2022a-r5  
[isc] @node4016 ~$ module load MATLAB/2022a-r5  
[isc] @node4016 ~$ matlab  
-ATLAB is selecting SOFTWARE: OPENGL rendering.
```

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, 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)

firewall.vscentrum.be

Vlaams Supercomputer Centrum Vlaanderen is supercomputing

Keep this browser tab open!

HPC Firewall

[IP Whitelist](#) | [Info](#)

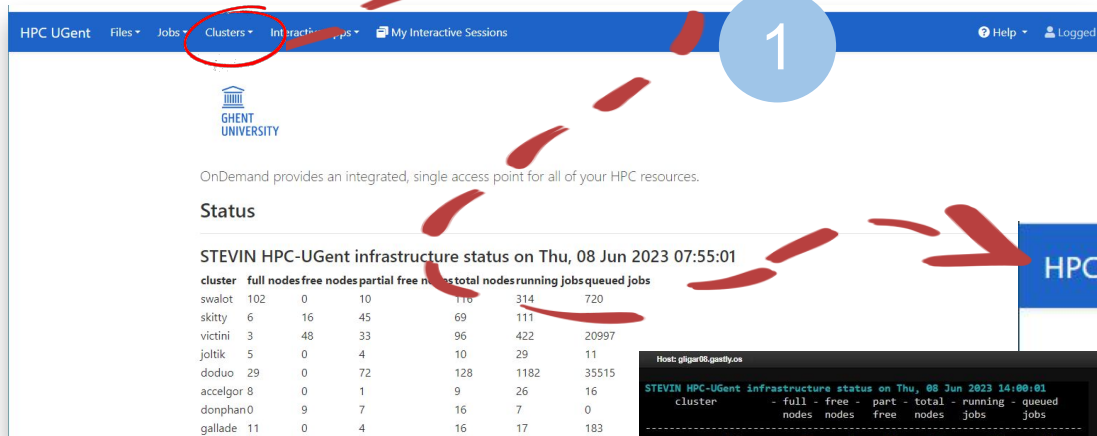
Logged on successfully as vsc40023.

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).

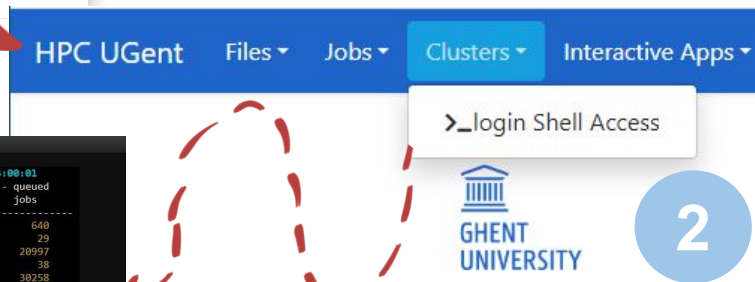
Getting shell access via web portal

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

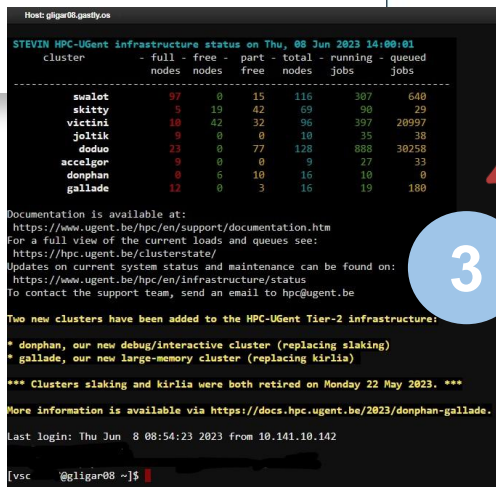


The screenshot shows the HPC UGent web portal interface. The navigation bar at the top includes 'Files', 'Jobs', 'Clusters', 'Interactive Apps', and 'My Interactive Sessions'. The 'Clusters' tab is highlighted with a red circle and a blue circle containing the number '1'. Below the navigation bar, the Ghent University logo is visible, followed by a message: 'OnDemand provides an integrated, single access point for all of your HPC resources.' The main content area displays the 'Status' section, titled 'STEVIN HPC-UGent infrastructure status on Thu, 08 Jun 2023 07:55:01'. A table lists various clusters with their respective node counts and job statuses.

cluster	full nodes	free nodes	partial free nodes	total nodes	running jobs	queued jobs
swalot	102	0	10	110	314	720
skitty	6	16	45	69	111	
victini	3	48	33	96	422	20997
joltik	5	0	4	10	29	11
deduo	29	0	72	128	1182	35515
accelgor	8	0	1	9	26	16
donphan0	9	7		16	7	0
gallade	11	0	4	16	17	183



The screenshot shows the HPC UGent web portal interface with the 'Clusters' tab selected in the navigation menu. A dropdown menu is open, showing the option '>_login Shell Access'. The Ghent University logo is visible below the navigation bar. A blue circle containing the number '2' is positioned to the right of the dropdown menu.



The screenshot shows a terminal window with the following content:

```
Host: glligar08.guestlyon
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
-----
swalot   97  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
deduo   13  0  77  128  888  30258
accelgor 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

[vs@ ~] glligar08 ~]$
```

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 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 (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__)'
```

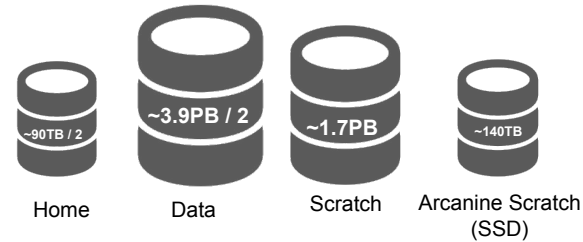
```
1.25.1
```


Useful environment variables for job scripts

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

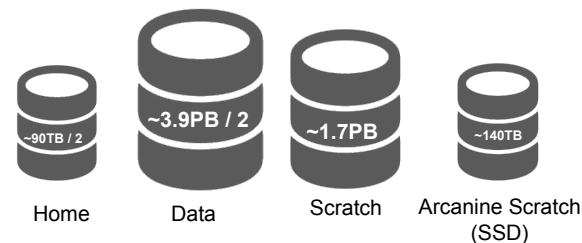
- **\$PBS_JOBID**: job id of running job
- **\$PBS_O_WORKDIR**: directory from which job was submitted on login node
 - It is common to use `cd $PBS_O_WORKDIR` at beginning of a job script
- **\$PBS_ARRAYID**: array id of running job
 - Only relevant when submitting array jobs (`qsub -t`)
- **\$TMPDIR**: 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

Input/output data and shared filesystems



- See [dedicated section 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 (disk space)



- 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, even TBs) available for *virtual organisations* (VOs);** see [dedicated section on VOs 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

⚠ Values can be outdated up to 1 hour.

Personal

Storage name	Used	Quota	%	Inodes used (files)
VSC_HOME	2.25 GiB	5.7 GiB	39.39%	77521
VSC_DATA	13.28 GiB	23.75 GiB	55.93%	234842
VSC_DATA_SHARED	n/a	972.8 MiB	n/a	n/a
VSC_SCRATCH_ARCANINE	0 B	974.0 MiB	0.00%	1
VSC_SCRATCH_KYUKON	15.17 GiB	23.75 GiB	63.88%	27467

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	%	Inodes used (files)
VSC_DATA_VO	gvo00002	0 B	7.67 TiB	0.00%	1
VSC_SCRATCH_ARCANINE_VO	gvo00002	0 B	7.25 TiB	0.00%	1
VSC_SCRATCH_KYUKON_VO	gvo00002	0 B	10.35 TiB	0.00%	1

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

⚠ Values can be outdated up to 1 hour.

Name	Used	Quota	%
VSC_DATA_VO	7.75 TiB	15.34 TiB	50.55%
VSC_DATA_SHARED_VO	0 B	1.9 GiB	0.00%
VSC_SCRATCH_ARCANINE_VO	8.23 TiB	14.5 TiB	56.72%
VSC_SCRATCH_KYUKON_VO	14.73 TiB	20.7 TiB	71.19%

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

# load Python 3.11, with batteries included (extra PyPI packages)
module load Python-bundle-PyPI/2023.06-GCCcore-12.3.0
# 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=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
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/donphan
```

```
$ 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	donphan

- 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 (hours, or even minutes/seconds)
- 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 [dedicated section 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`

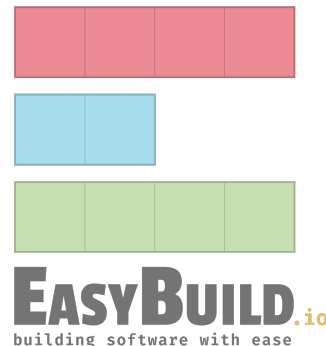
Software installations

- 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>



Questions, problems, getting help

Don't hesitate to contact the HPC-UGent Tier-2 support team via hpc@ugent.be

- 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 VSC account
 - Preferably don't send files in attachment, we prefer to look at it "in context"
 - Also mention job IDs, which cluster was used, how job was submitted, etc.
- Preferably use your UGent email address
- Alternatives:
 - Short (Teams) meeting (for complex problems, big projects)
 - `hpc-users` mailing list

Questions, problems, getting help (be patient...)

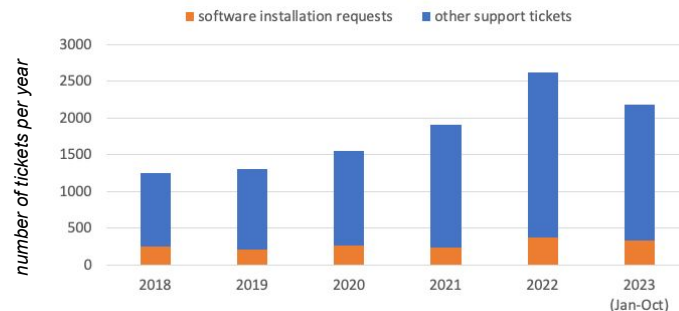
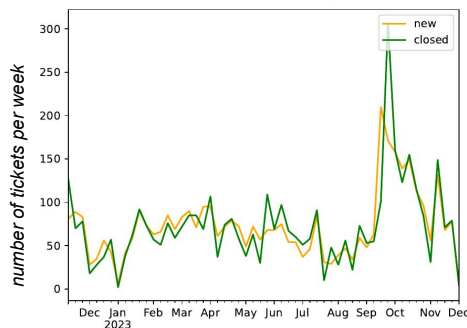
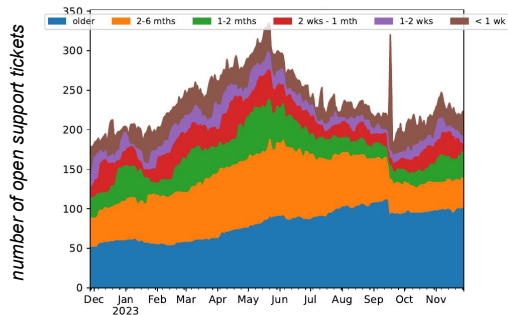
(Kenneth)

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

but be patient...



- We're doing what we can to keep up with incoming support questions + software installation req.
- We have been getting **50-100 new tickets per week** recently, and have a backlog of ~250 tickets
- **Help us help you:** read the docs, provide sufficient details (like job IDs, output files, etc.), ...
- Feel free to send a reminder in the same ticket or mail thread, especially if your work is blocked



Best Practices for HPC (@ VSC User Day 2023)



VLAAMS
SUPERCOMPUTER
CENTRUM



Vlaanderen
is supercomputing



Best Practices for HPC

or

How to get your work done faster?



24 Oct 2023 - VSC User Day 2023

Alex Domingo (VUB-HPC), Kenneth Hoste (HPC-UGent)

<https://www.vscentrum.be/usersday2023>

[direct link to slides \(PDF\)](#)

Agenda

- [10:00 - 12:00] *Introduction to HPC-UGent* presentation + Q&A
 - Overview of available hardware, getting a VSC account, using the systems, getting support, demos and examples, ...
- [12:00 - 13:00] Sandwich lunch
- [13:00 - 14:00] Guided tour of UGent datacenter 10,
incl. visit to HPC-UGent Tier-2 and VSC Tier-1 cluster
- [14:00 - 17:00] Hands-on session: Getting started with HPC-UGent
 - Login + submitting example jobs
 - Getting started with your own workloads + Q&A

Only for on-site attendees