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Introduction to HPC-UGent

March 27th 2019

https://www.ugent.be/hpc/en/training/materials/2019/introhpcugent

hpc@ugent.be

https://ugent.be/hpc

Vlaanderen is computing

About this training – purpose

- Inform you of HPC-UGent services and infrastructure
- Learn what the benefit can be for your research
- Get you started on the central HPC infrastructure at UGent
  - Successfully connect to the HPC infrastructure
  - Successfully launch your first job
  - Figure out how to leverage it for *your* research
- Answer any questions you may have

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About this training – HPC tutorial

- An HPC tutorial is available, applicable for all VSC infrastructure
- Download it here: **https://www.ugent.be/hpc/en/support/documentation.htm**
- *This is work in progress. If you find errors, do let us know.*
- We will specifically use information from these chapters:

1/ Introduction to HPC	4/ Running batch jobs
2/ Getting an HPC account	6/ Running jobs with input/output data
3/ Connecting to the HPC	8/ Fine-tuning job specifications

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What is High Performance Computing?

"***High Performance Computing***" **(HPC)** is computing 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 that work together so that in many respects they can be viewed as a single system.

(a.k.a. "supercomputing")

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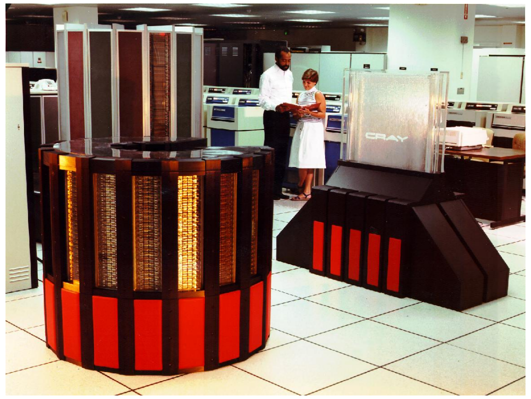
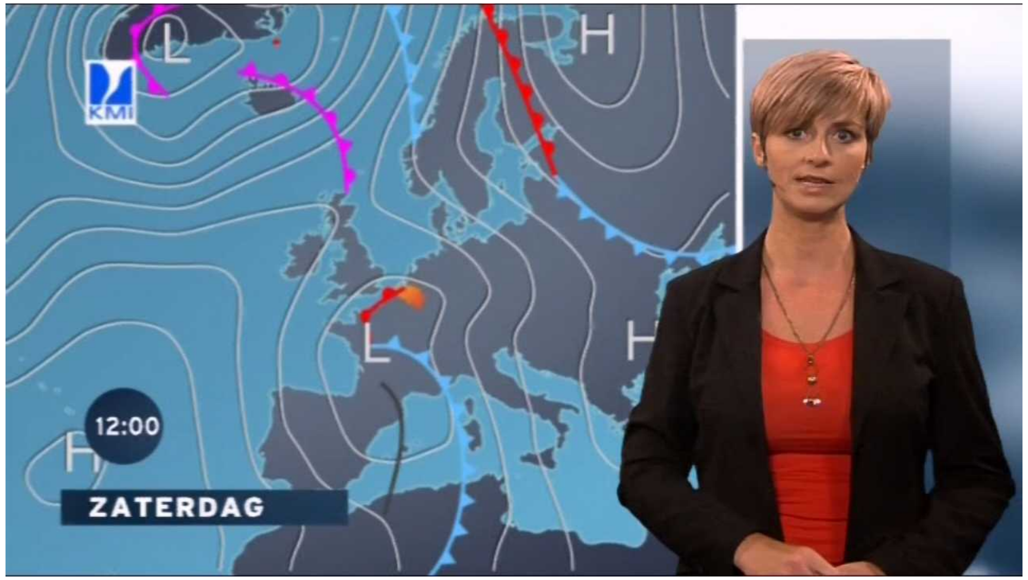
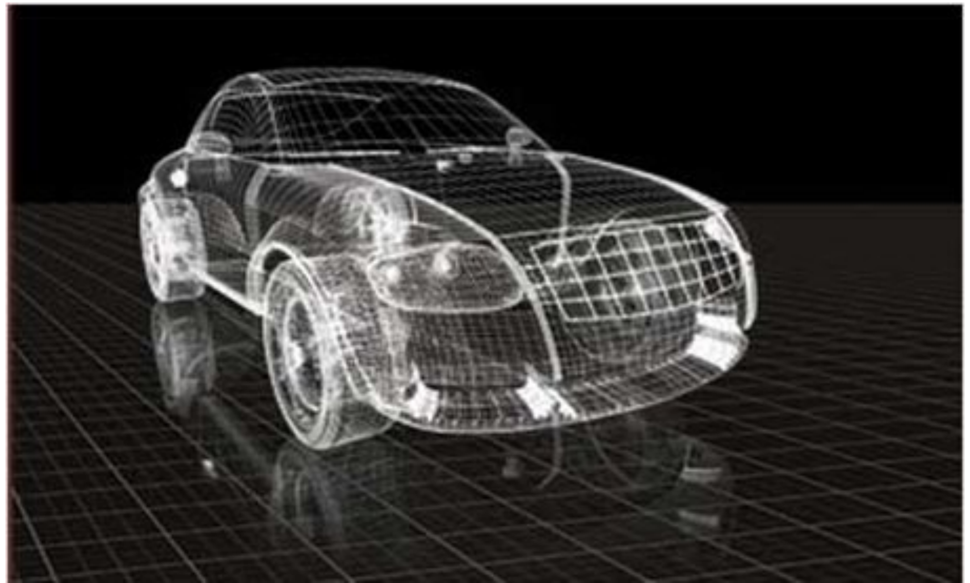
What is High Performance Computing?

harness power of multiple interconnected cores/nodes/processing units



Everyday applications of supercomputing





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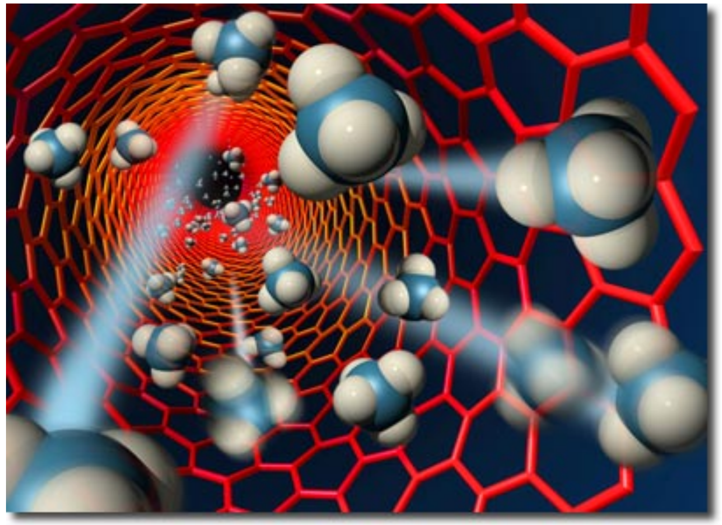
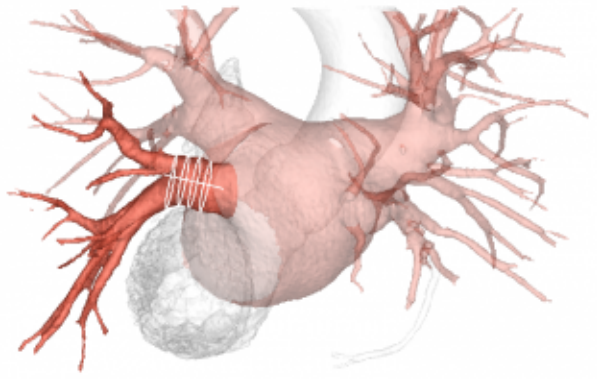
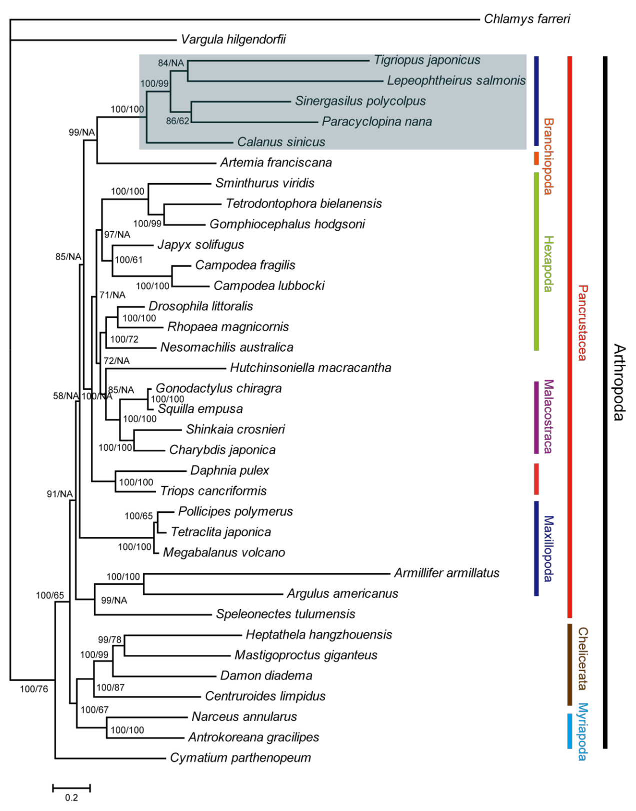
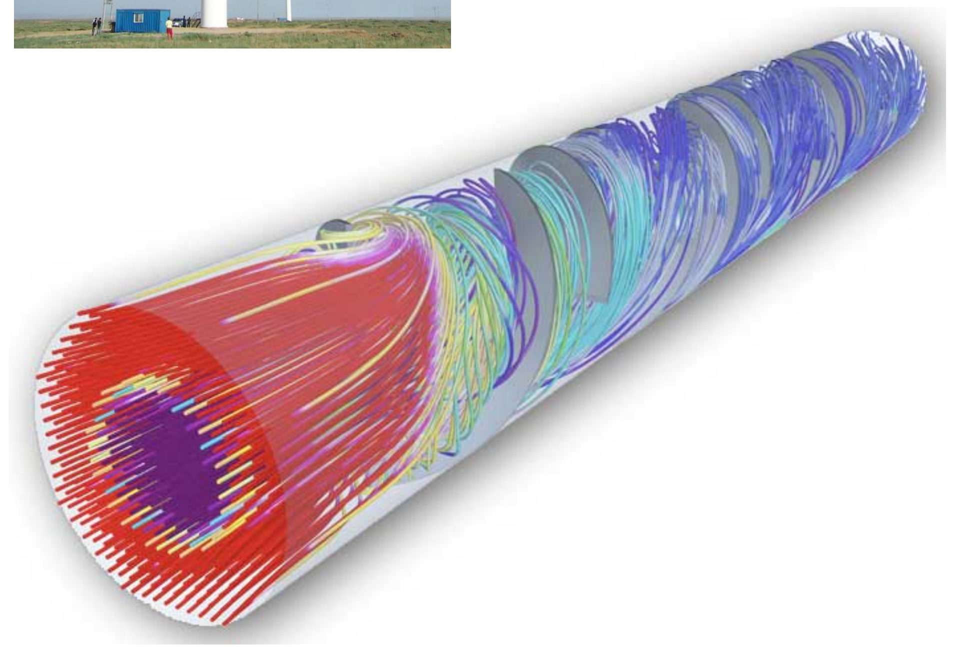
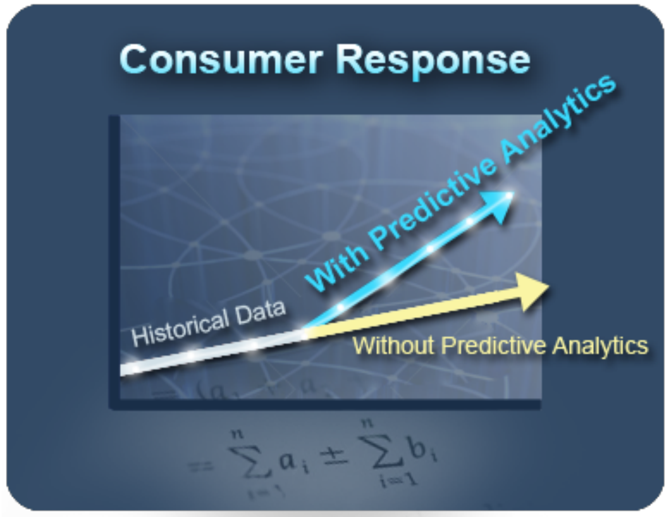
Scientific applications of supercomputing

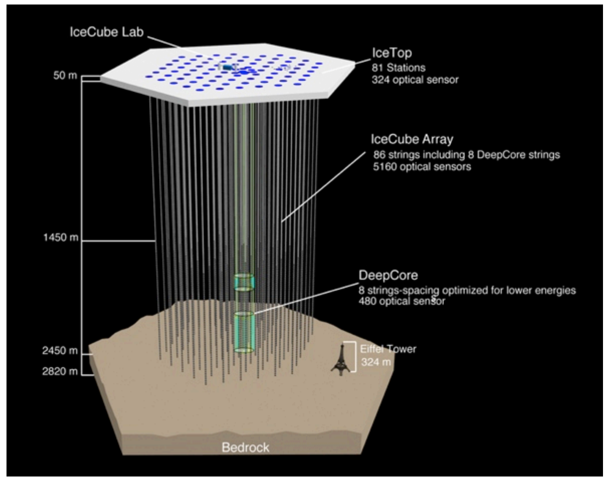









Consumer Response
With Predictive Analytics
Historical Data
Without Predictive Analytics
$\sum_{i=1}^{n} a_i \pm \sum_{i=1}^{n} b_i$

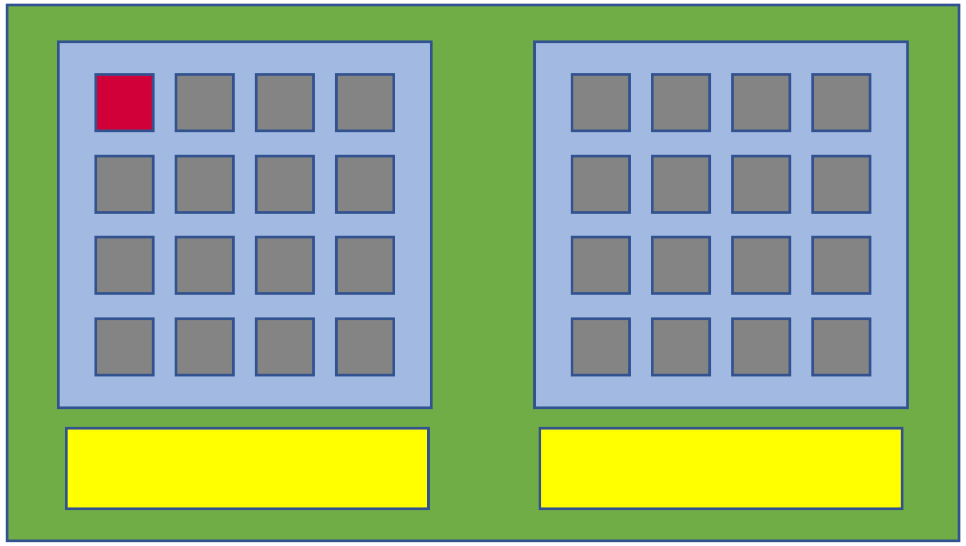


Cores, CPUs, processors, sockets, (worker)nodes

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 CPUs or **cores** that are used to execute *computations*.

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



🟩 *(worker)node*

🟦 *processor (in socket)*

⬛ *idle core*

🟥 *active core*

🟨 *memory (RAM)*

(not included in picture: local disk, network cards, ...)

Parallel vs sequential software

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").

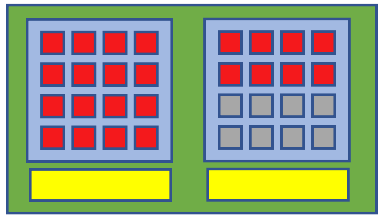
Example: OpenFOAM can easily use 160 cores at the same time to solve a CFD problem

Parallel programming paradigms:

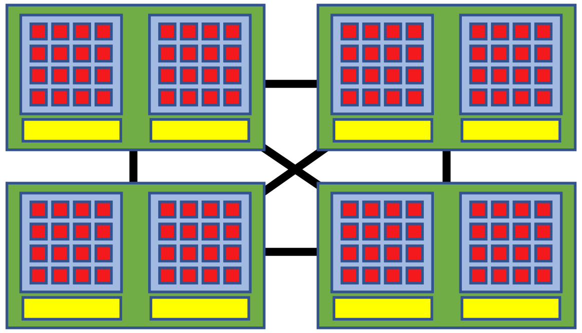
OpenMP for shared memory systems (*multithreading*) -> on cores of a *single* node

MPI for distributed memory systems (*multiprocessing*) -> 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*



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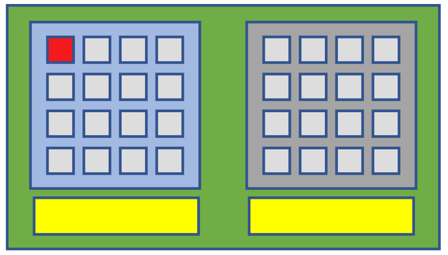
Parallel vs sequential programs

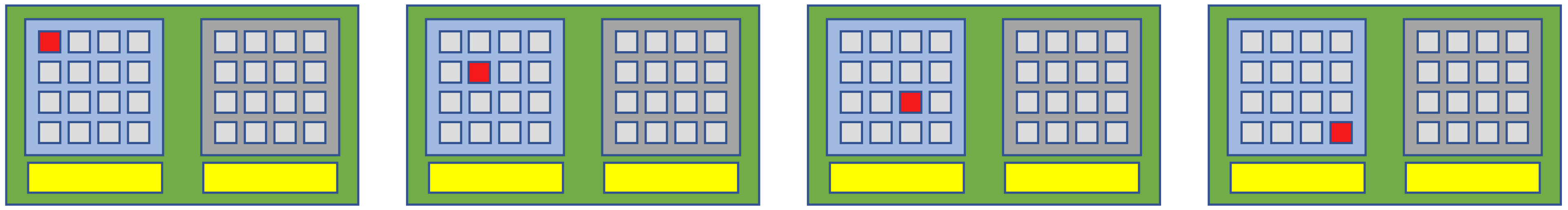
Sequential (a.k.a. serial) software does not do calculations in parallel, i.e. it only uses *one single core* of a single workernode.



This type of software does not run faster by just throwing cores at it...

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

e.g., you can run a Python script 100 times on 100 cores to quickly analyse 100 datasets



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HPC-UGent

hpc@ugent.be

Part of ICT Department of Ghent University

Our mission

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

Our core values

Empowerment - Centralisation - Automation - Collaboration

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HPC-UGent: staff

Stijn De Weirdt
technical lead

Ewald Pauwels
team lead

Kenneth Hoste
user support & training

Wouter Depypere
sysadmin, hardware

Andy Georges
sysadmin, tools

Kenneth Waegeman
sysadmin, storage

Balázs Hajgató
sysadmin, tools

Álvaro Simón García
cloud, user support

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

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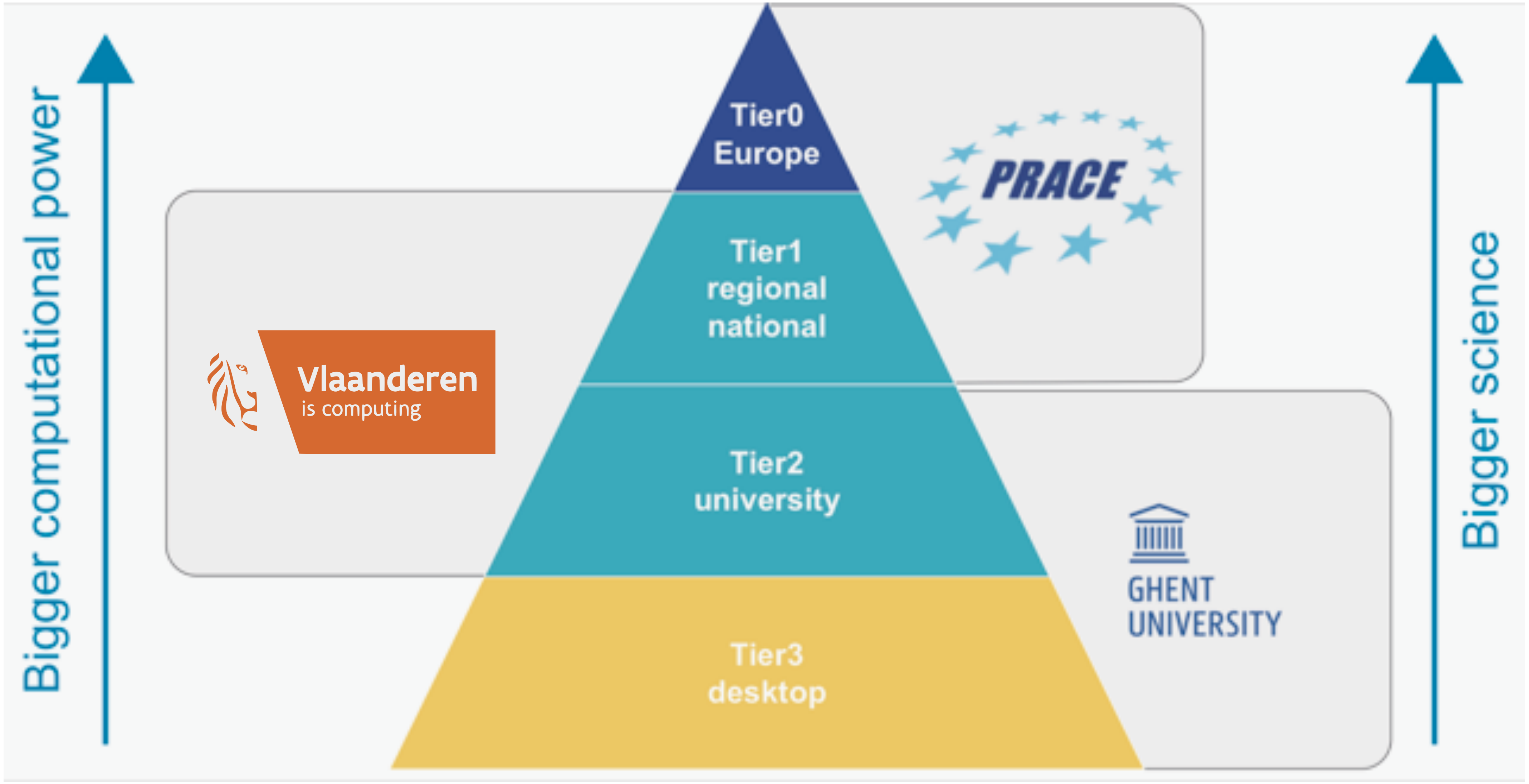
Centralised hardware



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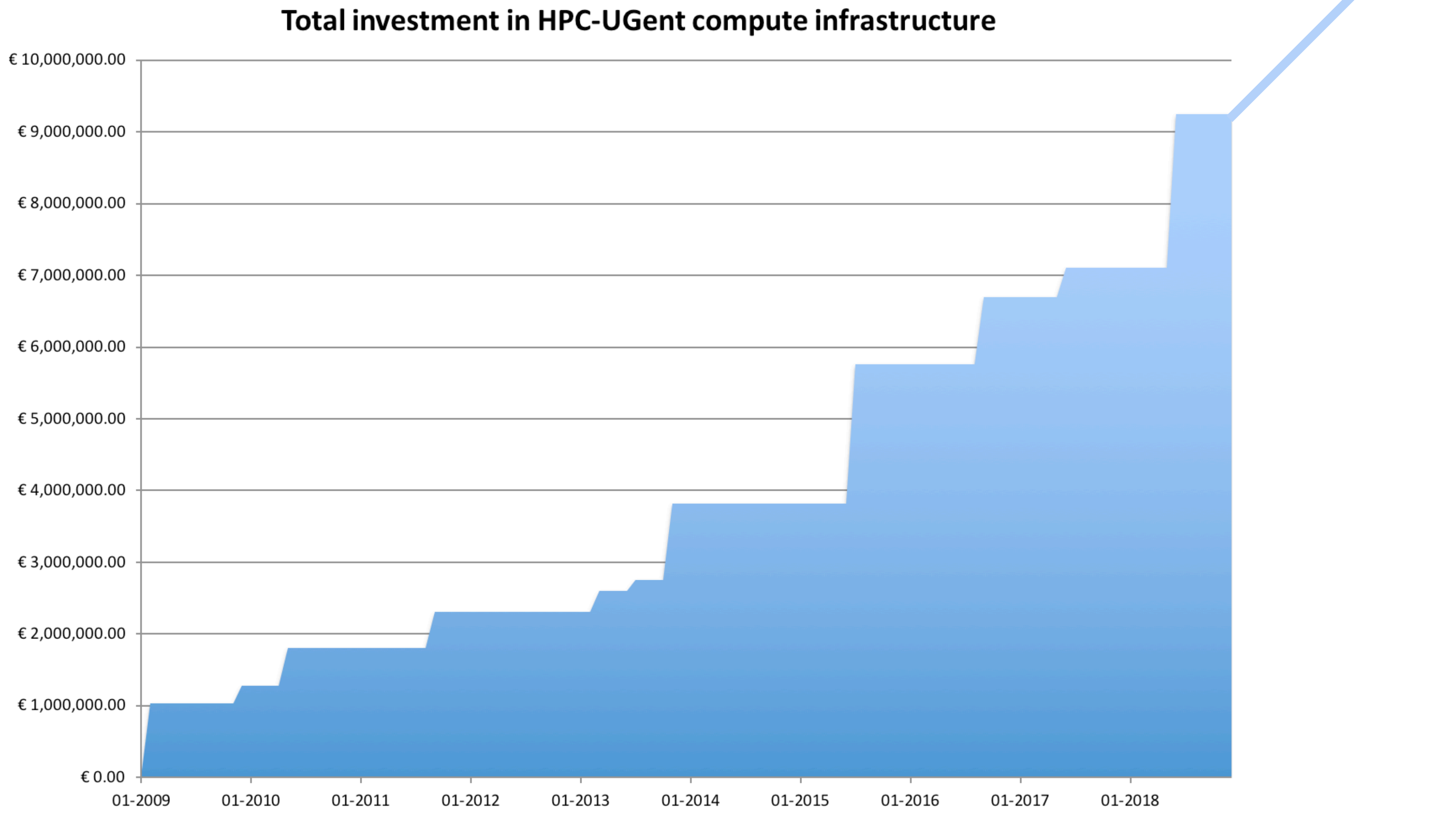
HPC-UGent Tier-2 (STEVIN): central investments

NATUS BRUGIS Anno 1548
DENATUS HAGÆ COMITIS Anno 1620
SIMON STEVIN.
MATHEMATICUS INSIGNIS
CONSILIAR. CELSISS: MAURITII PRINCIPIS ARAUSIONENSIUM.

1548 - 1620
°Bruges

STEVIN
HPC
infrastructure



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Financing by:

fwo

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HPC-UGent users

HPC-UGent Tier-2 (STEVIN)

https://www.vscentrum.be/infrastructure/hardware/hardware-ugent

6 Tier-2 clusters

> 600 workernodes, > 15,000 cores

Compute clusters

	#nodes	CPU	Mem/node	Diskspace/node	Network
delcatty	123	2 x 8-core Intel E5-2670 (Sandy Bridge @ 2.6 GHz)	64 GB	400 GB	FDR InfiniBand
phanpy	16	2 x 12-core Intel E5-2680v3 (Haswell-EP @ 2.5 GHz)	512 GB	3x 400 GB (SSD, striped)	FDR InfiniBand
golett	200	2 x 12-core Intel E5-2680v3 (Haswell-EP @ 2.5 GHz)	64 GB	500 GB	FDR-10 InfiniBand
swalot	128	2 x 10-core Intel E5-2660v3 (Haswell-EP @ 2.6 GHz)	128 GB	1 TB	FDR InfiniBand
skitty	72	2 x 18-core Intel Xeon Gold 6140 (Skylake @ 2.3 GHz)	192 GB	1 TB 240 GB SSD	EDR InfiniBand
victini*	96	2 x 18-core Intel Xeon Gold 6140 (Skylake @ 2.3 GHz)	96 GB	1 TB 240 GB SSD	10 GbE

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HPC-UGent Tier-2 (STEVIN)

Network connections between nodes ('interconnect')

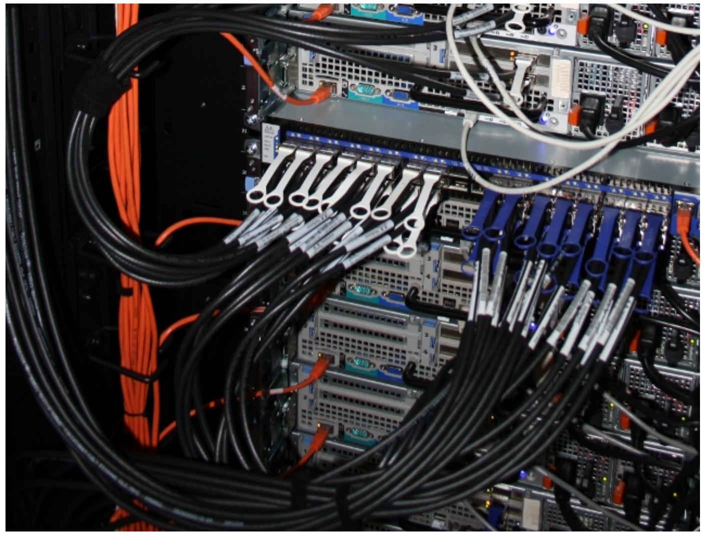
Ethernet: 1-10 Gbit/s

€

for single core/node jobs

(too slow for fast inter-node communication)

Infiniband: 50 - 100 Gbit/s



€€(€)

required for MPI jobs

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VSC Tier-2 infrastructure

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Vlaams Supercomputer Centrum

(Flemish Supercomputer Center)

https://www.vscentrum.be/en/access-and-infrastructure/tier-2

Antwerp University association
Brussels University association **+ Grid specialization**
Ghent University association **+ Big Data specialization**
KU Leuven association Limburg association University-Colleges **+ Shared memory, accelerator specialization (GPU)**

auha

universitaire associatie BRUSSEL

ASSOCIATIE UNIVERSITEIT GENT

ASSOCIATIE KU LEUVEN

ASSOCIATIE UNIVERSITEIT-HOGESCHOLEN LIMBURG

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VSC Tier-1 – BrENIAC (@ KUL)

For up to date information, see:
https://www.vscentrum.be/en/access-and-infrastructure/tier-1

Hardware

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

Extension is being installed currently, which should bring total compute power to ~1.5 petaflop.

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

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VSC Tier-1 – BrENIAC (@ KUL)

For academics (all Flemish research centers):

- *Free of charge*
- Starting Grant (100 node days)
    - https://www.vscentrum.be/en/access-and-infrastructure/tier1-starting-grant
    - Fill in application form, send it to hpc@ugent.be
- Project access (500-5000 nodedays)
    - 3 evaluation moments per year
    - Application form and more info

      https://www.vscentrum.be/en/access-and-infrastructure/project-access-tier1
- **Don't hesitate to contact hpc@ugent.be for help!**

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VSC Tier-1 – BrENIAC (@ KUL)

For industry:

- Exploratory access (100 node days)
  - *Free of charge*
  - Contact hpc@ugent.be
- Contract access
  - FWO/UGent/company contract
  - Payed usage (~13 euro / *node* / day)
  - Contact hpc@ugent.be

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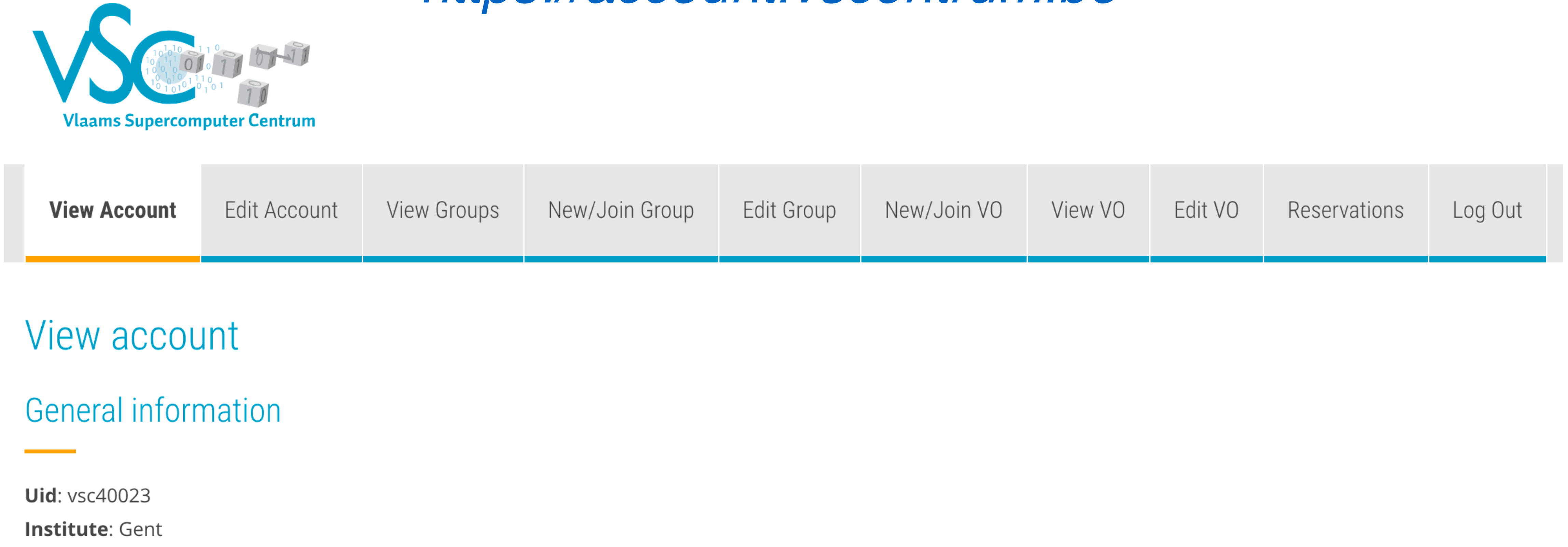
Getting a VSC account

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

Managing your VSC account

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

https://account.vscentrum.be



View account

General information

Uid: vsc40023

Institute: Gent

Workflow on HPC infrastructure

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

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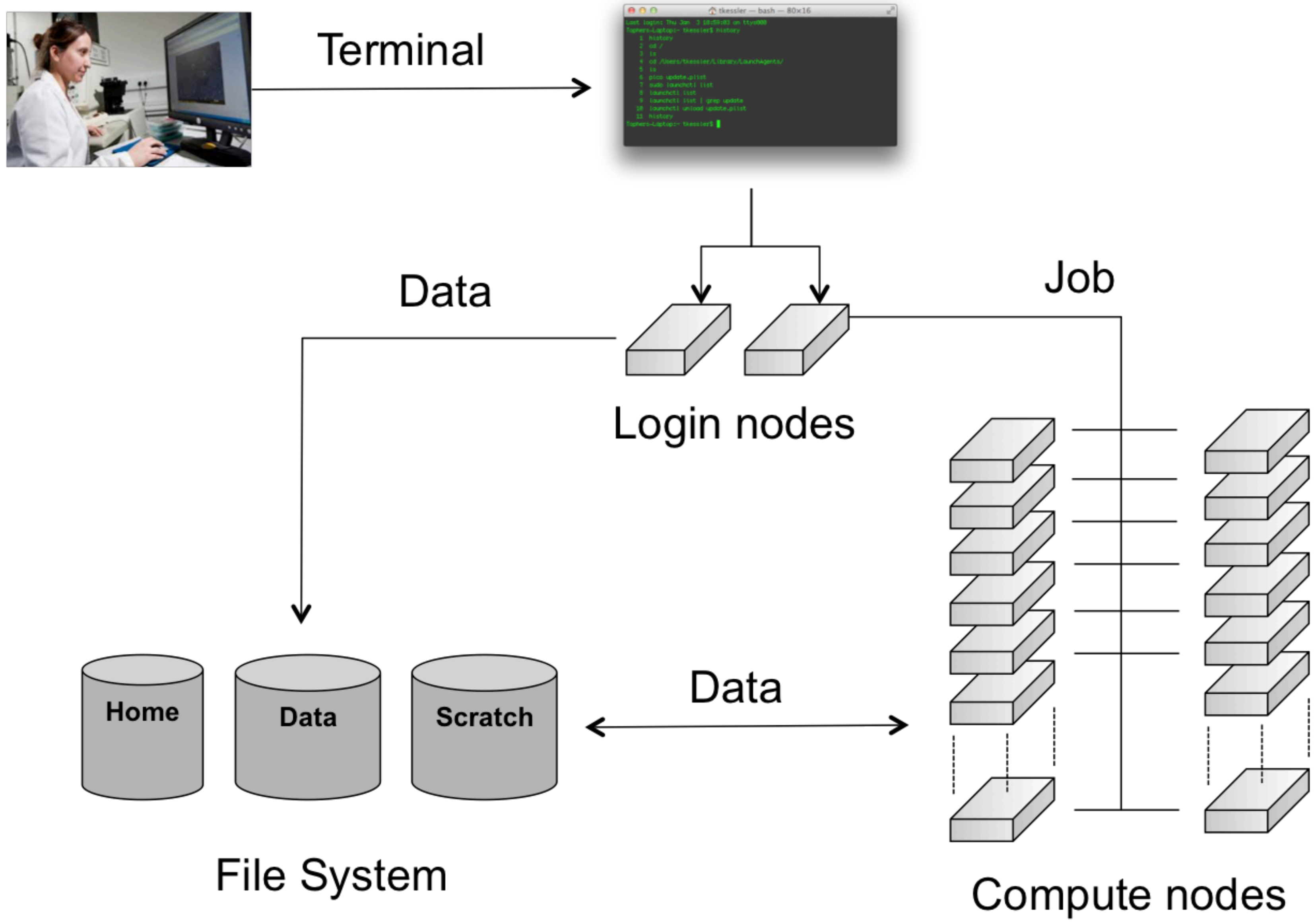
High-level overview of HPC-UGent infrastructure



```
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$ 
```

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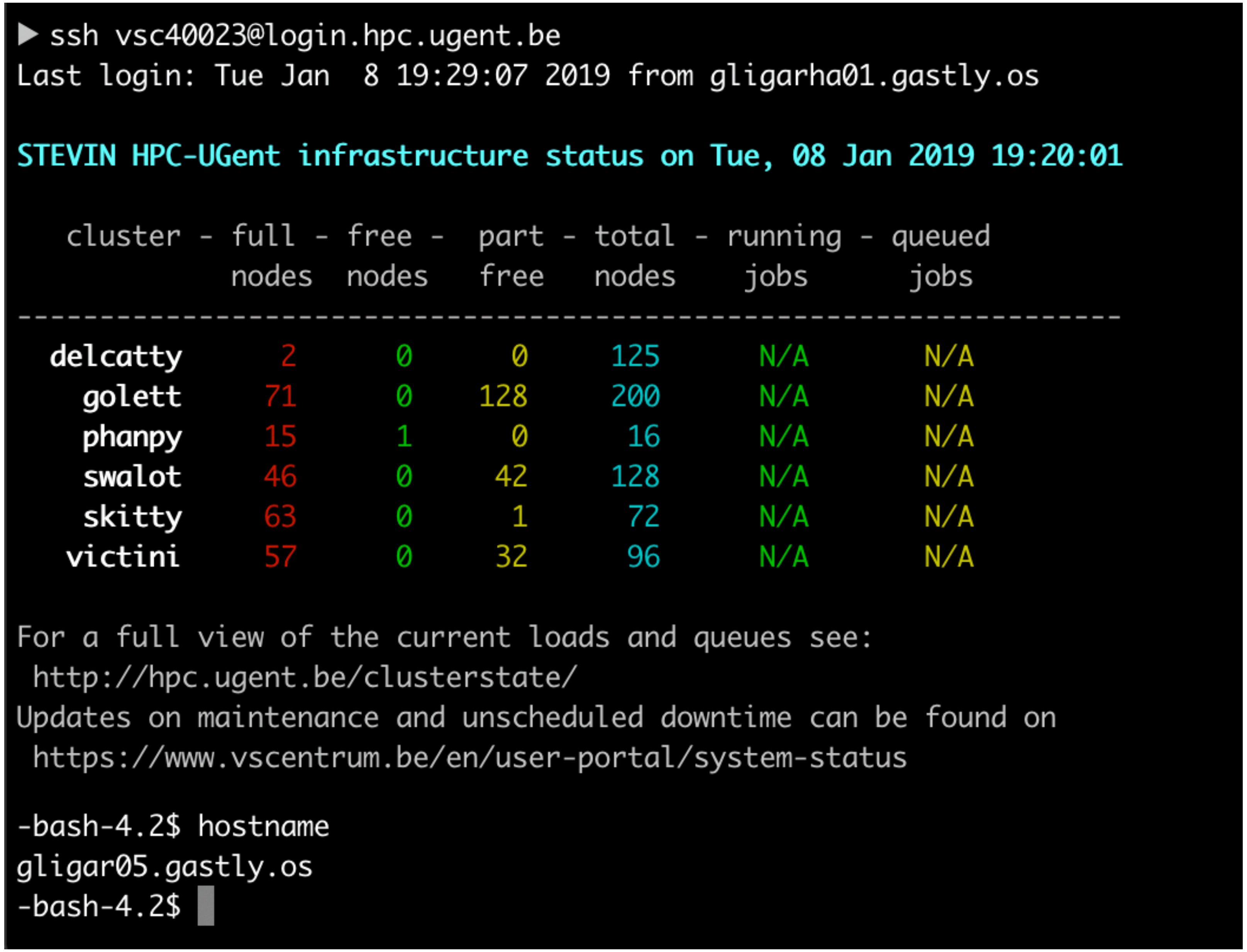
Connected to an HPC-UGent login node



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

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

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

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

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

Basic Linux shell usage (interactive)

- command line environment a.k.a. 'shell' a.k.a. `bash`
- type a command and hit "Enter" to execute it
  - ***think/double check before executing***, commands can be destructive!
- some commands take arguments or options (these start with `-` or `--`)
- right-left arrow keys : go forward/backward on current command line
- Ctrl-A / Ctrl-E: go to start/end of command line
- up/down arrow keys : access command history
- Ctrl-R: search through command history
- any line that starts with a '#' (hash) is a *comment* (not a command)

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Basic Linux shell commands: navigation

`ls`	list files/directories in current directory ("what's here?")
`ls -l`	long listing (more information)
`ls -lrt`	long listing and sorted by last changed (reversed)
`ls example`	show contents of directory named '`example`'
`cd`	change directory ("go to ...")
`cd example`	change to directory named '`example`'
`cd -`	change to previous directory
`cd`	(without any argument): change back to home directory
`pwd`	show present working directory ("where am I?")

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Basic Linux shell commands: files & directories

`mkdir`	create directory with specified name *(min. 1 argument required)*
`mkdir -p`	create directory + all missing parent directories
`cp`	copying of files/directories *(min. 2 arguments required)*
`cp -a`	*recursive* copy (& preserve permissions), required for directories
`mv`	moving/renaming of files/directories *(min. 2 arguments required)*
`ln -s`	create symbolic link between two locations *(2 arguments required)*
`rm`	removing files *(min. 1 argument required)* **BE CAREFUL!**
`rm -f`	forced removal (silent if there's nothing to remove)
`rm -r`	recursive removal (required for directories)
`rm -rf`	forced recursive removal ***(better think twice before using this...)***

There is no "trash bin", if you remove something with '`rm`', it's gone forever!

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Basic Linux shell: environment variables

- environment variables are basically "labeled boxes" (with something inside)
- defining an environment variable named `$EXAMPLE` with value `12345` :

  ```
  export EXAMPLE=12345
  ```

  (note: no output from '`export`' command, no `$`, no spaces around '=')
- showing the contents of an environment variable (`$` indicates name of env. var.)

  ```
  echo $EXAMPLE
  ```
- using non-existing environment variables does not produce errors!
- a non-existing environment variable is equivalent to an empty value **(be careful!)**
- environment variables are only defined in the current session/job (not persistent)!
- print all currently defined environment variables with `env | sort`

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Basic Linux shell: file paths

- *file paths* are locations to files & directories on a file system
- `.` is a shorthand for the current directory, `..` for the parent directory
- file paths can be either:
  - r*elative* to the current directory
    examples: `file1.txt` , `dir1/file2,txt` , `../../dir2/`
  - a*bsolute* (start from `/`, the 'root' of the filesystem)
    example: `/user/gent/400/vsc40000`
- environment variables often have file paths as a value
  examples: `$HOME`, `$VSC_DATA`, `$VSC_SCRATCH`, `$TMPDIR`, ...
- we strongly recommend to use the provides environment variables
  examples: `$VSC_DATA/project1`, `$VSC_SCRATCH/project1/12345.out`

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Basic Linux shell: file contents, editing, output redirection

- you can inspect the contents of (short) files using the `cat` command
- for long files, you can use:
  - `head` or `tail` to inspect the first/last lines of the file
  - a pager command like `less` (scroll with arrow keys or space bar, exit with '`q`')
- `nano` is a relatively easy-to-use command line editor (`^` means `Ctrl`)
- to capture the output of a command, you can use output redirection:
  - capturing *stdout* (normal output): `command > out.txt`
  - capturing *stderr* (errors & warnings): `command 2> err.txt`
  - capturing *both* in a single file: `command &> err.txt`

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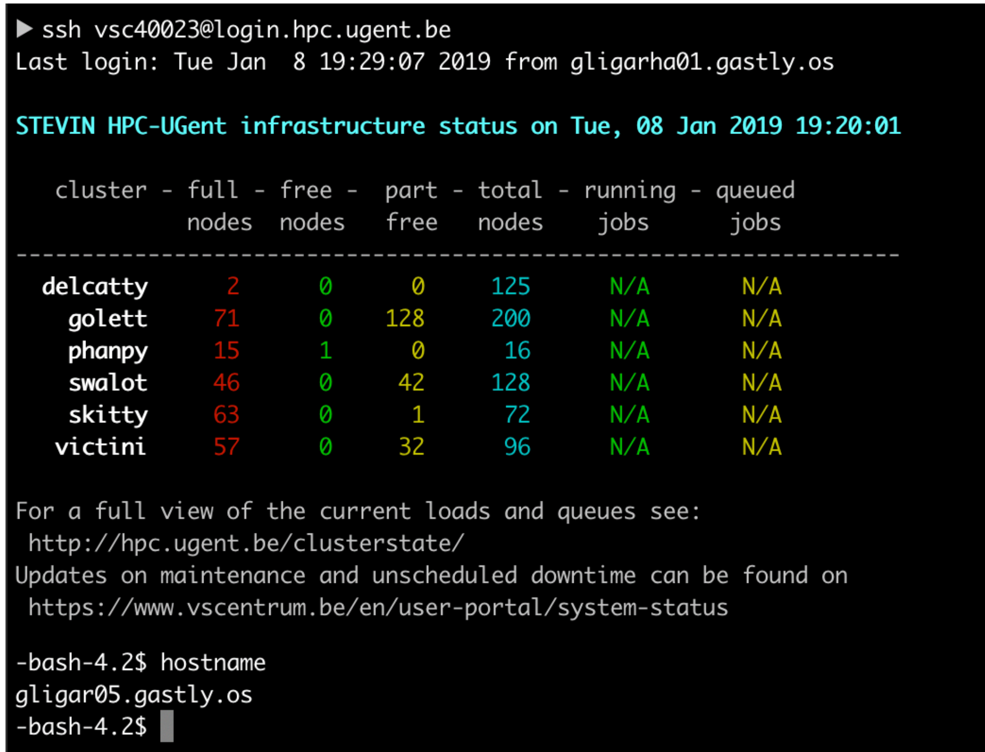
Basic Linux tutorial

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



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    phanpy     15      1      0      16      N/A       N/A
    swalot     46      0     42     128      N/A       N/A
    skitty     63      0      1      72      N/A       N/A
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For a full view of the current loads and queues see:
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-bash-4.2$ hostname
gligar05.gastly.os
-bash-4.2$ 
```

Workflow on HPC infrastructure

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

See Chapter 3 in HPC-UGent tutorial

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

  - Your job gets executed
  - Your job finishes

7. **Move your results**

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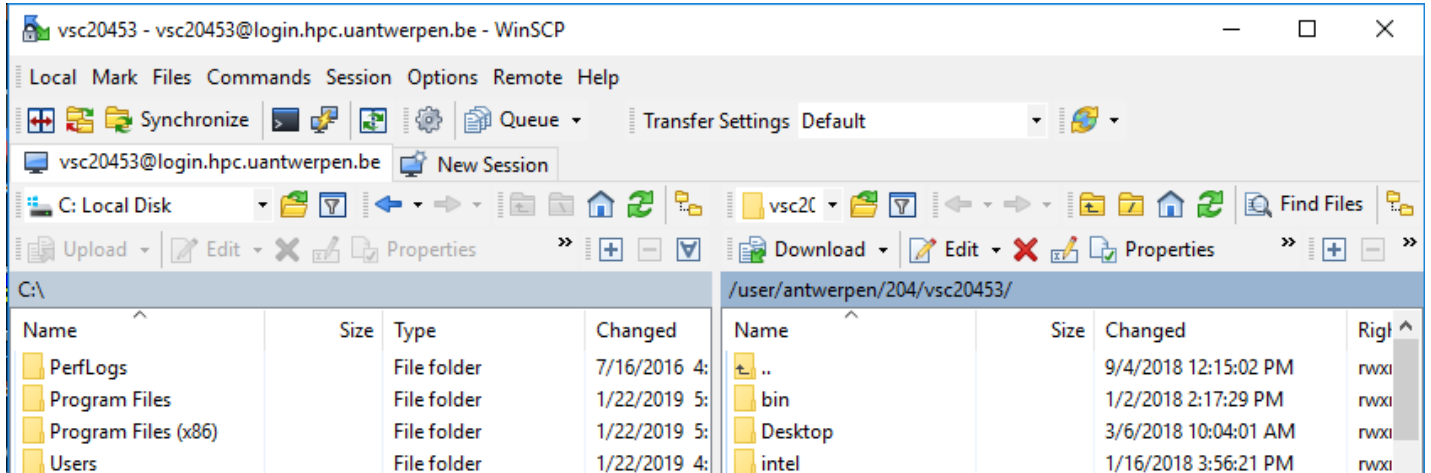
Transferring files to/from the HPC-UGent infrastructure

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


vsc20453 - vsc20453@login.hpc.uantwerpen.be - WinSCP

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

C:\

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

/user/antwerpen/204/vsc20453/

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

Workflow on HPC infrastructure

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

- Choose correct PBS directives (Chapter 4, 8)
- Load software modules (Chapter 3)
- Useful environment variables (Chapter 4)
- Access files on shared filesystems (Chapter 6)

7. Move your results

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What is a job script?

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

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

- the ***resources*** that are required by the calculation
  (number of nodes/cores, amount of memory, how much time, ...)
- the ***software*** that is used for the calculation
  (via `module load` commands)
- the steps that should be done to execute the calculation
  (starting from `$HOME`), specified as **shell *commands***, typically:
    - 1) staging in of input files
    - 2) running the calculation
    - 3) staging out of results

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Job scripts: required resources via `#PBS` directives

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

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

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Job scripts: software modules

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

Load a module to use the software:

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

See currently loaded modules using:

`$ module list` or `$ ml`

Get overview of available modules using:

`$ module avail` or `$ ml av`

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

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Job scripts: useful environment variables

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

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

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Job scripts: input data & filesystems

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

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

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Storage quota

- home directory (`$VSC_HOME`): 3GB (fixed)
- personal data directory (`$VSC_DATA`): 25GB (fixed)
- personal scratch directory (`$VSC_SCRATCH`): 25GB (fixed)
- current quota usage can be consulted on VSC accountpage https://account.vscentrum.be
- **more storage quota (GBs, TBs) available for virtual organisations (VOs)**
- see Section 6.6 in HPC-UGent tutorial
- additional quota can be requested via https://account.vscentrum.be/django/vo/edit
- shared directories with VO members: `$VSC_DATA_VO`, `$VSC_SCRATCH_VO`
- personal VO subdirectories: `$VSC_DATA_VO_USER`, `$VSC_SCRATCH_VO_USER`

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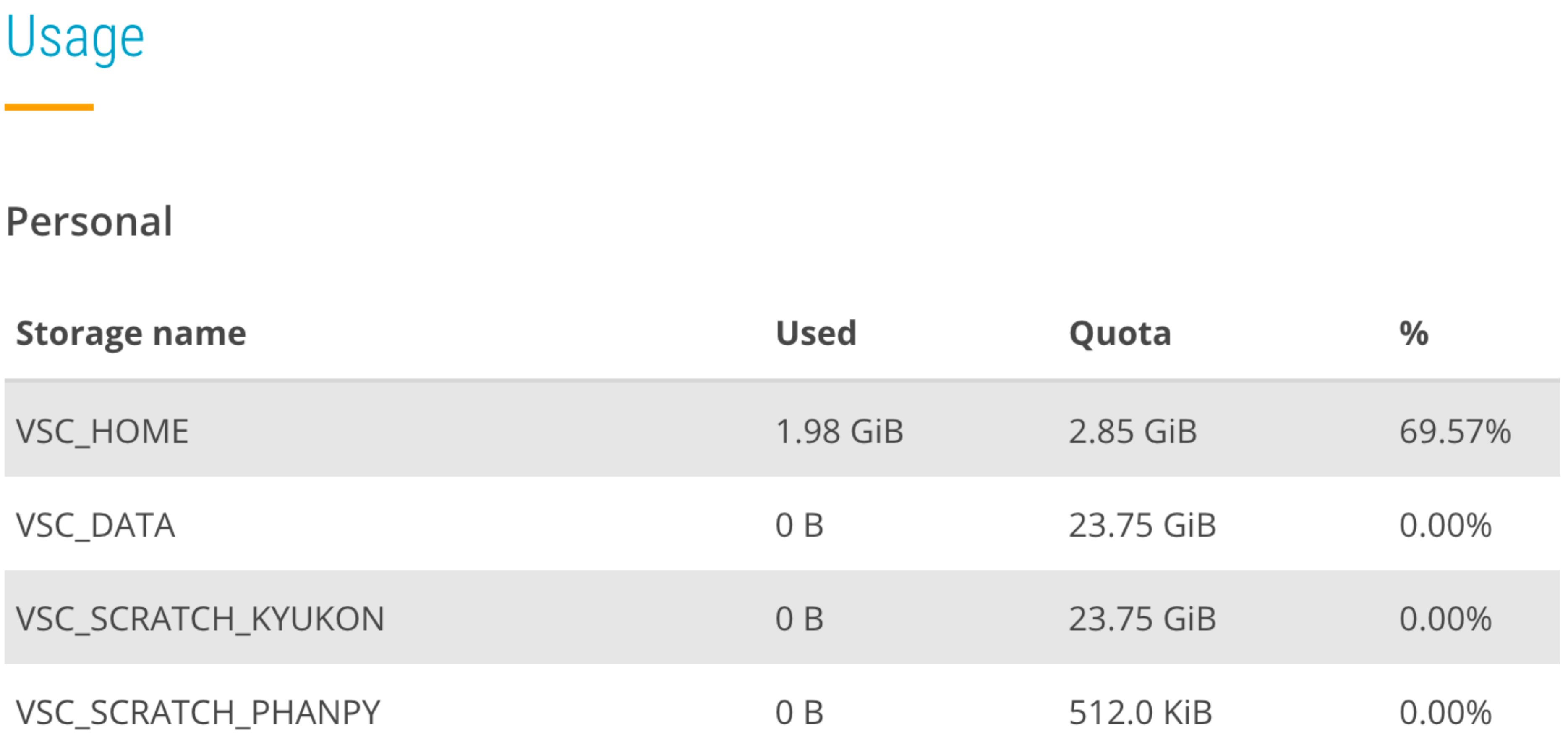
Current storage usage - personal directories

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



Usage

Personal

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

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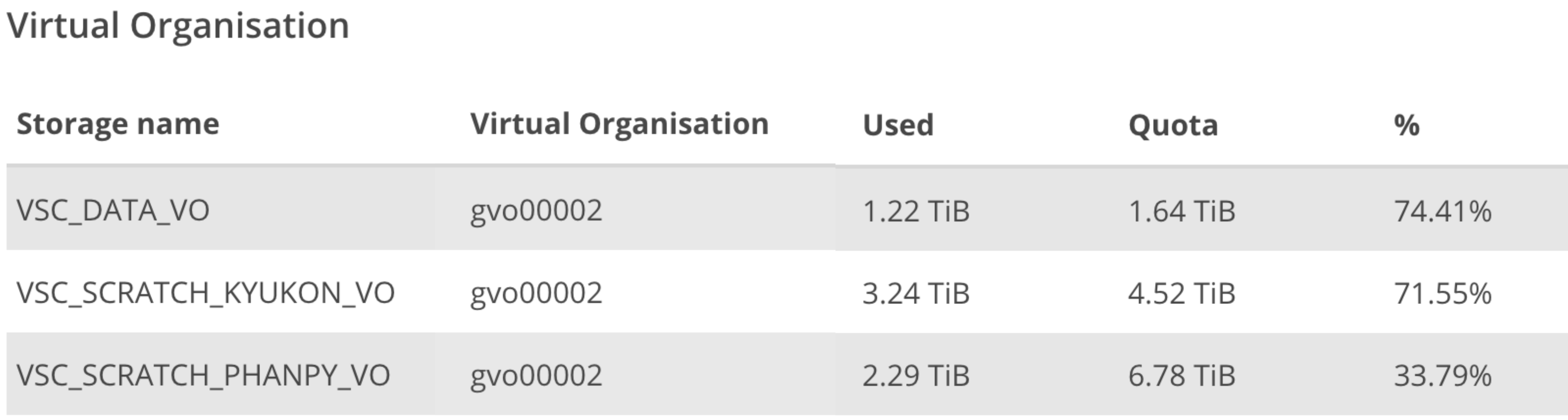
Current storage usage - own VO directories

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



Virtual Organisation

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

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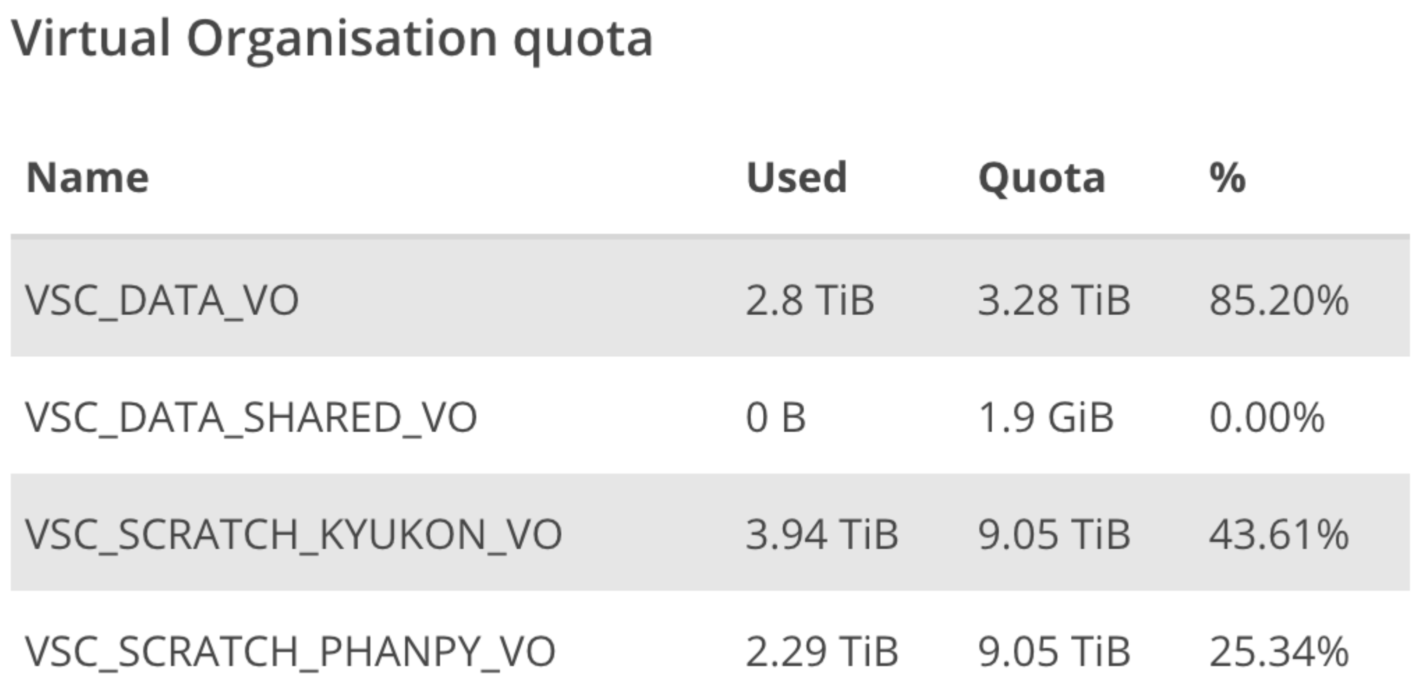
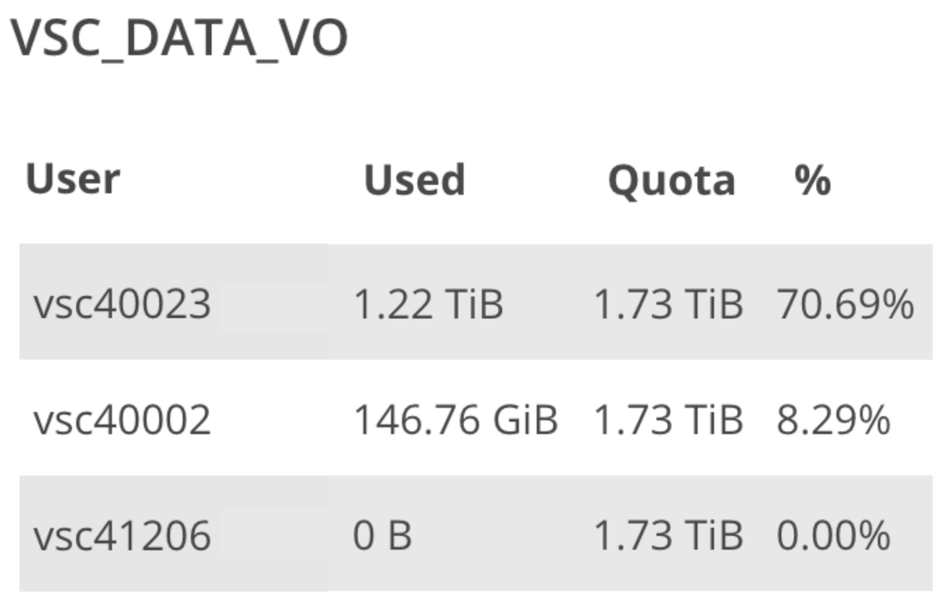
Current storage usage - total VO usage

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



Virtual Organisation quota

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



VSC_DATA_VO

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

Job scripts: full example (single-core job)

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

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

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Job scripts: full example (multi-node job)

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

module load intel/2018b
module load vsc-mympirun

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

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Jobs scripts: generated output files

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

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

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

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Workflow on HPC infrastructure

1. Connect to login nodes

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

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

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Demo: qsub, qstat, qdel

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

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

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

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

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

```
$ qdel 12345
```

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Job scheduling

- All our clusters use a *fair-share* scheduling policy.
- No guarantees on when job will start, so **plan ahead**!
- Job priority is determined by:
  - *historical usage*
    - aim is to balance usage over users
    - infrequent/frequent users => higher/lower priority
  - *requested resources* (# nodes/cores, walltime, memory, ...)
    - large 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

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Embarrassingly parallel jobs

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

Software installations

To submit a request for software installation:

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

Always include:

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

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

http://easybuilders.github.io/easybuild

Documentation & training

- **Documentation** is available at:
  - https://www.vscentrum.be/en/user-portal
  - https://www.ugent.be/hpc/en/support/documentation.htm
    - HPC tutorial, basic Linux tutorial

- **Training sessions -** https://www.vscentrum.be/en/education-and-trainings
  - upcoming sessions in Ghent (see also https://www.ugent.be/hpc/en/training/training)
    - *Introduction to multi-threading and OpenMP*: 2-3 April 2019
    - *Introduction to MPI*: 24 April 2019

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Questions, problems, getting help

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

Always include:

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

Preferably use your UGent email address.

Alternatives:

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

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Hands-on: pick your own adventure!

1) Create a (single-core) job script to:

- Calculate 2^n using using your favourite tool, e.g. Python, R, MATLAB, ...
- The value for *n* should be read from a file you pass to your program
- Print the result to a file named `result.txt` located in `$VSC_DATA`

2) Submit the job script to:

- *victini* (the default cluster)
- *golett*

3) Find the generated output files, and check the result

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Hands-on: pick your own adventure!

Copy one of these examples in a script, and create a job script to run it.

Python example

```
import sys
inputfile = sys.argv[1]
n = int(open(inputfile).read().strip())
print(2**n)
```

R example

```
args = commandArgs(trailingOnly=TRUE)
lines = readLines(file(args[1]))
n = strtoi(lines[1])
print(2^n)
```

MATLAB example

```
function x = two_n(inputfile)
fh = fopen(inputfile, 'r');
ns = fscanf(fh, '%d');
fclose(fh);
x = 2 ^ ns(1)
```

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Introduction to HPC-UGent

March 27th 2019

https://www.ugent.be/hpc/en/training/materials/2019/introhpcugent

hpc@ugent.be

https://ugent.be/hpc

Vlaanderen is computing