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Introduction to HPC-UGent

Nov 9th 2018

https://www.ugent.be/hpc/en/training/materials/2018/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 your questions

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About this training – HPC tutorial

- A 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.

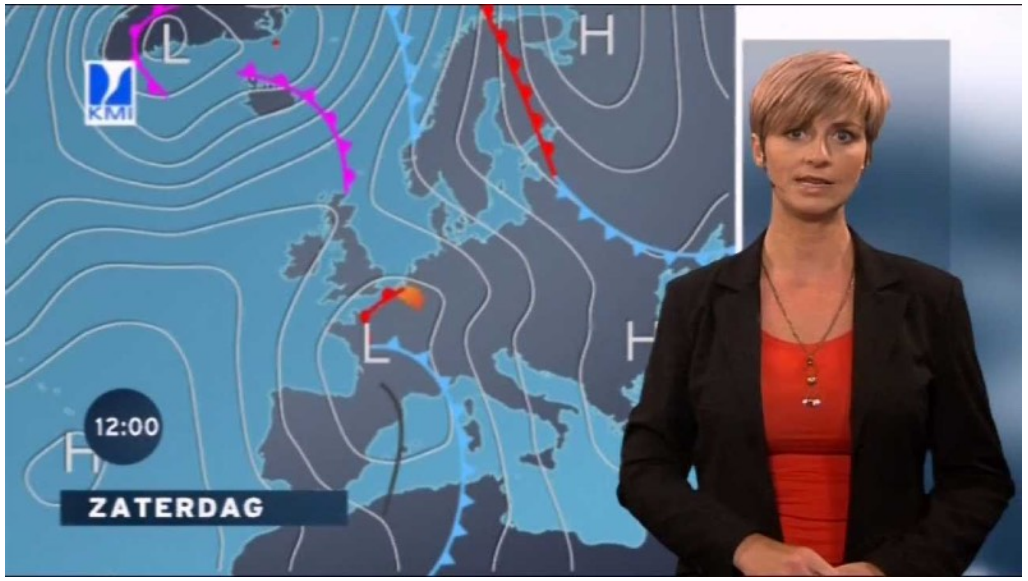
A computer ***cluster*** consists of a set of loosely or tightly connected computers that work together so that in many respects they can be viewed as a single system.

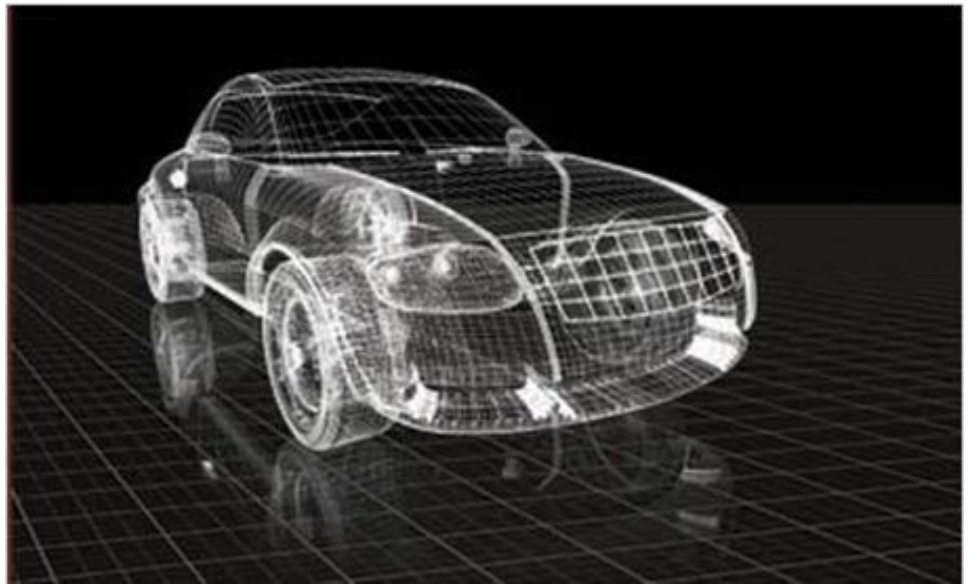
(a.k.a. "supercomputing")

What is High Performance Computing?

harness power of multiple interconnected cores/nodes/processing units

Everyday applications of supercomputing





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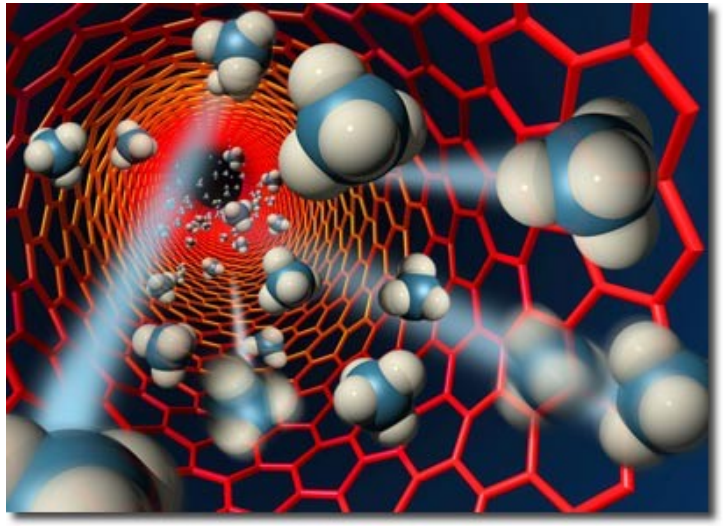
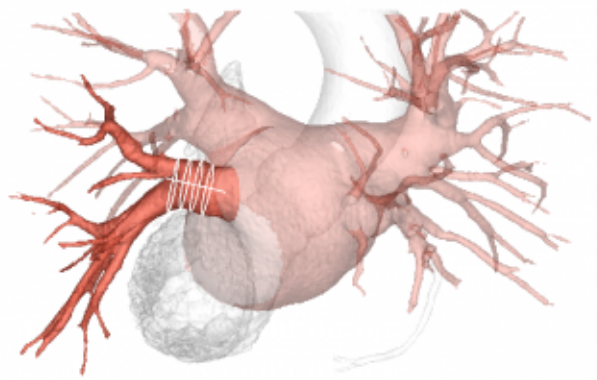
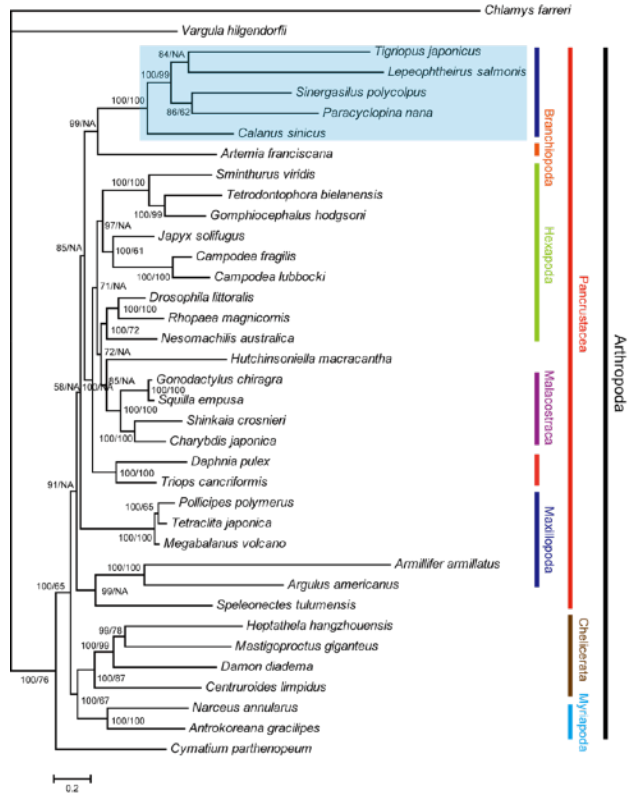
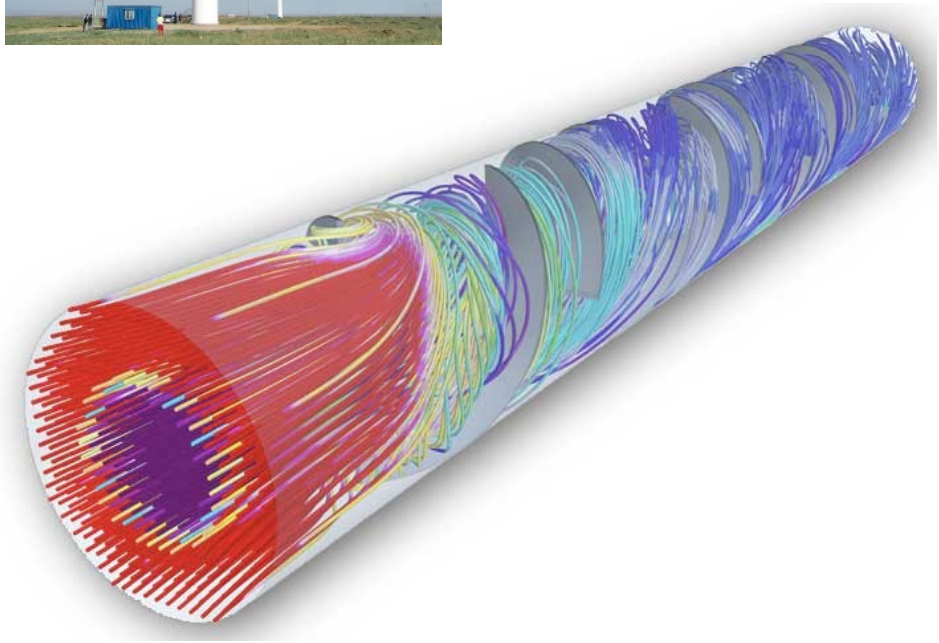
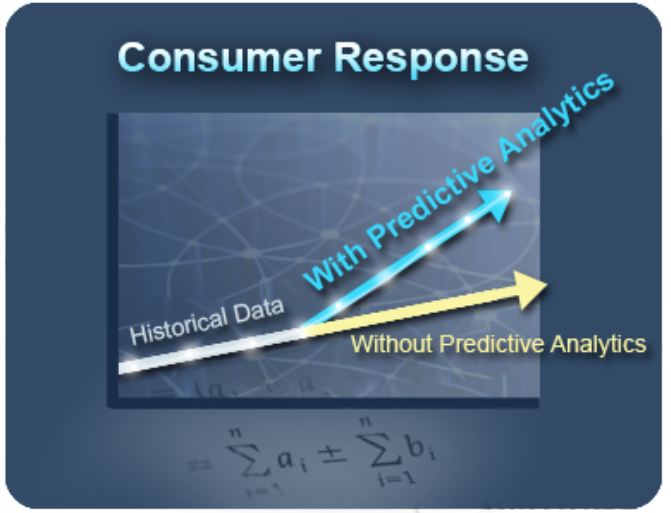
Scientific applications of supercomputing

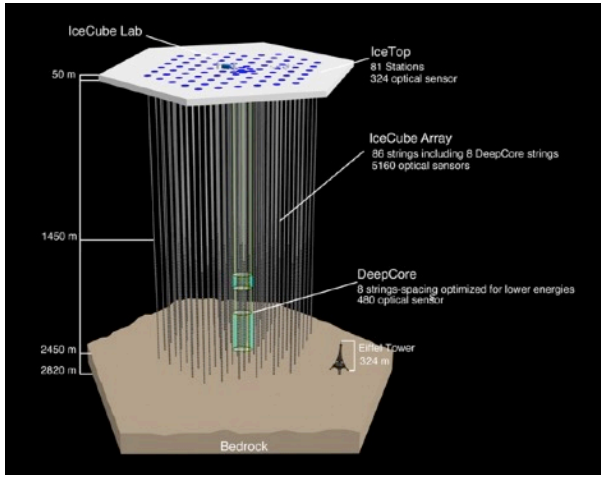










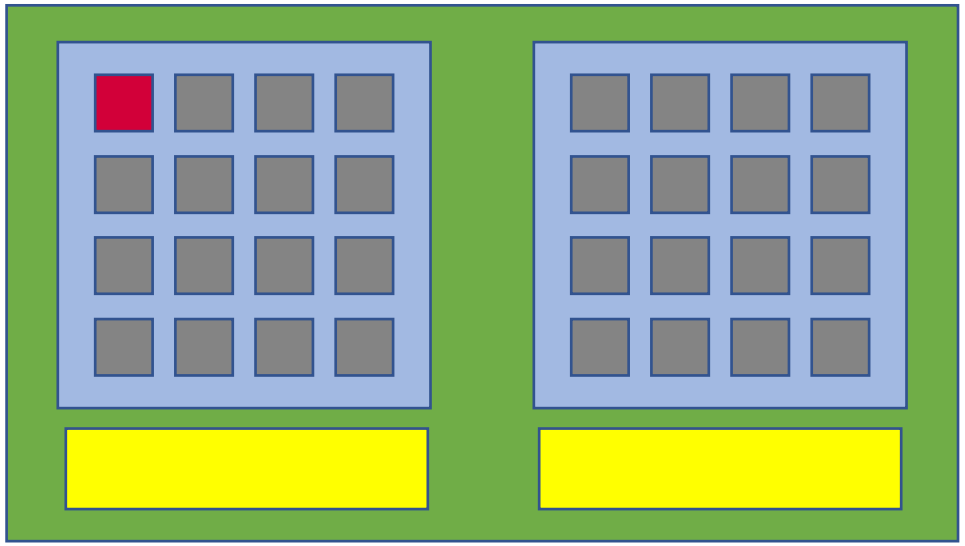


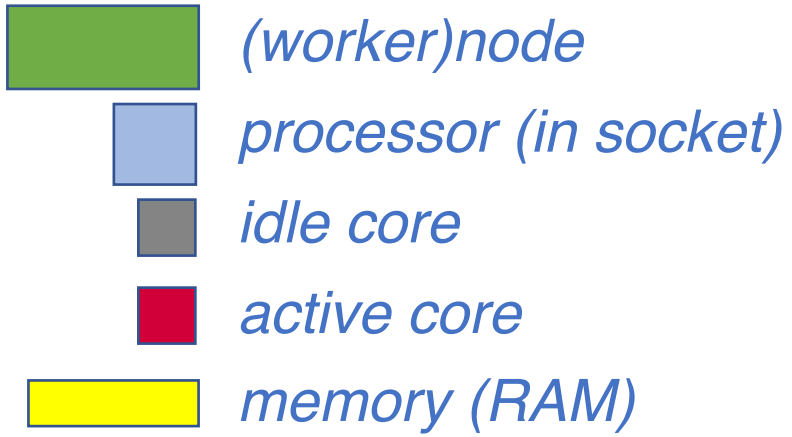
Cores, CPUs, processors, sockets, (worker)nodes

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”).

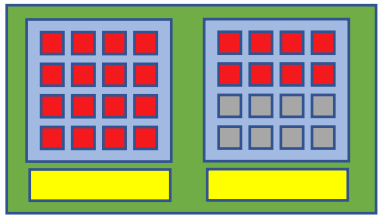
e.g., OpenFOAM can easily use 160 cores at the same time to solve a CFD problem

Parallel programming paradigms:

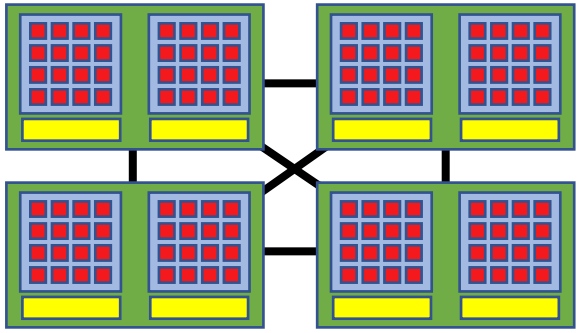
OpenMP for shared memory systems (*multithreading*) -> on cores of a *single* node

MPI for distributed memory systems (*multiprocessing*) -> on *multiple* nodes

OpenMP software can use multiple or all cores in a node



MPI software can use (all) cores in multiple nodes



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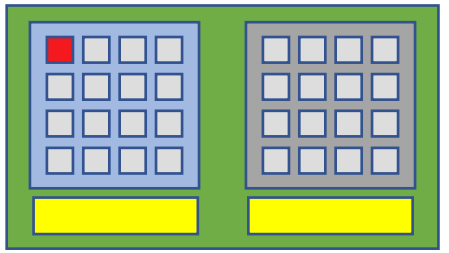
Parallel vs sequential programs

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

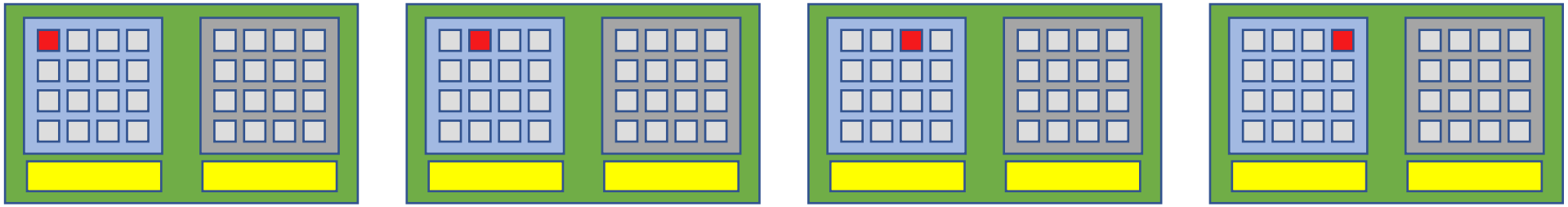
i.e. it only uses *one single core* of a single workernode.



(sequential) software does not become faster by just throwing cores at it...

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

e.g., you can run a Python script 1000 times at once to quickly analyse 1000 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 & testing

Ewald Pauwels
team lead

Wouter Depypere
sysadmin, hardware

Kenneth Waegeman
sysadmin, storage

Alvaro Simon Garcia
cloud, user support

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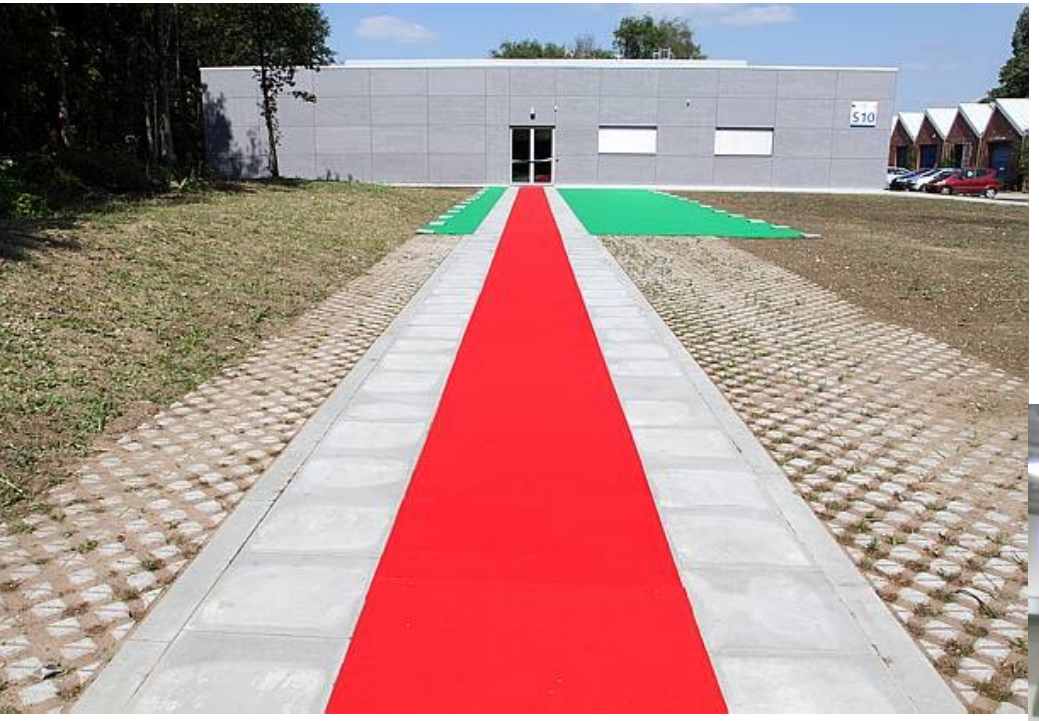
Centralised hardware



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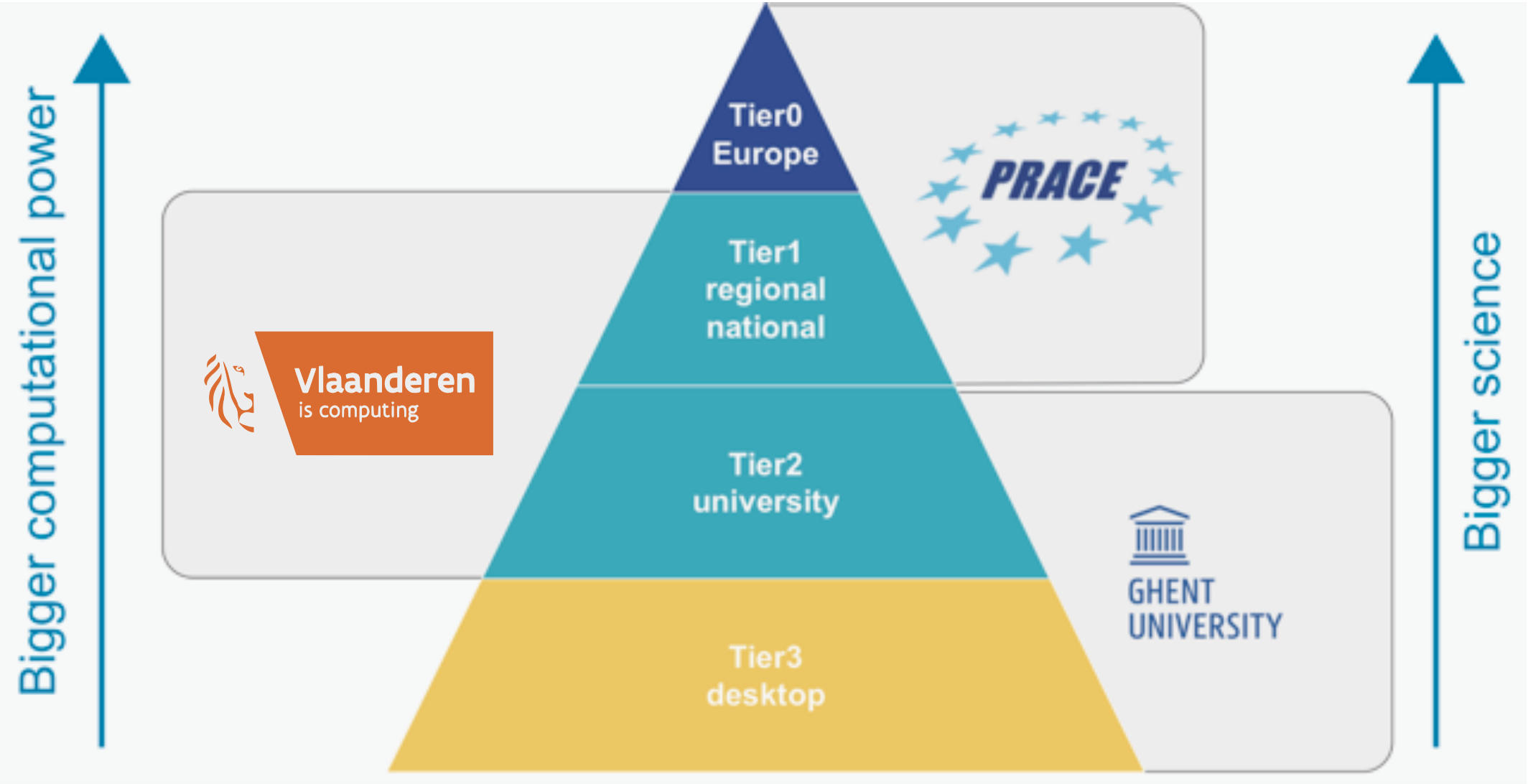
Centralised hardware



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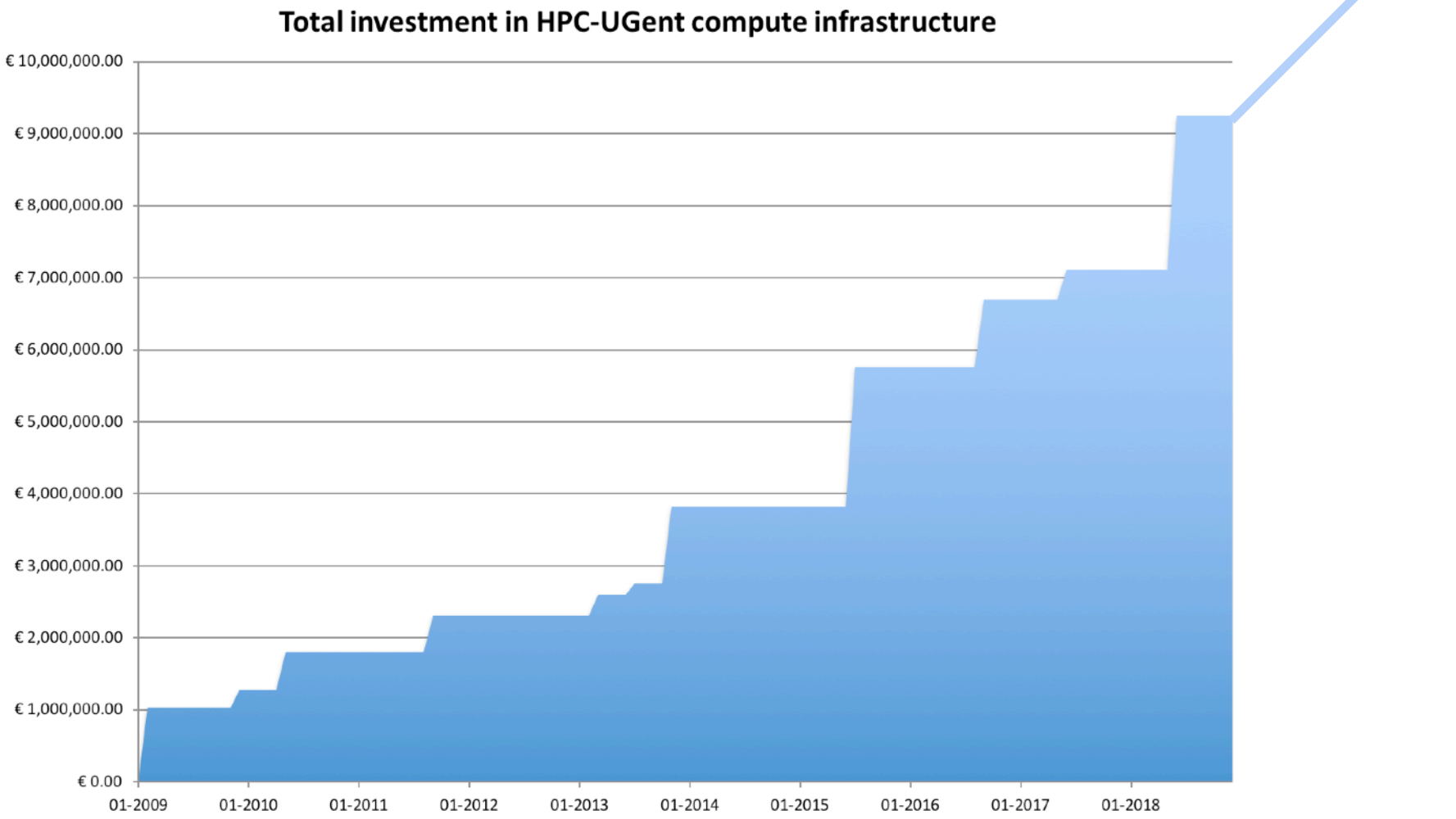
HPC-UGent Tier2 (STEVIN): central investments

1548 - 1620
°Bruges

STEVIN HPC infrastructure



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Financing by:

fwo

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HPC-UGent users

HPC-UGent Tier2 (STEVIN)

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

4 Tier2 clusters

in total ~~500~~ 470 workernodes, ~10k cores

Compute clusters

	#nodes	CPU	Mem/node	Diskspace/node	Network
Raichu	64	(retired on Jan 15th 2018) (Sandy Bridge @ 2.6 GHz)	32 GB	400 GB	GbE
Delcatty	~~160~~ 126	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)

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

2 new Tier2 clusters, replacements for raichu & delcatty

about 6000 extra compute cores, latest Intel processor generation

current status: operational since summer 2018

	#nodes	CPU	Mem/node	Diskspace/node	Network
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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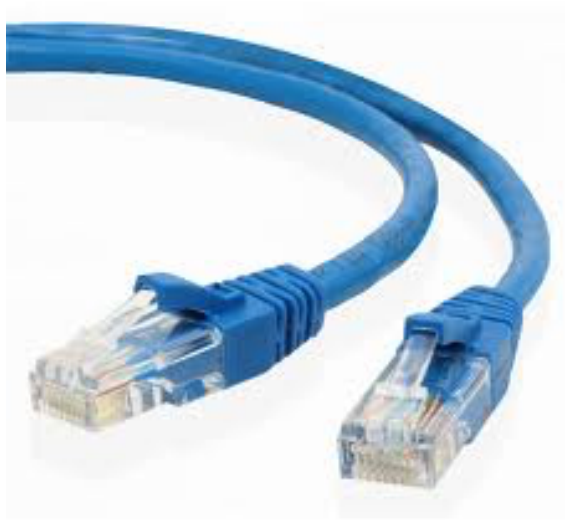
HPC-UGent Tier2 (STEVIN)

Network connections between nodes

Ethernet: 1-10 Gbit/s



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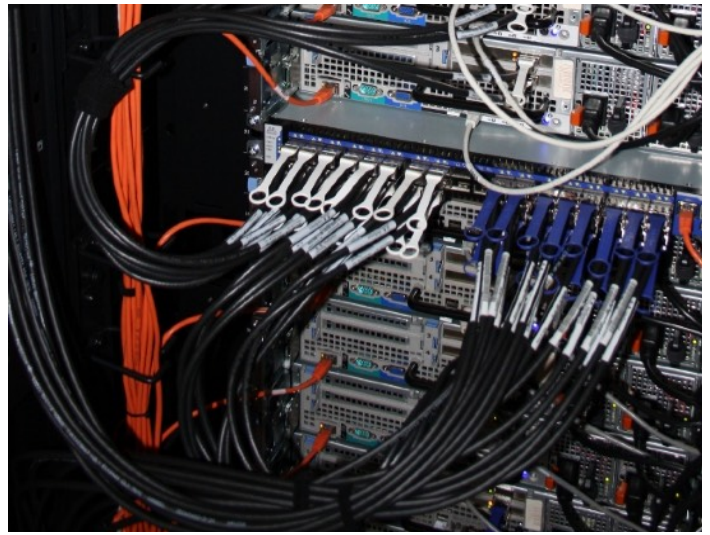
for single core/node jobs

(too slow for fast inter-node communication)

Infiniband: 50 - 100 Gbit/s



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required for MPI jobs

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VSC Tier2

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 Tier1 – muk (@ HPC-UGent)

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

retired on Jan 1st 2017

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

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

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- 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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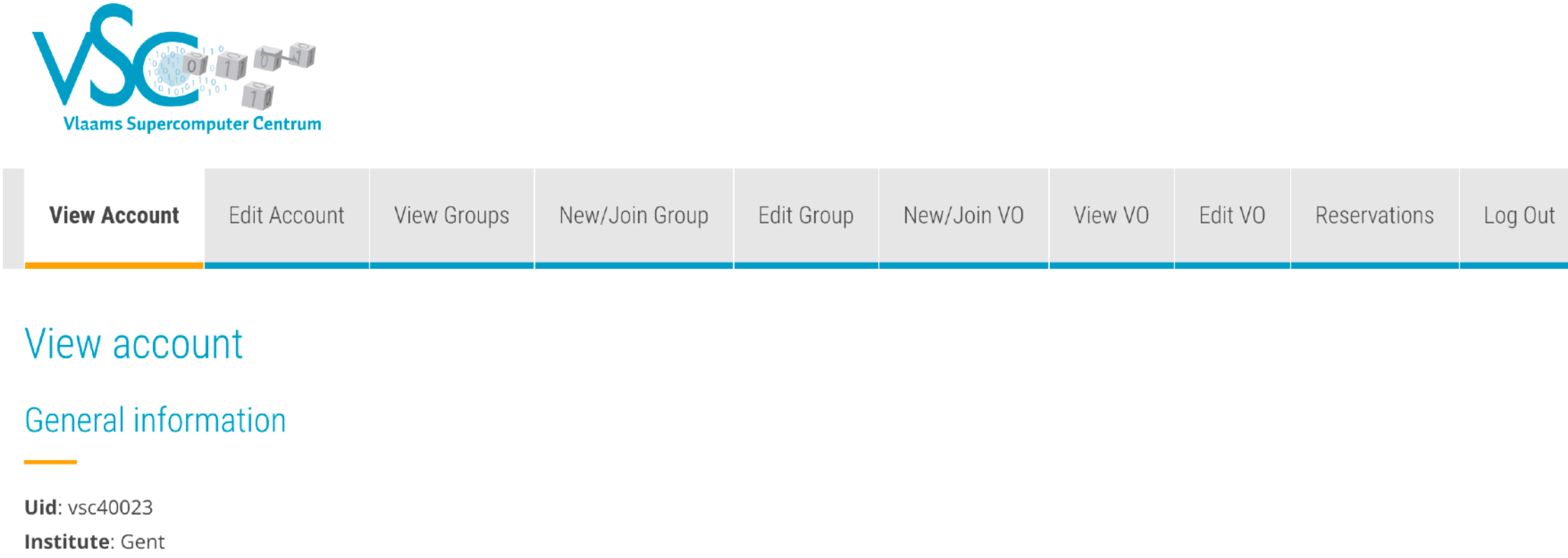
Account management

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

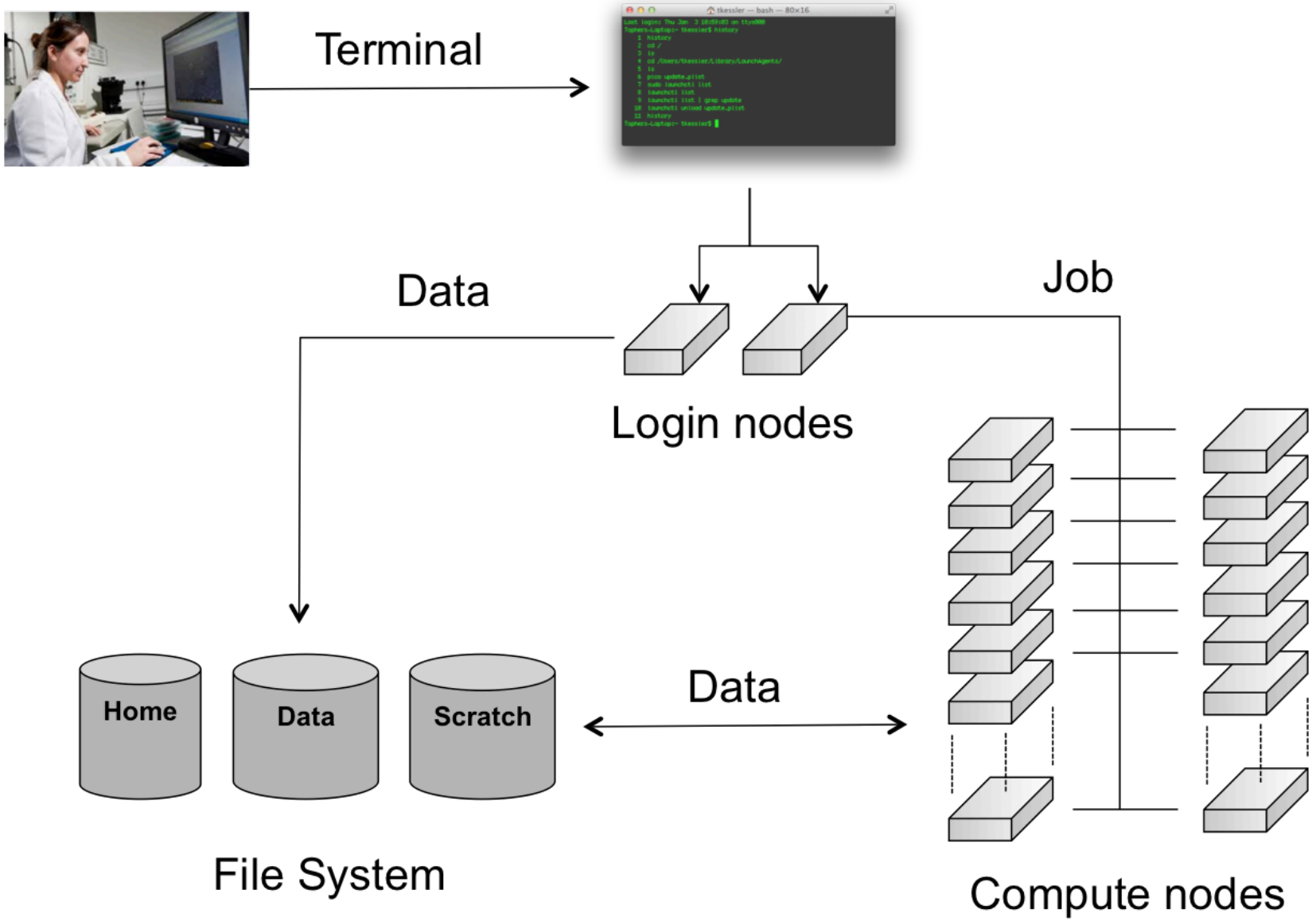
https://account.vscentrum.be



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 a login node

```
Last login: Thu Nov  8 22:52:34 2018 from gligar02.gligar.os

STEVIN HPC-UGent infrastructure status on Fri, 09 Nov 2018 08:05:01

   cluster - full - free -  part - total - running - queued
             nodes  nodes   free   nodes    jobs      jobs
-----------------------------------------------------------------
  delcatty    123      0      3     126      N/A       N/A
    golett    193      1      0     200      N/A       N/A
    phanpy      8      0      8      16      N/A       N/A
    swalot     44      0     77     128      N/A       N/A
    skitty     31      1     39      72      N/A       N/A
   victini     87      0      3      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
gligar03.gligar.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 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**
5. Submit your job

- Choose correct PBS directives (Chapter 4, 8)
- Load software modules (Chapter 3)
- Useful environment variables (Chapter 4)
- Select correct data volume (Chapter 6)

7. Move your results

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Job scripts: 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 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/2.7.14-intel-2018a` 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 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

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Storage quota

- home directory (`$VSC_HOME`): 3GB (fixed)
- personal data directory (`$VSC_DATA`): 25GB (fixed)
- personal scratch directory (`$VSC_SCRATCH`): 25GB (fixed)
- current quota usage can be consulted on VSC accountpage https://account.vscentrum.be
- **more storage quota (GBs, TBs) available for members of virtual organisations (VOs)**
- see Chapter 6 (section 6.6)
- additional quota can be requested via https://account.vscentrum.be/django/vo/edit
- shared with VO: `$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/3.6.4-intel-2018a
# 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/2017b
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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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 jobs (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)

- **HPC-UGent user meeting**: Mon Jan 28th 2019 (more information soon)

- **Training sessions -** https://www.vscentrum.be/en/education-and-trainings
  - upcoming sessions in Ghent:
    - Introduction to multi-threading (OpenMP)

      (April-May 2019, to be planned)
    - Introduction to MPI

      (April-May 2019, to be planned)

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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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Introduction to HPC-UGent

Nov 9th 2018

https://www.ugent.be/hpc/en/training/materials/2018/introhpcugent

hpc@ugent.be

https://ugent.be/hpc

Vlaanderen is computing