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DIRECTIE ICT
AFDELING INFRASTRUCTUUR

HPC-UGENT UPDATE

HPC-UGent user meeting

8 July 2022

Dr. Ewald Pauwels

hpc@ugent.be

https://www.ugent.be/hpc

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VLAAMS SUPERCOMPUTER CENTRUM

Vlaanderen is supercomputing

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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ABOUT HPC-UGENT

Personnel

- 9 dedicated UGent staff
- Regular consultancy assistance (4-5 people)
- Student interns
- Help from other DICT staff and teams

Funding

- FWO – Vlaams Supercomputer Centrum (VSC)
- EuroHPC
- Ghent University

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fwo

VLAAMS SUPERCOMPUTER CENTRUM

Vlaanderen is supercomputing

EuroHPC Joint Undertaking

inuits OPEN SOURCE INNOVATORS

OPERATIONS 2021 - NOW

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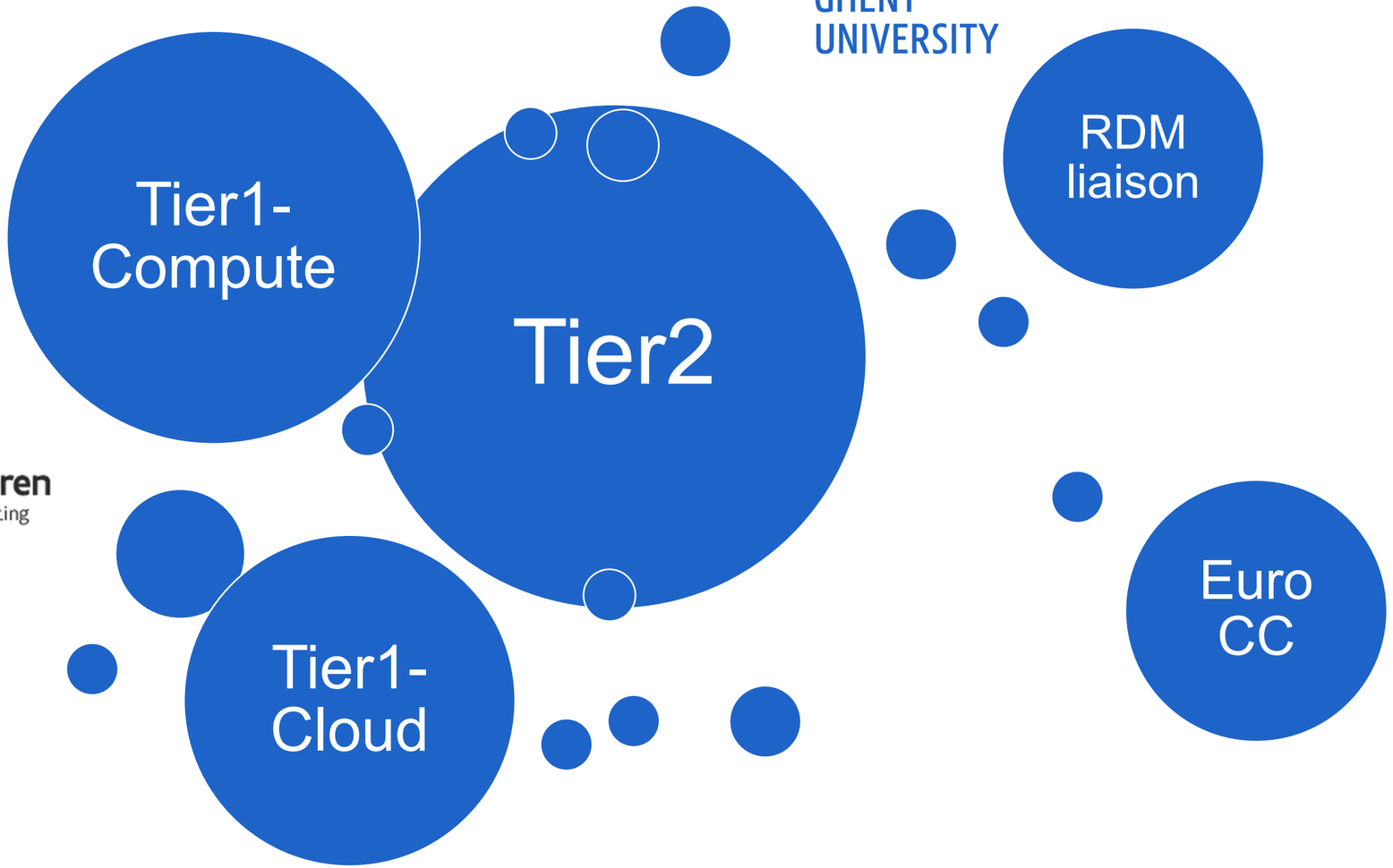

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Vlaanderen
is supercomputing

EURO

EuroHPC
Joint Undertaking

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OPERATIONS 2021 - NOW

ANNUAL REVIEW HPC-UGENT

2021

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

OPERATIONS – TIER2 2021 - NOW

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TIER2 – UGENT HPC INFRASTRUCTURE

Infrastructure


- cluster *doduo* in production (MPI, 12.288 cores)
- cluster *phanpy* decommissioned
  - cluster *kirlia* takes over (big-memory 738GiB/node, 576 CPU cores)

- new GPU cluster *accelgor* (36 Nvidia Ampere A100 GPUs)
  - co-investment with Center for Molecular Modeling
  - ~600.000 euro investment

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

TIER2 – UGENT HPC INFRASTRUCTURE

Cluster name	#nodes	CPU per node	Mem/node	Storage/node	Interconnect	OS
doduo 	128	96-core AMD EPYC 7552 (Rome) Total: 12.288 CPU cores	250 GiB (2.6 GiB/core)	180GB SSD	HDR-100 Infiniband	RHEL8
accelgor 	9	48-core AMD EPYC 7413 (Milan) 4x NVIDIA Ampere A100 GPUs (80GB GPU memory) Total: 432 CPU cores 36 GPUs	500 GiB (10.4 GiB/core)	180GB SSD	HDR-100 InfiniBand	RHEL 8

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TIER2 – UGENT HPC INFRASTRUCTURE

User experience

- New job command wrappers
  - We only support Torque PBS style commands (qstat, qsub, qdel, etc.)

- Webportal https://login.hpc.ugent.be
- Interactive debug cluster *slaking* (no waiting time in queue, limited resources)

- 2022: migration of all clusters to Red Hat Enterprise Linux 8 (RHEL8)

TIER2 – UGENT HPC INFRASTRUCTURE

Cluster name	Compute time consumed		Effective use percentage	
	CPU hours	GPU hours	CPU	GPU
~~Phanpy~~	242 117		34%	
Swalot	16 066 093		72%	
Skitty	16 632 156		73%	
Victini	20 292 526		67%	
Kirlia	3 540 566		70%	
Doduo	77 542 561		72%	
Joltik	2 072 339	217 221	74%	62%
Accelgor (pilot)	434 123	34 985	39%	38%

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TIER2 – UGENT HPC INFRASTRUCTURE

Consumed compute time by affiliation		
	CPU time	GPU time
UAntwerpen	0.10%	0.01%
VUB	0.39%	2.68%
UGent	98.62%	96.86%
KULeuven / UHasselt	0.51%	0.00%
Other research institutes	0.30%	0.00%
Industry	0.08%	0.46%

Students/researchers		
	CPU time	GPU time
Ma/Ba students	17.55%	11.83%
Researchers	82.45%	88.17%

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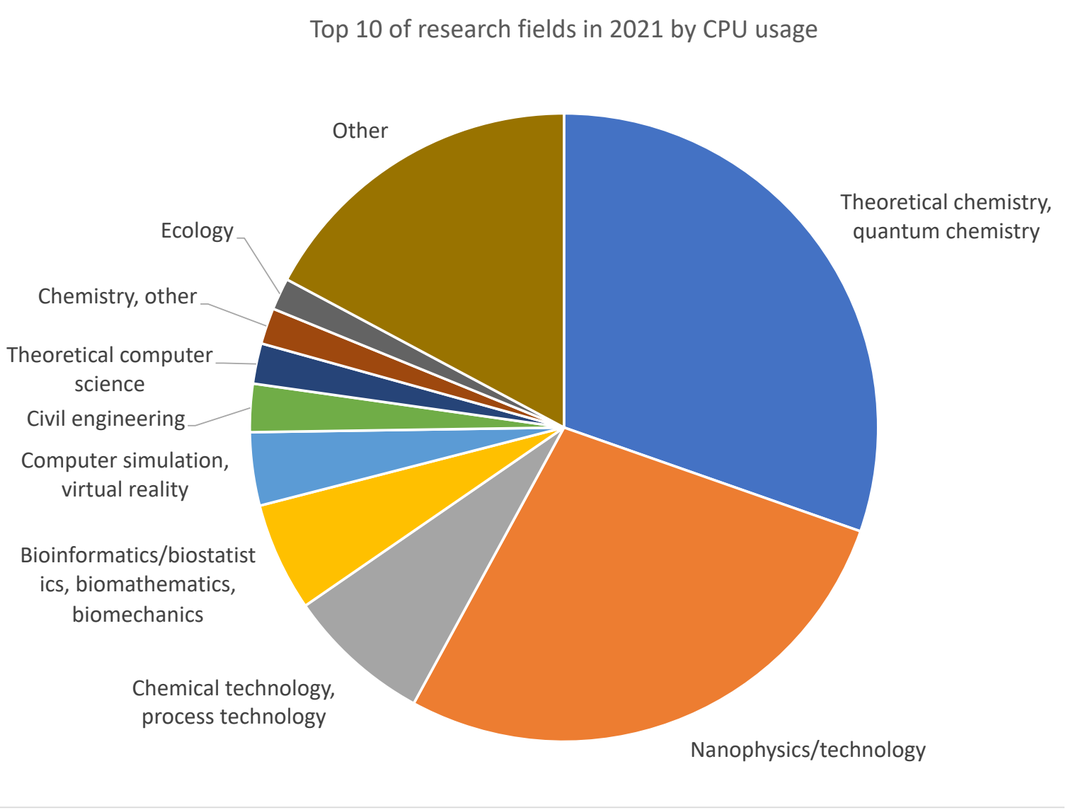
TIER2 – UGENT HPC INFRASTRUCTURE



145 Virtual Organisations

Faculty	# VOs
Engineering and Architecture	34
Sciences	42
Engineering and Architecture & Sciences	1
Economics and Business Administration	6
Medicine and Health Sciences	20
Psychology and Educational Sciences	5
Pharmaceutical Sciences	2
Bioscience Engineering	13
Arts and Philosophy	2
Law and Criminology	1
Veterinary Medicine	3
Industry	15

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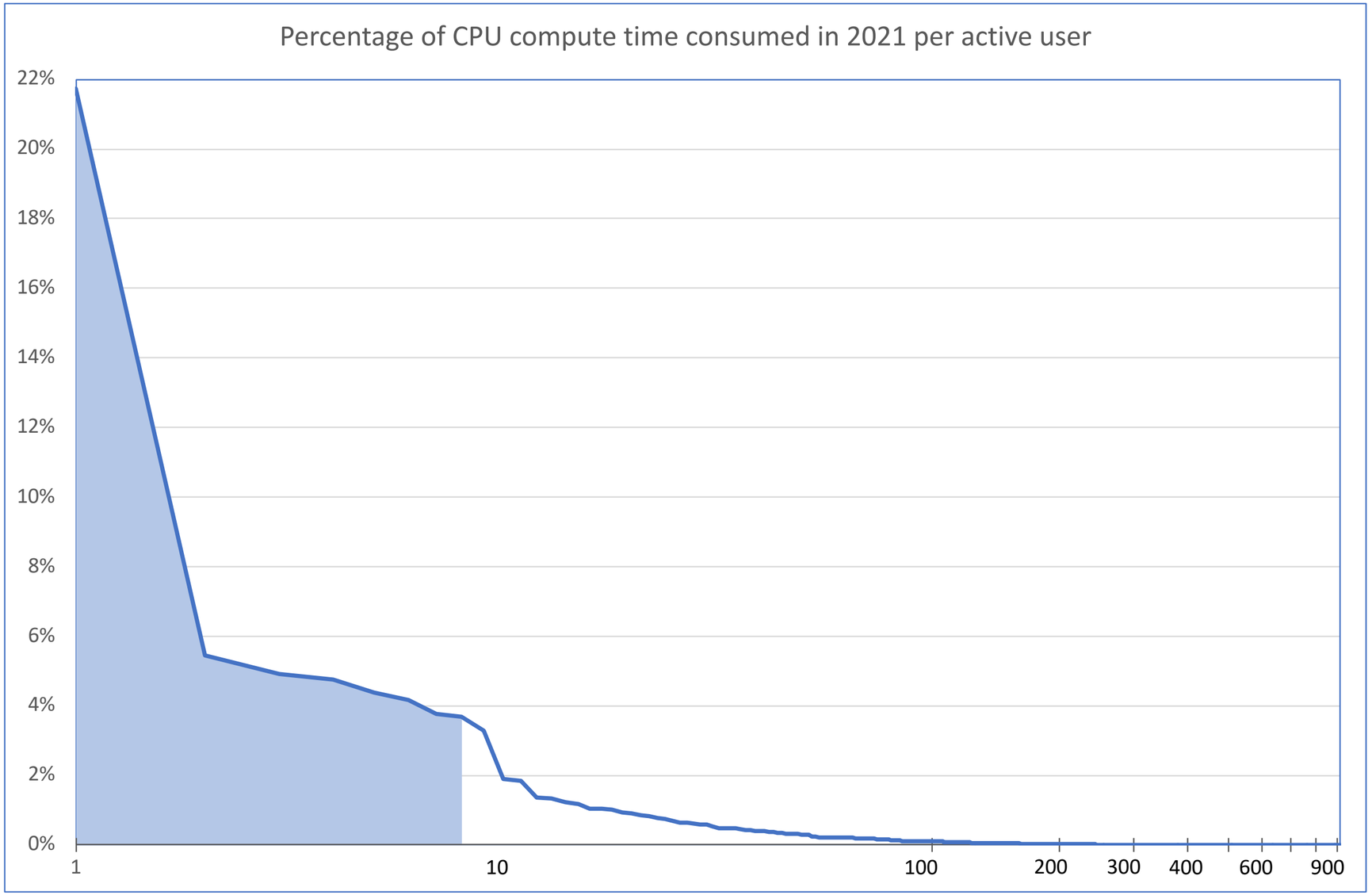
TIER2 – UGENT HPC INFRASTRUCTURE

Active users

2019
608 (100%)

2020
691 (114%)

2021:
915 (150%)



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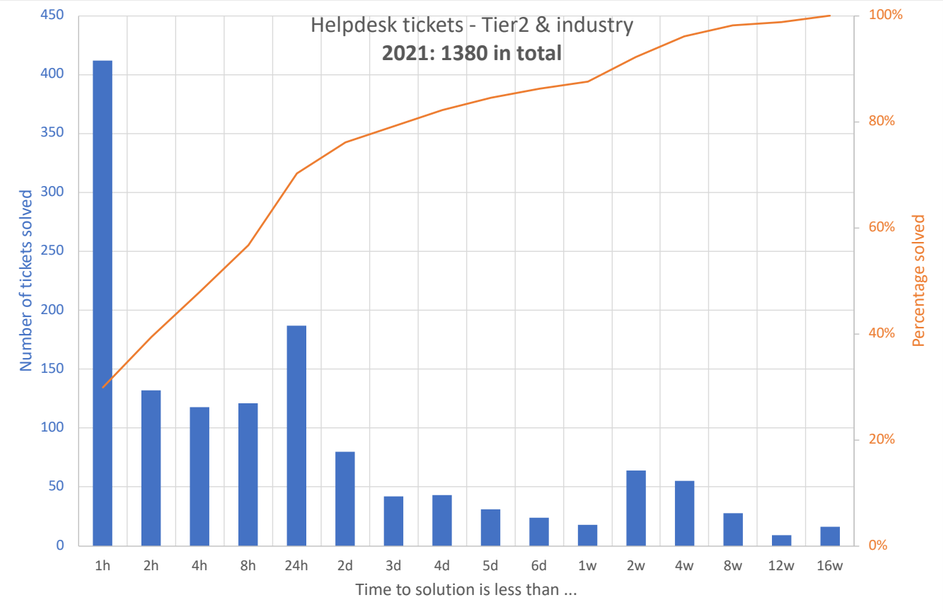
HPC-UGENT HELPDESK

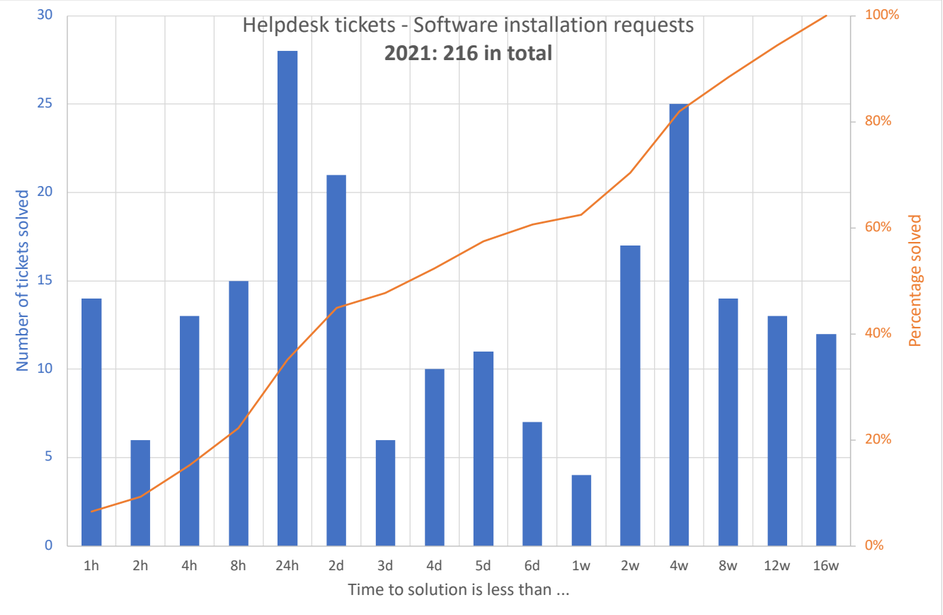
2019
1533 closed
(100%)

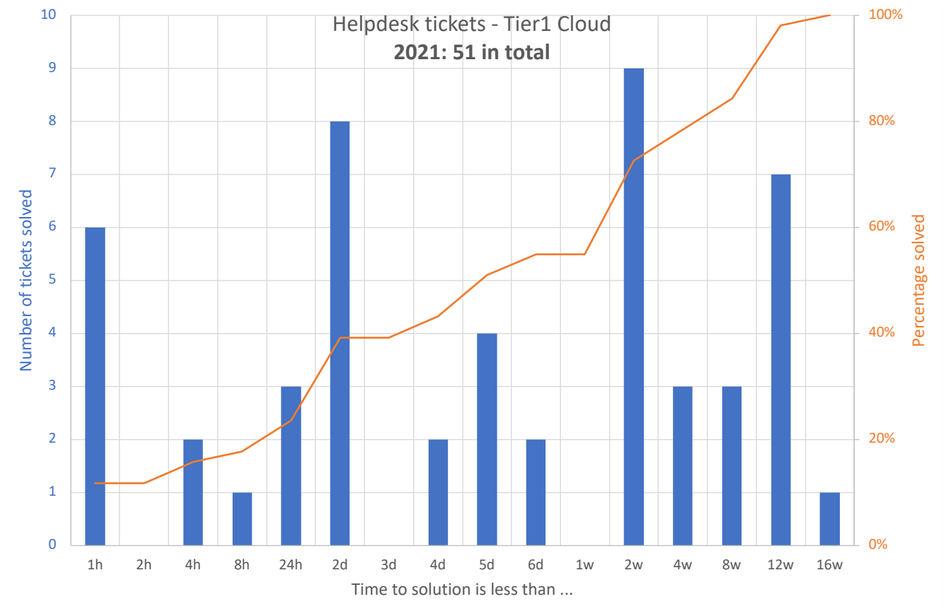
2020
1798 closed
(117%)

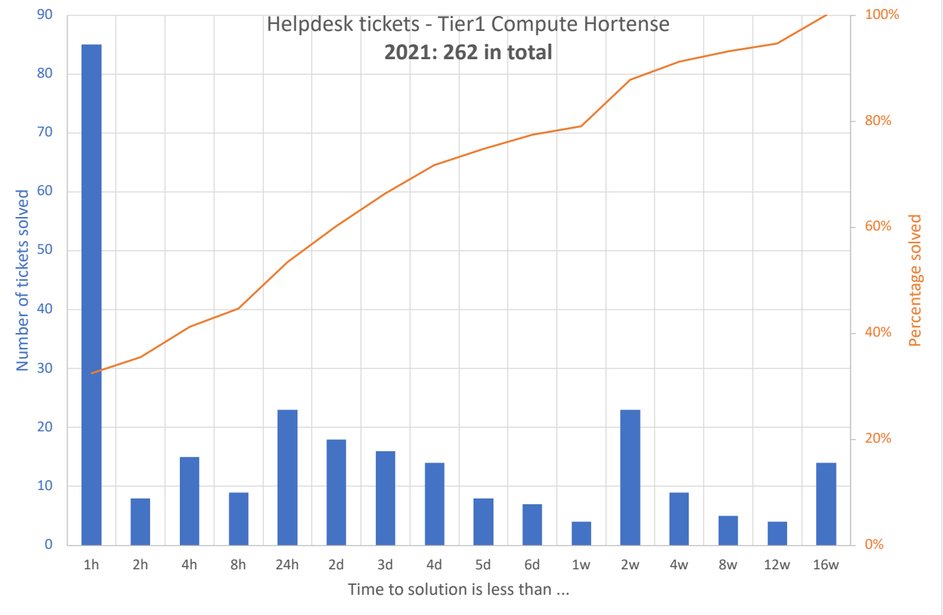
2021:
1909 closed
(125%)

2022 H1:
1474
(96%)









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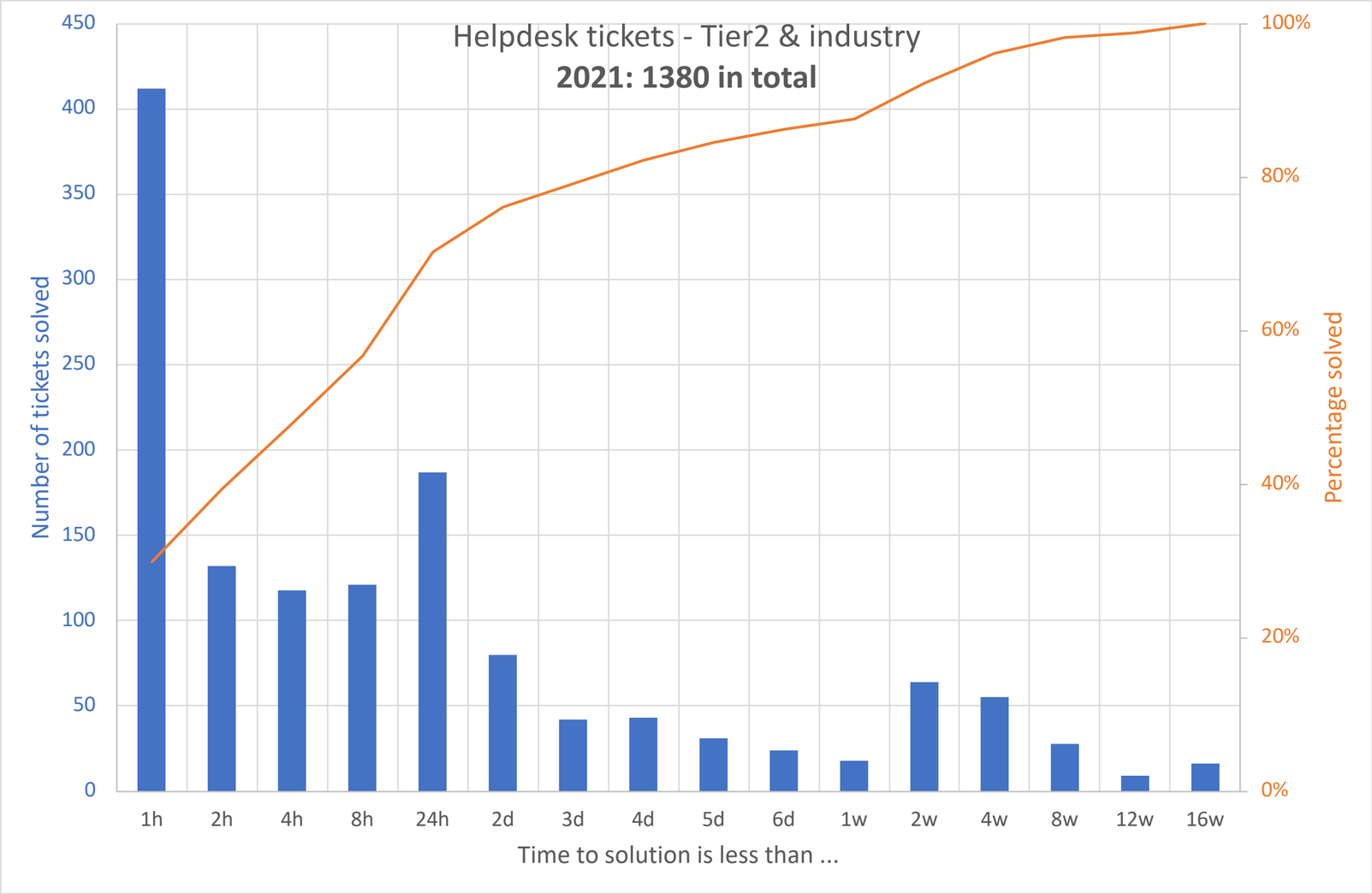
HPC-UGENT HELPDESK



In 2021:

~80% of tickets got resolved within 3 days

~90% of tickets got resolved within 1 week

‘regular’ Tier2 helpdesk tickets

NOT including software install requests

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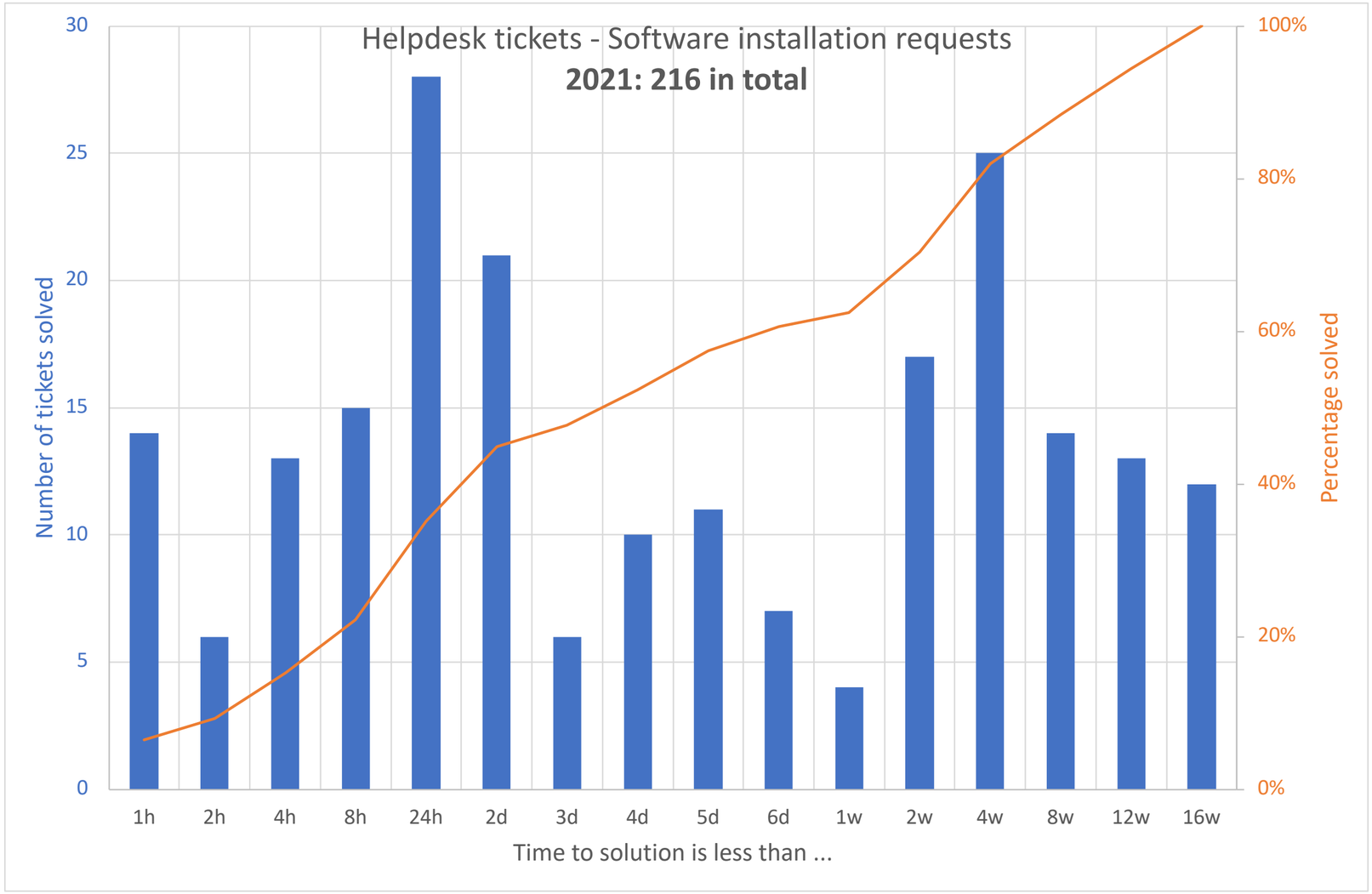
HPC-UGENT HELPDESK



Swiftness of install depends on

- whether software is new or not
- complexity of software install
  - framework e.g. MPI
  - dependencies
  - cluster architecture
  - GPU
  - ...

EXPERTS required

Effort invested:

- 2 dedicated HPC-UGent staff
- 3 Inuits consultants
- + help from other HPC-UGent staff

2022:
VSC project to improve sharing effort of software installation

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OPERATIONS – TIER1 2021 - NOW

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TIER1 – VSC INFRASTRUCTURE

Tier-1 Compute

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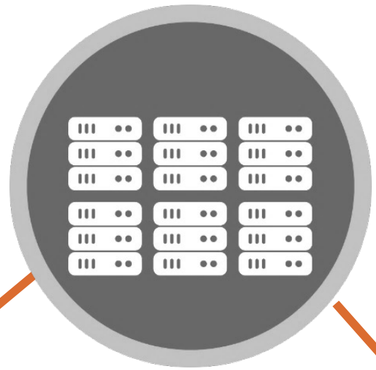
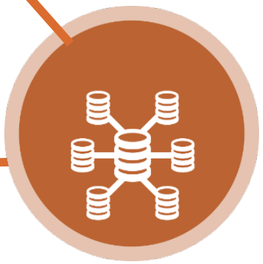
ASSOCIATIE KU LEUVEN



Compute Power



Flexibility

Tier-1 Cloud

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Tier-1 Data

ASSOCIATIE KU LEUVEN

Storage capacity

Data management

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TIER1 – VSC INFRASTRUCTURE

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

9 UPSv1 hypervisors

- AMD Epyc 7542 2.9GHz
- 128 Cores
- 512 GB RAM
- Connected to UPS
- 25 Gb ethernet

67 CPUv1 hypervisors (older)

- Intel Xeon CPU E5-2670 2.60GHz
- 16 Cores
- 128 GB RAM
- 10 Gb ethernet

9 GPUv1 hypervisors

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

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

Project management by HPC-UGent team
1 public IP per project
Various VM images/flavors/instance types

Results from calls:

- 5 starting grants
- 16 academic projects
- 2 exploratory industry projects

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TIER1 – VSC INFRASTRUCTURE

Tier-1 Compute ‘Hortense’ https://www.vscentrum.be/compute

336 CPU nodes
- AMD Epyc 7H12 CPU 2.6 GHz
- RAM: 256 GiB / 512 GiB
- Total of 43.008 cores

20 GPU nodes
- AMD Epyc 7402 CPU 2.8 GHz
- NVIDIA A100 NVLink3 (40 GB)
- RAM: 256 GiB
- Total of 960 cores and 80 GPUs

InfiniBand HDR-100 interconnect
3 PB shared storage based on Lustre

Pilot phase: 23 November 2021

Production: 15 March 2022

71 academic projects
59 starting grants
19 industry projects

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TIER1 – VSC INFRASTRUCTURE

Tier-1 Compute 'Hortense' https://www.vscentrum.be/compute

Academic user	Commercial user
A. Starting Grant B. Project access C. Collaborative Grant Free of charge – project based	D. Free exploratory access E. Full access

Next project call deadline for B. = **3 Oct 2022**

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Success depends on quality of your proposal
Send your proposal to hpc@ugent.be for prior review

OPERATIONS – EU 2021 - NOW

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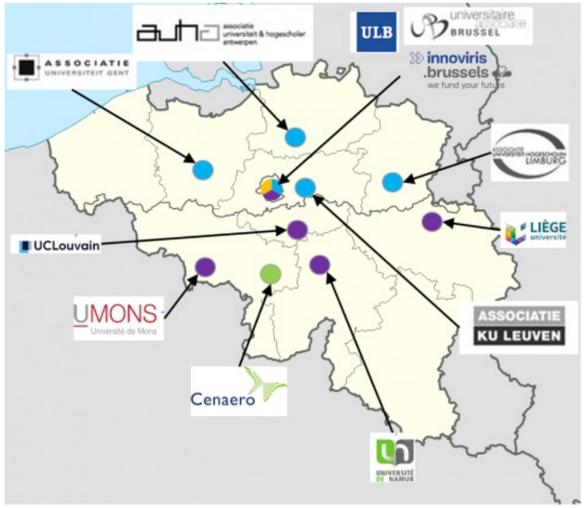
EUROPEAN PARTICIPATION AND ASPIRATION

- EuroCC National Competence Center Belgium (https://enccb.be)
  - 2020-2022
  - Map HPC competences and institutions
  - Act as gateway for industry and academia
  - Collect HPC training offers
  - Foster industrial uptake of HPC



- *EuroCC 2.0 in the making, but without UGent as structural partner*

- *S4 - Scientific Software Stacks as a Service (NEIC)*
- *MultiXscale (HORIZON-EUROHPC-JU-2021-COE-01-02)*

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EUROPEAN PARTICIPATION AND ASPIRATION

10+ years of easybuild

easybuild.io

(April 2012)
First public release of EasyBuild
+ **start of EasyBuild community**

(Nov. 2012)
EasyBuild v1.0 (released *at* SC'12)

(mid-2009)
EasyBuild is created
by Stijn De Weirdt
(HPC-UGent tech lead)
as an in-house project

in-house development
(incl. redesigns, test suite, ...)

(2013 - 2019)
Getting Scientific Software Installed
SC/ISC Birds-of-a-Feather sessions

(March 2015)
EasyBuild v2.0
Backwards-incompatible changes

(Nov. 2016)
EasyBuild v3.0
Lmod as default modules tool
Stable GitHub integration

(2015)
Integration with Cray PE
EasyBuild @ cscs

(Sept. 2019)
EasyBuild v4.0
Compatible with Python 3
Only requires Python std. lib.

(Jan. 2021)
EasyBuild selected as installation tool for LUMI
(see EUM'22 talk)

(Nov. 2014)
Proper documentation
easybuild.readthedocs.org

(2012 - 2016)
11 EasyBuild hackathons
across Europe (Univ. of Cyprus, JSC, CSC.fi, CSCS, ...) + TACC

(2016 - 2022)
7 EasyBuild User Meetings
(easybuild.io/eum**)**
@ Ghent, Jülich, Amsterdam, Louvain-la-Neuve, Barcelona
+ 2x via Zoom/YouTube/Slack

(2020 - 2022)
EasyBuild tutorial at ISC
(easybuild.io/tutorial**)**
Online tutorial in June'20
Half-day tutorial @ ISC'21
Half-day tutorial @ ISC'22

USER POLL RESULTS

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USER POLL RESULTS

- 63 respondents
- Average completion time: 2 minutes

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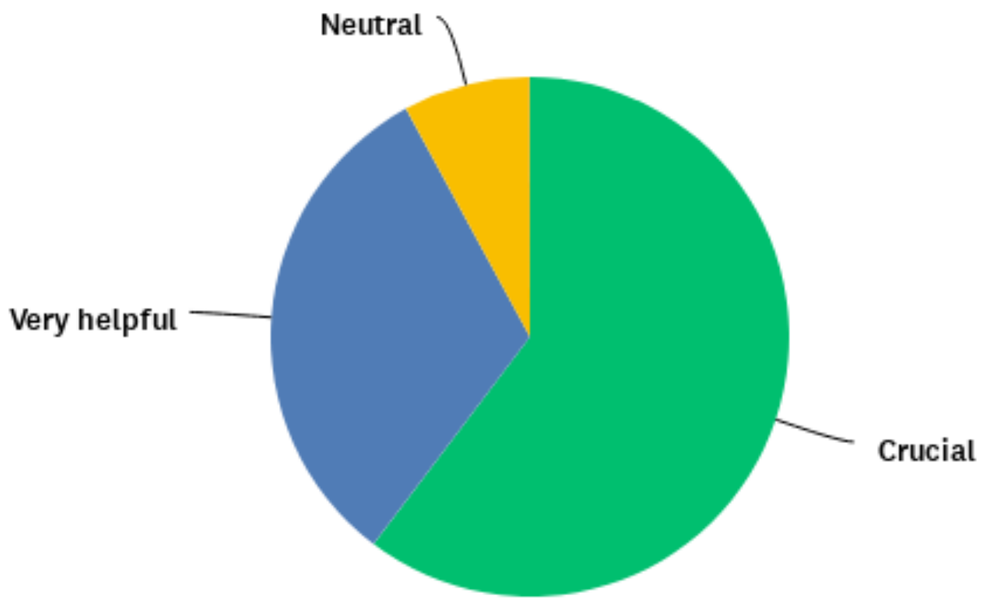
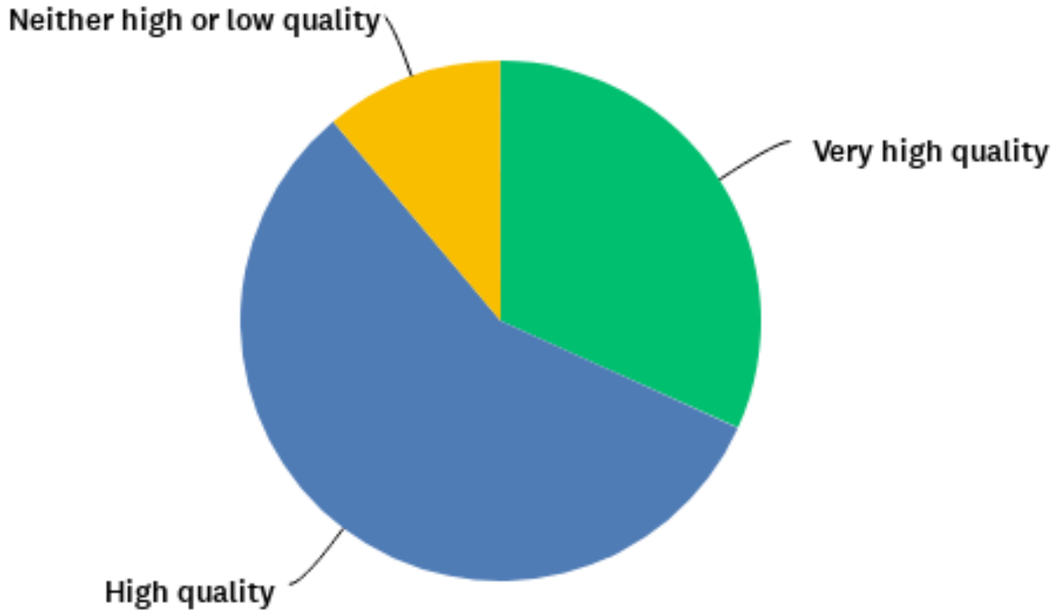
USER POLL RESULTS

How important is HPC-UGent for your research?



92% Very helpful or crucial to research

How would you overall rate HPC-UGent services?



89% High quality or better

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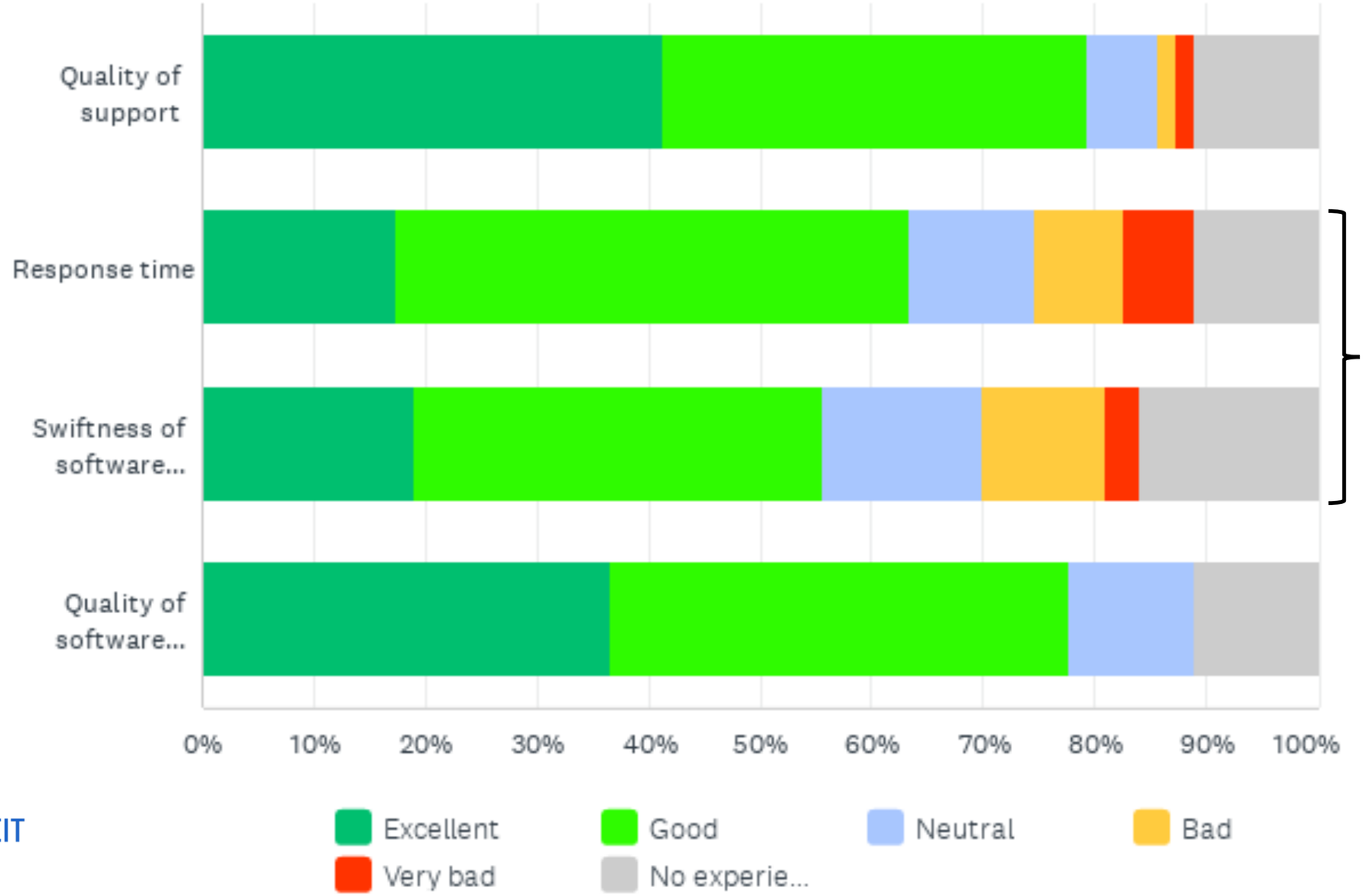
USER POLL RESULTS

Rate aspects of HPC-UGent user support:



At least 9 out of 63 people are not happy

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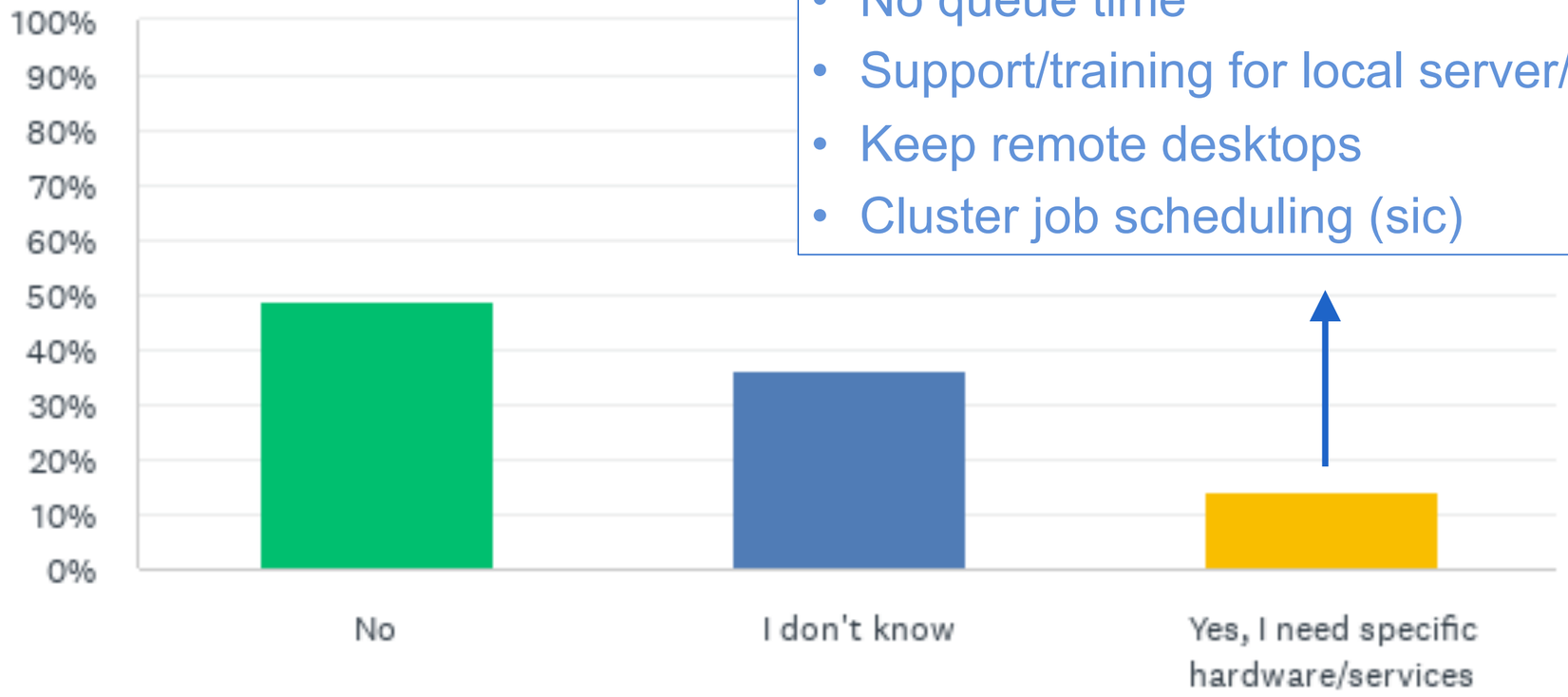
USER POLL RESULTS

Would your research benefit from specific IT hardware or services that HPC-UGent currently does not provide?

- More GPU hardware
- Specific scientific software packages
- No queue time
- Support/training for local server/cloud install
- Keep remote desktops
- Cluster job scheduling (sic)



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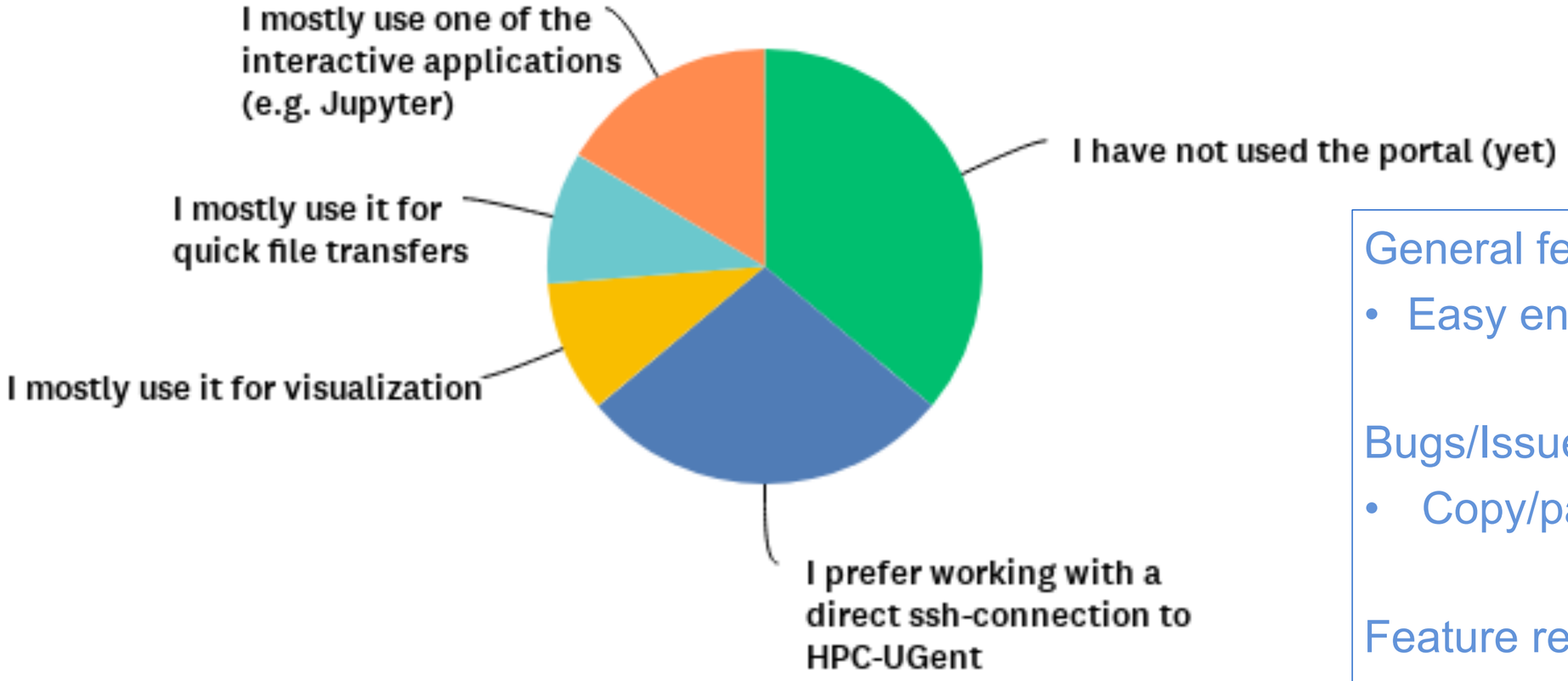
USER POLL RESULTS

Have you tried using the HPC via the webportal?

https://login.hpc.ugent.be



General feedback

- Easy entry for starting users

Bugs/Issues

- Copy/paste does not work

Feature requests

- slaking with a GPU
- run for more than 72h

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USER POLL RESULTS

How could we further improve HPC-UGent services?

Infrastructure

- More clusters and nodes
- More GPU hardware
- Slaking with GPU functionality

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USER POLL RESULTS

How could we further improve HPC-UGent services?

Training

- Training and instruction on using specific software packages
- More low to mid level training for newcomers with limited experience (current training is high/expert level)
- Focused course on setting up local server / cloud instance in UGent network

Documentation

- Real-world actual research examples in the manual
- Video demonstration for beginners

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USER POLL RESULTS

How could we further improve HPC-UGent services?

User experience

- High uptimes
- Visualisation GPU support
- Option to extend wall time of an active job
- Way to run jobs with wall-clock of +50 days
- Way to estimate queue time (if not exact, upper limits)
- Old software modules should still work and be available on RHEL8

USER POLL RESULTS

How could we further improve HPC-UGent services?

User support

- More time to help people with specific questions
- Feedback or meeting with specific research teams
- Swifter response time on hpc@ugent.be helpdesk
- Swifter software installation
- Instant service, like a chat
- Better support – hire people

OUTLOOK
2022 - BEYOND

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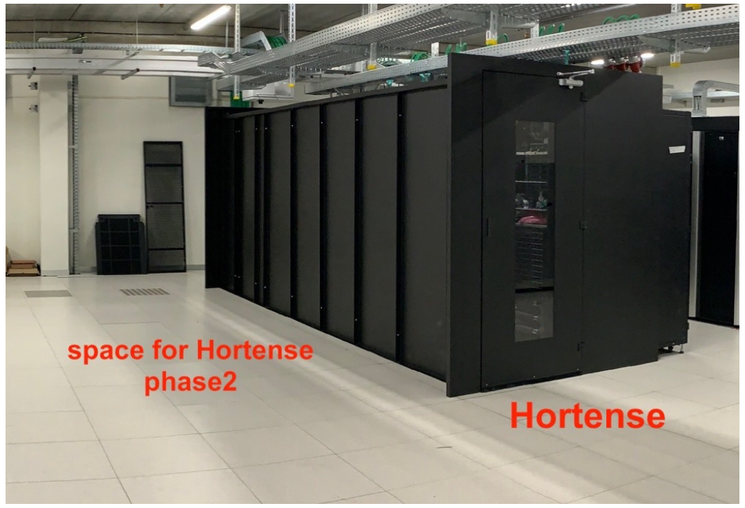
OUTLOOK 2022 - BEYOND

- **Extend Tier1 Compute** infrastructure Hortense
  - ~ 6.000.000 euro investment (FWO budget)
  - Order initiated, in accord with VSC
  - Equip datacenter with additional heat recuperation ”LoopC”
  - ATOS: hardware and rack and stack
  - HPC-UGent: software installation and integration, upkeep



Phase1
- +48 CPU nodes, each with 2 x 64-core AMD Epyc 7H12 Rome CPUs

Phase2
- 384 CPU nodes, each with 2 x 64-core AMD 7763 Milan CPUs
- 20 GPU nodes, each with 4 A100 Nvidia GPUs (80GB)

Storage
- 3 PB -> 6 PB

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OUTLOOK 2022 - BEYOND

- **Maintain Tier2** infrastructure and keep up to date
  - ~ 1.000.000 euro / year (recurring FWO budget)

- Complete roadmap “compute for research and education”
  (delays incurred because of Tier-1 Hortense)
  - Better integration of student lists and accountpage
  - Access without ssh keys ✅
  - Easier reservations
    - Free for teaching
    - Pay-what-you-reserve for research

OUTLOOK 2022 - BEYOND

- Further promote and invest in **HPC webportal and debug cluster**
  - In training, in helpdesk, in manual
  - More supporting infrastructure if needed

- Lessons learned so far: **webportal complements features of Cloud**
  - Users (mostly) actually want features of webportal, not Cloud
  - Cloud is useful, but only for power users

- Complement **VSC Tier1 Cloud** with similar webportal for **Tier1 Compute**
  - Webportal in Tier1 Hortense ✅
  - Debug partition (similar to *slaking*)

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OUTLOOK – VSC 2.0 2023 - BEYOND

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VSC 2.0

VLAAMS SUPERCOMPUTER CENTRUM
Vlaanderen is supercomputing

- Follow-up to the Tier1-Supercomputing-As-A-Service plan (2018)
- Result of a lengthy strategic exercise

"Towards an all-tier recurrent budget for supercomputing in Flanders to become a respected element of the European HPC ecosystem"

"The mission of VSC 2.0 is clearly an extension of that of VSC 1.0: the aim is to contribute to innovation in Flanders by offering services and infrastructure on Tier-2 and Tier-1 level for all RD&I activities in the academic environment, in industry and government in order to team up with the European HPC aspirations."

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VSC 2.0

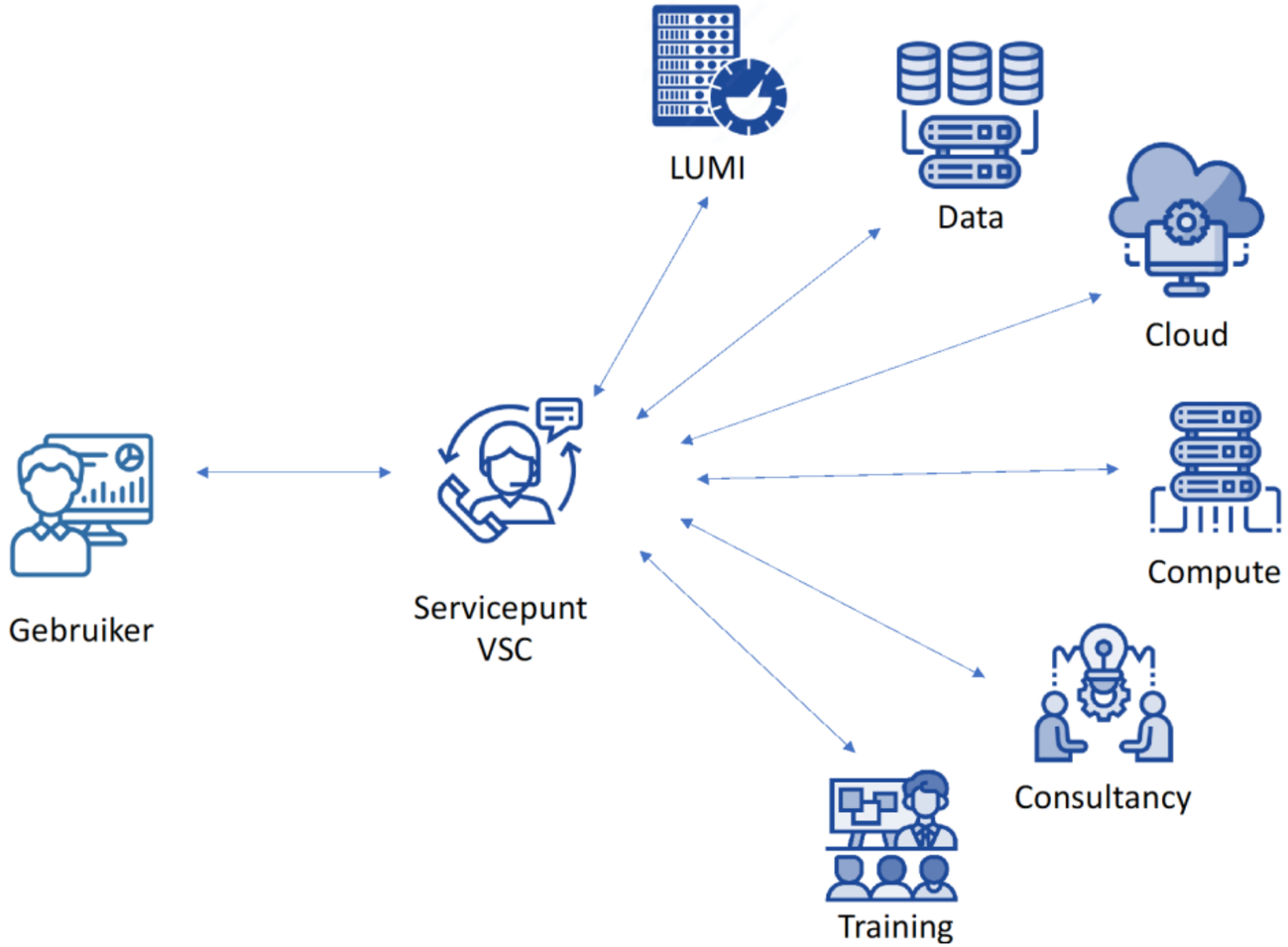
VLAAMS SUPERCOMPUTER CENTRUM | Vlaanderen is supercomputing

- VSC remains a virtual center: 5 academic institutions, 4 equipment hubs
- Activities across all tiers:

  Tier-2 local / Tier-1 regional / Tier-0 European

- Front office:

  towards single point of contact



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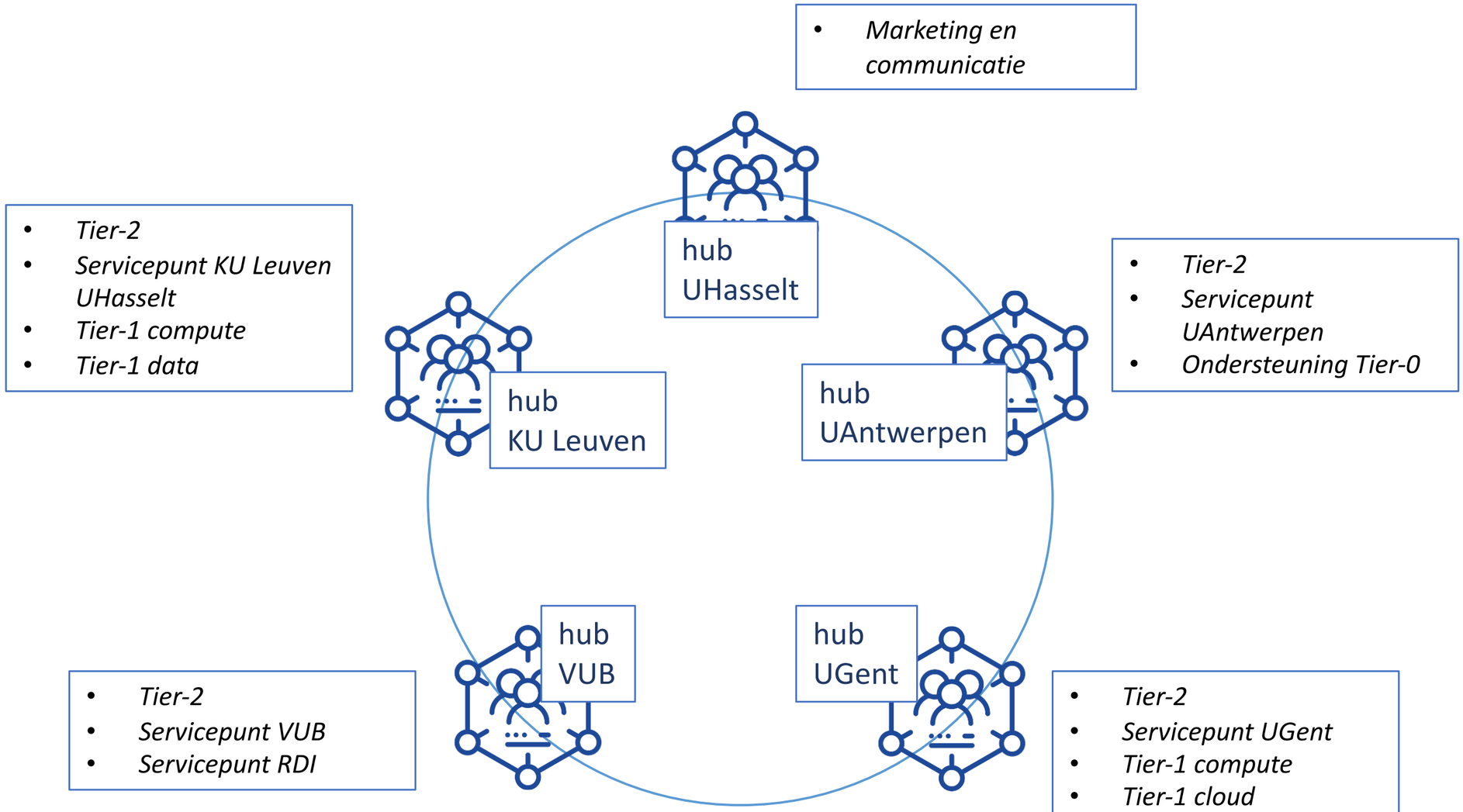
VSC 2.0

VLAAMS SUPERCOMPUTER CENTRUM | Vlaanderen is supercomputing

- Well-defined responsibilities



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SPOTLIGHT: HPC WEBPORTAL DEBUG CLUSTER

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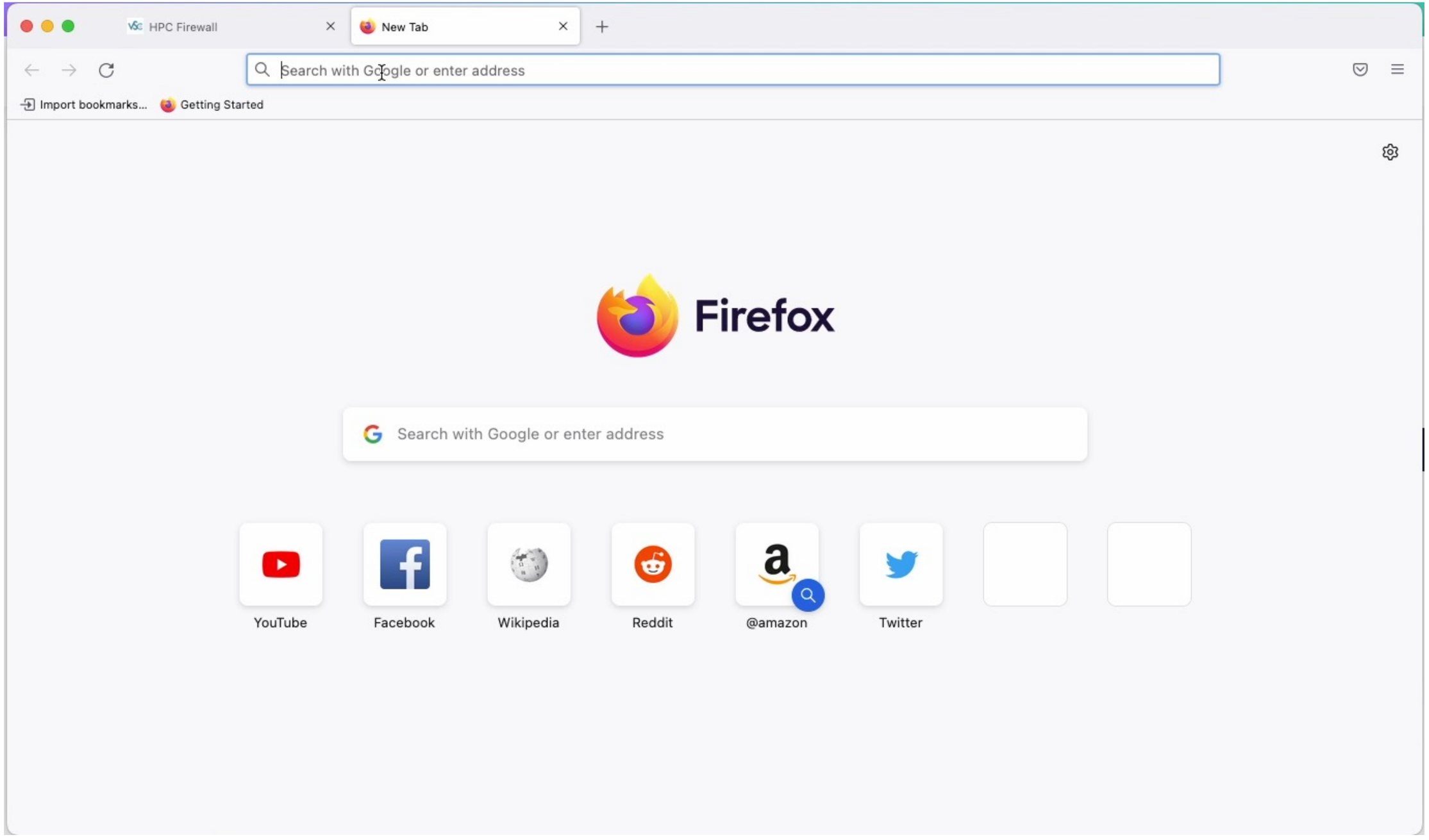
HPC WEBPORTAL + DEBUG CLUSTER

- HPC webportal is gamechanger, especially in combination with debug cluster *slaking*
- *slaking*: zero wait time (but limited resources)
- No system administration required
- Possibility for remote virtual desktop
- Ideal for interactive and visualisation tasks
- Custom interactive applications are possibility
  - Easy to do it yourself
  - In context of course, e.g. one app with fixed parameters for students

HPC WEBPORTAL



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