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Introduction to HPC-UGent

March 20th 2019 - GhEnToxLab

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
2/ Getting an HPC account
3/ Connecting to the HPC
4/ Running batch jobs
6/ Running jobs with input/output data
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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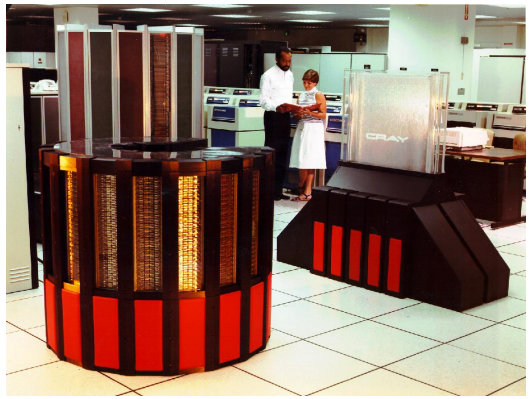
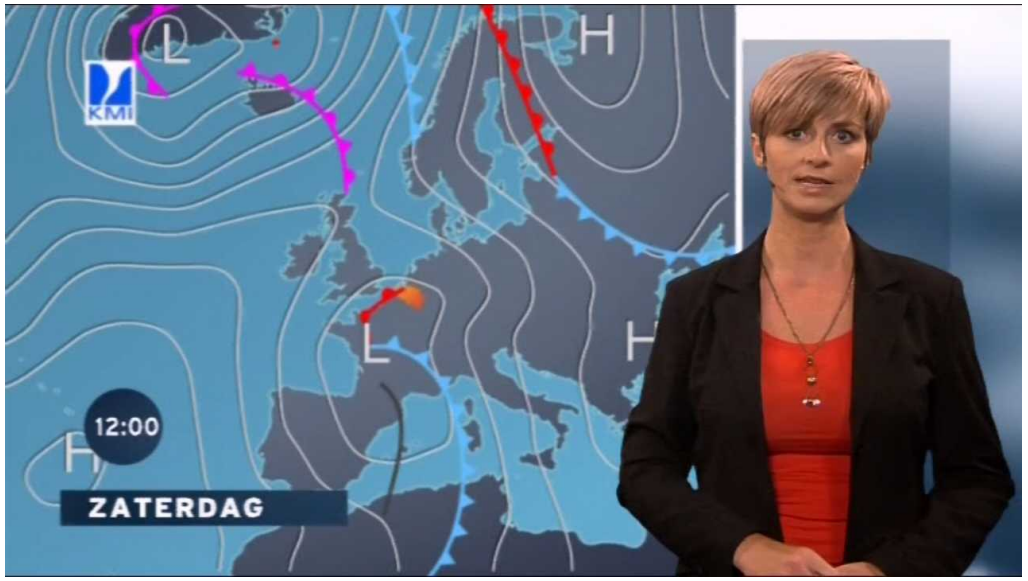
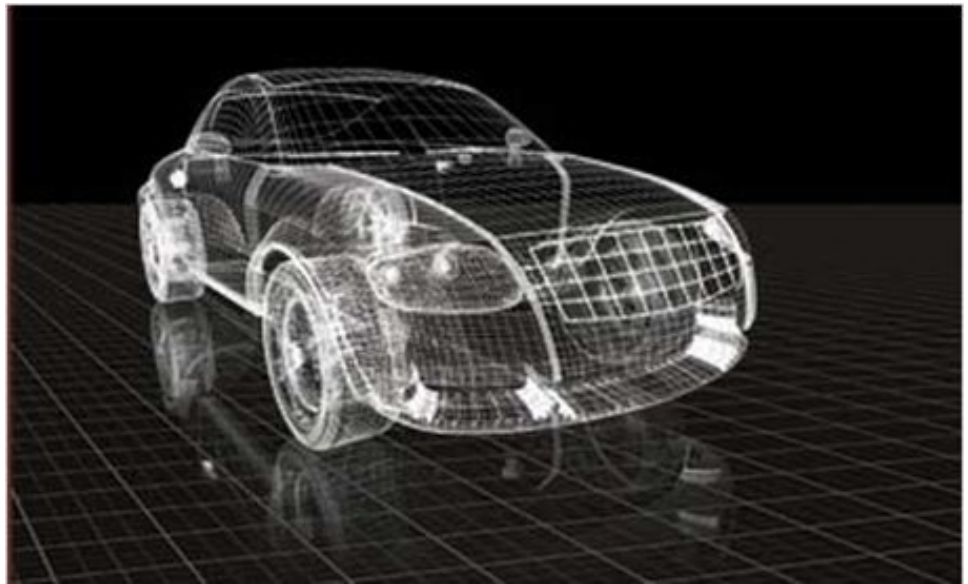
What is High Performance Computing?

harness power of multiple interconnected cores/nodes/processing units



Everyday applications of supercomputing





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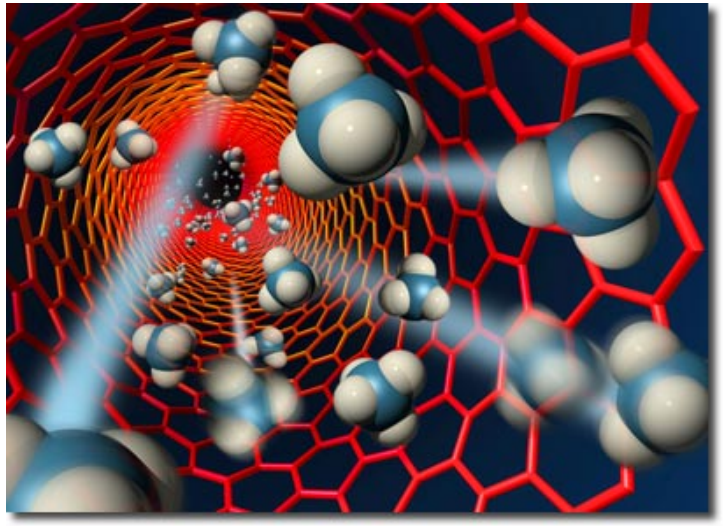
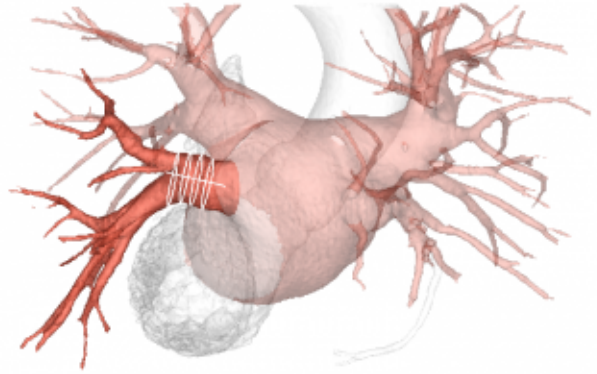
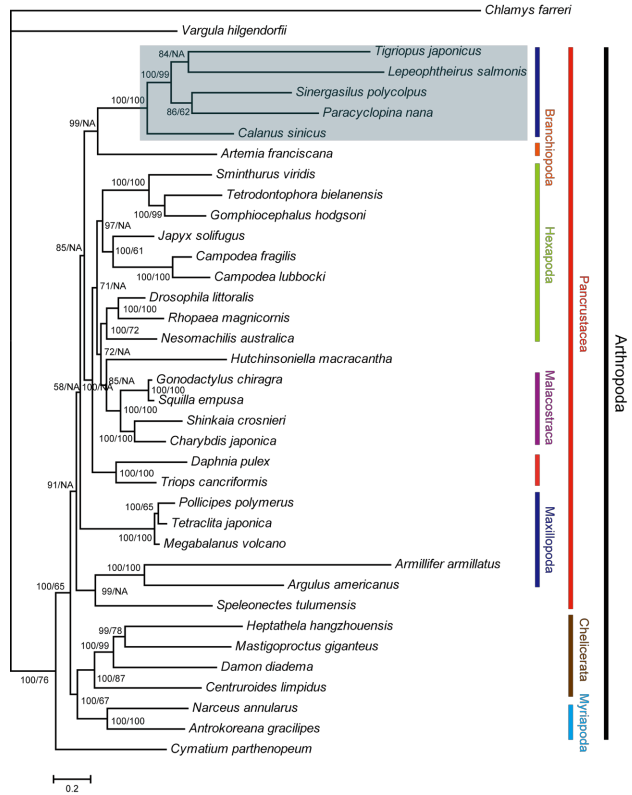
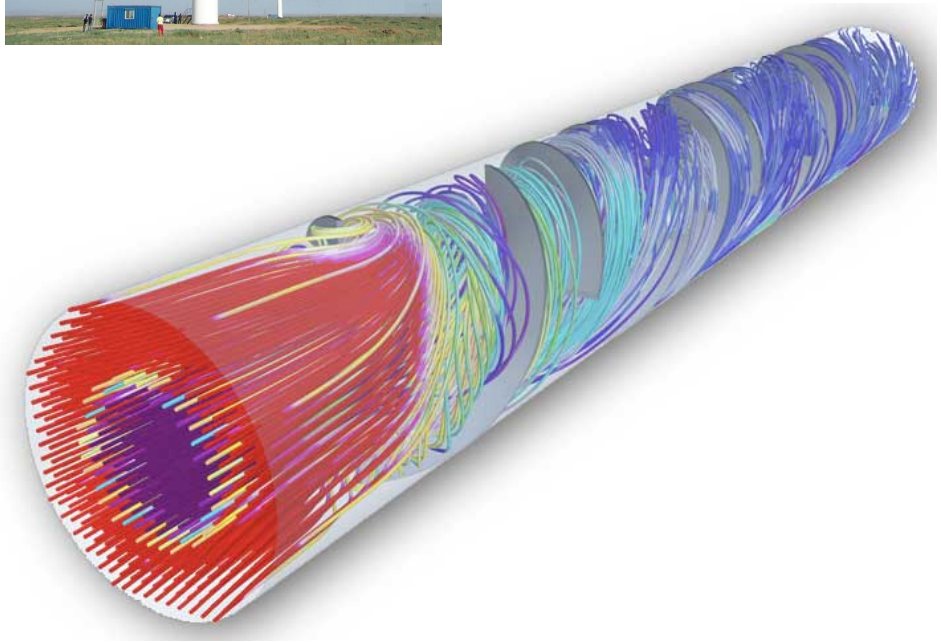
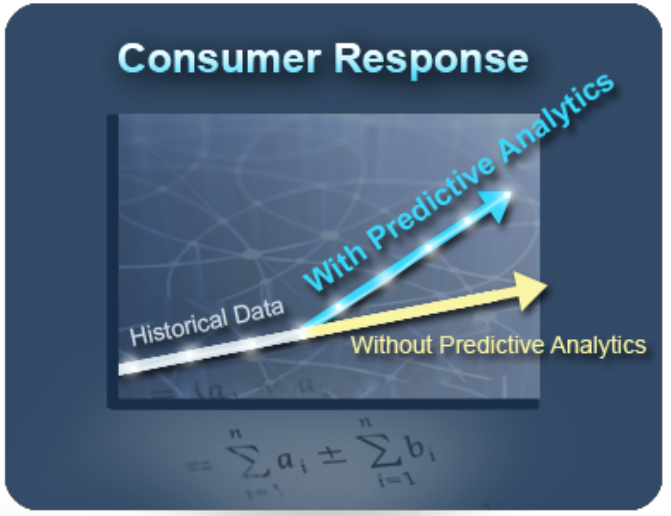
Scientific applications of supercomputing

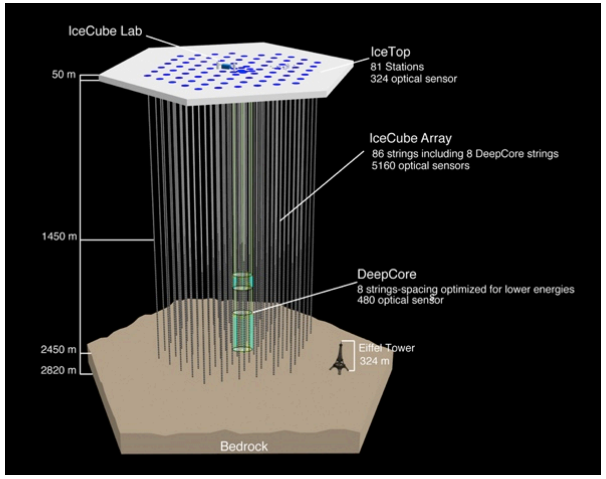










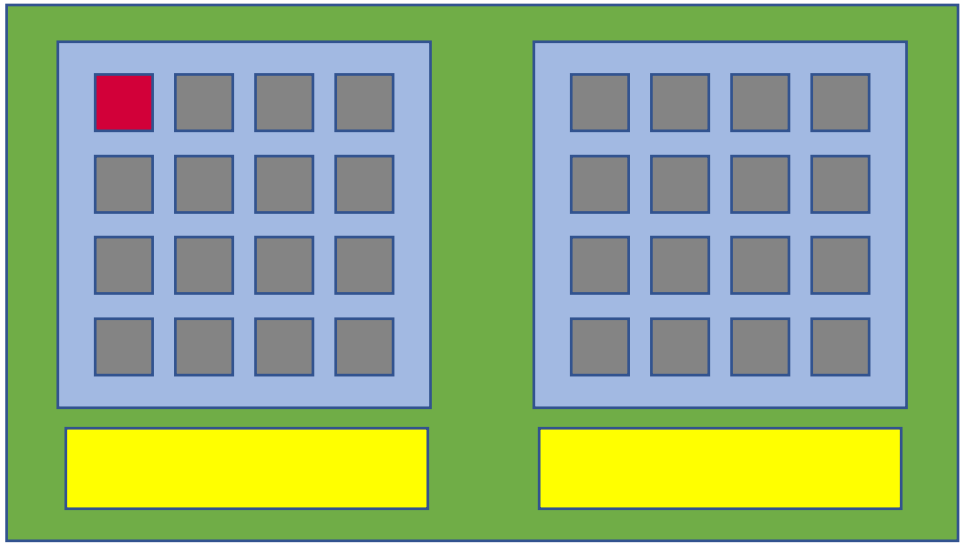


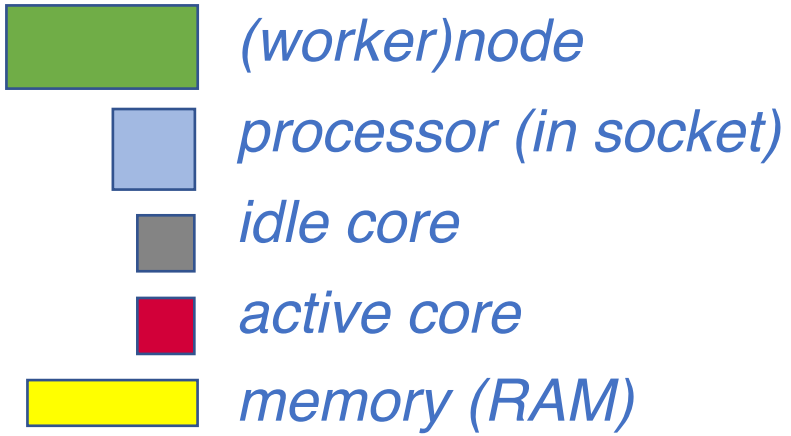
Cores, CPUs, processors, sockets, (worker)nodes

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





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

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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").

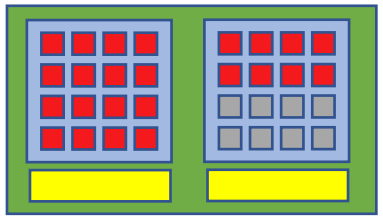
Example: OpenFOAM can easily use 160 cores at the same time to solve a CFD problem

Parallel programming paradigms:

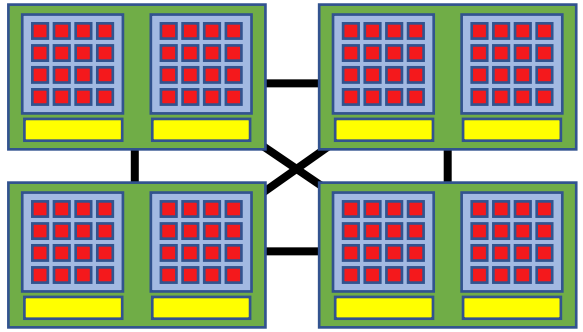
OpenMP for shared memory systems (*multithreading*) -> on cores of a *single* node

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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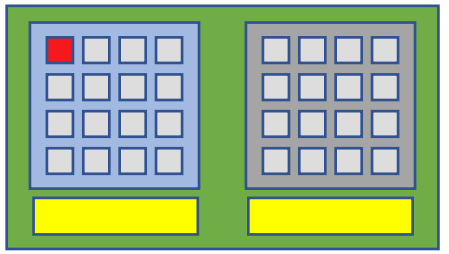
Parallel vs sequential programs

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

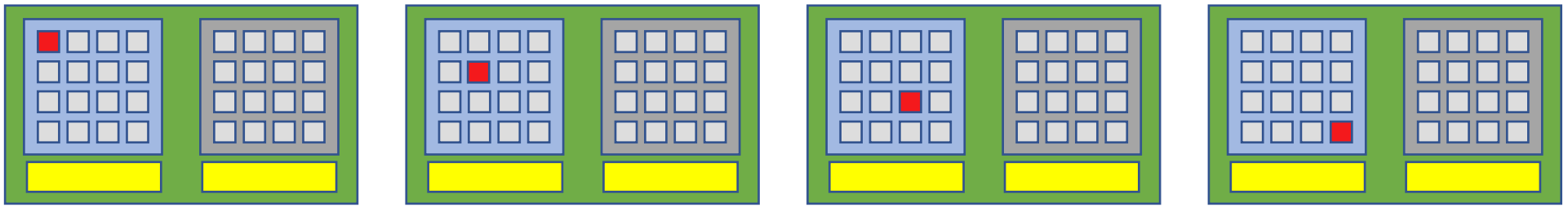
i.e. it only uses *one single core* of a single workernode.



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

Kenneth Hoste
user support & training

Andy Georges
sysadmin, tools

Balázs Hajgató
sysadmin, tools

Ewald Pauwels
team lead

Wouter Depypere
sysadmin, hardware

Kenneth Waegeman
sysadmin, storage

Álvaro Simón García
cloud, user support

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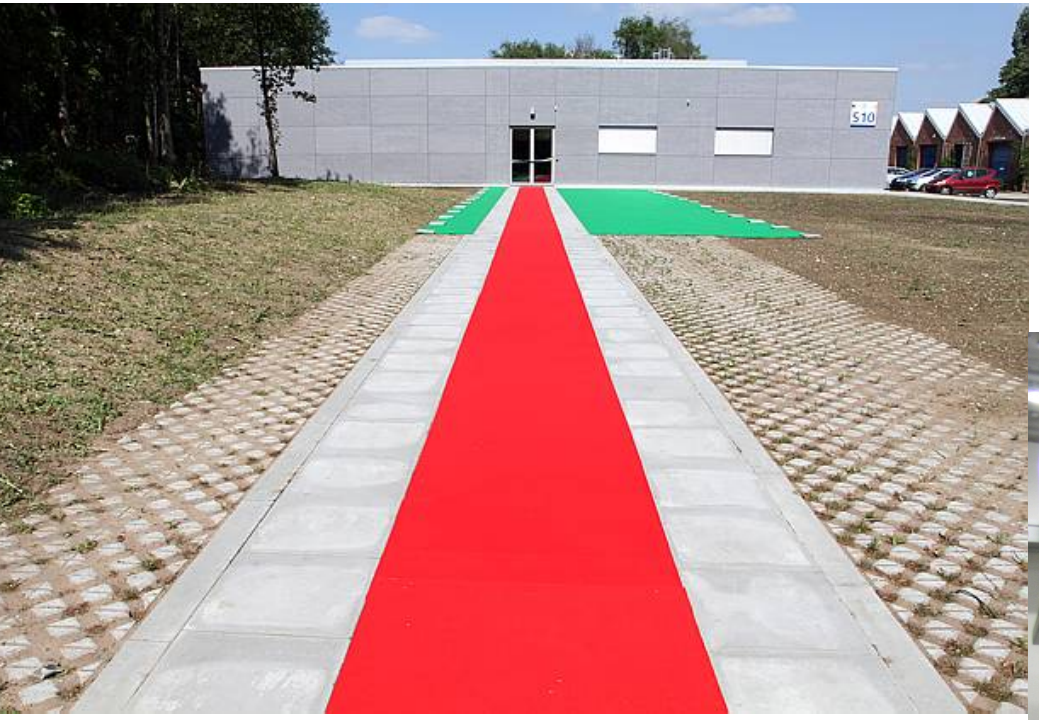
Centralised hardware
in the UGent datacenter
at campus Sterre (building S10)



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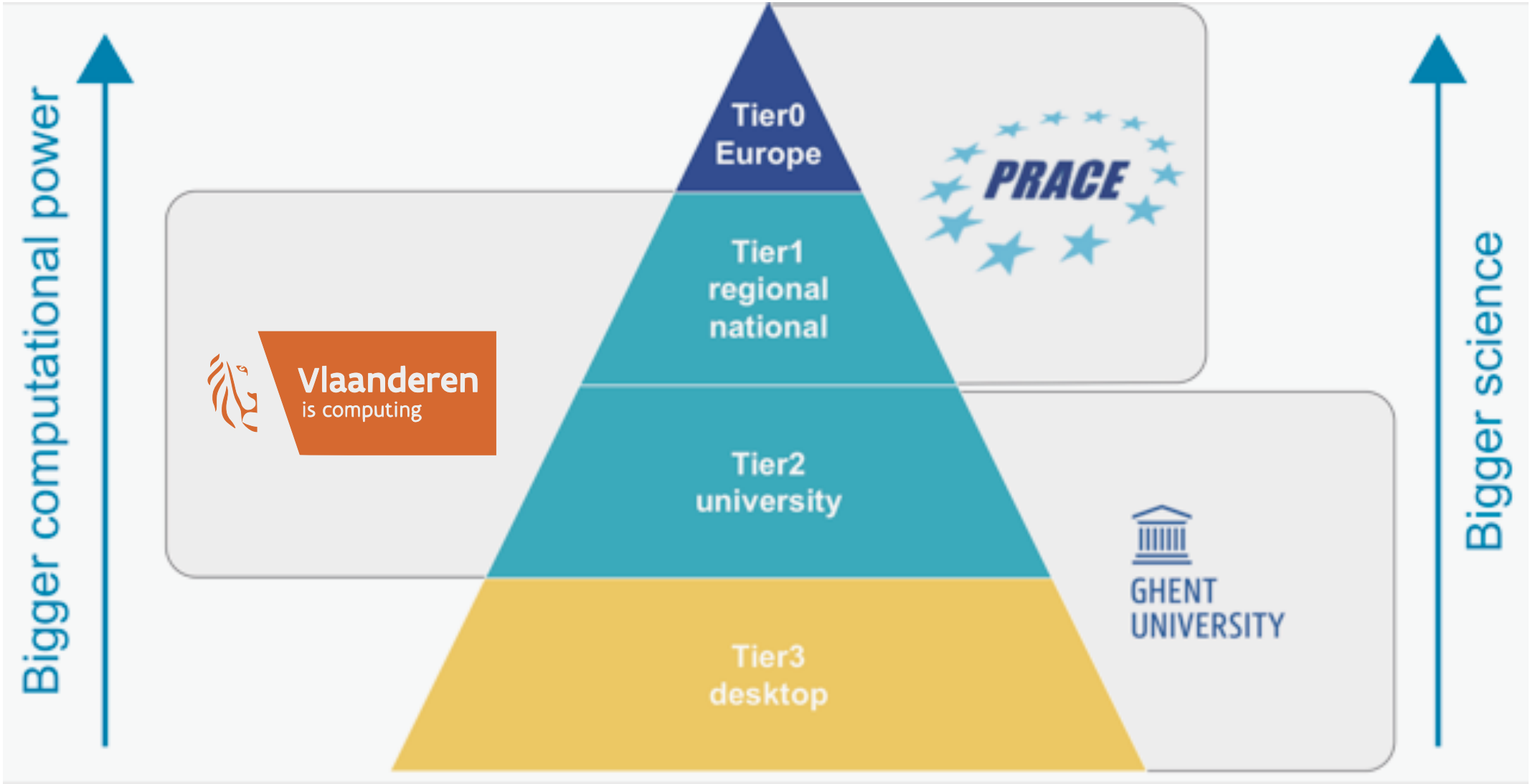
Centralised hardware



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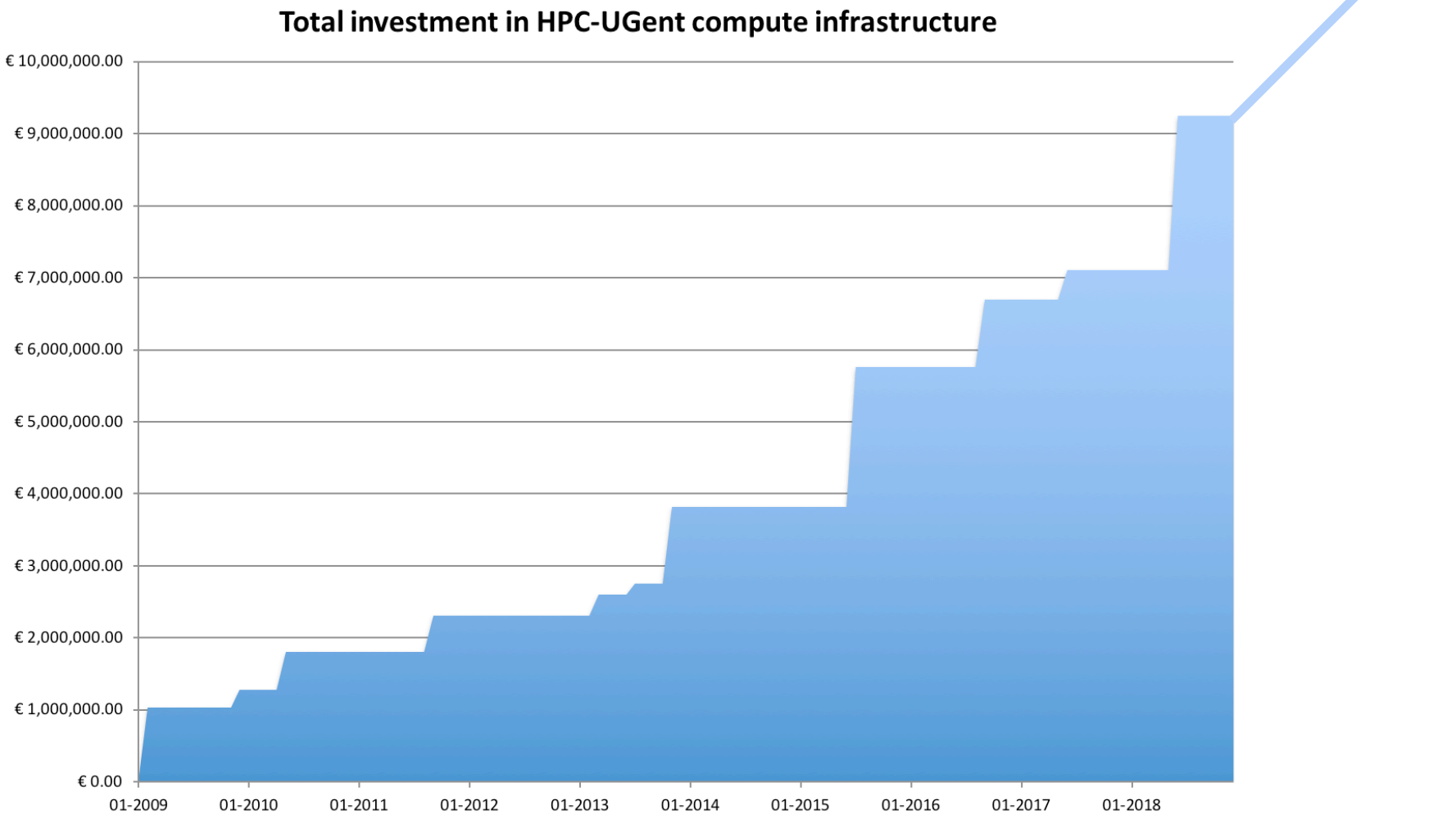
HPC-UGent Tier-2 (STEVIN): central investments

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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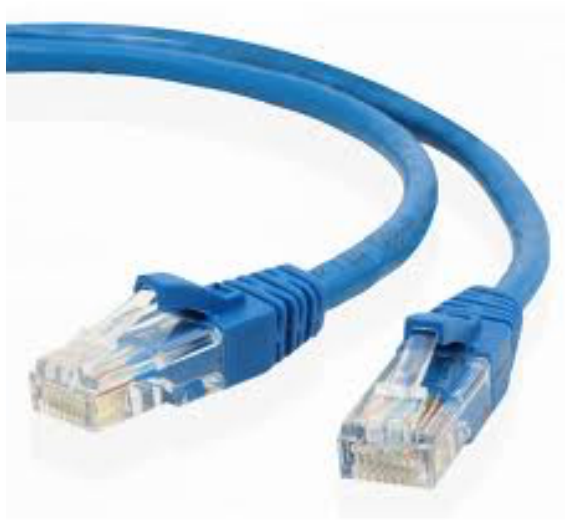
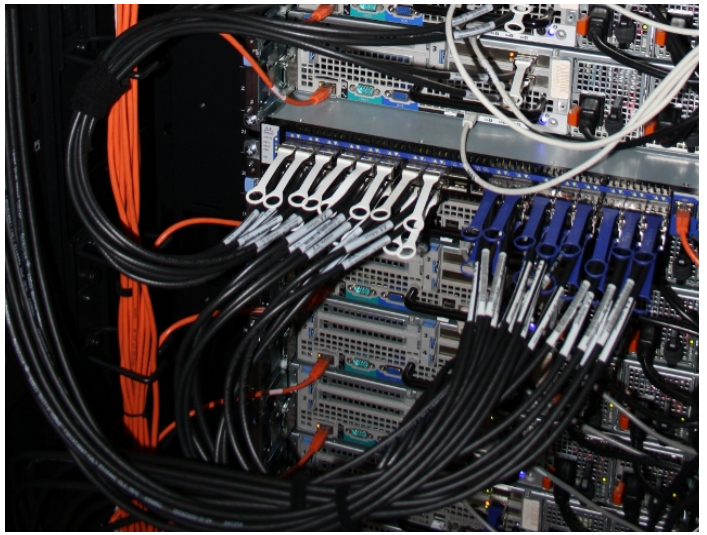
HPC-UGent Tier-2 (STEVIN)

Network connections between nodes ('interconnect')

Ethernet: 1-10 Gbit/s

Infiniband: 50 - 100 Gbit/s





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for single core/node jobs

(too slow for fast inter-node communication)

€€(€)

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)**

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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

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- **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

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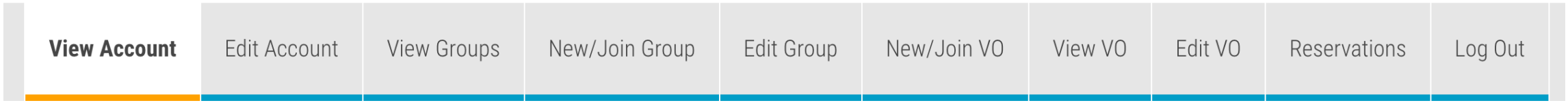
Account management

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

https://account.vscentrum.be



View account

General information

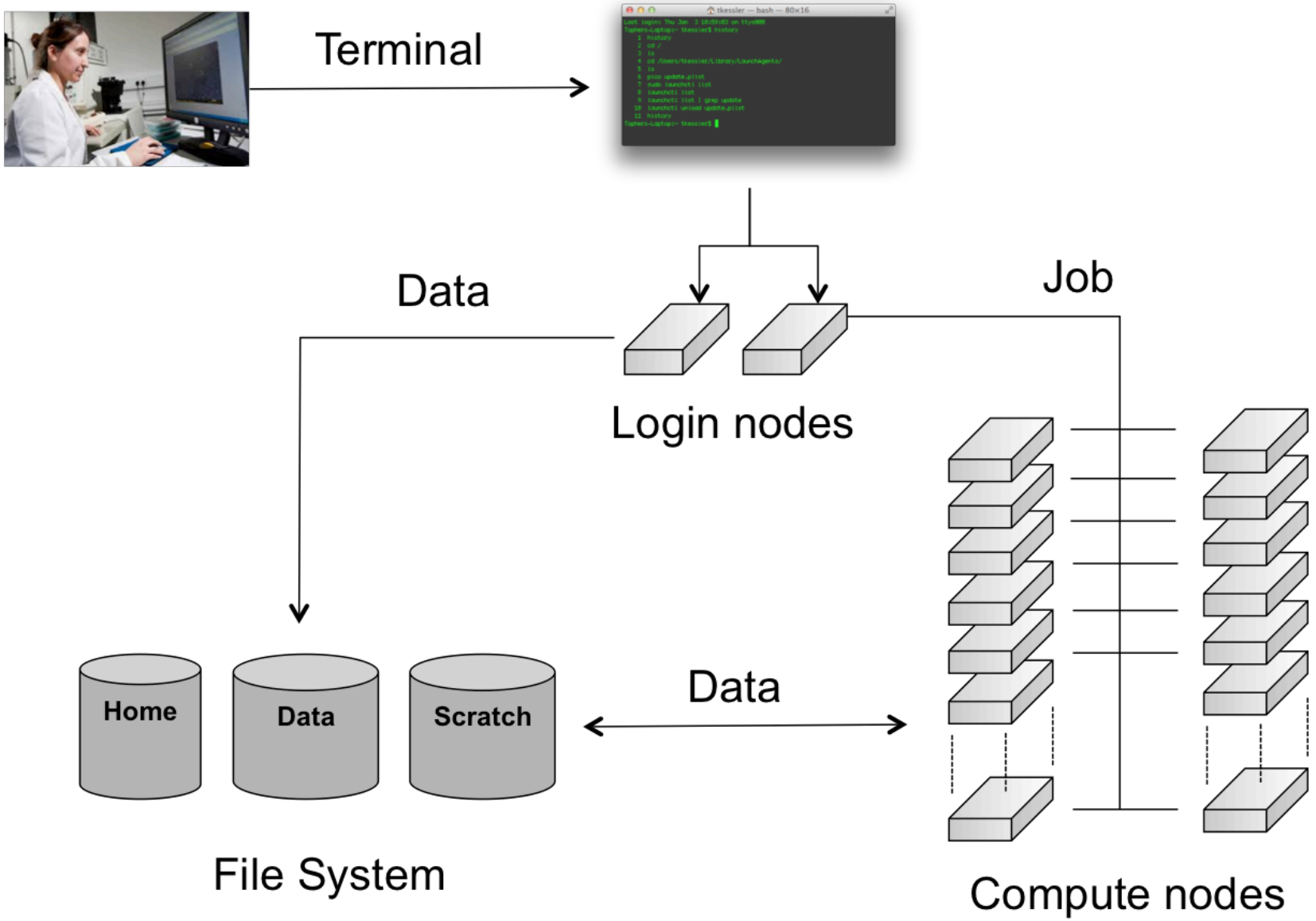
Uid: vsc40023

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

High-level overview of HPC-UGent infrastructure



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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$
```

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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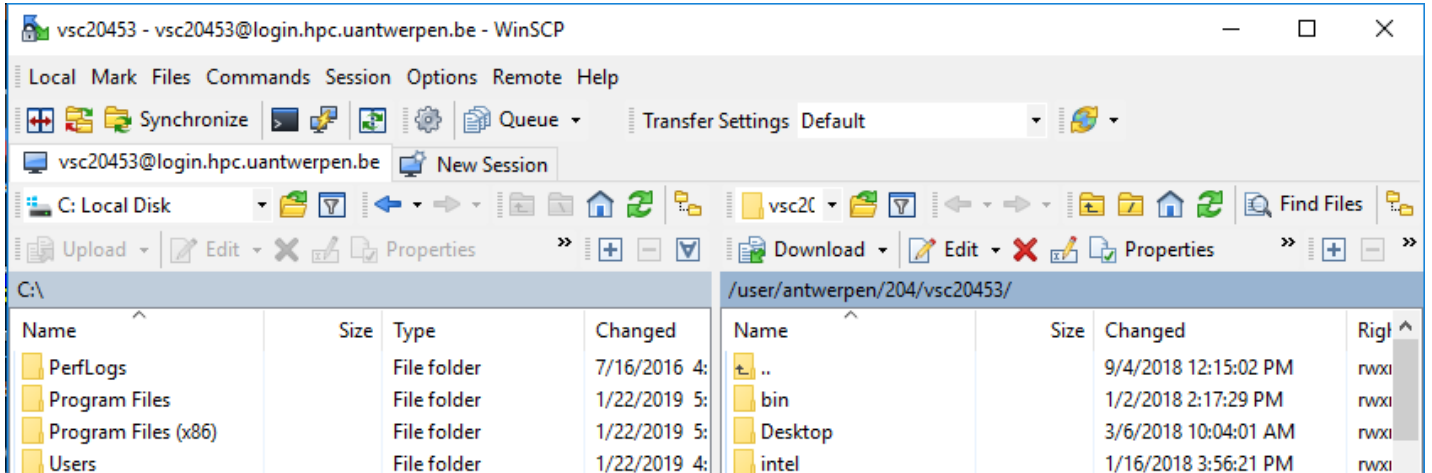
Transferring files to/from the HPC-UGent infrastructure

- **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



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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Basic Linux shell usage (interactive)

- 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)

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)!
- some environment variables are special: `$HOME`, `$USER`, `$PATH`, `$PYTHONPATH`, ...

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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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
```
or `$ ml Python/...`

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%

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

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

1. Connect to login nodes
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

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`'

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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!

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 HPC-UGent*: 27 March 2019
    - *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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Example job script to run a **Python** script

- **use a recent Python installation available via modules:**

  `module load Python/2.7.15-intel-2018b` ***or*** `module load Python/3.6.6-intel-2018b`

- our Python installations come with batteries included: `numpy`, `scipy`, `pandas`, ...
- additional modules may need to be loaded for some Python packages: `matplotlib`, `Seaborn`, ...
- use the `python` command to run your Python script file
- **using Anaconda is discouraged,** because it is not properly optimised for HPC-UGent clusters)
- **we do *not* recommend to install missing Python packages yourself**
  - so don't use "`pip install`" to install stuff in your home directory
  - instead, submit a software installation request for missing libraries
    via *https://www.ugent.be/hpc/en/support/software-installation-request*

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Example job script to run a **Python** script

```
#!/bin/bash
#PBS -l nodes=1:ppn=1
#PBS -l walltime=1:0:0

module load Python/2.7.15-intel-2018b
module load matplotlib/2.2.3-intel-2018b-Python-2.7.15
module load Seaborn/0.9.0-intel-2018b-Python-2.7.15

cd $PBS_O_WORKDIR

python HPC_Workshop.py > ${PBS_JOBID}.out 2> ${PBS_JOBID}.err
```

- we request a single core for 1 hour
- job is run in directory where it was submitted from (`$PBS_O_WORKDIR`)
- output messages from script are redirected to `<jobid>.out`
- warnings & errors from script are redirected to `<jobid>.err`

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Example job script to run an **R** script

- **use the most recent R installation available via modules:**

```
module load R/3.5.1-foss-2018b
```

- also consider additional bundles of R libraries: `R-bundle-Bioconductor`
- use the `Rscript` command to run your R script file
- **we do *not* recommend to install missing R libraries yourself**
  - so don't use install.packages in your R script
  - instead, submit a software installation request for missing libraries via *https://www.ugent.be/hpc/en/support/software-installation-request*

Example job script to run an **R** script

```
#!/bin/bash
#PBS -l nodes=1:ppn=1
#PBS -l walltime=1:0:0

module load R/3.5.1-foss-2018b

cd $PBS_O_WORKDIR

mkdir -p Graphs
Rscript S_HPCWorkshop.R > ${PBS_JOBID}.out 2> ${PBS_JOBID}.err
```

- we request a single core for 1 hour
- job is run in directory where it was submitted from (`$PBS_O_WORKDIR`)
- required `Graphs` directory is created (if it's not there yet)
- output messages from script are redirected to `<jobid>.out`
- warnings & errors from script are redirected to `<jobid>.err`

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Introduction to HPC-UGent

March 20th 2019 - GhEnToxLab

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

hpc@ugent.be

https://ugent.be/hpc

Vlaanderen is computing