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Introduction to HPC-UGent

January 25th 2017

http://users.ugent.be/~kehoste/hpcugent-intro-ILVO-20170125.pdf

hpc@ugent.be

http://ugent.be/hpc

Vlaams Supercomputer Centrum

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 platform
  - Successfully connect to the HPC
  - Successfully launch your first job

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About this training – schedule

- 1pm – 2.30pm: Info/demo session
- 2.30pm: Hands-on session
  - Logging in
  - Launch your first jobs
  - Discuss user-specific applications
  - Q&A

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About this training – course notes

- A manual is available, applicable for all VSC infrastructure
- Download it here: http://www.ugent.be/hpc/en/support/hpctutorial
- *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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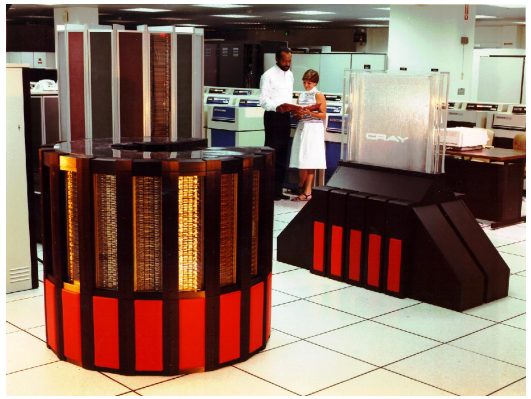
What is High Performance Computing?

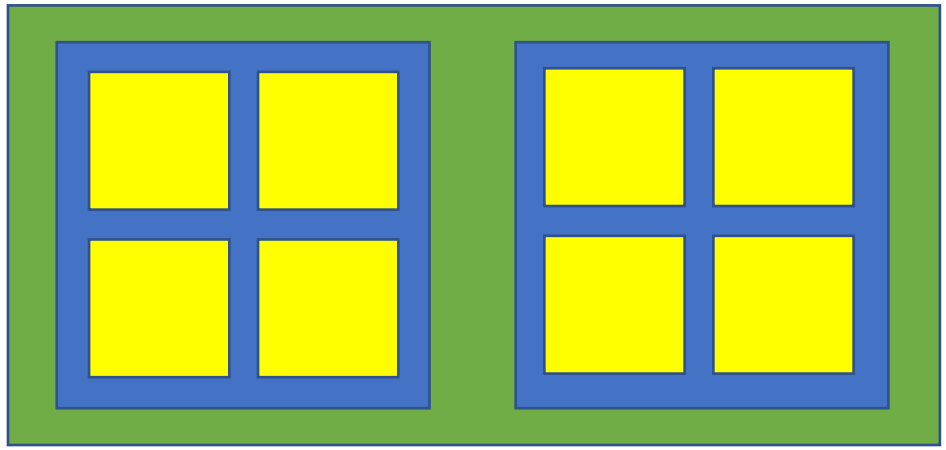
harness power of multiple interconnected cores/nodes/processing units

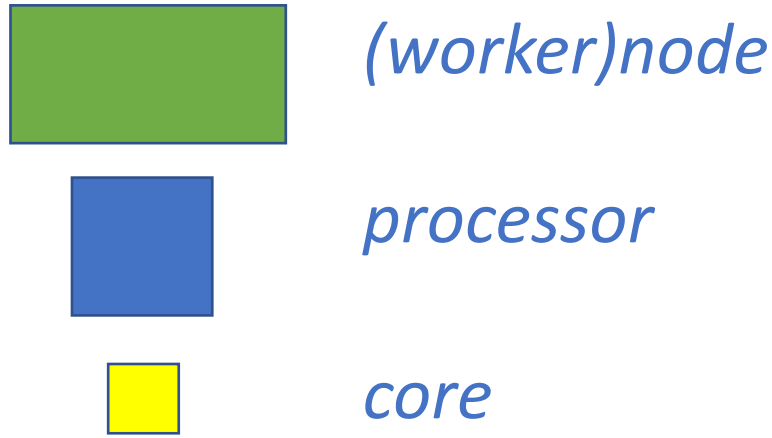


Cores vs processors vs nodes

Modern systems, often referred to as **(worker)nodes**, include one or more *multi-core processors* (next to memory, disk(s), network cards, …).

A modern **processor** consists of multiple CPUs or **cores** that are used to execute *computations*.





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Parallel vs sequential software

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

They are based on the principle that large problems can often be divided

into smaller ones, which are then solved concurrently (“in parallel”).

e.g., 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 *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 uses only *one single core* of a single workernode.

But, you can run *multiple instances* at the same time on a supercomputer.

e.g., you can easily run 1000 times a simple Python script to swiftly analyze 1000 datasets

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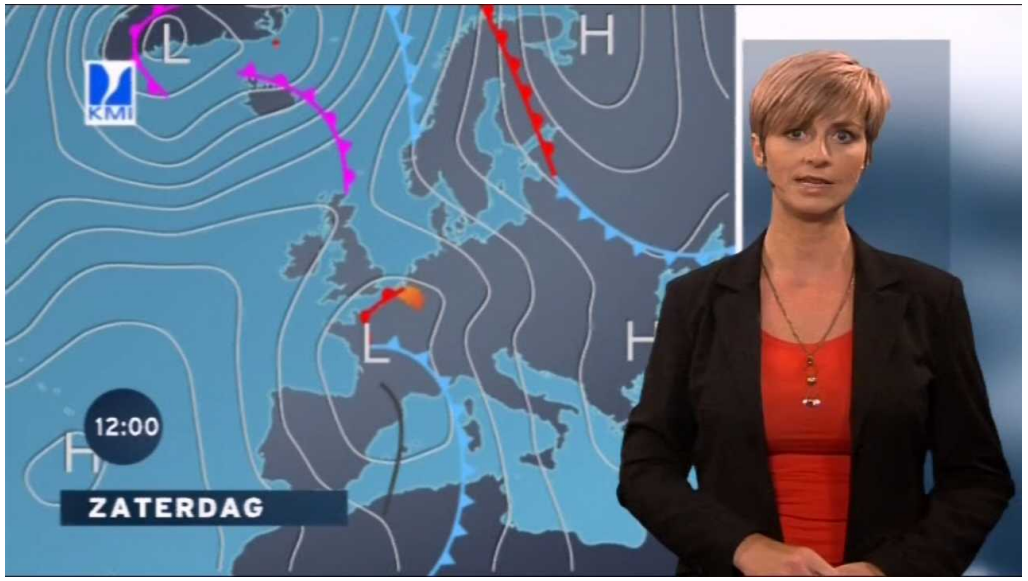
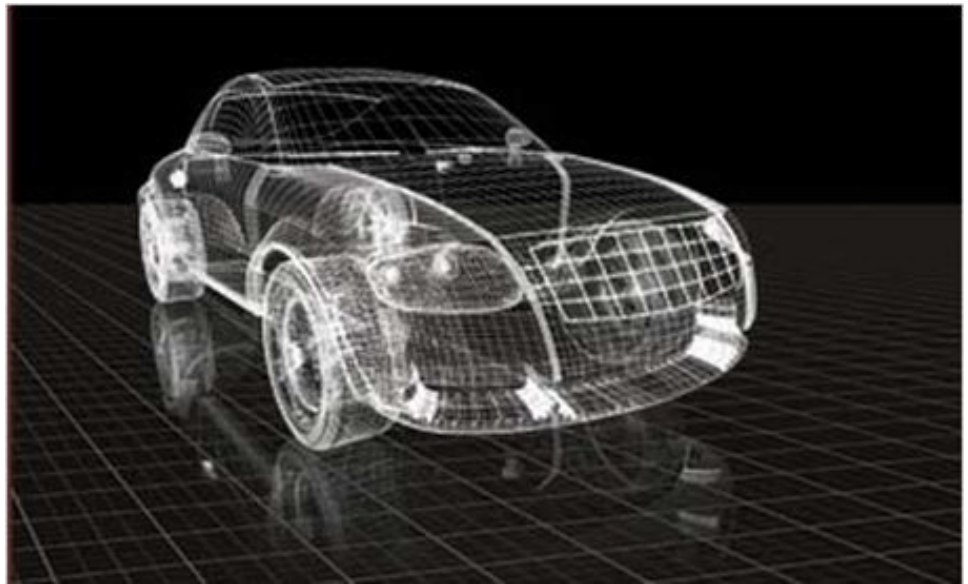
Everyday applications of supercomputing





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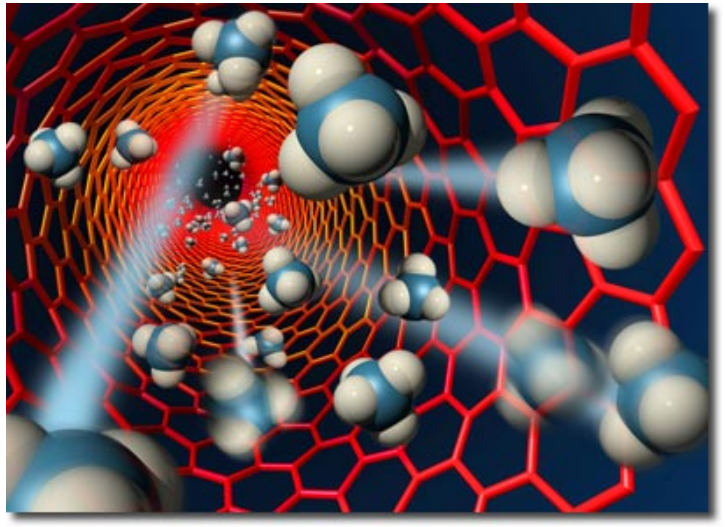
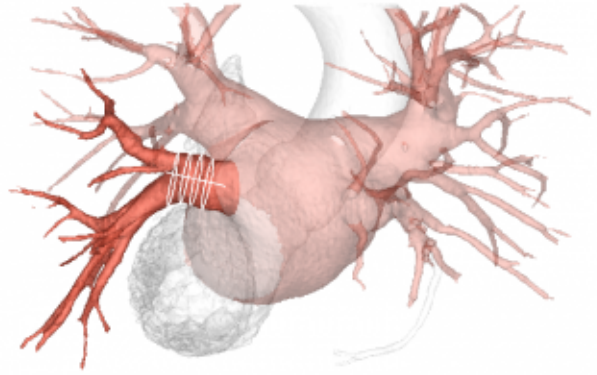
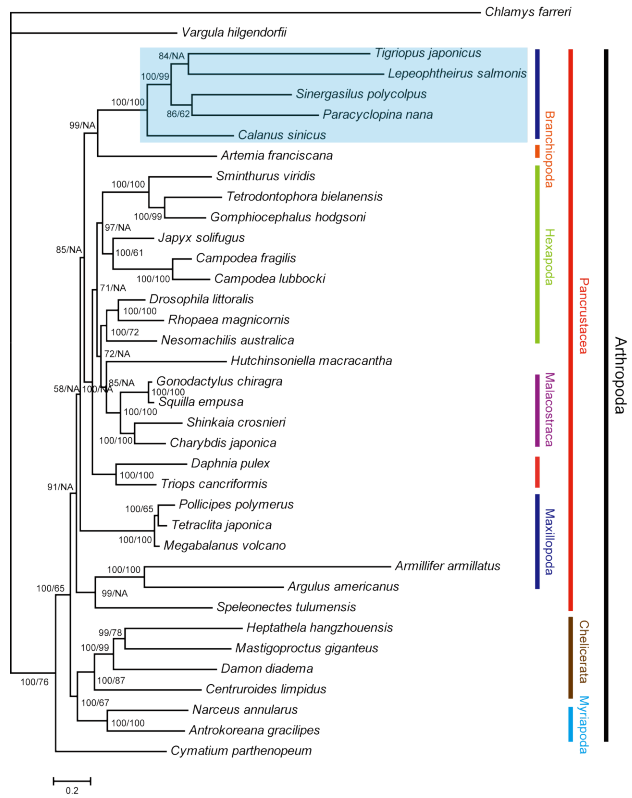
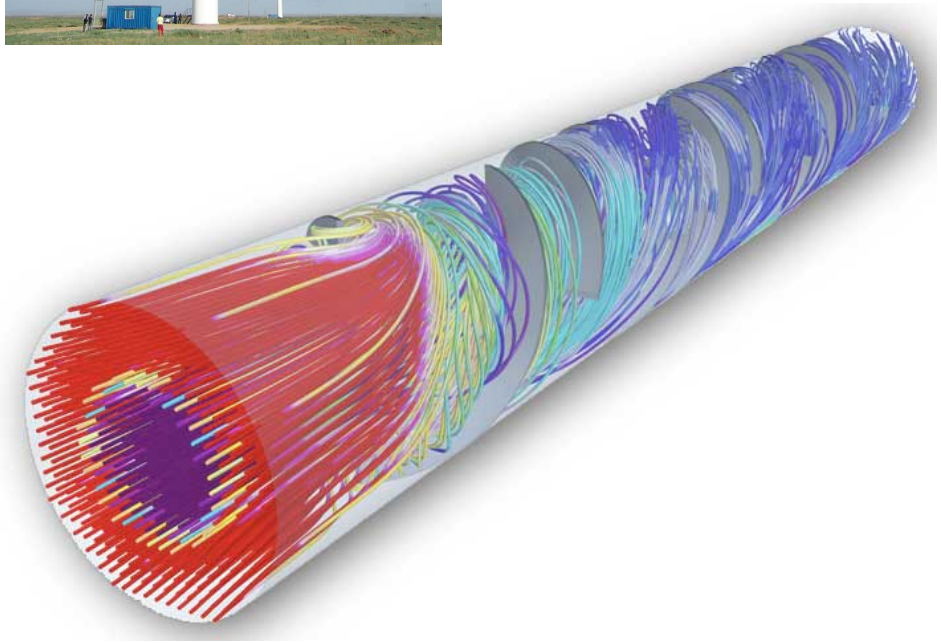
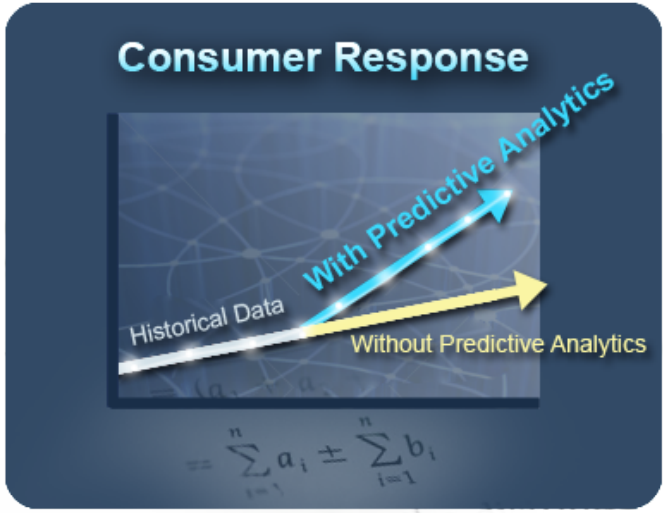
Scientific applications of supercomputing

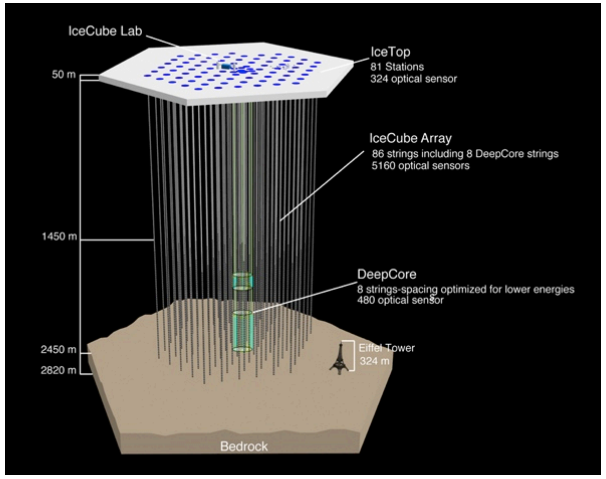












HPC-UGent

Part of ICT Department of Ghent University

Our mission

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

Our core values

Empowerment - Centralization - 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

Jens Timmerman
user support, *sysadmin, security*

Kenneth Waegeman
sysadmin, storage

Andy Georges
user support, sysadmin

Alvaro Simon Garcia
sysadmin, cloud

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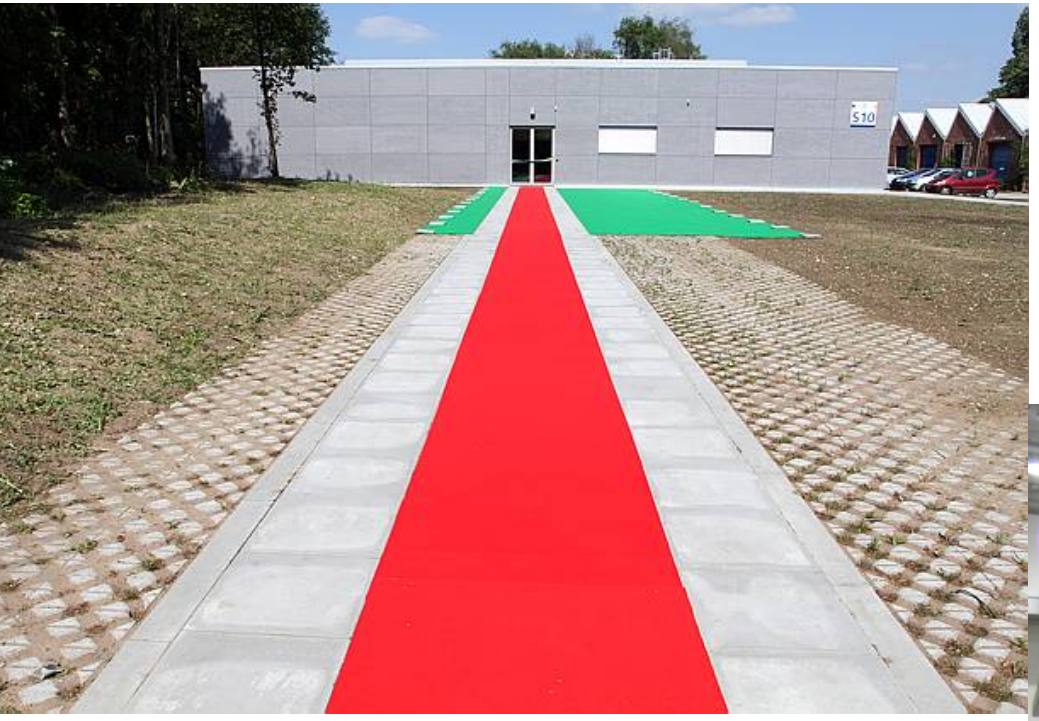
Centralized hardware



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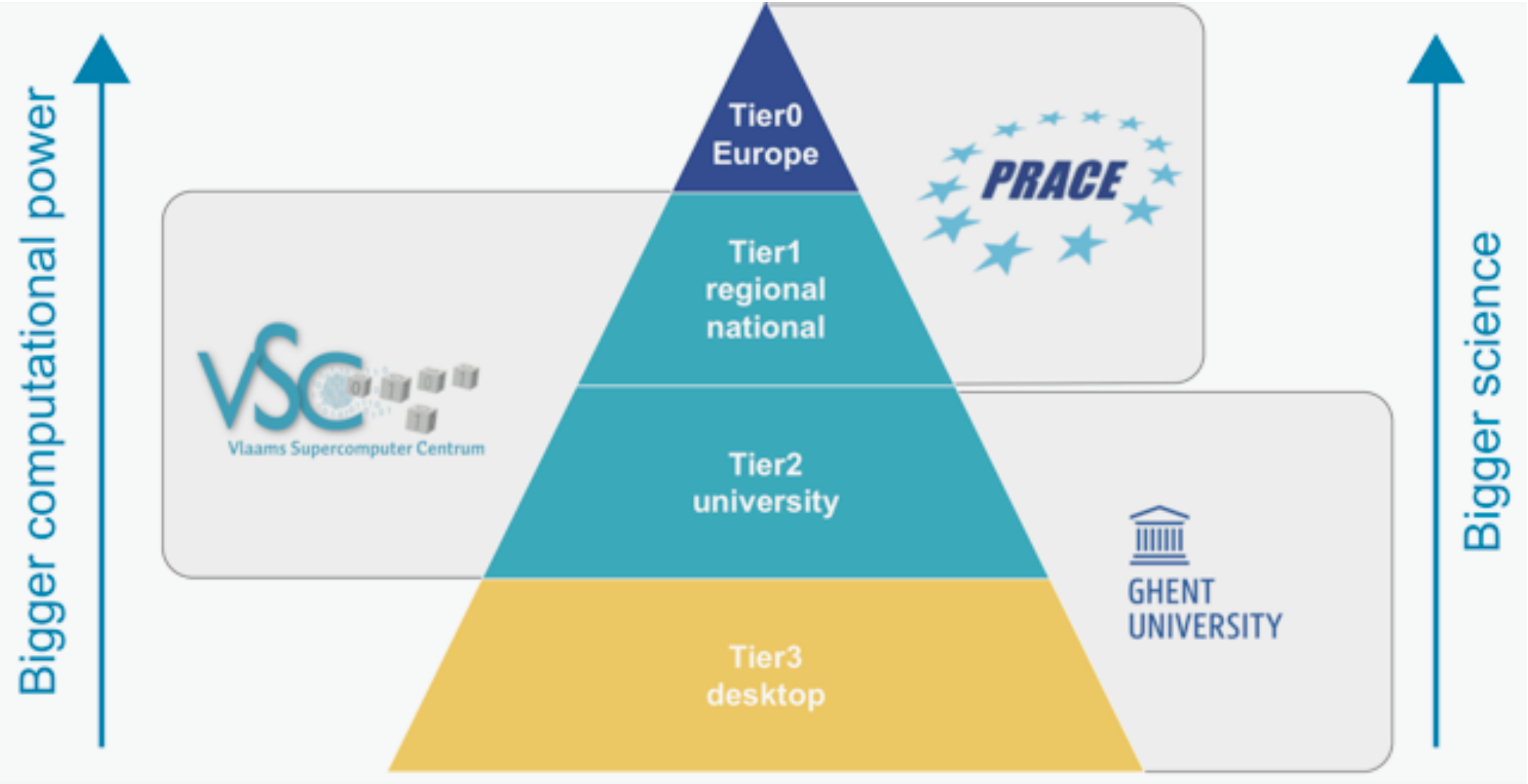
Centralized hardware



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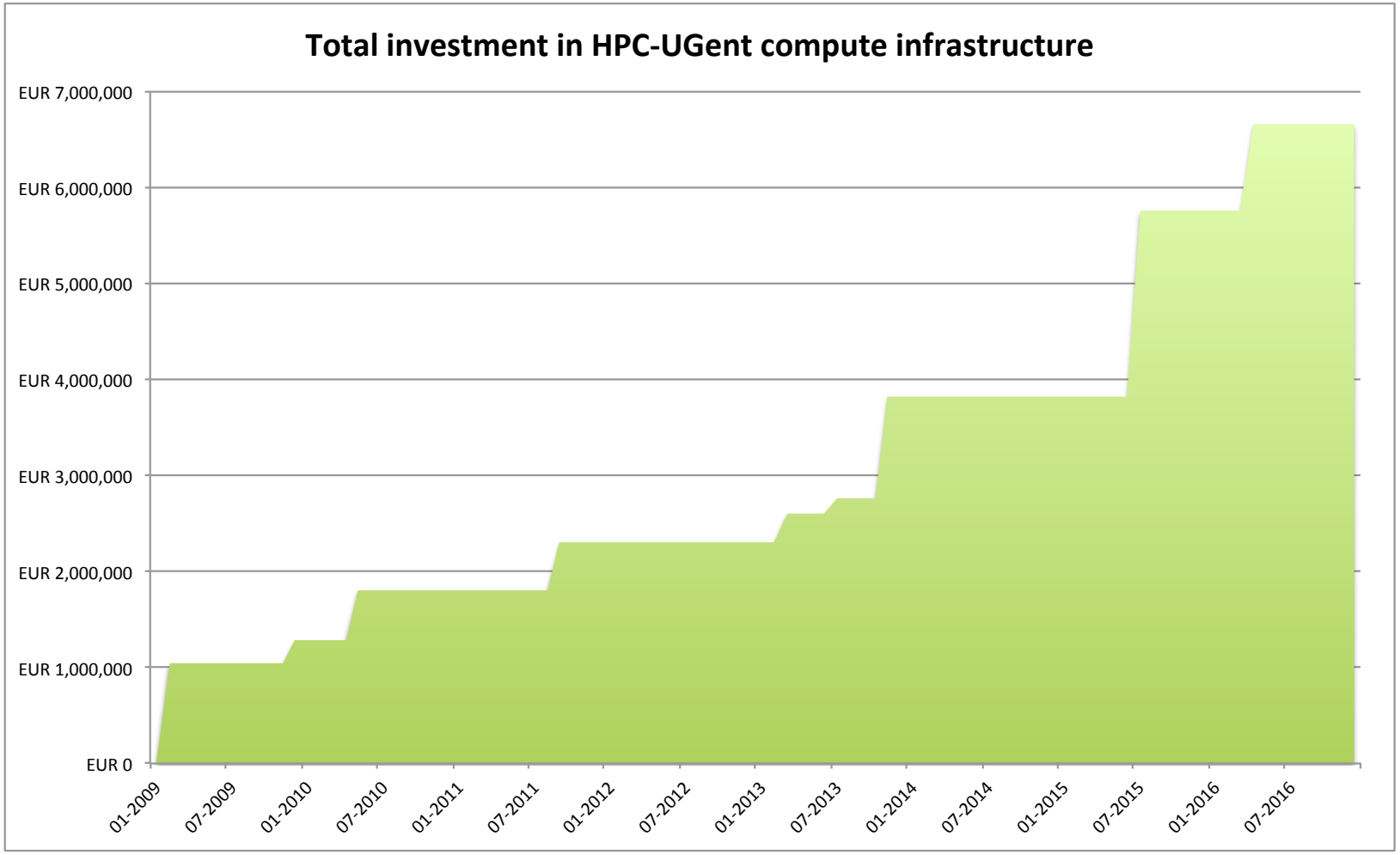
HPC-UGent Tier2 (STEVIN)

1548 - 1620
°Bruges

STEVIN
HPC
infrastructure



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Financing bodies:

fwo

VSC Vlaams Supercomputer Centrum

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HPC-UGent users

HPC-UGent Tier2 (STEVIN)

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

Compute clusters

5 Tier2 clusters; in total 500+ workernodes, 11k+ cores

	#nodes	CPU	Mem/node	Diskspace/node	Network
 **Raichu**	64	2 x 8-core Intel E5-2670 (Sandy Bridge @ 2.6 GHz)	32 GB	400 GB	GbE
 **Delcatty**	160	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

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HPC-UGent Tier2 (STEVIN)

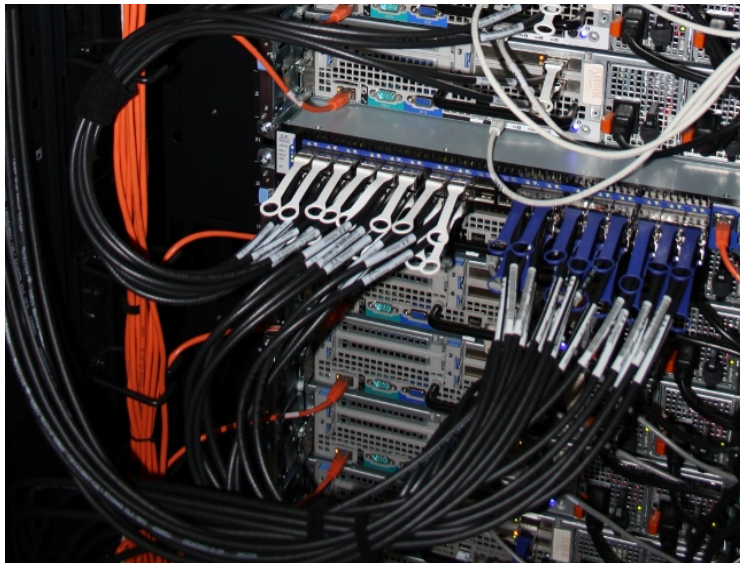
Network connections between nodes

Ethernet: 1 - 10 Gbit/s

€

for single core/node jobs

Infiniband: 24 - 54 Gbit/s



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required for MPI jobs

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VSC Tier2

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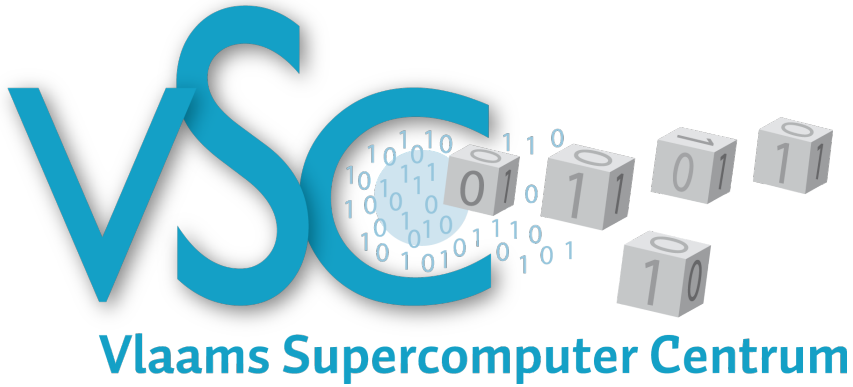
(Flemish Supercomputer Center)



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

(GPGPU systems @ KUL: http://hpc.ugent.be/userwiki/index.php/Tips:Software:GPGPU)

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**

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VSC Tier1 – muk (@ HPC-UGent)

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

Hardware

- 528 computing nodes
  - Two 8-core Intel Xeon processors (Sandy Bridge, E5-2670, 2.6 GHz)
  - 64 GiB RAM
- FDR InfiniBand interconnect with a fat tree topology
  - High bandwidth (6.5 GB/s per direction, per link)
  - Low latency
- Storage system
  - Capacity of 400 TB
  - Peak bandwidth of 9.5 GB/s

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VSC Tier1 – BrENIAC (@ KU Leuven)

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

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VSC Tier1

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 Tier1

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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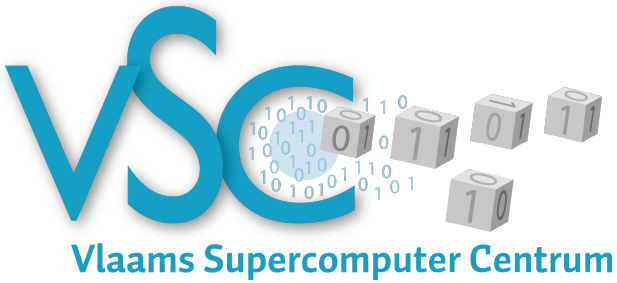
Getting a VSC account



- See Chapter 2 in HPC-UGent intro course notes
- https://www.vscentrum.be/en/access-and-infrastructure/requesting-access
- All users of AUGent can request an account
  - Researchers
  - Master/Bachelor students (after motivation of ZAP)
  - Staff
- 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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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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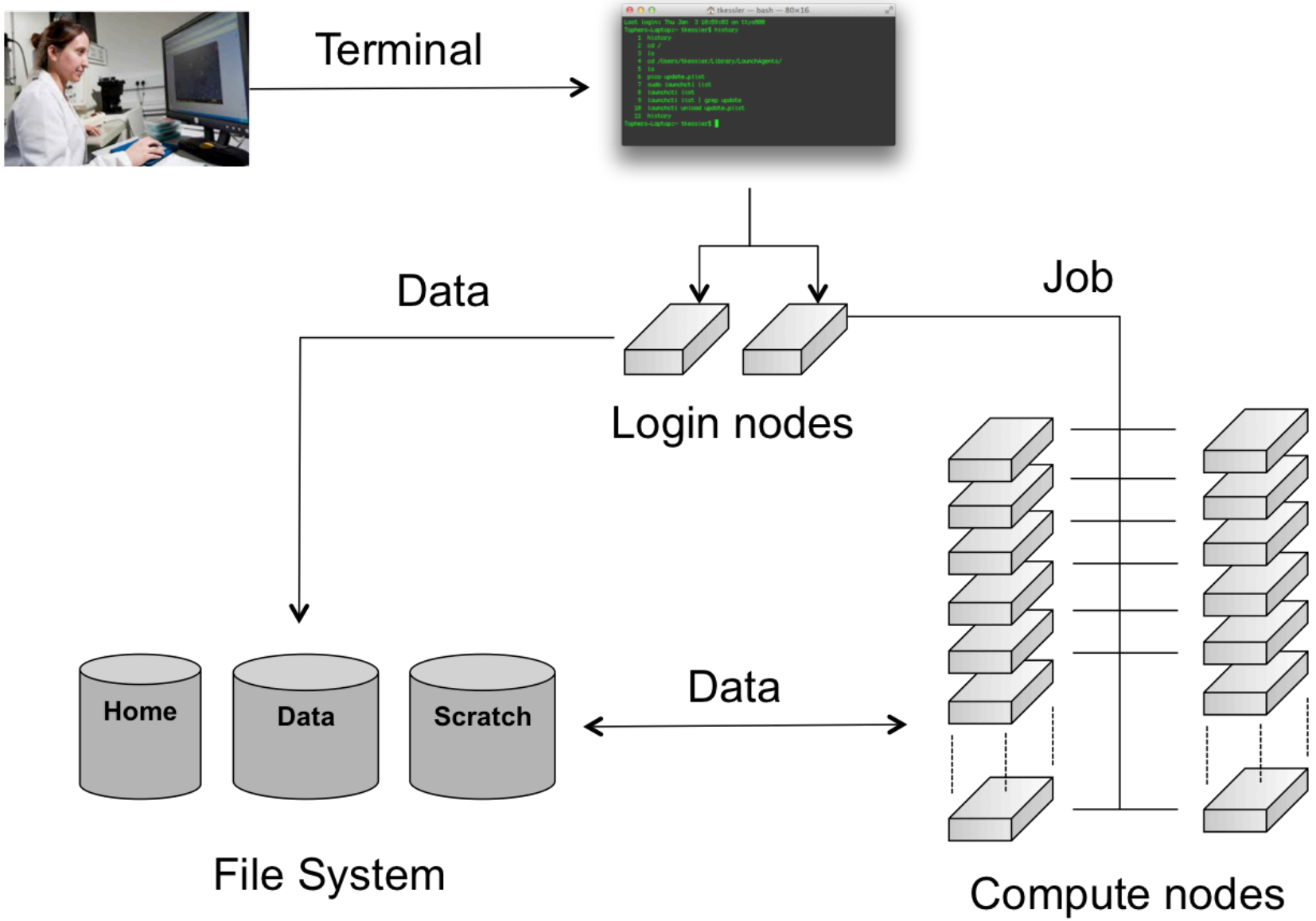
Workflow on HPC infrastructure



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Workflow on HPC infrastructure

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

See Chapter 3 in course notes

- Users interact with the 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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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**

- Choose correct PBS directives (Chapter 4, 8)
- Load software modules (Chapter 3)
- Useful environment variables (Chapter 4)
- Select correct data volume (Chapter 6)
- http://hpc.ugent.be/userwiki/index.php/User:VscScripts

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Job scripts: PBS directives

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

- **maximal walltime: 72 hours**
- for longer jobs, use *checkpointing*
  - preferable internal/application checkpointing
  - external checkpointing
    - see http://hpc.ugent.be/userwiki/index.php/User:Checkpointing

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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/2.7.12-intel-2016b
```

See currently loaded modules using:

```
$ module list
```

Get overview of available modules using:

```
$ module avail
```

- Only mix modules built with the same compiler toolchain.

  e.g., `intel` (Intel compilers, Intel MPI, Intel MKL (BLAS, LAPACK))
- See also https://www.vscentrum.be/cluster-doc/software/modules/lmod

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Job scripts: useful environment variables

- **`$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_JOBID`**
  - job id of running job
- **`$PBS_ARRAYID`**
  - array id of running job
  - only relevant when submitting array jobs (`qsub -t`)
- **`$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 is loaded

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Job scripts: input data & filesystems

- See Section 6.2 in course notes
- Think about I/O:
  - How will you *stage in* your data and input files?
  - How will you *stage out* your output files?
- Manually (on login nodes) 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
- Storage limits / quota:
  - Home: 3GB (fixed)
  - Data/scratch: 25GB by default, more via VO by request (TBs if needed)

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Workflow on HPC infrastructure

- 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 fibo.pbs
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      job1     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
  - Some overhead involved with each job (job scheduling, node health check, …)
  - Results in lots of bookkeeping (job scripts, failed jobs, output files, …)
- Better approach:
  - Array jobs (http://hpc.ugent.be/userwiki/index.php/User:VscScripts#Array_Example)
    - 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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Documentation & training

- Documentation is available at:
  - https://www.vscentrum.be/en/user-portal
  - http://hpc.ugent.be/userwiki
- HPC tutorial: http://www.ugent.be/hpc/en/support/hpctutorial
- Basic Linux: http://hpc.ugent.be/userwiki/index.php/Tips:Introduction_to_Linux
- **Training sessions -** https://www.vscentrum.be/en/education-and-trainings
  - Singularity: Containers in HPC (Tue Feb 7th 2017)
  - Introduction to Linux (Wed March 15th 2017)
  - Specialist Workshops in Scientific Computing (SWSC)
    - *Introduction to multithreading and OpenMP* (April 18-19th 2017)
    - *Introduction to MPI* (May 3rd 2017)

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Software installations

Request for new software installations: hpc@ugent.be

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!

Getting help

Contact HPC-UGent support: **hpc@ugent.be**

Always include:

- 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
- VSC login id

Preferably use your UGent email address

Alternatives:

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

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Hands-on session (ILVO)

- Logging in
- Create and submit a simple job script
  - A handful of workernodes are reserved
  - **Submit in reservation *(only today!):***

    `qsub -W x=FLAGS:ADVRES:ILVO.278`
- Figure out your workflow
- Available software (see modules):
  - Python 2.7.12 (incl. numpy)
  - R 3.3.1
  - OpenCV 3.1.0
  - h5py 2.6.0 (w/ HDF5 1.8.17)
  - mahotas 1.4.3
  - hyperspy 1.1.1
  - GroIMP 1.5
  - ImageJ 1.51i
  - QGIS 2.8.12 [PENDING]
  - Photoscan [PENDING]
  - ArcMap [PENDING]

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Hands-on session (ILVO): GRECOS use case

```
module load R/3.3.1-intel-2016b
Rscript GECROS_Sensitivity.R
```

- R module already provides required `FME` package

- 2 trivial changes in `GECROS_Sensitivity.R`:
  - '`setwd`' is not required, current working directory is by default correct on Linux
  - to load `FME` library, just use: `library("FME")`

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Hands-on session (ILVO): CreateCube use case

```
module load Python/3.5.2-intel-2016b
module load matplotlib/1.5.3-intel-2016b-Python-3.5.2
python CreateCube.py
```

Example output (on a swalot workernode):

```
Took 1630.00ms to create the cube.
Took 260.00ms to get response.
Took 110.00ms to get Confidence Interval.
Took 150.00ms to add a value.
Took 120.00ms to multiply a value.
Took 210.00ms to subtract mask.
Took 120.00ms to convert the cube.
```

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Hands-on session (ILVO): ImageJ

```
module load ImageJ/1.51i
java -jar $EBROOTIMAGEJ/ij.jar –macro <script> <image>
```

Extra “Morphological Operators” plugins required?

http://www.mecourse.com/landinig/software/software.html

Strictly requires graphical user environment (also with `-batch`)? ☹

- X-forwarding:
  - macOS/Linux: connect with ‘`ssh -X`’ (macOS requires XQuartz: https://www.xquartz.org/)
  - Windows requires XMing: https://www.vscentrum.be/client/windows/xming
    - enable X11 in PuTTy: https://www.vscentrum.be/client/windows/console-putty
- VNC: http://hpc.ugent.be/userwiki/index.php/User:VNC

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January 25th 2017

http://users.ugent.be/~kehoste/hpcugent-intro-ILVO-20170125.pdf

hpc@ugent.be

http://ugent.be/hpc

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