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DEPARTMENT ICT

HPC-UGENT USER MEETING

Dr. Ewald Pauwels
hpc@ugent.be
http://hpc.ugent.be

28/06/2021

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VLAAMS SUPERCOMPUTER CENTRUM

Vlaanderen is supercomputing

PROGRAM

- 10h00: Overview of HPC-UGent activities, future plans, VSC opportunities
- 10h30: Review of user poll results, Q&A
- 11h00: User in the spotlight
  - Nick Vereecke on Mycoplasma & Brachyspira

ABOUT HPC-UGENT

Part of ICT department, Infrastructure office

Mission

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


Alvaro Simon Garcia


Andy Georges


Ewald Pauwels


Bart Verheyde


Balazs Hajgato


Kenneth Hoste


Kenneth Waegeman


Stijn De Weirdt


Wouter Depypere

Part-time consultancy

Jobstudents

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ABOUT HPC-UGENT

Tasks

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

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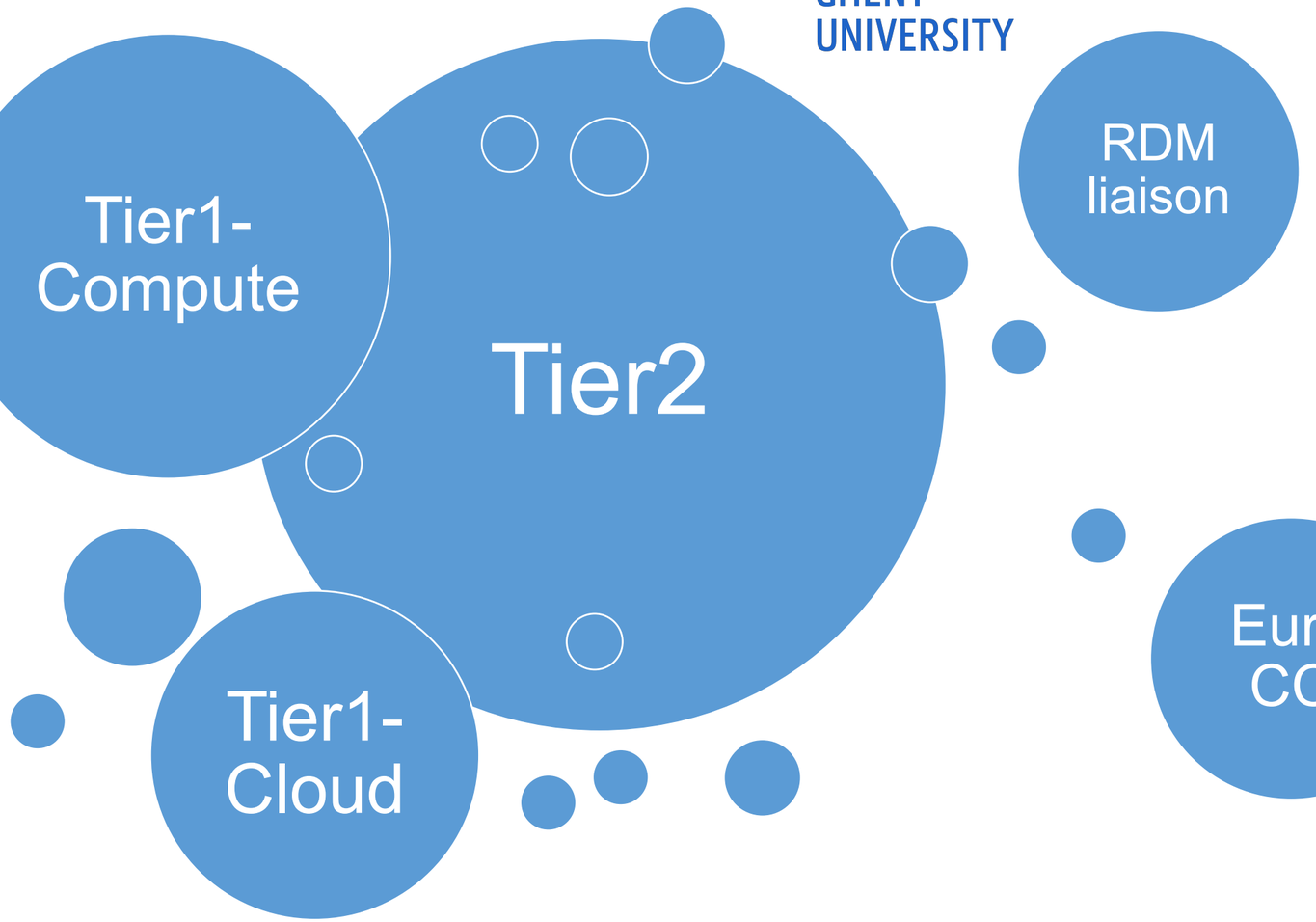
OPERATIONS



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RDM liaison

VLAAMS SUPERCOMPUTER CENTRUM

Vlaanderen is supercomputing

EURO

Euro CC

EuroHPC Joint Undertaking

INFRASTRUCTURE CHANGES IN 2020-2021

- InfiniBand network rewiring/extension
- General maintenance and update works

- New, larger storage for HOME/DATA/SCRATCH – 3.75 PB
- Fast scratch area *arcanine* in production – 70 TB NVMe
- HPC storage – DICT shares connection, Globus

- Clusters *phanpy* and *golett* end of life
- GPU cluster *joltik* in production
- Big-memory cluster *kirlia* in production
- CPU cluster *doduo* in pilot and productiono

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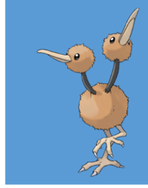
NEW CLUSTERS

Cluster name	#nodes	CPU per node	Mem/node	Storage/node	Interconnect	OS
joltik 	10	32-core Intel Xeon Gold 6242 4x NVIDIA Volta V100 GPUs (32GB GPU memory) Total: 320 CPU cores, 40 GPUs	256 GiB (8 GiB/core)	800GB SSD	double EDR Infiniband	CentOS 7
kirlia 	16	36-core Intel Xeon Gold 6240 Total: 576 CPU cores	738 GiB (20.5 GiB/core)	1.6 TB NVME	HDR-100 InfiniBand	CentOS 7
doduo 	128	96-core AMD EPYC 7552 Total: 12.288 CPU cores	250 GiB (2.6 GiB/core)	180GB SSD	HDR-100 InfiniBand	RHEL 8

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CLUSTER USAGE IN 2020

Cluster name	Compute time consumed		Effective use percentage	
	CPU hours	GPU hours	CPU	GPU
~~Phanpy~~	2 024 716		60%	
~~Golett~~	22 765 468		62%	
Swalot	18 111 027		81%	
Skitty	17 210 229		76%	
Victini	22 696 689		75%	
Joltik	1 499 605	229 124	53%	65%
Kirlia	1 862 691		37%	
Doduo (pilot)	5 870 828		22%	

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CLUSTER USAGE IN 2020

Consumed compute time by affiliation		
	CPU time	GPU time
UAntwerpen	0.05%	0.00%
VUB	0.16%	5.51%
UGent	99.47%	94.43%
KULeuven / UHasselt	0.01%	0.00%
Other research institutes	0.20%	0.00%
Industry	0.10%	0.06%
Total	100.00%	100.00%

Students/researchers		
	CPU time	GPU time
Ma/Ba students	2.60%	5.32%
Researchers	97.40%	94.68%
Total	100.00%	100.00%

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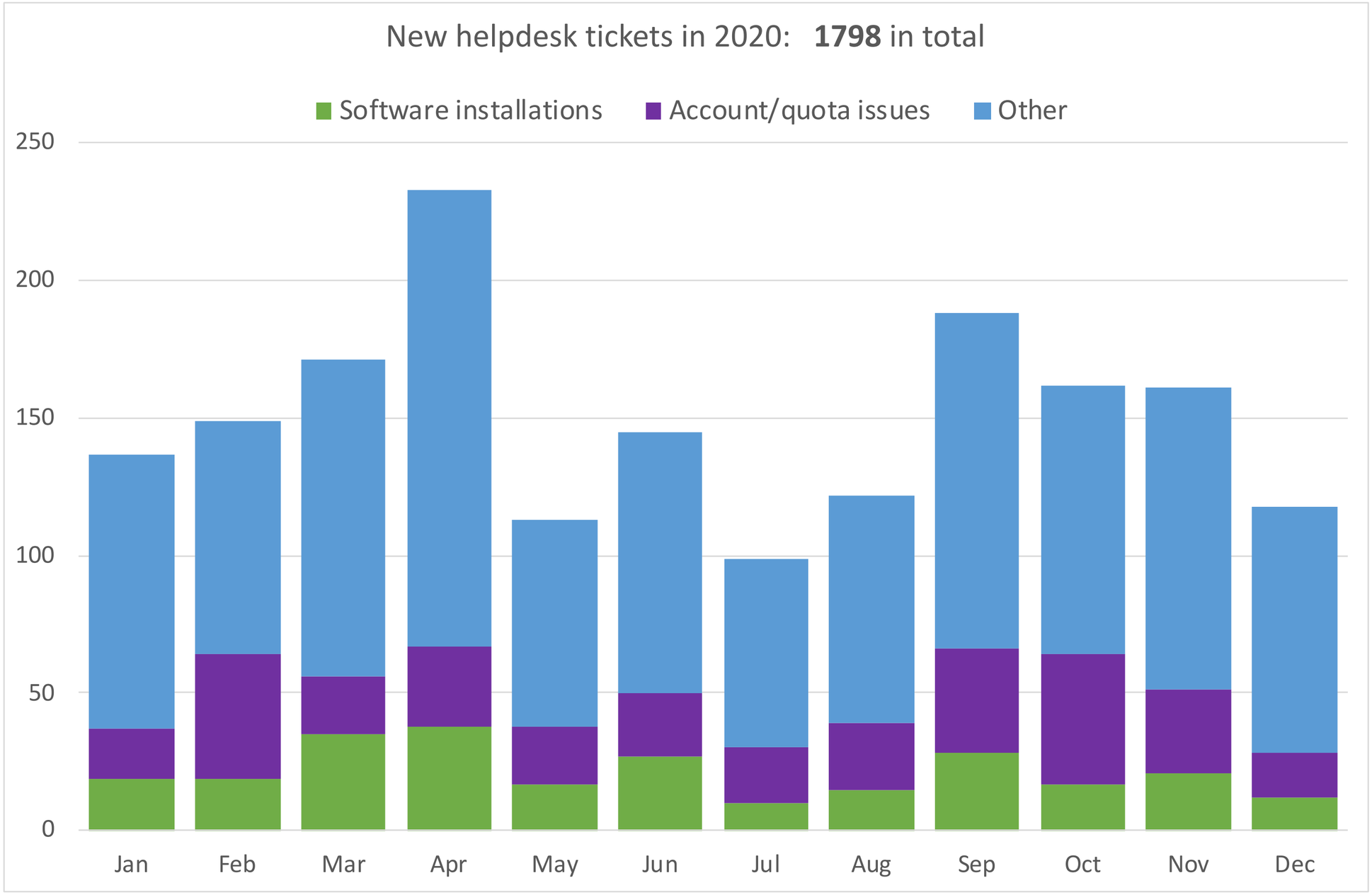
HELPDESK



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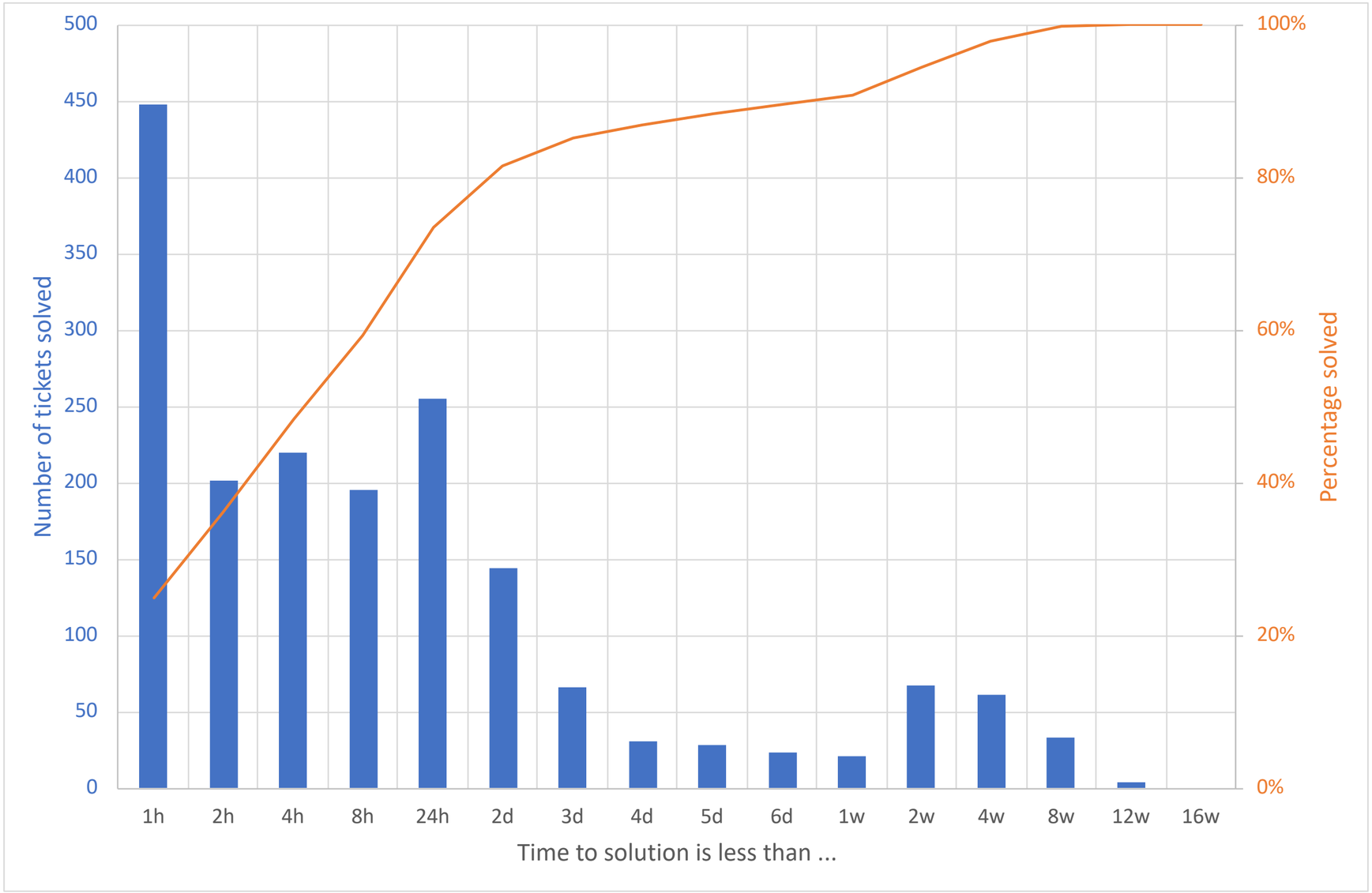
Average time to resolution – overall



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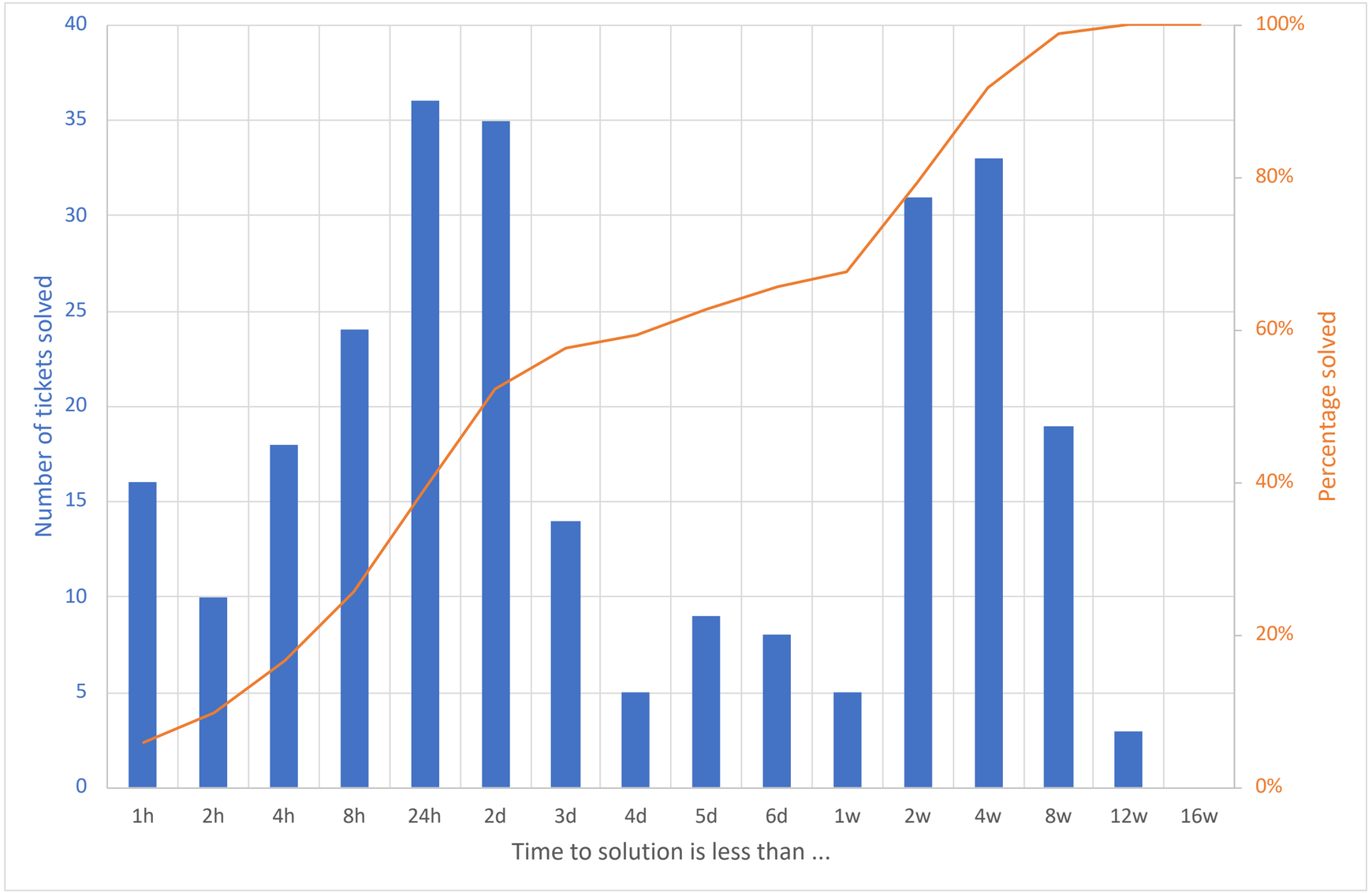
HELPDESK

Average time to resolution – 266 software installation requests

On average, every software installation takes **~7 hours of time**



MORE INFO – ANNUAL REVIEW 2020

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

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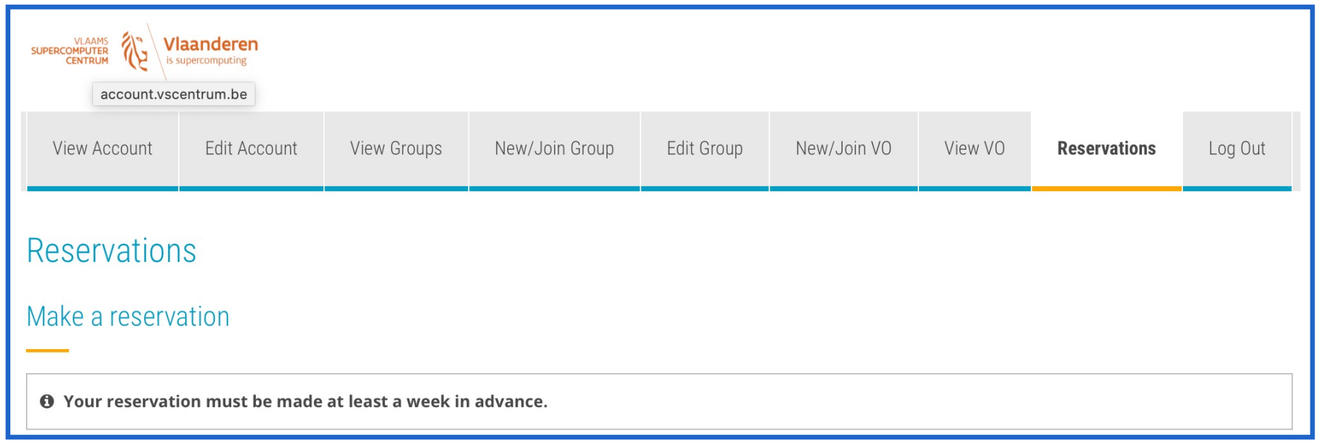
HIGHLIGHTED (NEW) FEATURES

- Students and courses
- UGent shares – HPC-UGent connection
- Globus
- XDMoD
- HPC-UGent webportal

HIGHLIGHT – STUDENTS AND COURSES

- HPC-UGent IS available for students, but SLA remains best effort
- Student account requests no longer require ZAP approval
- Reservations for practical sessions



Dedicated resources for duration of practical session

Registration form:

https://account.vscentrum.be/django/reservation

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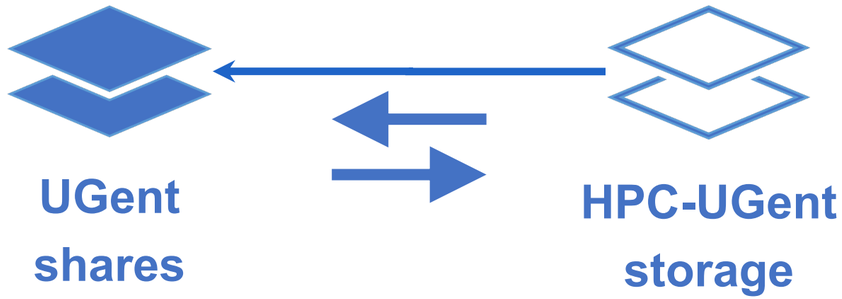
HIGHLIGHT – CONNECT TO UGENT SHARES

https://www.ugent.be/hpc/en/support/documentation.htm

Chapter 6.2.5 *'Your UGent home drive and shares'*

- Mount shares on HPC storage
- Allows file manipulations to/from via HPC platform interface
- Caveat: file systems differ
  - Set permissions separately on platforms
  - Zip to preserve attributes when backing up

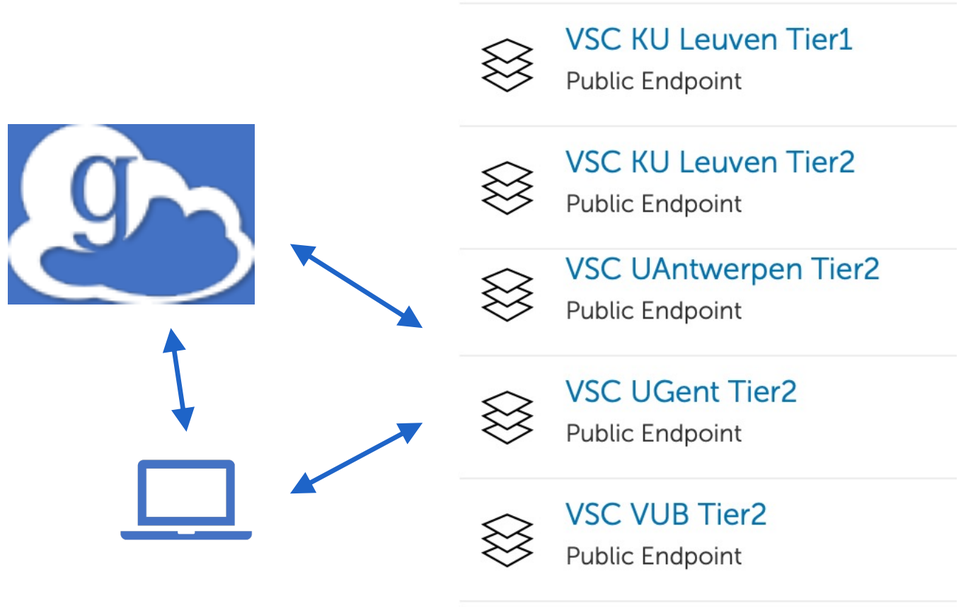


RDM
liaison

HIGHLIGHT – GLOBUS

https://docs.vscentrum.be/en/latest/globus/globus_main_index.html

- Easier transfer of files between (VSC) endpoints
  - In background
  - Doesn’t (necessarily) involve user device
- Possibility to define multiple endpoints



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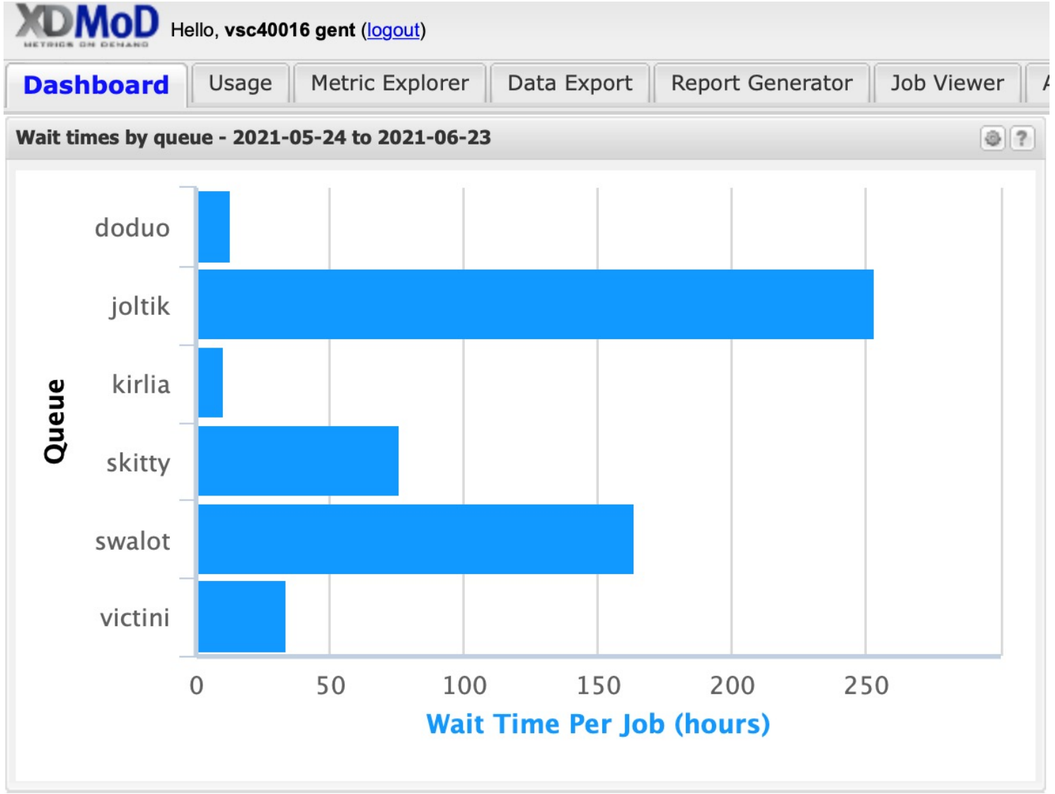
HIGHLIGHT – XDMOD

https://www.ugent.be/hpc/en/support/documentation.htm

Chapter 9 *'XDMoD portal'*



- Get information on completed jobs, e.g.
  - total amount of CPU/GPU hours used
  - waiting time
  - job size
  - resource usage (clusters)
  - …
- Information only for your personal vsc-id

> UGent VPN

> Connect to https://shieldon.ugent.be/xdmod

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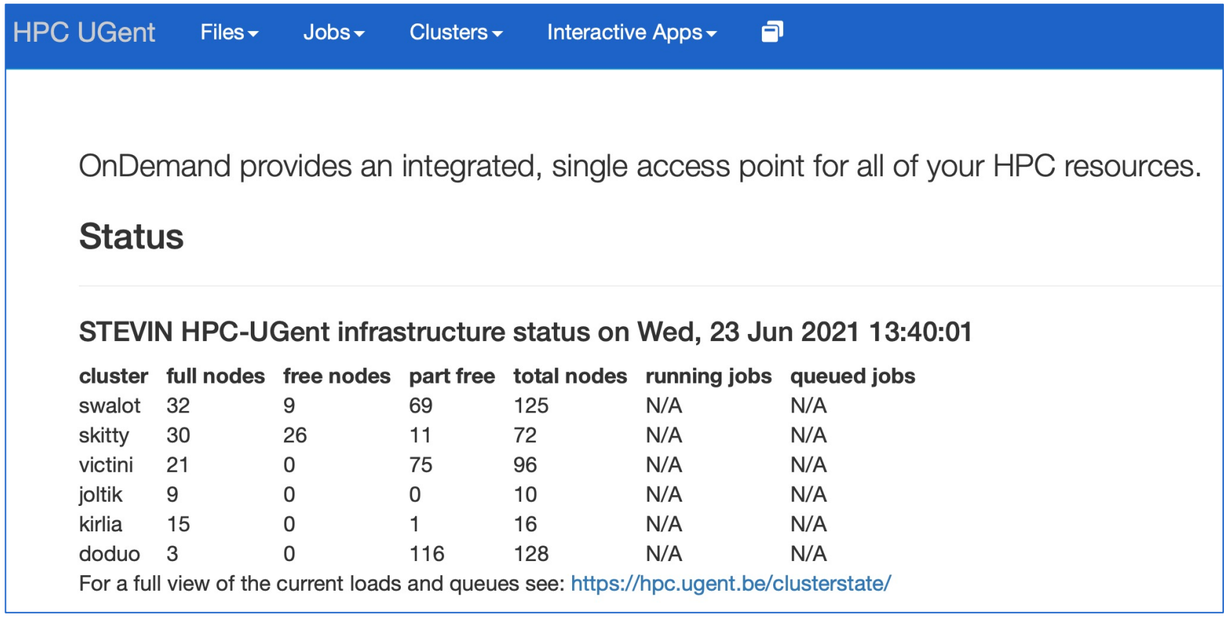
HIGHLIGHT – HPC-UGENT WEB PORTAL

https://www.ugent.be/hpc/en/support/documentation.htm

Chapter 8 '*Using the HPC-UGent web portal*'

- Web portal
- Upload/download files
- Create/edit/submit/monitor jobs
- Run Interactive/GUI applications
- Connect via SSH



> UGent VPN or VSC firewall app (https://firewall.hpc.kuleuven.be)

> Connect to https://login.hpc.ugent.be

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OUTLOOK 2021

- New GPU cluster
- Debug/interactive cluster *slaking*
- Consolidation of HPC web portal
- UGent cloud

- VSC Tier1-Compute ‘Hortense’ – operations and management
- VSC Tier1-Cloud – operations and management

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VSC – VLAAMS SUPERCOMPUTER CENTRUM

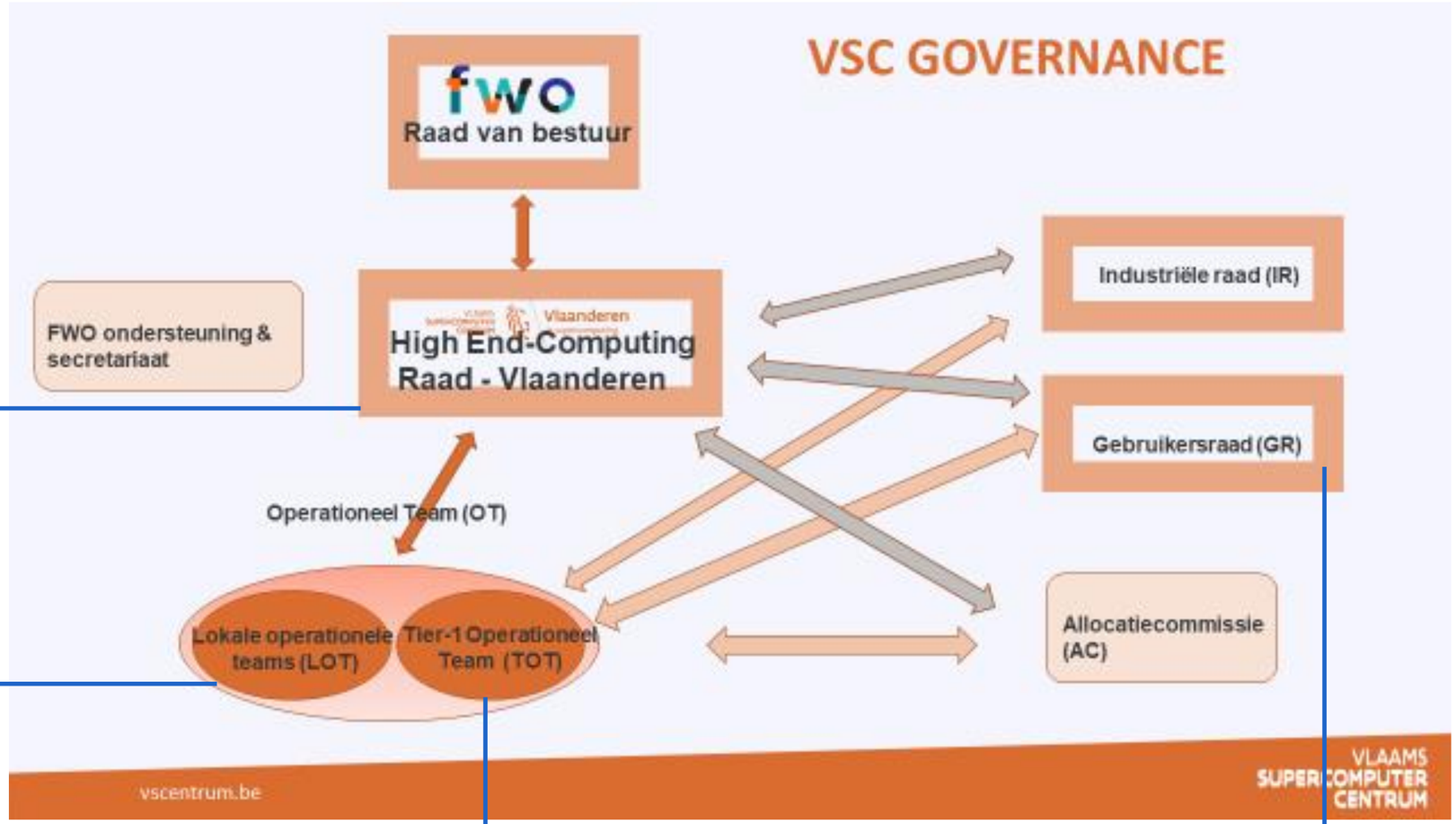
VSC – Flemish Supercomputer Center

- Partnership between Flemish university associations
- Tier1 + Tier2 Infrastructure in four hubs
- Managed by FWO

Mission

The VSC encourages the use of scientific and technical computing in the Flemish academic and industrial landscape. To this end, it offers infrastructure, training and services. In addition, VSC acts as a lever to promote the importance of scientific and technical computing and its added value to society.

VSC – GOVERNANCE



Johan Van Camp

Ewald Pauwels

Stijn De Weirdt

Dr. Jan Goedgebeur

Department of Applied Mathematics, Computer Science and Statistics

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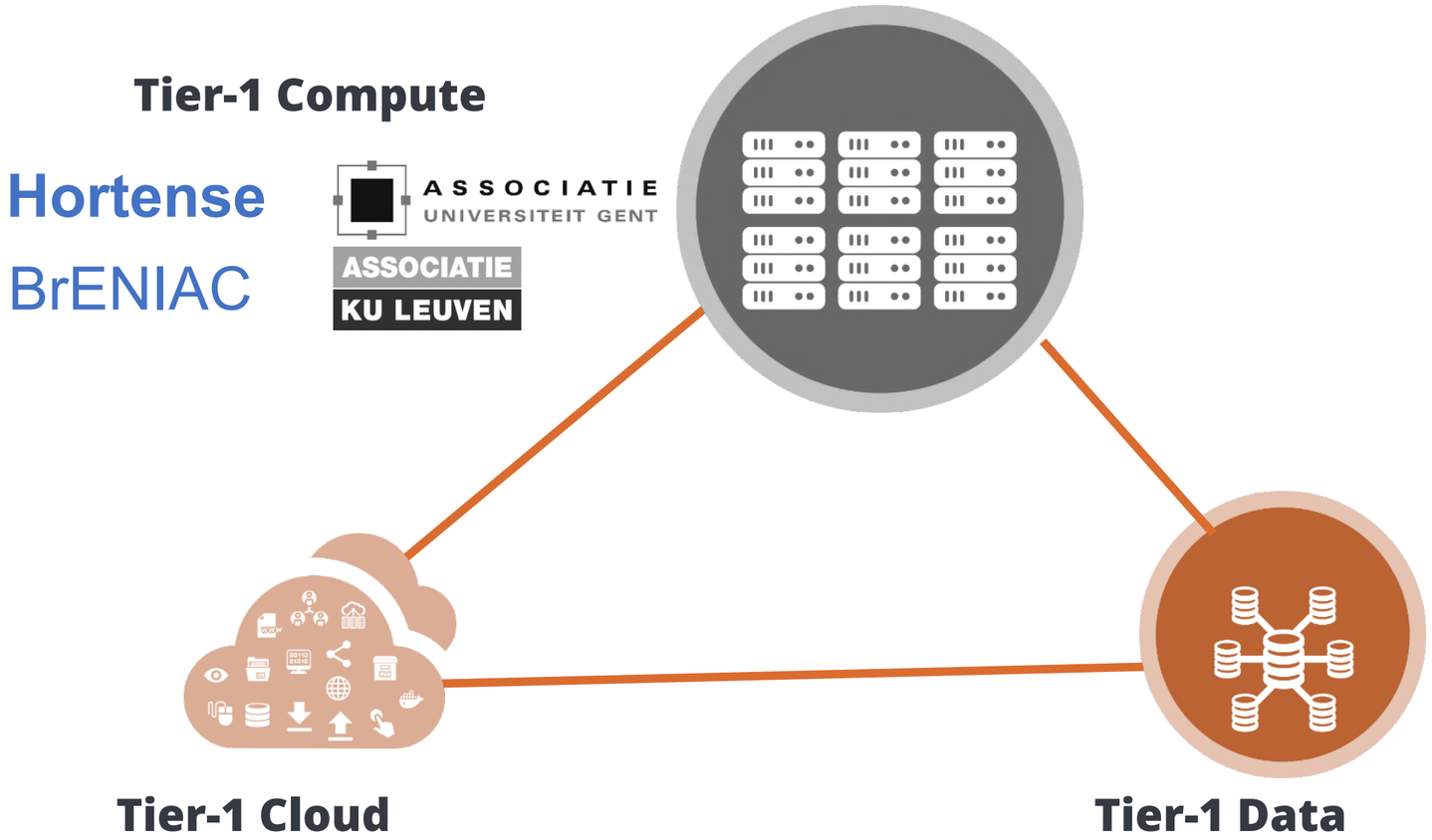
VSC PRIME INFRASTRUCTURE: TIER-1 SAAS

30 Meuro impulse investment “Supercomputing as a service” 2018-2022



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VSC TIER-1 COMPUTE “HORTENSE”

https://www.vscentrum.be/compute

336 CPU nodes

- 2x 64-core AMD Epyc 7H12 CPU 2.6 GHz
- RAM: 294 nodes @ 256 GiB, 42 nodes @ 512 GiB
- Total of 43.008 cores

20 GPU nodes

- 2x 24-core AMD Epyc 7402 CPU 2.8 GHz
- 4x NVIDIA Ampère NVLink3 (40 GB)
- RAM: 256 GiB
- Total of 960 cores and 80 GPUs

InfiniBand HDR-100 interconnect

3 PB shared storage based on Lustre

Availability: *likely* Oct-Nov 2021

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VSC TIER-1 COMPUTE ACCESS MODELS

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

https://www.vscentrum.be/compute

Next project call deadline for B. = **4 Oct 2021**

Success depends on quality of your proposal

Send your proposal to hpc@ugent.be for prior review

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VSC TIER-1 CLOUD

https://www.vscentrum.be/cloud

- On-demand resources in a flexible and cloud-like manner
- Platform-as-a-Service for power users that can deploy resources and adapt them to their scientific use case:
  - virtual machines
  - storage systems
  - private/public networks
- Ready-to-use catalog of templates
  - databases
  - web servers

Access is project-based and open to all
Project call deadlines: 28 June 2021
4 October 2021

Send your proposal to hpc@ugent.be for prior review

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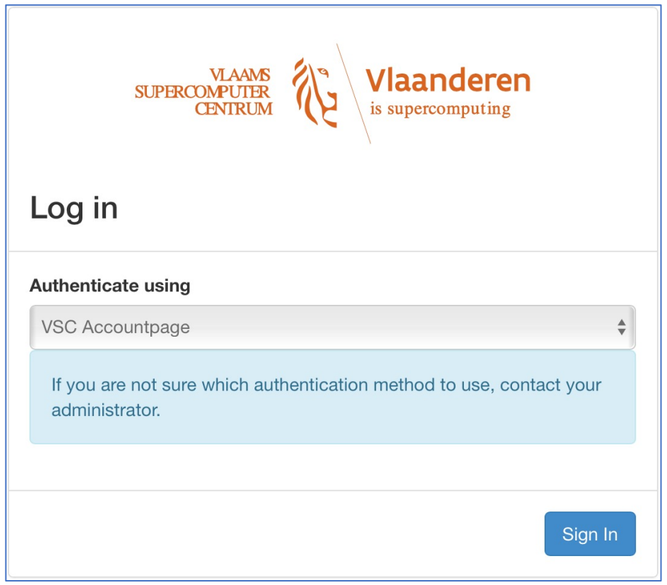
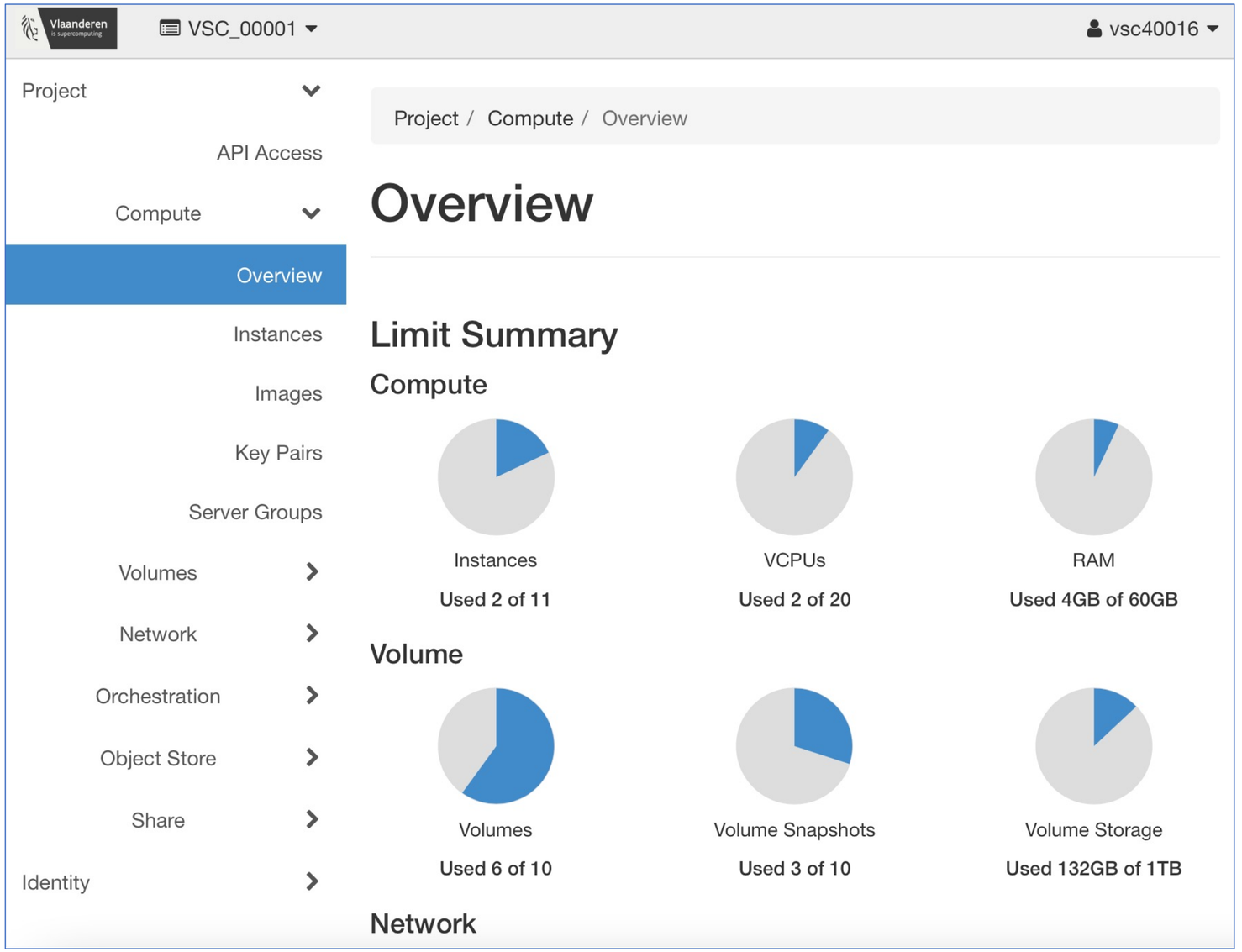
VSC TIER-1 CLOUD



openstack™



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EUROPEAN OPPORTUNITIES

EuroCC – European Competence Centers

> National single points of contact for HPC/HPDA/AI competences

> map competences, visibility of service offering, spoc

- HPC-UGent part of Belgian NCC (12 partners)
- WP-leader ‘Competence mapping’
- Contributor to ‘Tech Transfer/Business Development’
  ‘Collaboration with industry’

FF4EUROHPC CALL

- For small consortia that work together with industry or SMEs on HPC, BigDATA or AI/ML projects
- Financing up to 200.000 euro (incl. personnel)
- HPC-UGent can provide compute resources

https://www.ff4eurohpc.eu/en/open-calls/open-call/

PROGRAM

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  - Nick Vereecke on Mycoplasma & Brachyspira

REVIEW OF USER POLL RESULTS

- 118 respondents
- Average completion time: 3 minutes

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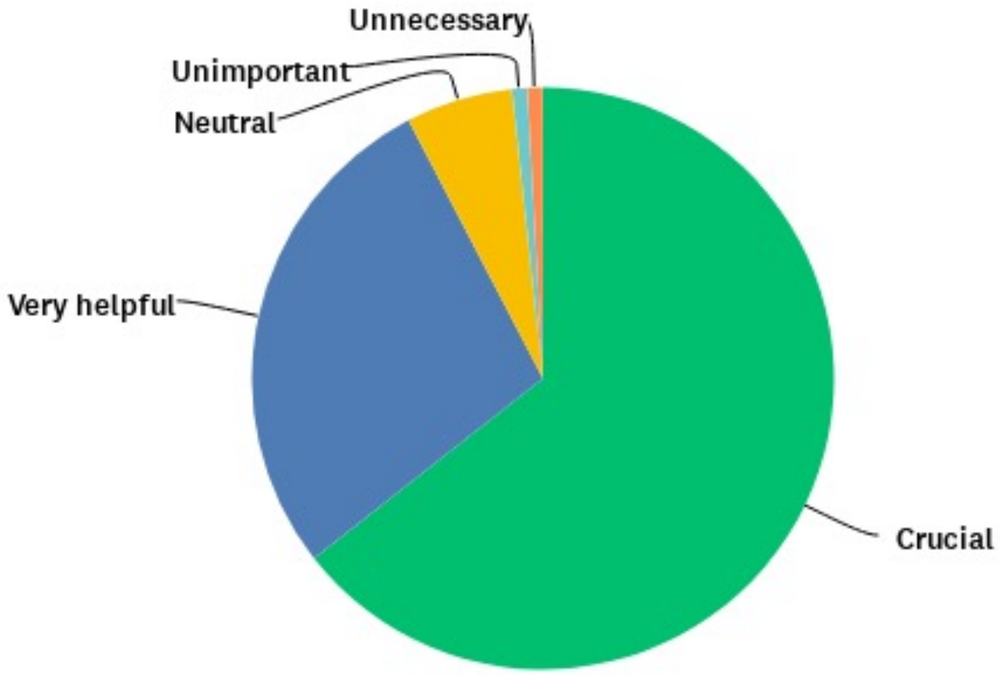
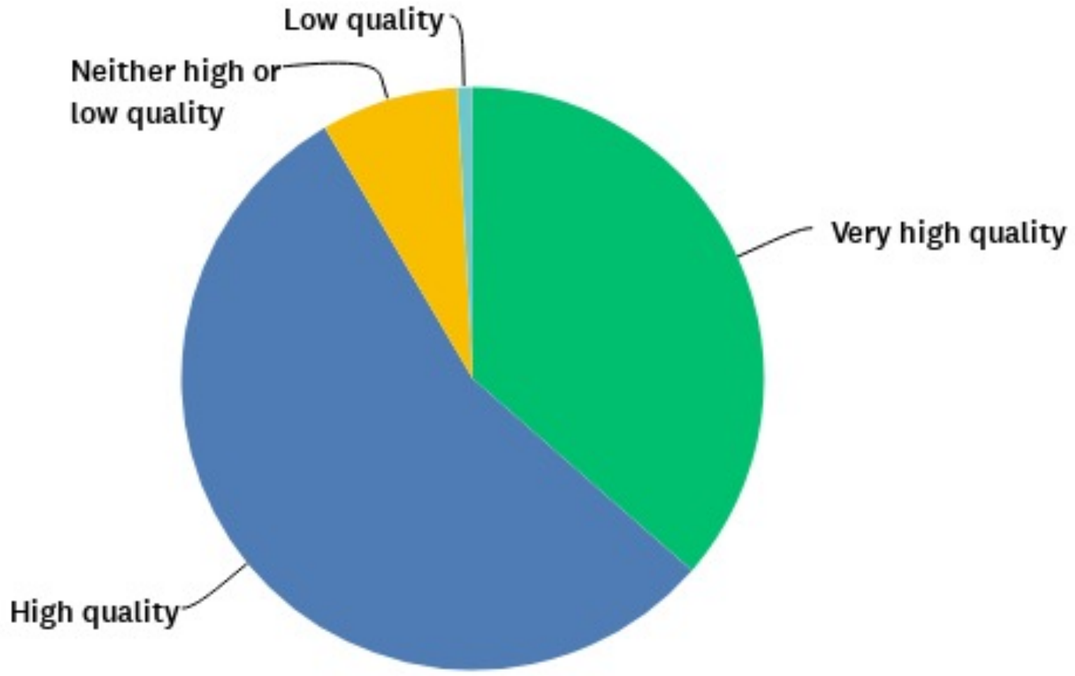
REVIEW OF USER POLL RESULTS

How important is HPC-UGent for your research?



92% Very helpful or crucial to research

How would you overall rate HPC-UGent services?



91% High quality or better

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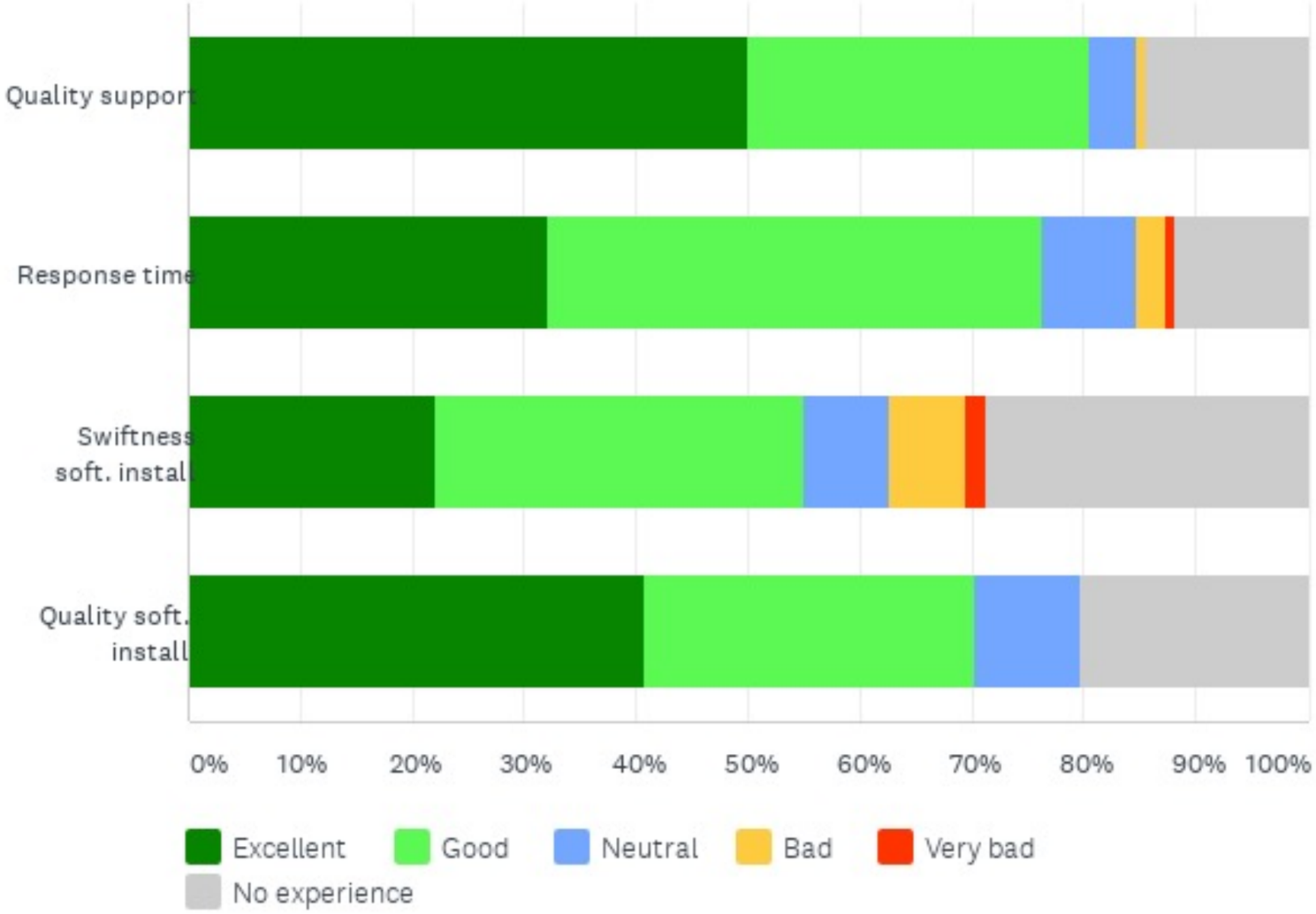
REVIEW OF USER POLL RESULTS

Rate aspects of HPC-UGent user support:



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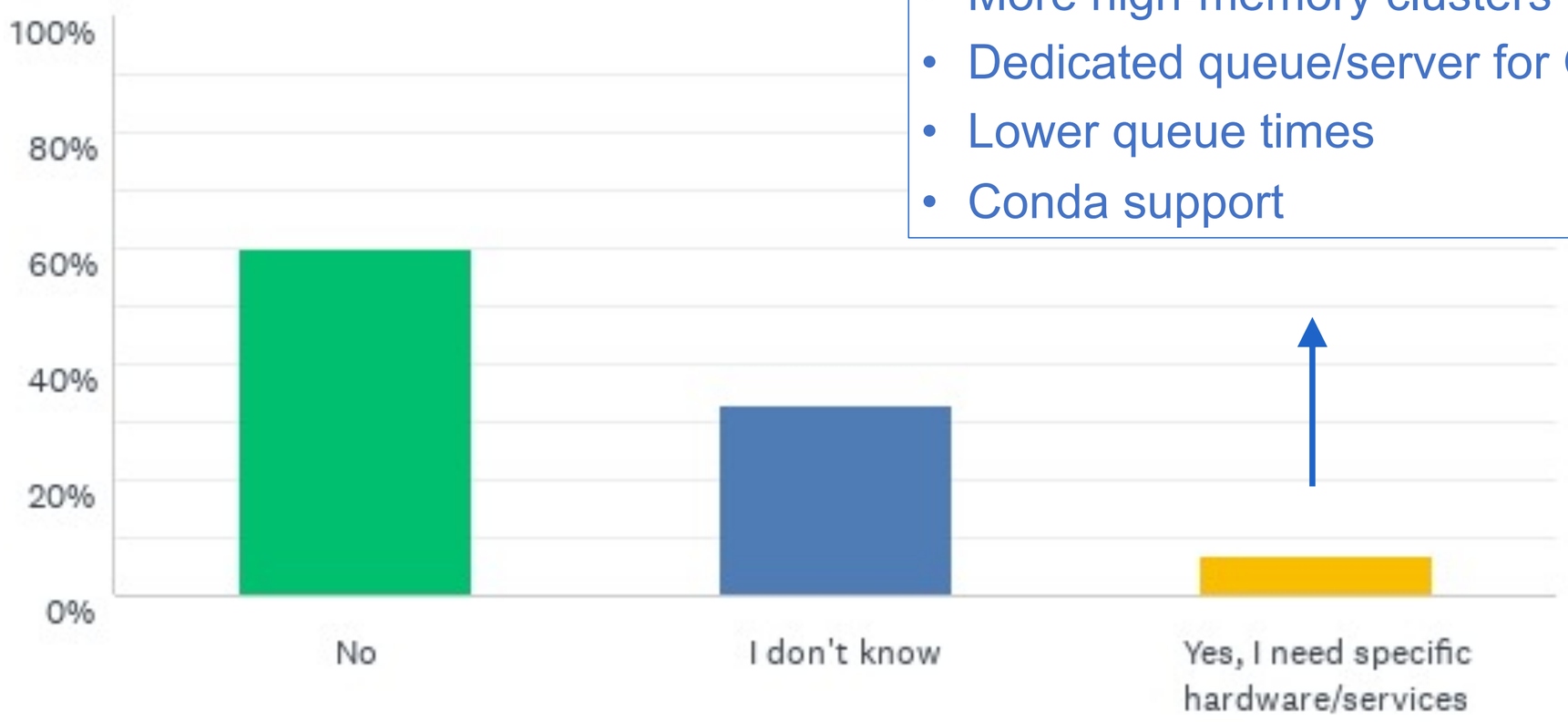
REVIEW OF USER POLL RESULTS

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

- More GPUs
- More high-memory clusters
- Dedicated queue/server for GPU porting
- Lower queue times
- Conda support



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REVIEW OF USER POLL RESULTS

How could we further improve HPC-UGent services?

Infrastructure

- More nodes/clusters
- More GPUs
- Higher file transfer speeds
- Fast parallel and accessible communication to SCRATCH on victini
- More storage in HOME directory

REVIEW OF USER POLL RESULTS

How could we further improve HPC-UGent services?

User support

- Speed up software installation
- Speed up response time in general
- (Better) support for first time users and non-computational science researchers
- More staff

REVIEW OF USER POLL RESULTS

How could we further improve HPC-UGent services?

”… months for a single installation just takes too long …
A … researcher cannot invent … months of alternative work when the software is not available.”

- Having software in place is CRUCIAL for (starting) researchers
- (Proper) software installations CAN take a lot of time

https://easybuild.io

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REVIEW OF USER POLL RESULTS

How could we further improve HPC-UGent services?

User experience

- Shorter queue times (for companies)
- Way to estimate queue time
  - See number of jobs/corehours requested per cluster by all users
- Project applications for VOs to get compute time (to reduce load)
- Automatic distribution of jobs across clusters in terms of occupancy and efficiency
- Longer wall-clock time
- Better estimate of the impact of maintenance on e.g. license servers

REVIEW OF USER POLL RESULTS

How could we further improve HPC-UGent services?

Training

- Online courses/recordings on how to use HPC efficiently
- Specific workshops, targeted to specific research groups
- Introduction to parallel programming
- How-to lecture on compiling your own complex software model
- Using git
- Jupyter notebooks on HPC web portal
- More mails with suggested courses (e.g. PRACE)

REVIEW OF USER POLL RESULTS

How could we further improve HPC-UGent services?

Software

- Easy local module installation
- Permit installation of published R packages without separate manual requests
- Update all the software on a regular basis

REVIEW OF USER POLL RESULTS

How could we further improve HPC-UGent services?

Documentation

- Expand documentation with links to external sources
- Step-by-step documentation on e.g. pip and conda
- Workflows including git/github
- Workflows including jupyter notebooks

REVIEW OF USER POLL RESULTS

How could we further improve HPC-UGent services?

Consultancy

- Advanced programing support (e.g. testing and improving code)
- Support for compiling complex software models

Q&A

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