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TRAIN-THE-TRAINER: TEACHING USING HPC-UGENT

Info session 22 June 2023

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ABOUT HPC-UGENT

Mission

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

Tasks
- User support
- Training
- Infrastructure installation & upkeep (software & hardware)
- Outreach + marketing
- Collaboration with other supercomputing centers

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TEACHING USING HPC-UGENT – TL;DR

- Use the HPC-UGent Tier2 web portal https://login.hpc.ugent.be
- Jobs start instantly on cluster *donphan* (with limited resources)

- Lots of scientific software is preinstalled as modules (*module load*)
- Custom interactive applications on web portal are possible
- Students make VSC account themselves, or we do based on UGent course id

- Always prepare a plan B – e.g. in case of unexpected power failure

- Still need a dedicated server? Request VSC Tier1 Cloud VM(s)
  https://www.vscentrum.be/cloud

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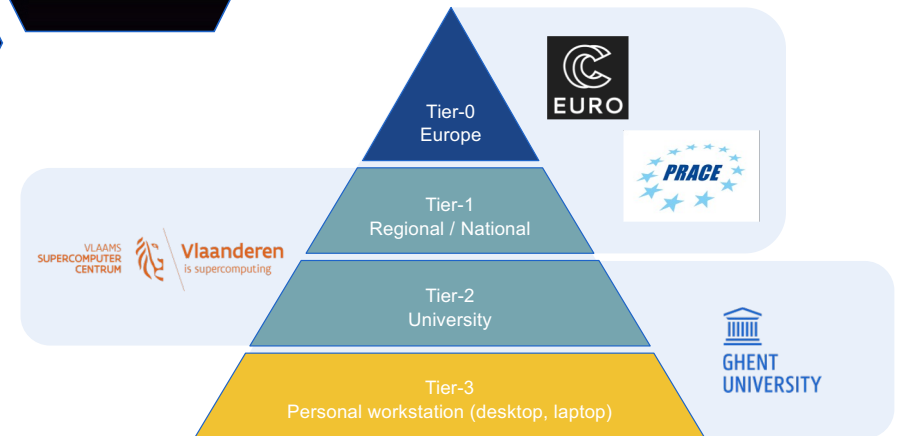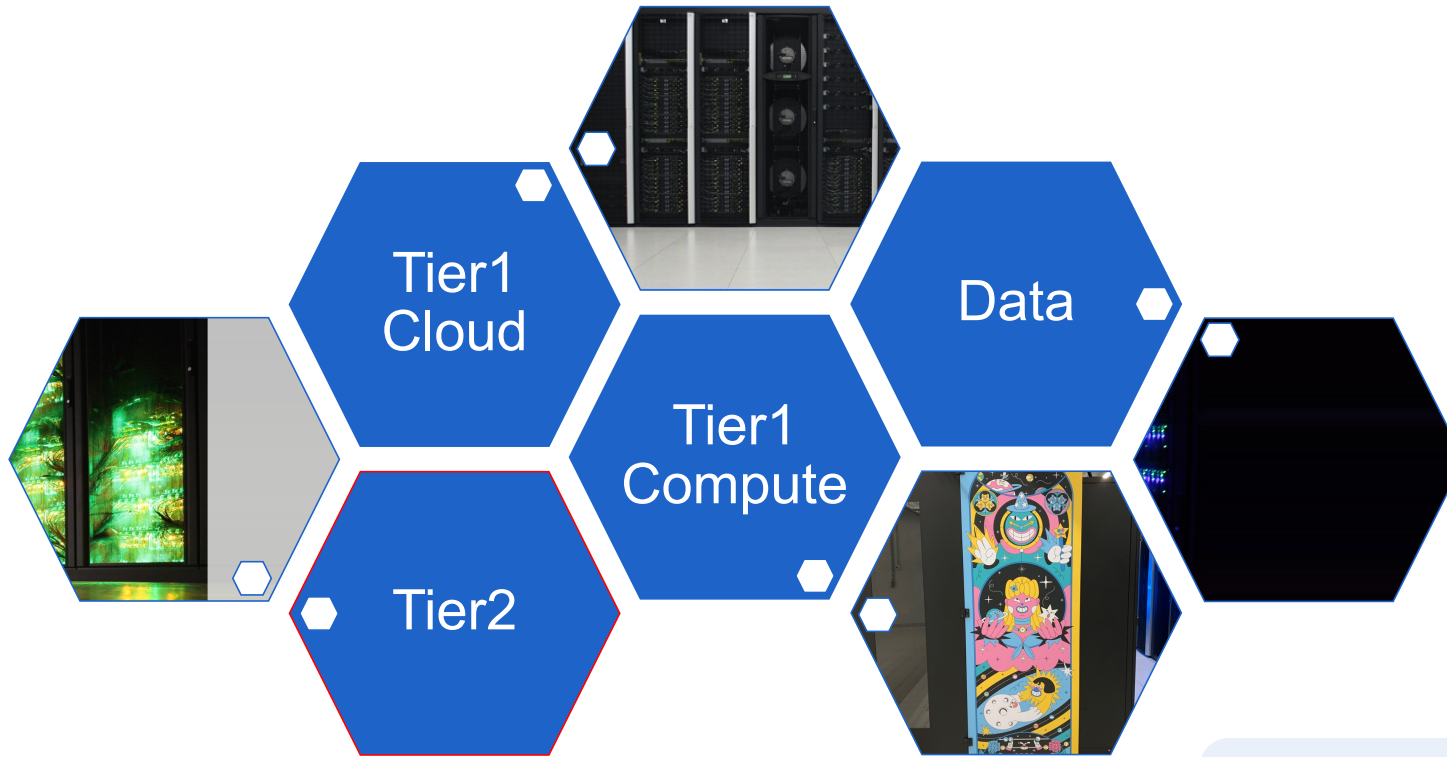GENT

TEACHING USING HPC-UGENT – TL;DR

Inform hpc@ugent.be about your course

- Start- and end date of hands-on/course
- UGent course ID
- VSC account of group moderators
- Need for customized web portal application

Please do this **well in advance** of start of your course
(weeks to months, not days/hours)

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INFRASTRUCTURE

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INFRASTRUCTURE MANAGED BY HPC-UGENT

Tier1 Cloud

Tier1 Compute

Tier2

Data

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Tier-0 Europe	EURO / PRACE
Tier-1 Regional / National	VLAAMS SUPERCOMPUTER CENTRUM / Vlaanderen is supercomputing
Tier-2 University	
Tier-3 Personal workstation (desktop, laptop)	GHENT UNIVERSITY

TIER2 – UGENT HPC INFRASTRUCTURE

See https://www.ugent.be/hpc/en/infrastructure

8 clusters
- CPU-only batch cluster
  (no high-speed network, no fast access to shared storage)
- CPU-only compute clusters
- GPU clusters
- CPU-only interactive + debug cluster

All running Red Hat Enterprise Linux 8 (RHEL8) as operating system

Free of charge for academic researchers
Pay-what-you-use for industry (after free exploratory period)

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TIER2 – UGENT HPC INFRASTRUCTURE

Example CPU cluster: *doduo*

128 workernodes, each with:

- 96 cores (AMD Rome)
- 250 GB of RAM

= 12.288 compute cores & 24 TB RAM available for you !

High-speed InfiniBand network between nodes

Fast access to shared filesystems
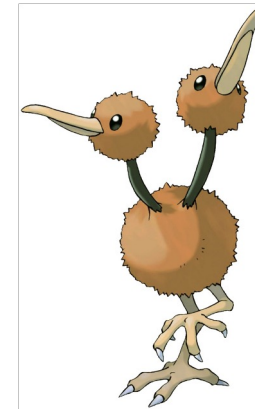
TIER2 – UGENT HPC INFRASTRUCTURE

Example GPU cluster: *accelgor*

9 workernodes, each with:

- 48 CPU cores (AMD Milan)
- 4 NVIDIA A100 GPUs (80GB GPU memory)
- ~500 GB of RAM

High-speed InfiniBand network between nodes
Fast access to shared filesystems

And there are many more, check out:

https://www.ugent.be/hpc/en/infrastructure

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TIER2 – UGENT HPC INFRASTRUCTURE

Interactive/debug cluster *donphan*

16 workernodes, each with:

- 36 CPU cores (Intel Cascade Lake)
- 1 shared NVIDIA Ampere A2 GPU (16GB GPU memory)
- ~700 GB of RAM

High-speed InfiniBand network between nodes

Fast access to shared filesystems

Strict user limits (max 3 jobs running, 5 in queue, 8 cores in use at a time)

No waiting time for jobs to start!
Ideal for debugging/visualization and for teaching.

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TIER2 – UGENT HPC INFRASTRUCTURE

- Go-to cluster for **teaching/exams**: interactive cluster *donphan*
- Need more resources? Request a reservation on another cluster
  https://account.vscentrum.be/django/reservation/

! Reservations currently require manual intervention by HPC-UGent staff
  Issue them well in advance (weeks to months, not days/hours)

TIER2 – UGENT HPC INFRASTRUCTURE

Using Tier2 for teaching/exam purposes – disclaimer

- Definitely possible, but caution!
- No guarantee on HPC availability (e.g. power outage)
- Have a backup plan at hand
- Advisable teaching/exam formula = longer-term project work

- HPC-UGent abides by UGent "sperperiode" rules
- Uptime of HPC-UGent infrastructure is relatively high
- But unexpected outages DO happen
  - in 2022, there was an extended maintenance window 28/11-14/12
  - 16/6/2023, there was a power outage during sperperiode

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GETTING ACCESS

VSC ACCOUNT

See https://www.ugent.be/hpc/en/access

- ALL UGent staff + students can request a VSC account
  can be used to access HPC infrastructure throughout VSC

- VSC account does NOT require SSH key
  (e.g. not needed for webportal access)

- https://account.vscentrum.be to manage your VSC account:
  - Join/leave user groups
  - Consult storage usage
  - Request more storage quota
  - Manage virtual organisation (VO)
  - ...
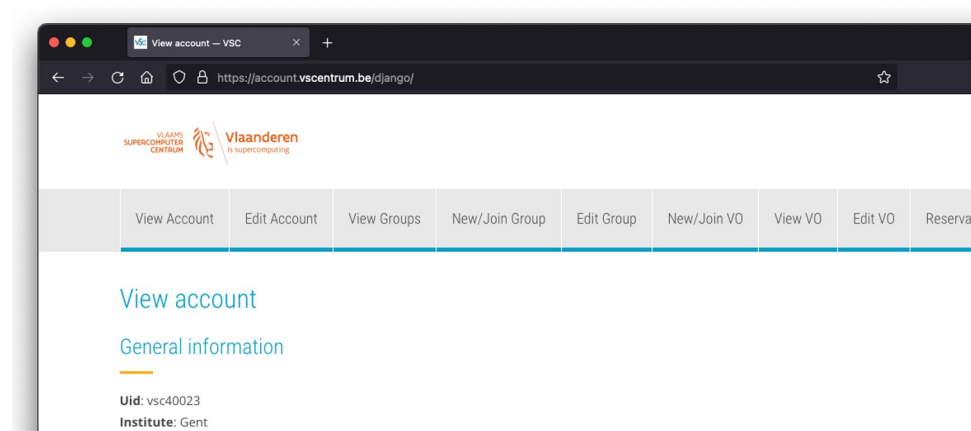
UP FRONT ACCOUNT MANAGEMENT

Provide hpc@ugent.be information (well in advance)

- Start- and end date of hands-on/course

- UGent course ID

- Group moderator vsc-ids

HPC-UGent offloads your VSC account management

- We make a dedicated group for the course

- We assign chosen moderators to the group

- We create VSC accounts (without ssh keys) for all registered students

SCIENTIFIC SOFTWARE

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SCIENTIFIC SOFTWARE

THE first question of a researcher when starting on an HPC system:

"Is my software available?"

Tier2 @ UGent

~1350 unique CPU software packages

~4000 incl. different versions & builds
~6000 incl. R, perl, python extensions
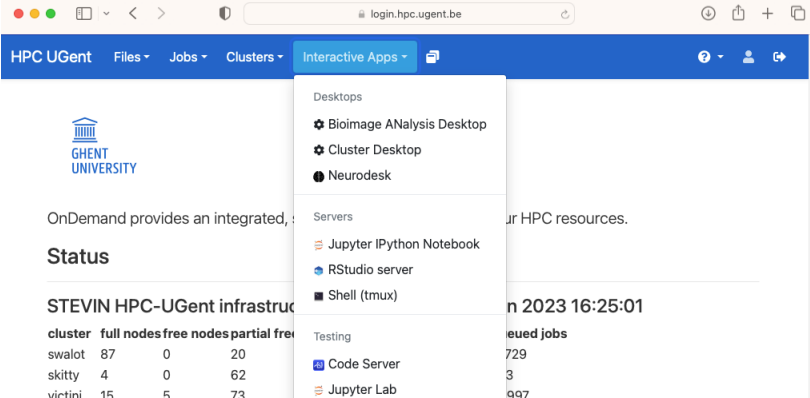
~150 unique GPU software packages

~200 incl. different versions & builds

List of all software: > **module avail**

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SCIENTIFIC SOFTWARE

Interactive applications on web portal

- Popular generic applications are already available

- Customized interactive applications are possible

  (but also take time to install)

  - Options are locked down and prefilled

  - Benefit: students make less mistakes, no slow down

  - Downside: students don't learn to use the generic application
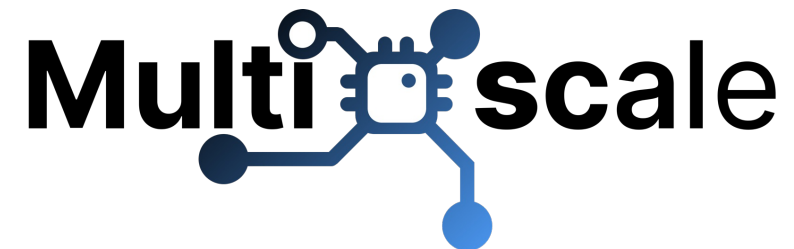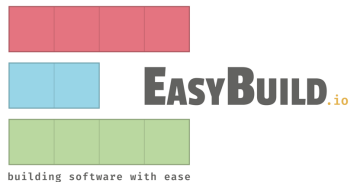
  - Removed at end of course

SCIENTIFIC SOFTWARE INSTALLATION

Installation of scientific software is a tremendous problem for researchers and HPC sites all around the world.

HPC-UGent invests in collaborative initiatives to share 'build recipes' so other HPC centers, researchers don't have to reinvent the wheel

SCIENTIFIC SOFTWARE INSTALLATION

At HPC-UGent:

- Central software installation as a service

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

- As much and as swiftly as possible

- Researcher saves time and can focus on research

Limitations:

- Windows software

  - Consider Linux alternatives

  - Try on VSC Tier1 Cloud

- Licensed software = bring your own license

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SCIENTIFIC SOFTWARE INSTALLATION

HPC-UGent invests A LOT of effort

- 3 dedicated staff
- 3 regular consultants
- Other HPC-UGent staff

But still we're struggling !

HPC-UGent software installation requests by year (Tier-2 + Tier-1)

Helpdesk tickets - Software installation
2022: 272 in total
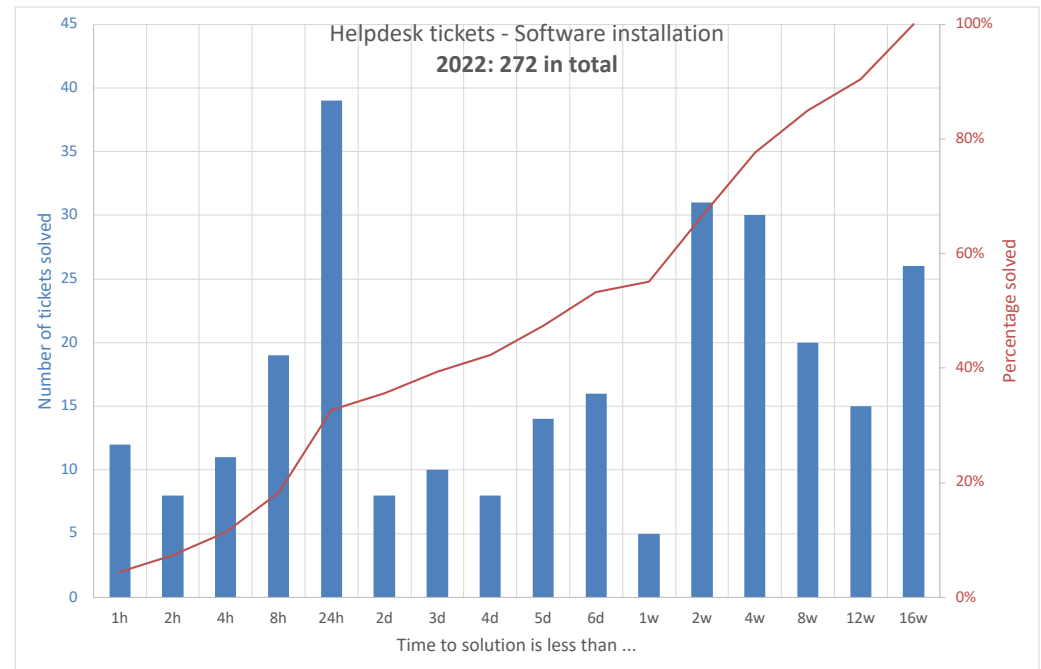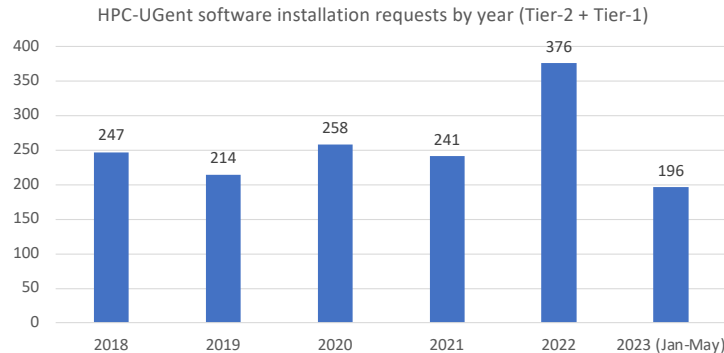
Requesting software? Do it well in advance and have patience

Make sure you will actively use the software

USER SUPPORT TRAINING

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USER SUPPORT & TRAINING

HPC-UGent tutorial documentation:
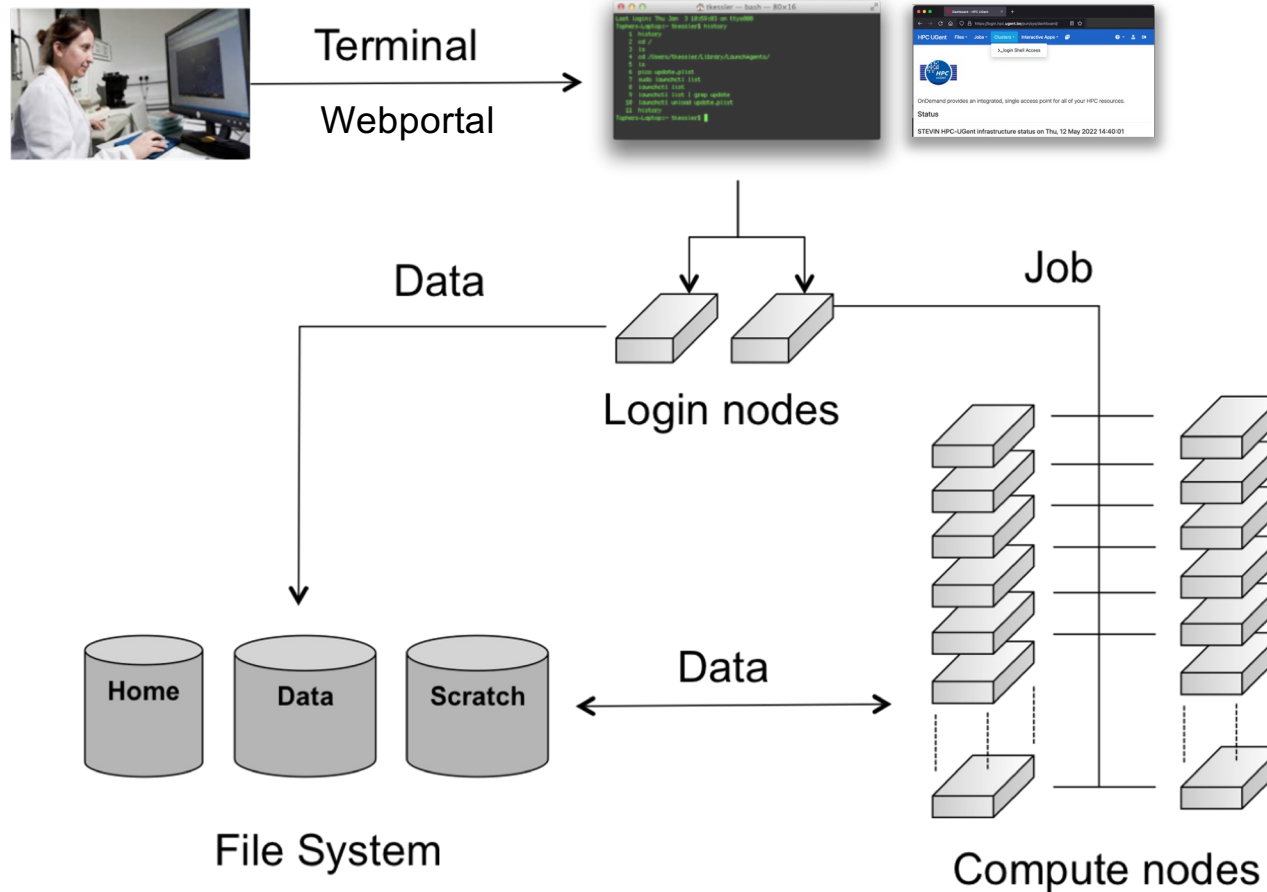
https://docs.hpc.ugent.be

Introductory training (recording available):

https://www.ugent.be/hpc/en/training/2023/introhpcugent

Dedicated helpdesk: hpc@ugent.be

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HOW TO USE ?

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HIGH-LEVEL OVERVIEW

WORKFLOW IN A NUTSHELL

See https://www.ugent.be/hpc/en/training/2022/introhpcugent

- Connect to login nodes (ssh / webportal)
- Wrap your computational task in a jobscript
  - Specify resources (#cores, #mem, wallclock time, etc.)
  - Load relevant software module
- Submit it to the job scheduler

- Or use web portal and interactive apps that hide this complexity

- **Maximum wallclock time of jobs: 72 hours (3 days)**
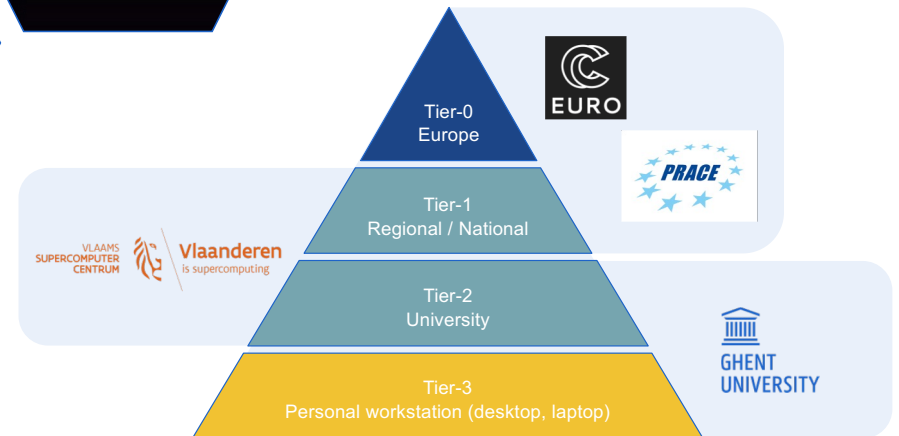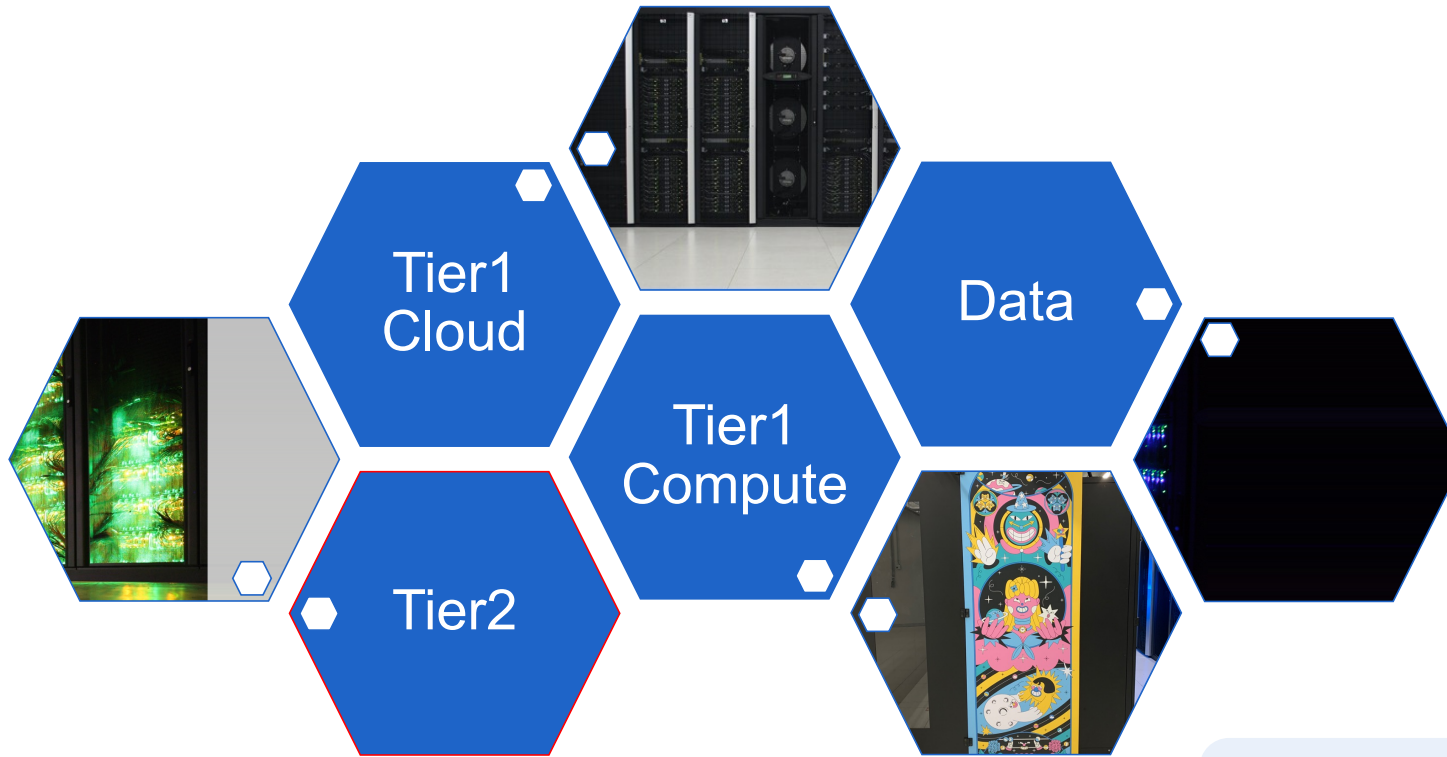
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SOUNDS COMPLICATED?

DEMO TIME

- Connection via webportal (in a browser)
- Easy file access, drag and drop
- Terminal shell in a browser, submitting a job
- Interactive application (Jupyter notebook)
- Interactive GUI usage on cluster desktop

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VSC INFRASTRUCTURE

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INFRASTRUCTURE MANAGED BY HPC-UGENT

Tier1 Cloud

Tier2

Tier1 Compute

Data

Tier-0
Europe

Tier-1
Regional / National

Tier-2
University

Tier-3
Personal workstation (desktop, laptop)

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GHENT UNIVERSITY

EURO

PRACE

VLAAMS SUPERCOMPUTER CENTRUM

Vlaanderen
is supercomputing

TIER1 CLOUD – VSC INFRASTRUCTURE

Tier-1 Cloud https://www.vscentrum.be/cloud

9 UPSv1-GPUv2 hypervisors

- AMD Epyc 7542 2.9GHz
- 128 Cores
- 512 GB RAM
- 3 NVIDIA Ampere 2
- Connected to UPS

80 CPUv1 hypervisors (older)

- Intel Xeon CPU E5-2680 2.40GHz
- 28 Cores
- 512 GB RAM

9 GPUv3 hypervisors

- AMD Epyc 7542 2.9GHz
- 128 Cores
- 512 GB RAM
- 2 NVIDIA Tesla 4
- Connected to UPS

Deployed with Red Hat OpenStack Platform
Supported by HPC-UGent team and Red Hat
Public dashboard & APIs: https://cloud.vscentrum.be

1 public IP per project
Various VM images/flavors/instance types

Tier-1 Cloud = platform for power users
You are responsible for

- Installation
- Maintenance
- user management
- ...

Project-based access (free of charge)

Starting grants: continuously open

3 cut-off dates per year for submitting larger project proposals

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Q&A

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