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DEPARTMENT ICT

# HPC-UGENT USER MEETING

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

28/01/2019

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VSC Vlaams Supercomputer Centrum

# PROGRAM

- (13h00: Optional tour of datacenter)
- 14h00: Overview of HPC-UGent usage, status of the VSC, future plans
- 14h30: Review of user poll results, Q&A
- 15h00: User in the spotlight – Chiara Caratelli, CMM
- 15h45: Slots for 1-minute poster presentations
- 16h15 - 18h00 Networking reception & poster session

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# 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.

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# ABOUT HPC-UGENT

## Personnel

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


Alvaro Simon Garcia


Andy Georges


Ewald Pauwels


Jens Timmerman


Kenneth Hoste


Kenneth Waegeman

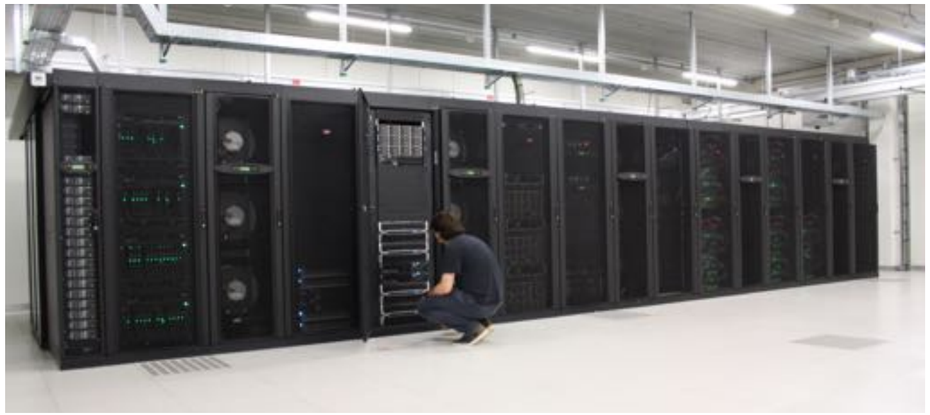

Stijn De Weirdt


Wouter Depypere


Balazs Hajgato

New vacancy opening soon

# HPC-UGENT INFRASTRUCTURE



| Shared storage | Size |
|---|---|
| $VSC_HOME | 35 TB |
| $VSC_DATA | 702 TB (can grow to 1 PB) |
| $VSC_SCRATCH<br>$VSC_SCRATCH_KYUKON | 1 PB |
| $VSC_SCRATCH_PHANPY | 35 TB SSD |

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| Cluster name | #nodes | CPU per node | Memory per node | Interconnect |
|---|---|---|---|---|
| Raichu | 56 | 2 x 8-core Intel E5-2670 (Sandy Bridge @ 2.6 GHz) | 32 GB | Gb Ethernet |
| Delcatty | 124 | 2 x 8-core Intel E5-2670 (Sandy Bridge @ 2.6 GHz) | 64 GB | FDR InfiniBand |
| Phanpy | 16 | 2 x 12-core Intel E5-2680v3 (Haswell-EP @ 2.5 GHz) | 512 GB | FDR InfiniBand |
| Golett | 200 | 2 x 12-core Intel E5-2680v3 (Haswell-EP @ 2.5 GHz) | 64 GB | FDR-10 InfiniBand |
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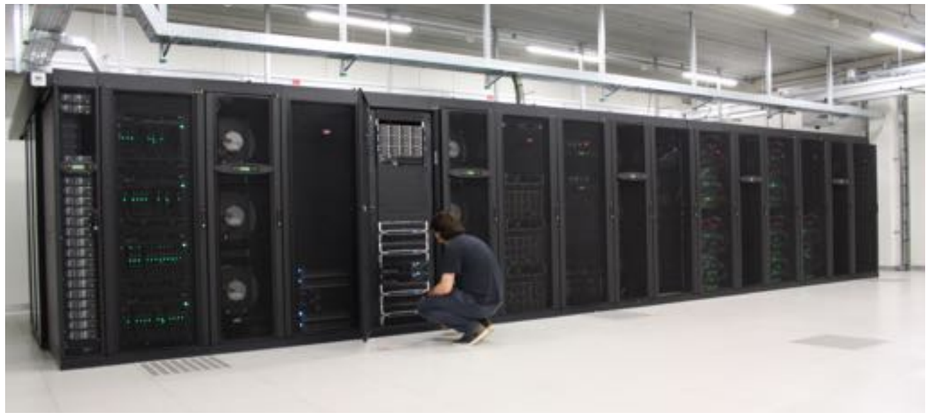
| Victini | 96 | 2 x 18-core Intel Xeon Gold 6140 (Skylake @ 2.3 GHz) | 96 GB | 10 Gb ethernet |

# HPC-UGENT INFRASTRUCTURE



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Standard cluster

SLURM

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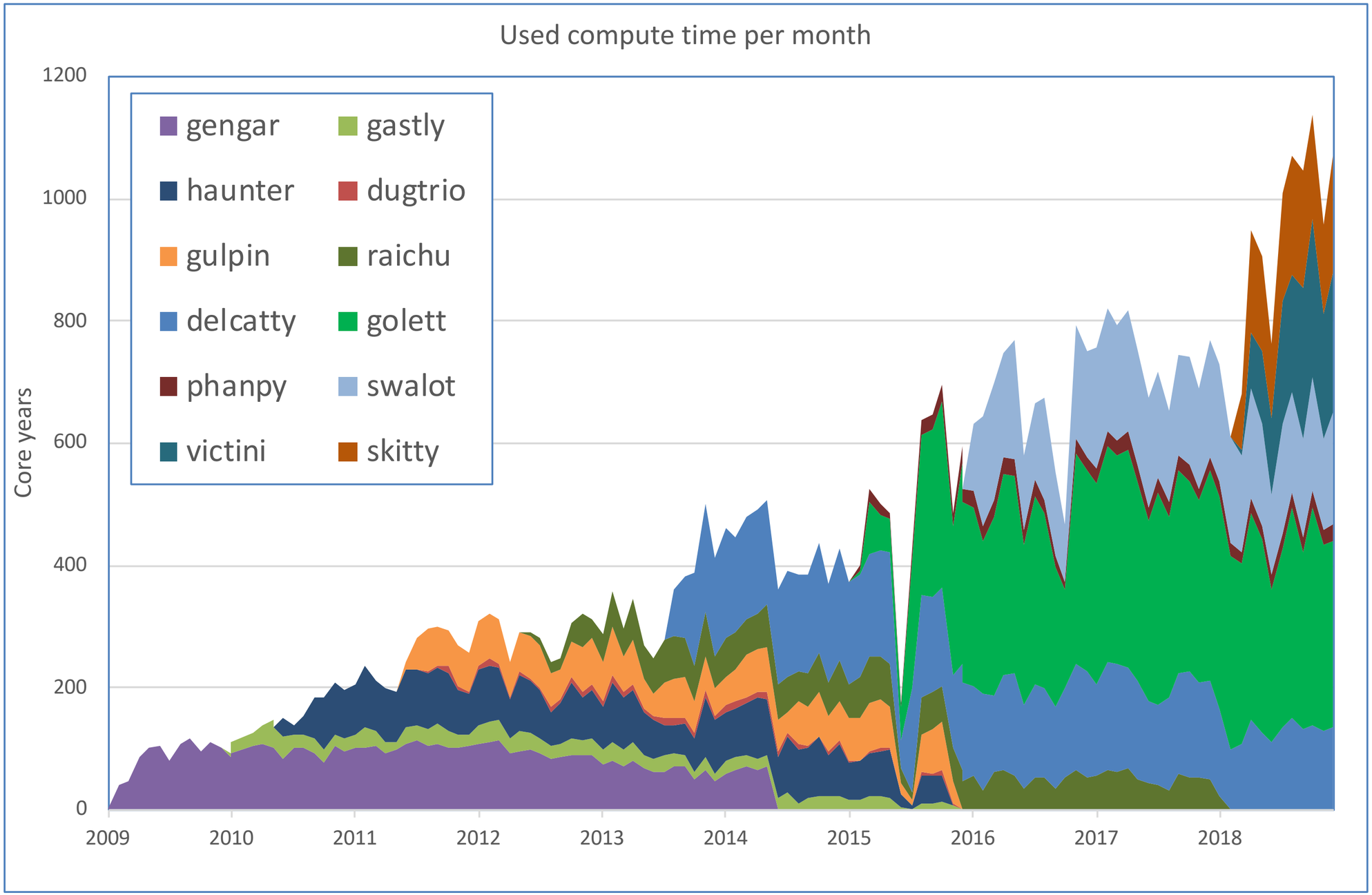
# OVERVIEW OF HPC-UGENT USAGE

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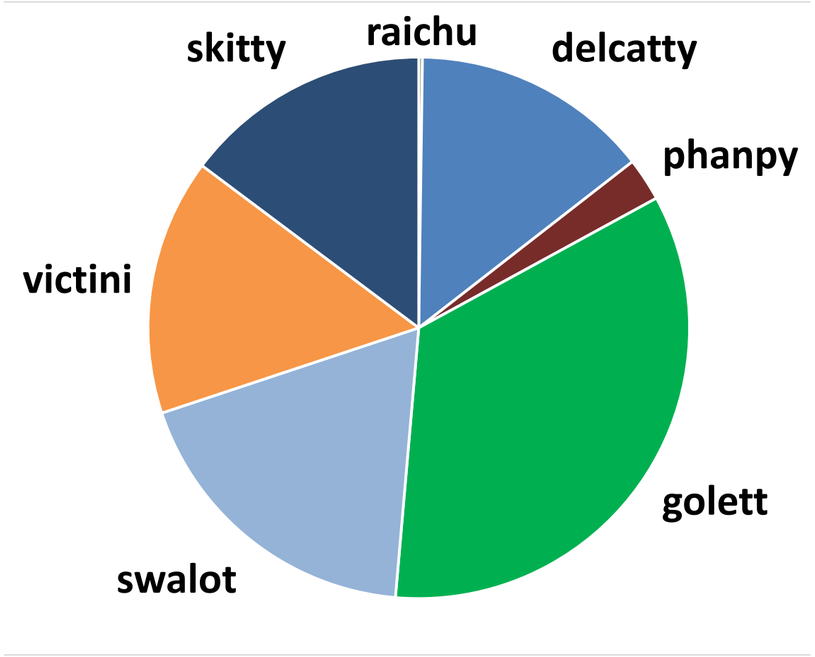
# OVERVIEW OF HPC-UGENT USAGE

## Consumed compute time in 2018, per compute cluster




| Cluster name | Compute time consumed (in core years) | | Effective use percentage |
|---|---|---|---|
| Raichu | (until 15/01/2018) | 24 | 65% |
| Delcatty | | 1559 | 79% |
| Phanpy | | 281 | 73% |
| Golett | | 3753 | 78% |
| Swalot | | 2026 | 79% |
| Victini | (from 1/03/2018) | 1676 | 58% |
| Skitty | (from 1/03/2018) | 1615 | 74% |
| **Total** | | **10933** | **74%** |

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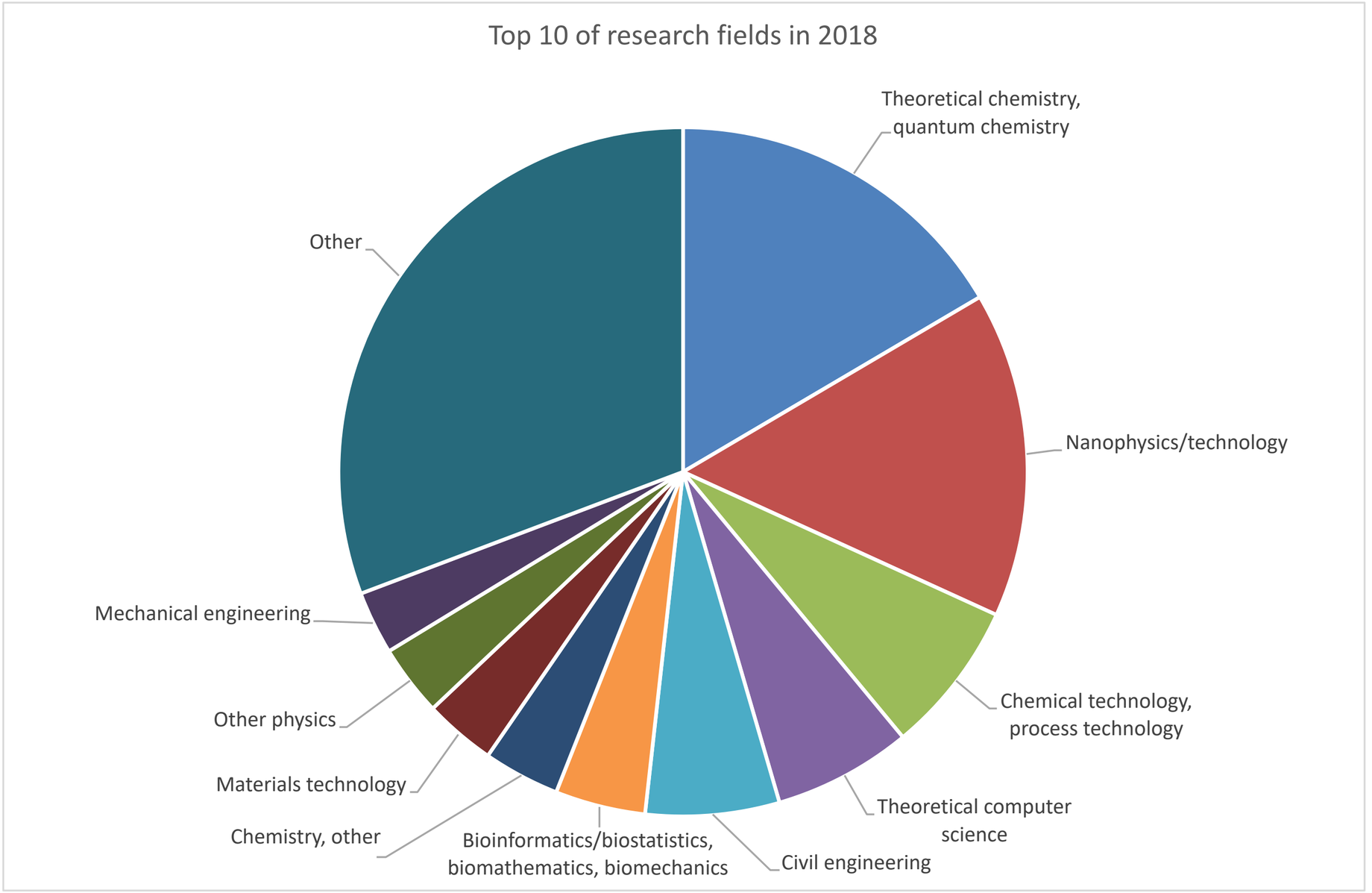
# OVERVIEW OF HPC-UGENT USAGE

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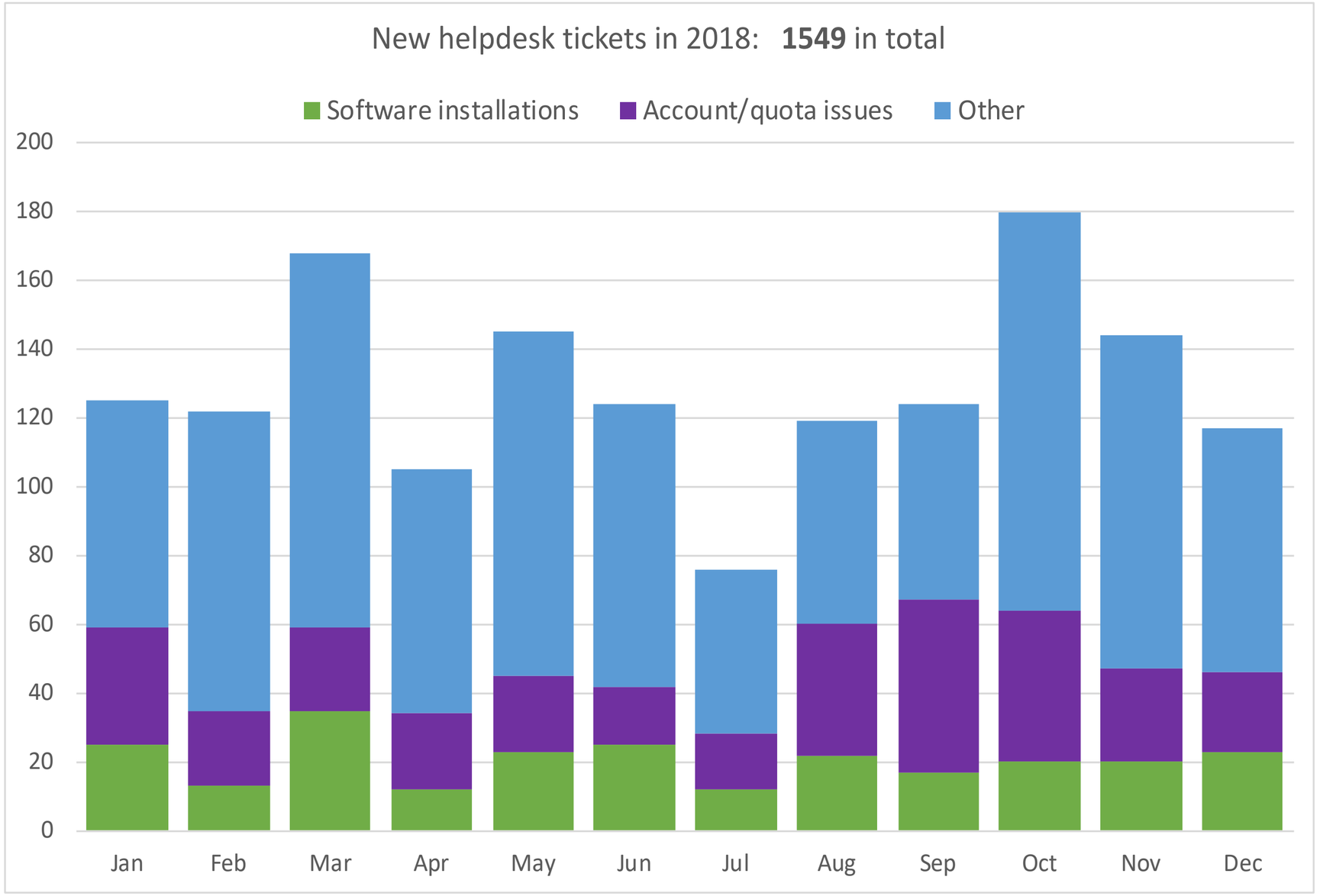
# HPC-UGENT – REALIZATIONS IN 2018

- 2 additional clusters
- Introduction of SLURM scheduler
- Elimination of (outdated) userwiki in favour of VSC usermanual
- Portal rewrite
- General maintenance and update works

# HPC-UGENT – HELPDESK IN 2018

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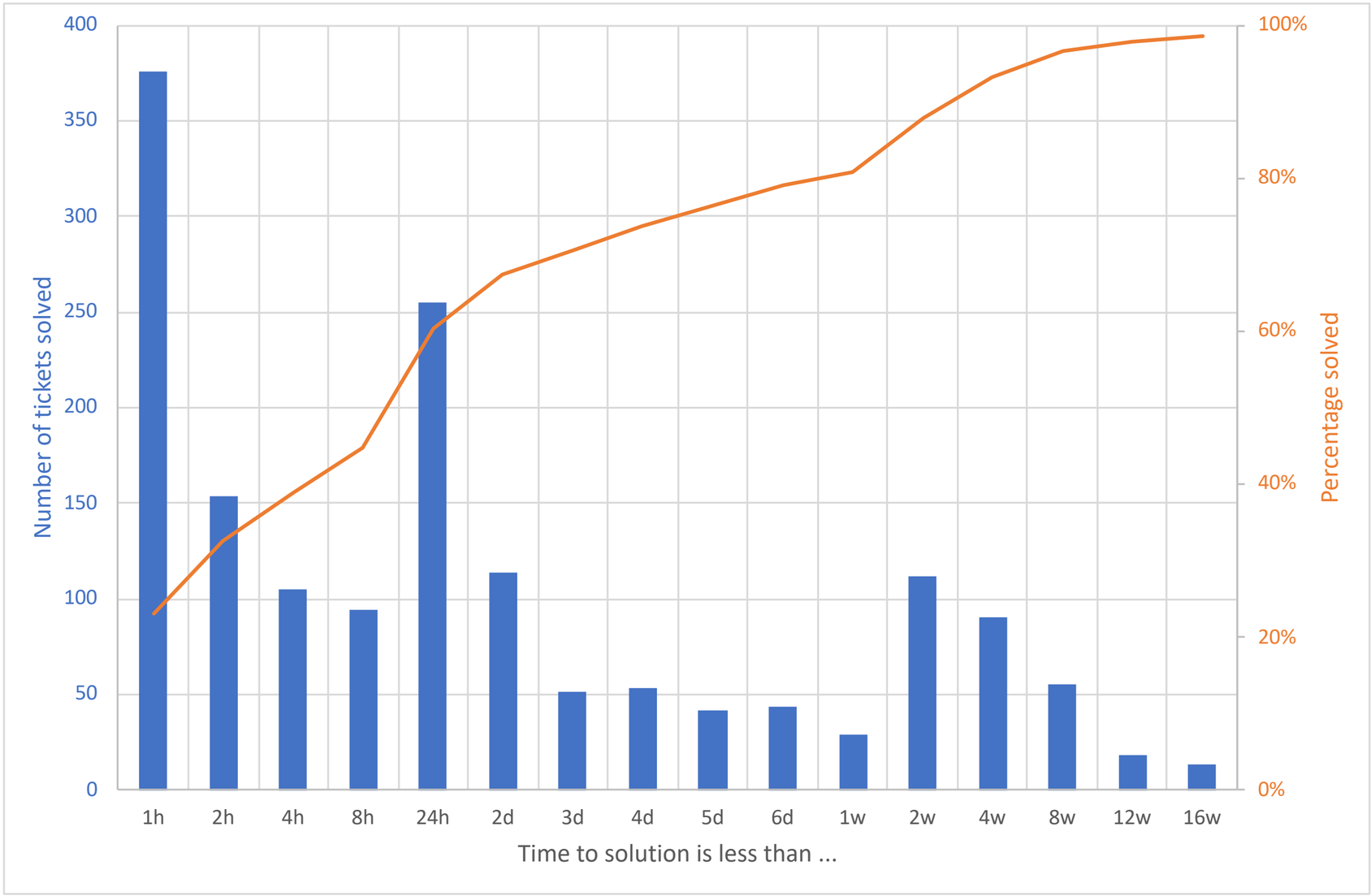
# HPC-UGENT – HELPDESK IN 2018

## Average time to resolution – overall

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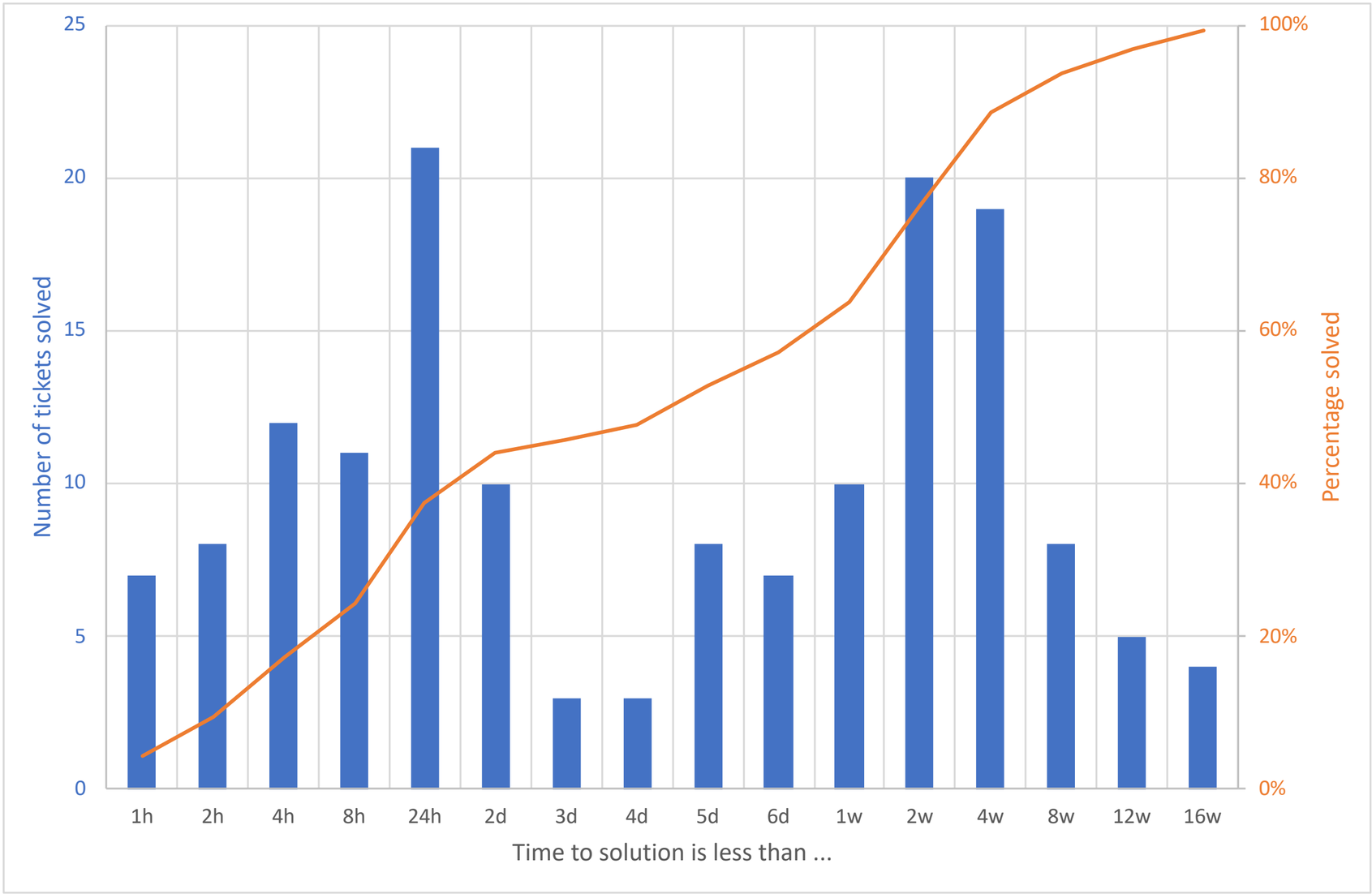
# HPC-UGENT – HELPDESK IN 2018

## Average time to resolution – software installation requests

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# HPC-UGENT – ANNUAL REVIEW 2018

UNIVERSITEIT
GENT

## ANNUAL REVIEW HPC-UGENT

2018

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# HPC-UGENT – NEW DEVELOPMENTS 2019+

- Tier-2 storage extension 2019Q2
- Switch all clusters to SLURM 2019Q2
- Decommission delcatty 2019Q2
- Additional clusters
  - golett replacement 2019Q4
  - phanpy replacement 2020Q1

- GPU partition 2019Q3

~ 2 Meuro investment in 2019

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# HPC-UGENT – PLANNED EVENTS 2019Q1Q2

| | |
|---|---|
| Introduction to HPC @ UGent | 9 Jan<br>27 Mar |
| Scientific Python | 16 Jan |
| Introduction to Linux | 25 Jan |
| HPC-UGent user meeting | 28 Jan |
| Tech talks on scientific computing | 4 Feb |
| Introduction to CP2K | 11-13 Mar |
| Scientific computing Social Sciences & Humanities | 26 Mar |
| Introduction to multithreading and OpenMP | 2-3 Apr |
| Introduction to MPI | 24 Apr |

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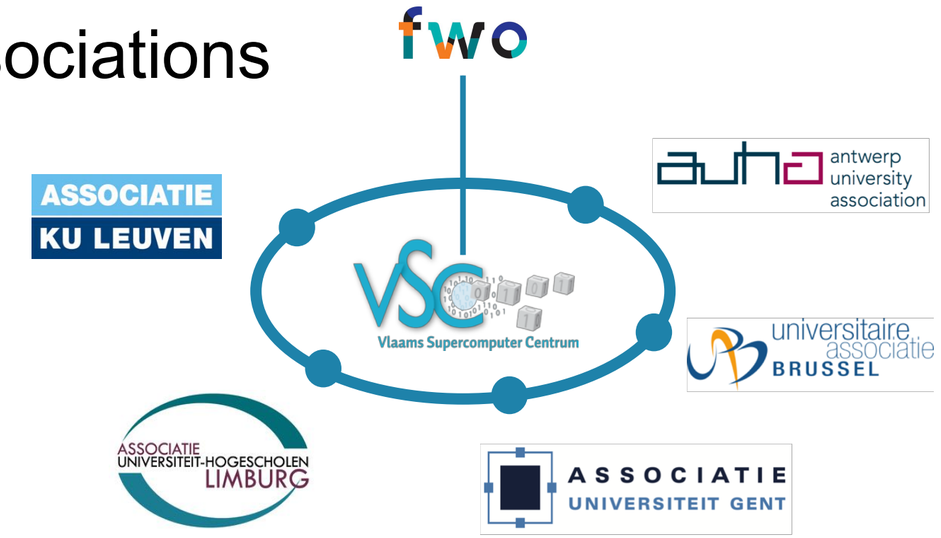
# VSC – VLAAMS SUPERCOMPUTER CENTRUM

**VSC – Flemish Supercomputer Center**

- Partnership between Flemish university associations
- 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 INFRASTRUCTURE

Bigger (super)computer
Bigger science

Vlaams Supercomputer Centrum

PRACE

Tier-0

Tier-1

BrENIAC

Tier-2

Tier-3

Laptop, workstation

HPC-UGent

ICTS KULeuven

CalcUA UAntwerpen

SISC VUB

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# VSC INFRASTRUCTURE – TIER-2

**Using other Tier-2 VSC infrastructure**

- Don't hesitate
- If unsure about pricing,
  ask KULeuven for quote
  (usually 5% of full cost)

| HPC-UGent Tier-2 usage | |
|---|---|
| Breakdown of consumed compute time by affiliation | |
| UAntwerpen | 0.251% |
| VUB | 0.000% |
| UGent | 97.647% |
| KULeuven / UHasselt | 1.886% |
| Other research institutes | 0.216% |
| Industry | 0.001% |
| Total | 100.000% |

- Feel free to ask support at another VSC site, e.g.
  - Error reporting
  - Trouble with credit system
  - Software installation
- **Always** put hpc@ugent.be in cc

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# VSC INFRASTRUCTURE – TIER-1

| #nodes | #cores | Mem/node | Storage | Network |
|---|---|---|---|---|
| 580 | 16.240 | 128 / 256 GB | 634 TB | EDR InfiniBand |

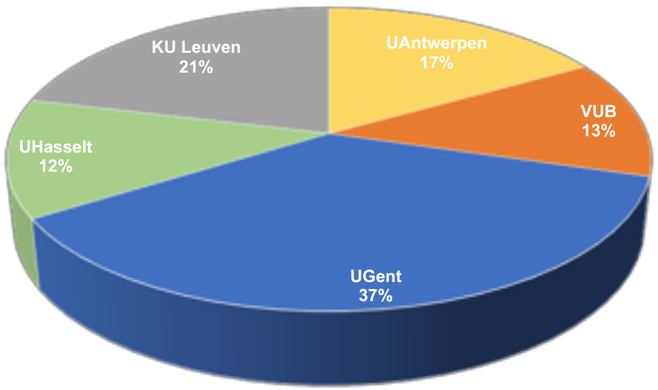
1 month on 5% of BrENIAC = 33 years on an average laptop

Access = project based

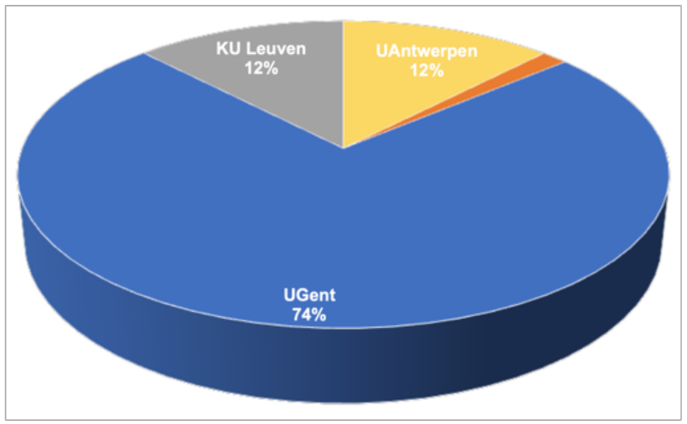
**Free of charge**

- Starting Grant
- Full project access

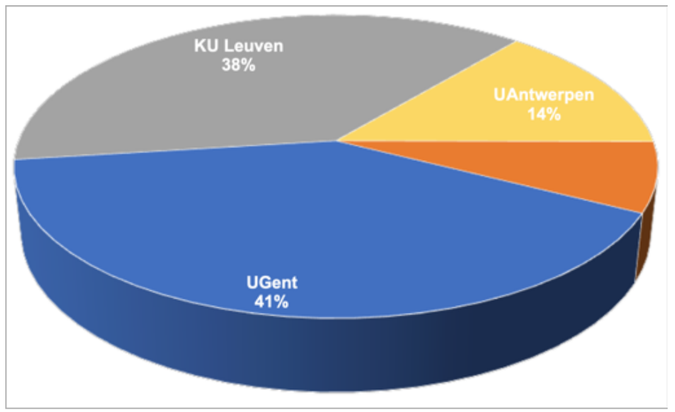
*Feb 2018*




*June 2018*




*Oct 2018*

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# TIER-1 ACCESS – STARTING GRANT

https://www.vscentrum.be/en/access-and-infrastructure/tier1-starting-grant

- Purpose = explore, do scaling tests of your software, prepare for project
- **500 node days** (= 500 x 28 x 24 = 336.000 core hours)
- Available for **4 months**
- Personal grant
- Fast submission procedure, very short proposal
- Constantly reviewed
- Success rate = 100%

- FREE OF CHARGE

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# TIER-1 ACCESS – PROJECT ACCESS

https://www.vscentrum.be/en/access-and-infrastructure/project-access-tier1

- 500 - 5000 node days (= 336.000 – 3.360.000 core hours)
- **Upper limit may be exceeded if justification is provided**
- Can be granted to multiple researchers
- Available for **8 months**
- Reviewed 3x per year by Tier-1 Evaluation Committee
  - Deadlines in 2109:
    - 4 Feb
    - 3 June
    - 7 Oct
- Success depends on quality of your proposal
  - Send your proposal to hpc@ugent.be for prior review

- FREE OF CHARGE

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# VSC - FUTURE PLANS

- New website
- LinkedIn - https://www.linkedin.com/company/vschpc/



Contact hpc@ugent.be if you want to contribute

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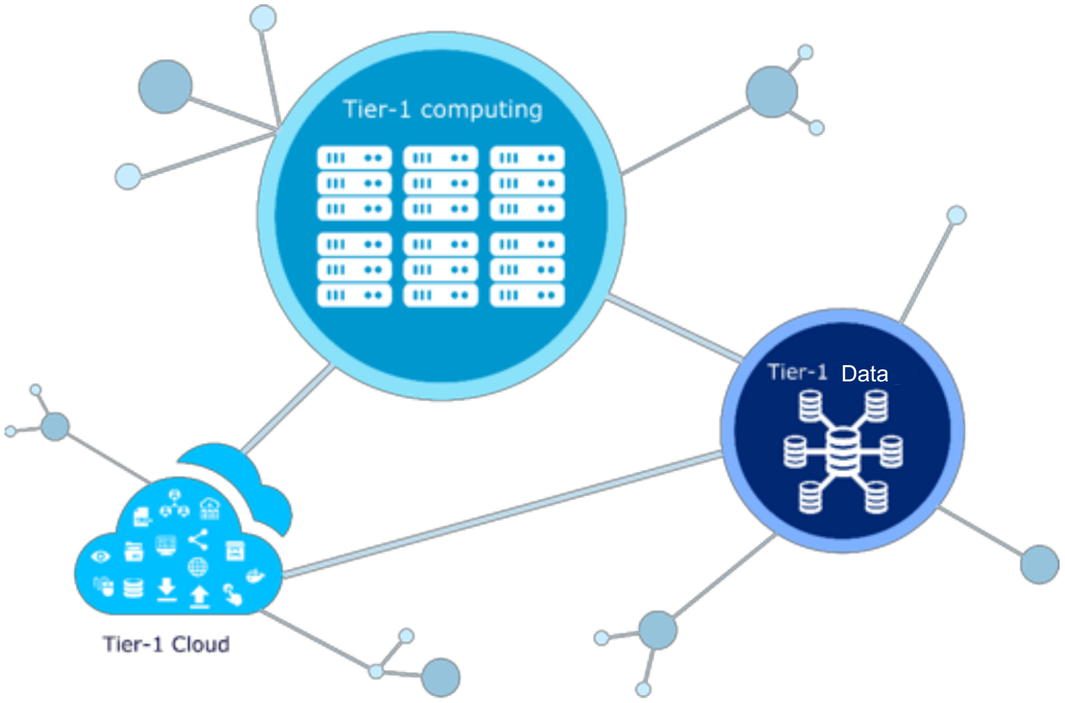
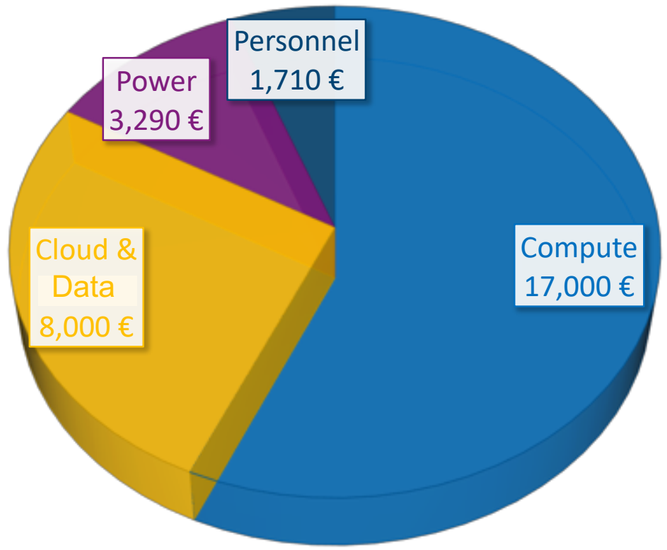
# VSC - FUTURE PLANS

## Tier-1 impulse investment - “Supercomputing as a service” platform



**2018 - 2022**

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# VSC - FUTURE PLANS

## Tier-1 impulse investment - “Supercomputing as a service” platform

### 2019


### End 2020

**New Tier-1 installation**

**~ 7 Meuro**

### 2022

**Upgrade Tier-1 installation**

**~ 5 Meuro**

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# PROGRAM

- (13h00: Optional tour of datacenter)
- 14h00: Overview of HPC-UGent usage, status of the VSC, future plans
- 14h30: Review of user poll results, Q&A
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- 16h15 - 18h00 Networking reception & poster session

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# REVIEW OF USER EVALUATION

- 93 respondents
- Average completion time: 3 minutes

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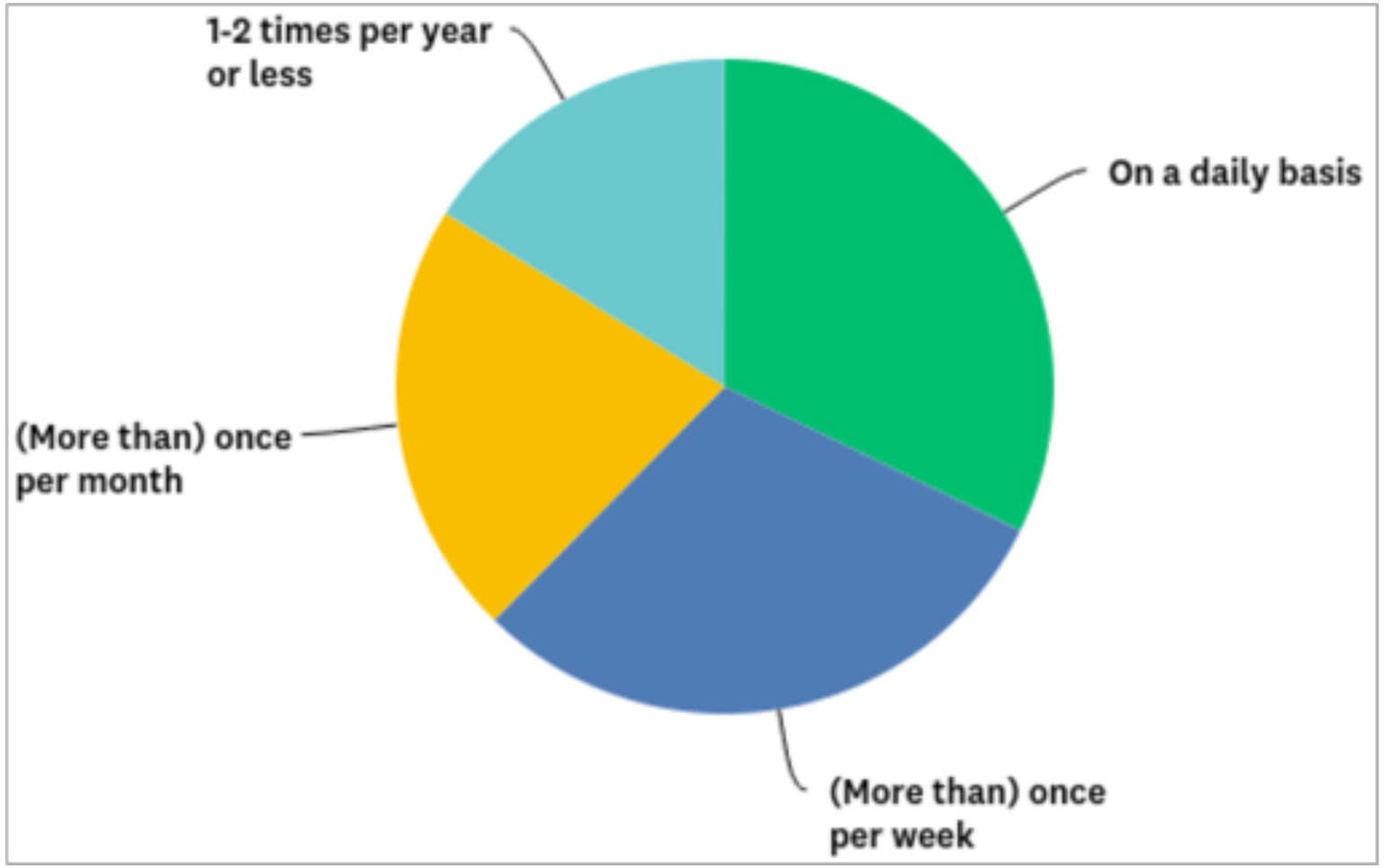
# REVIEW OF USER POLL RESULTS

## How often do you use HPC-UGent?

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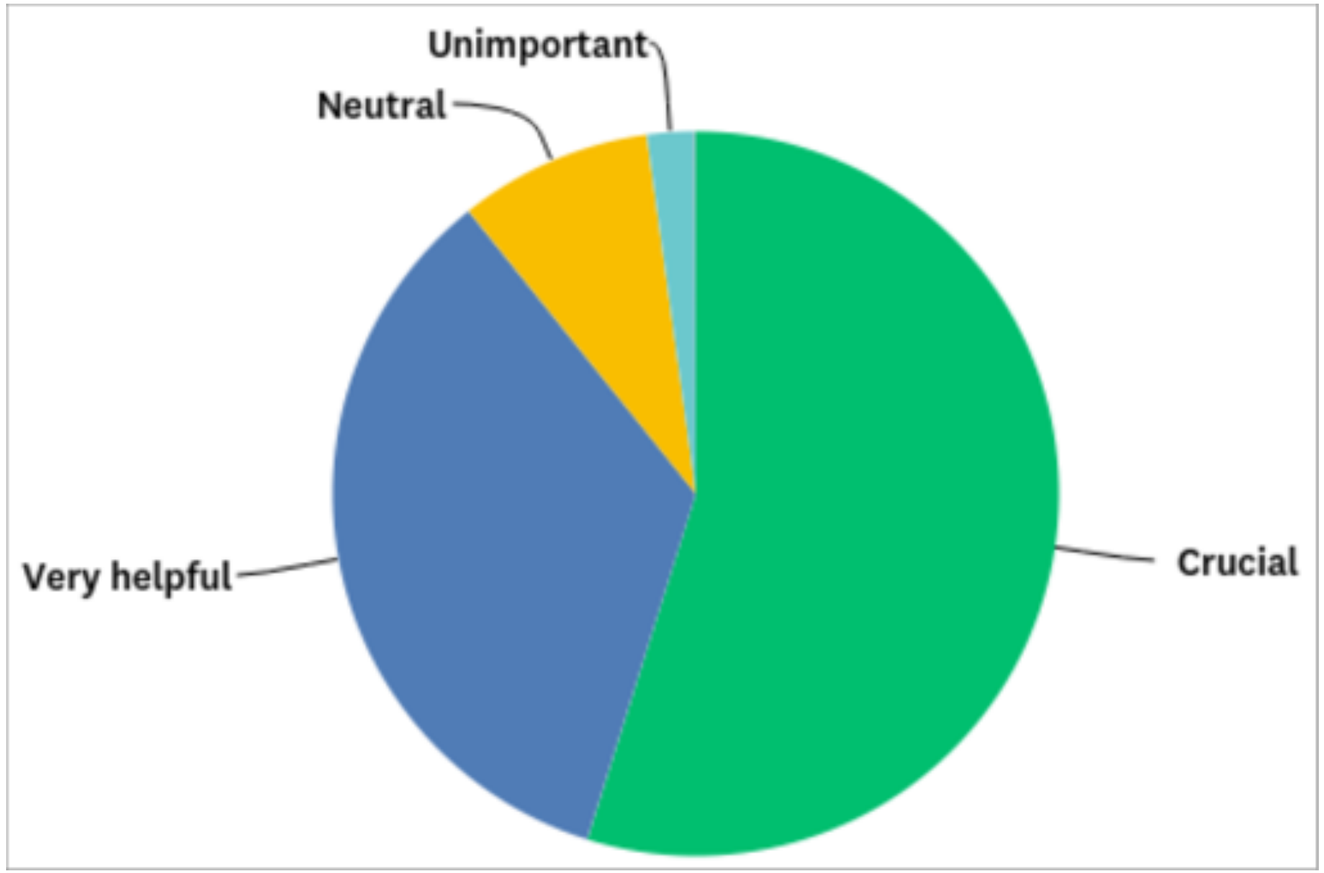
# REVIEW OF USER POLL RESULTS

**How important is HPC-UGent for your research?**




89% Very helpful or crucial to research

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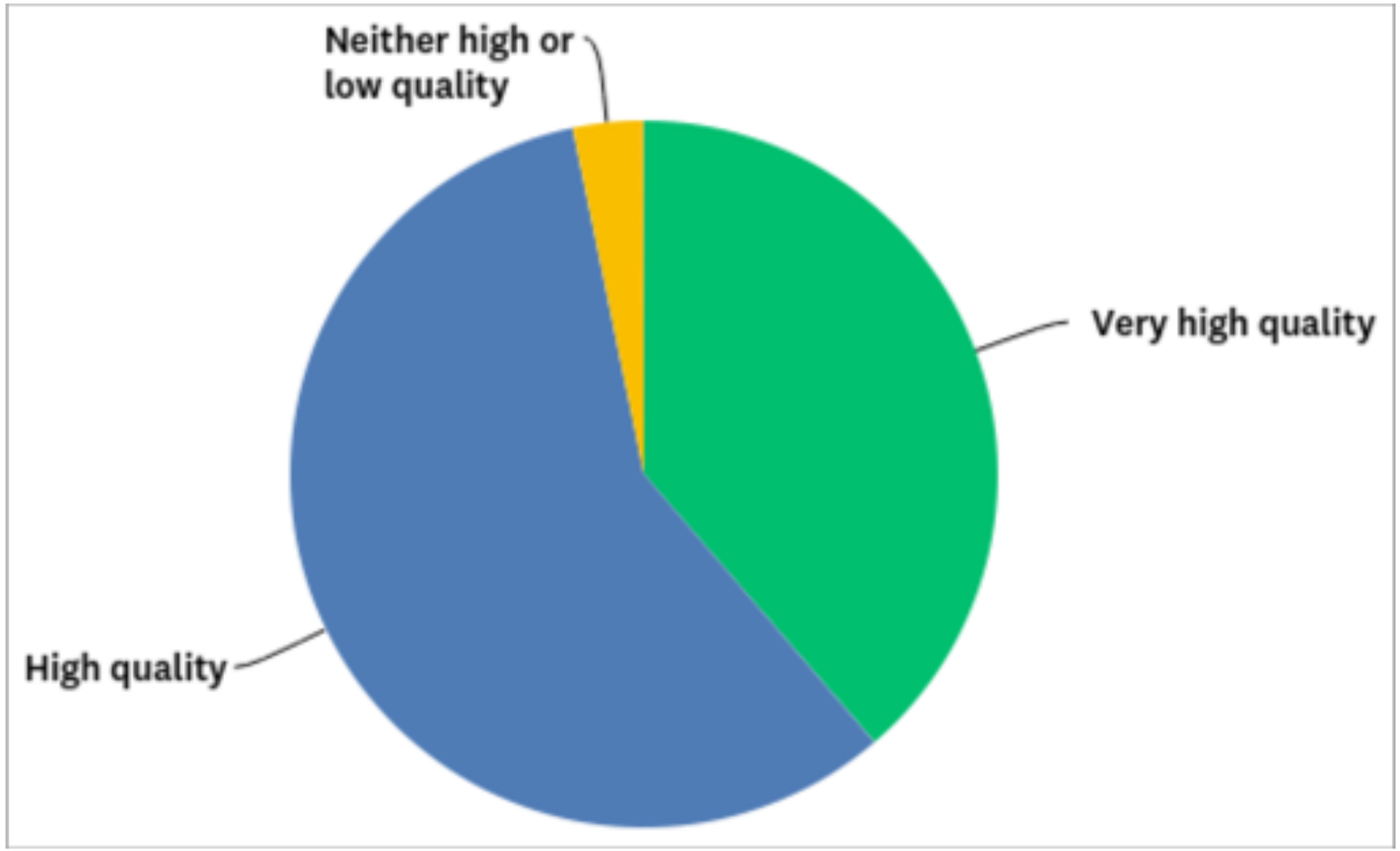
# REVIEW OF USER POLL RESULTS

**How would you overall rate the services that HPC-UGent provides?**




97% High quality or better

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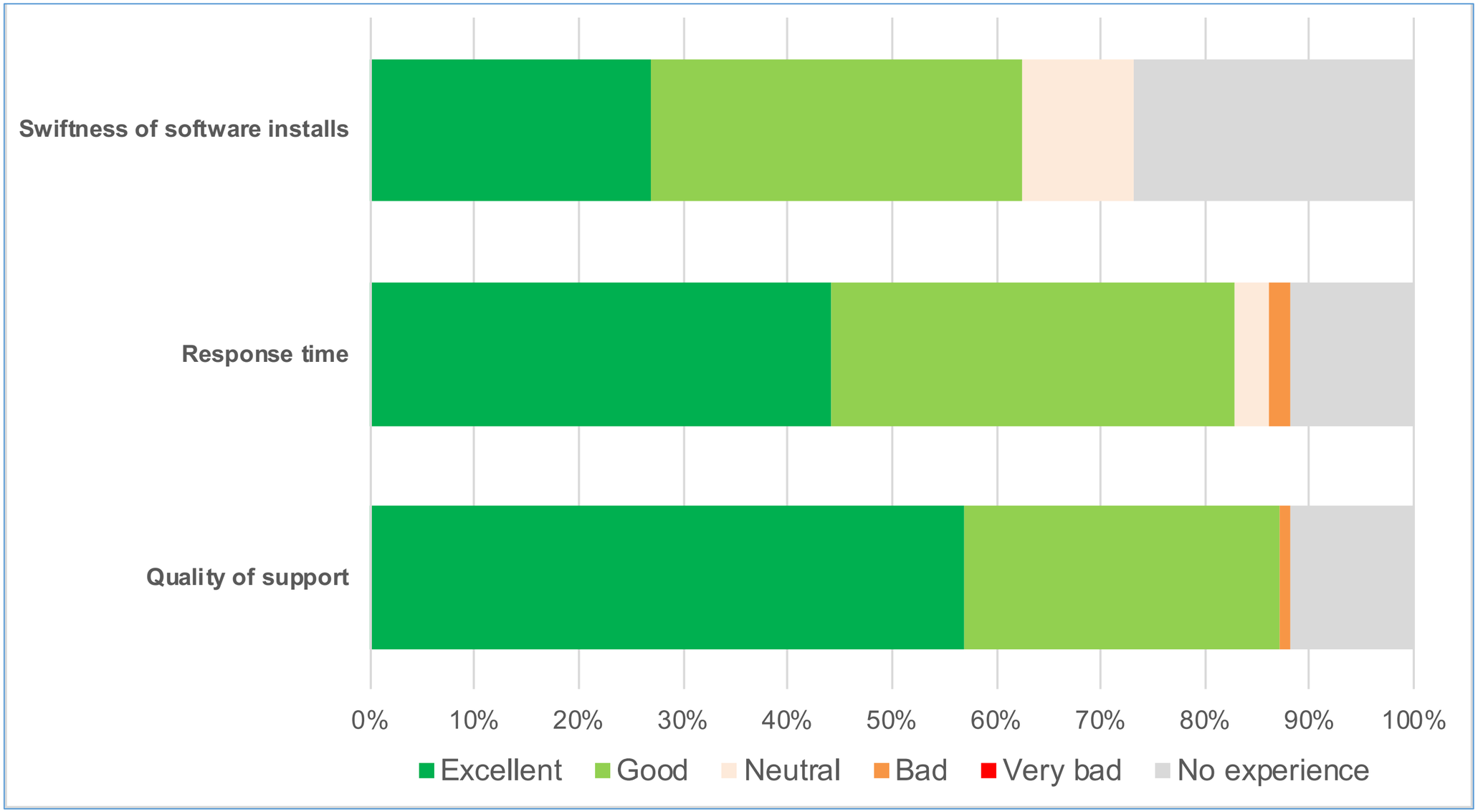
# REVIEW OF USER POLL RESULTS

## Rate aspects of HPC-UGent user support:

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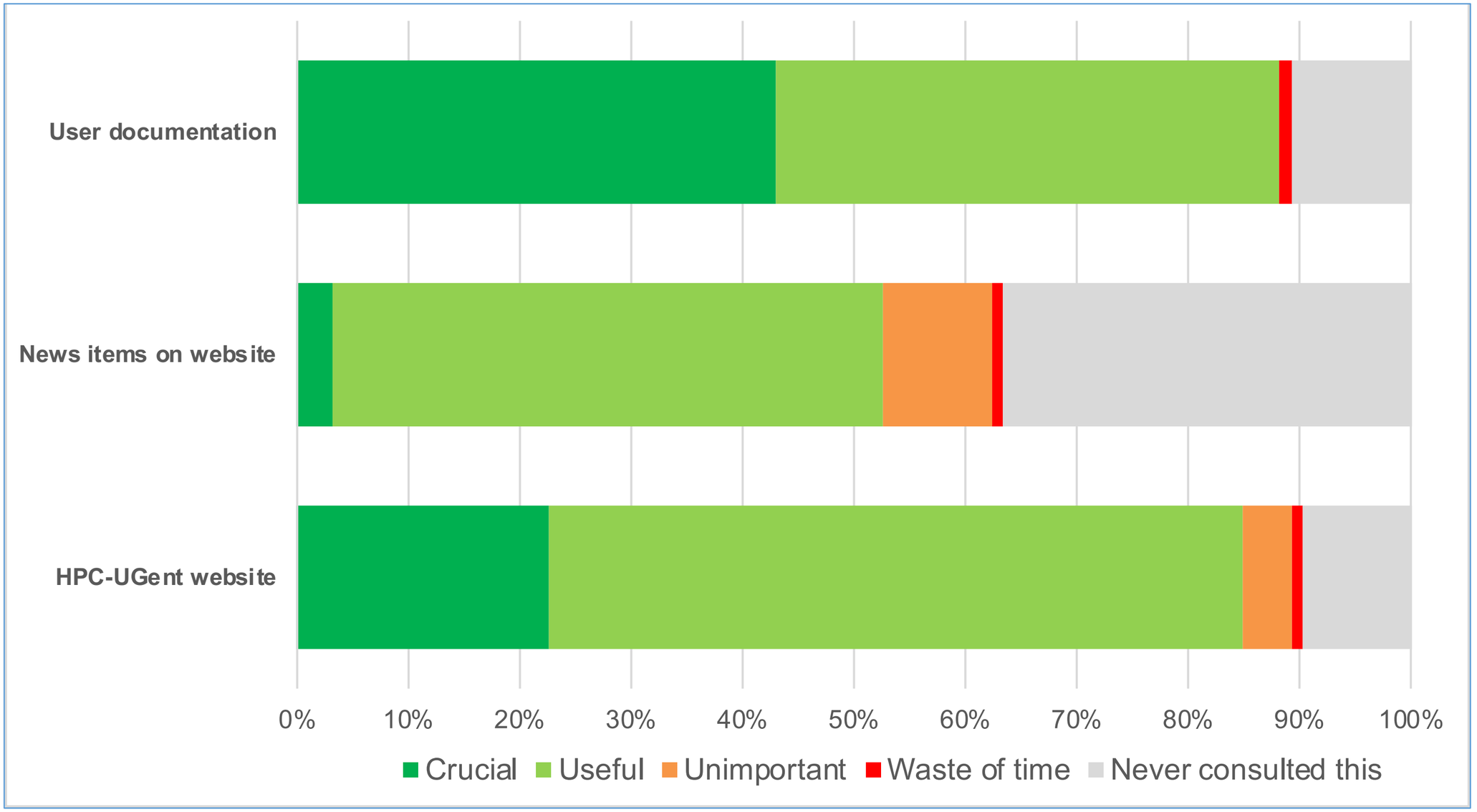
# REVIEW OF USER POLL RESULTS

## Rate aspects of HPC-UGent documentation sources:

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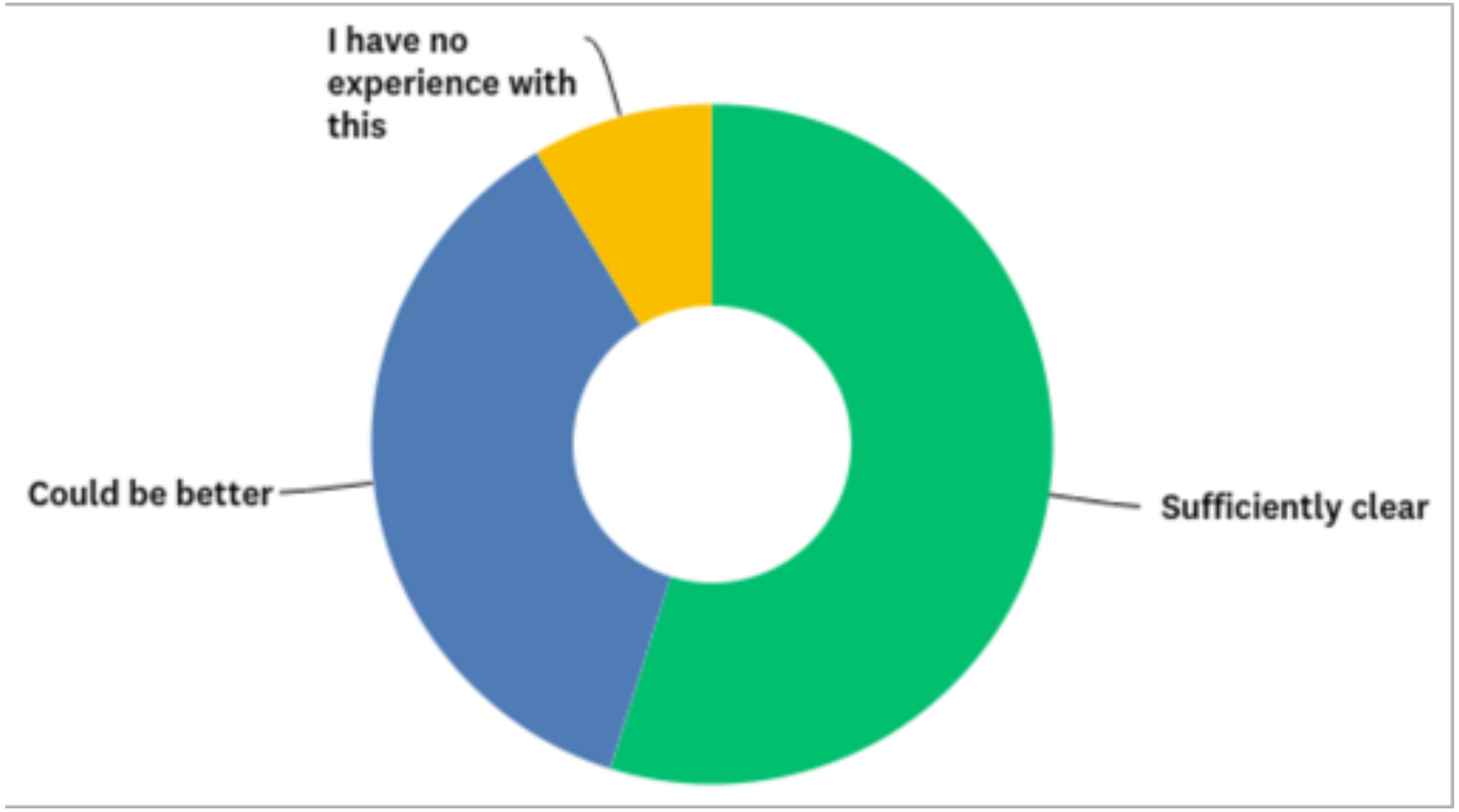
# REVIEW OF USER POLL RESULTS

**Is the purpose of the diverse compute clusters sufficiently clear?**

- multi-node jobs: skitty, swalot, golett, delcatty, phanpy
- single-node jobs: victini
- big memory jobs: phanpy




Only clear enough for 55 %

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# REVIEW OF USER POLL RESULTS

**Is the purpose of the diverse compute clusters sufficiently clear?**

| | Cluster name | #nodes | CPU per node | Memory per node | Interconnect |
|---|---|---|---|---|---|
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Big memory jobs

Multi-node jobs

Single-node jobs

Only clear enough for 55 %

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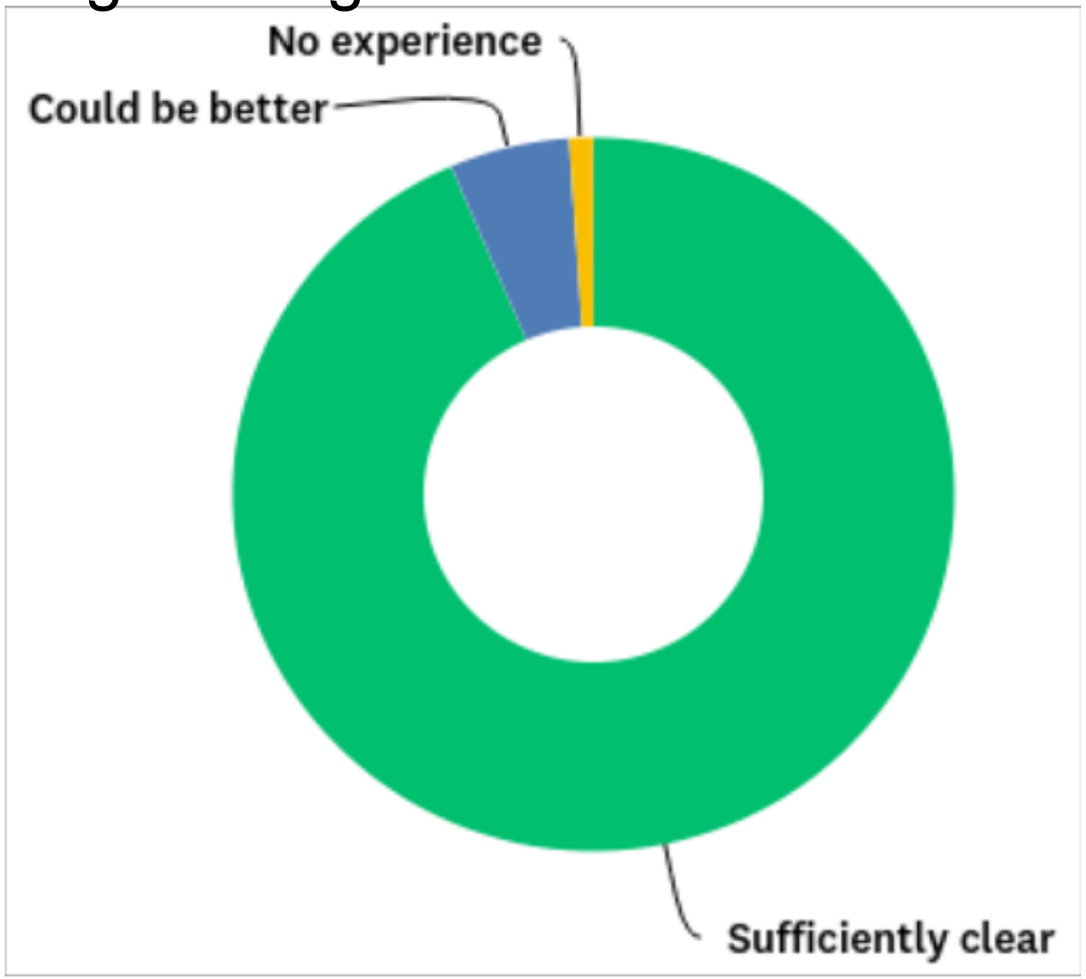
# REVIEW OF USER POLL RESULTS

**Is our communication w.r.t. maintenance/downtime sufficiently clear?**

- via VSC status page
- message-of-the-day login message on login nodes
- mail to hpc-announce

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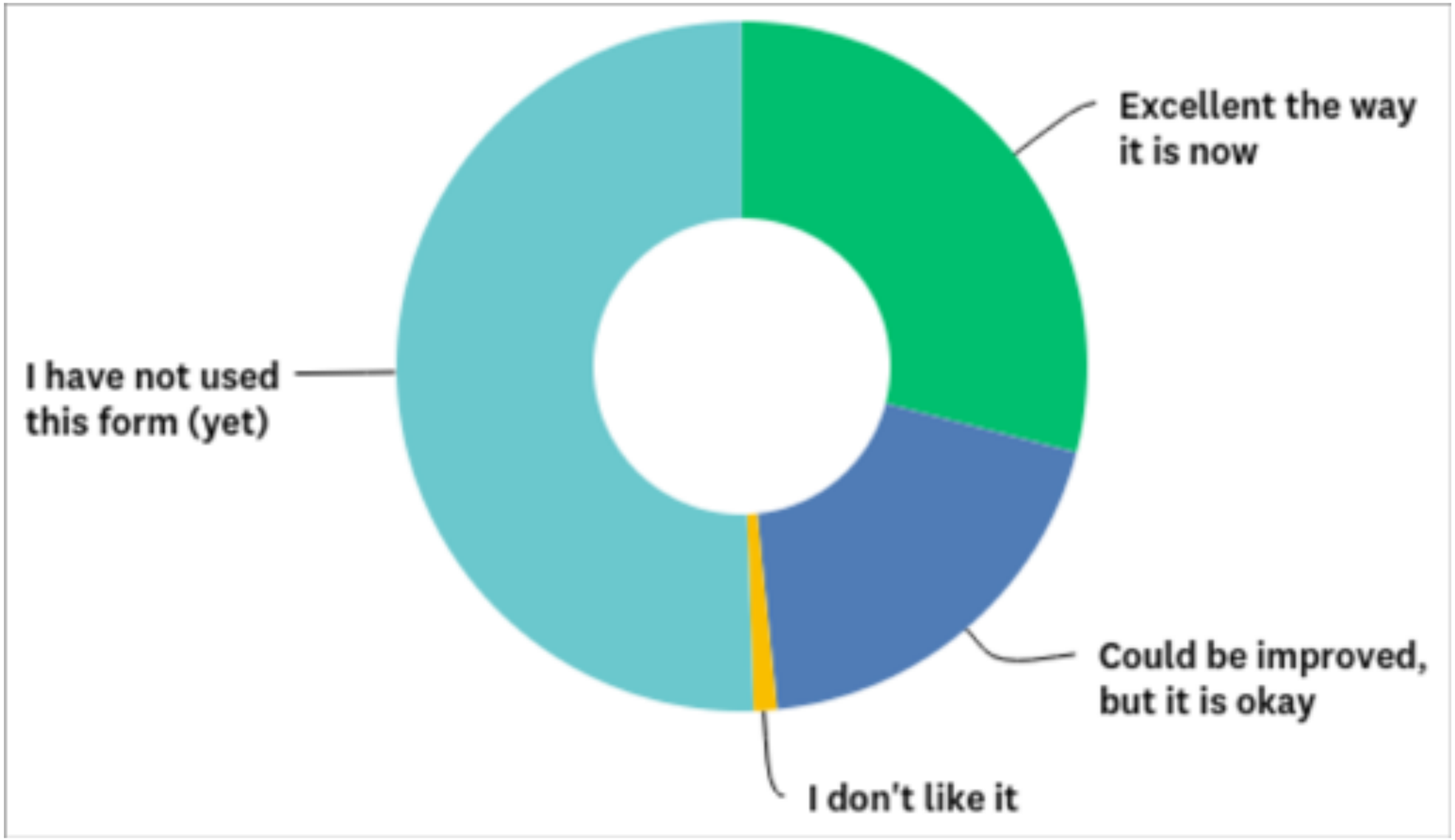
# REVIEW OF USER POLL RESULTS

**How do you like the form for software installation requests?**

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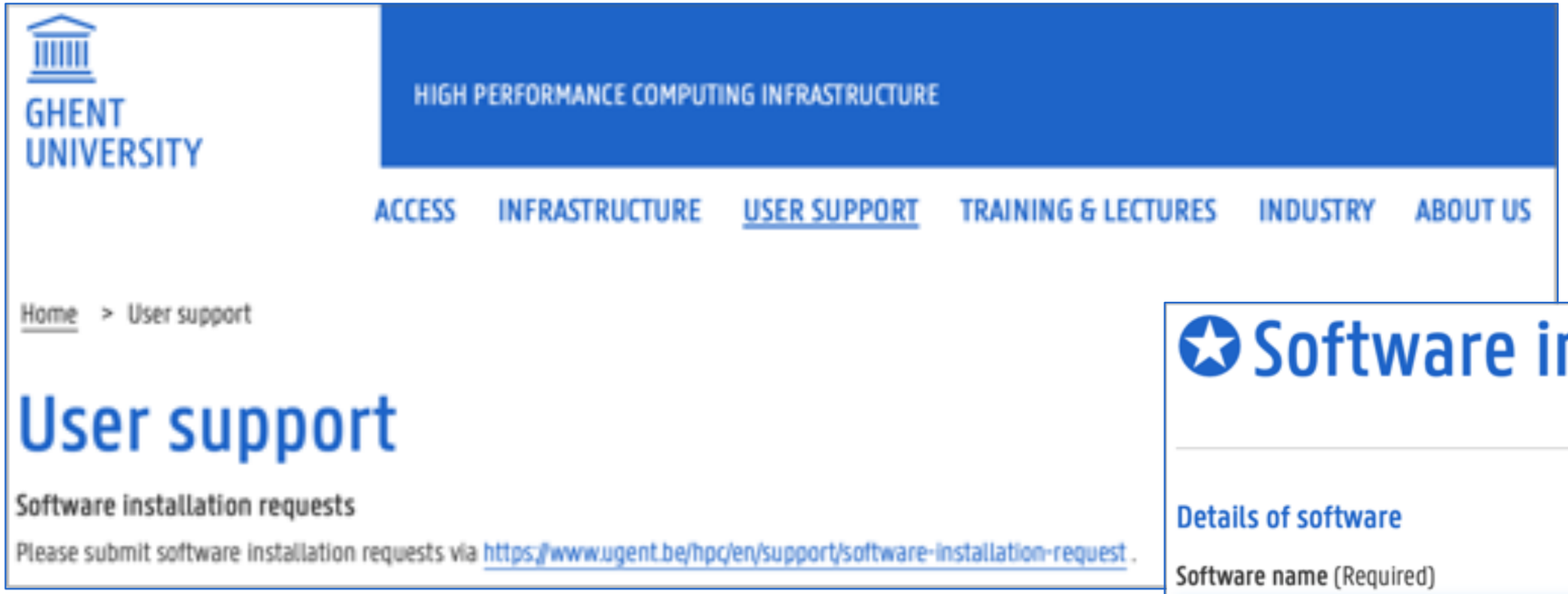
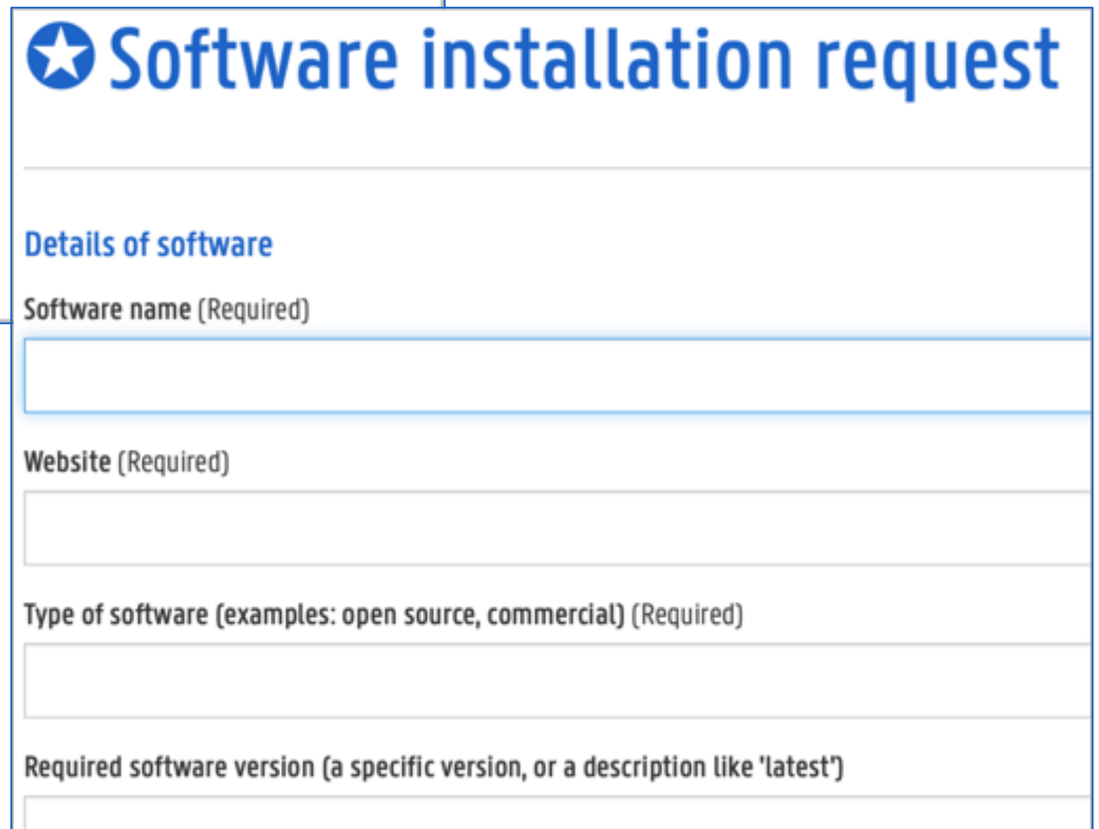
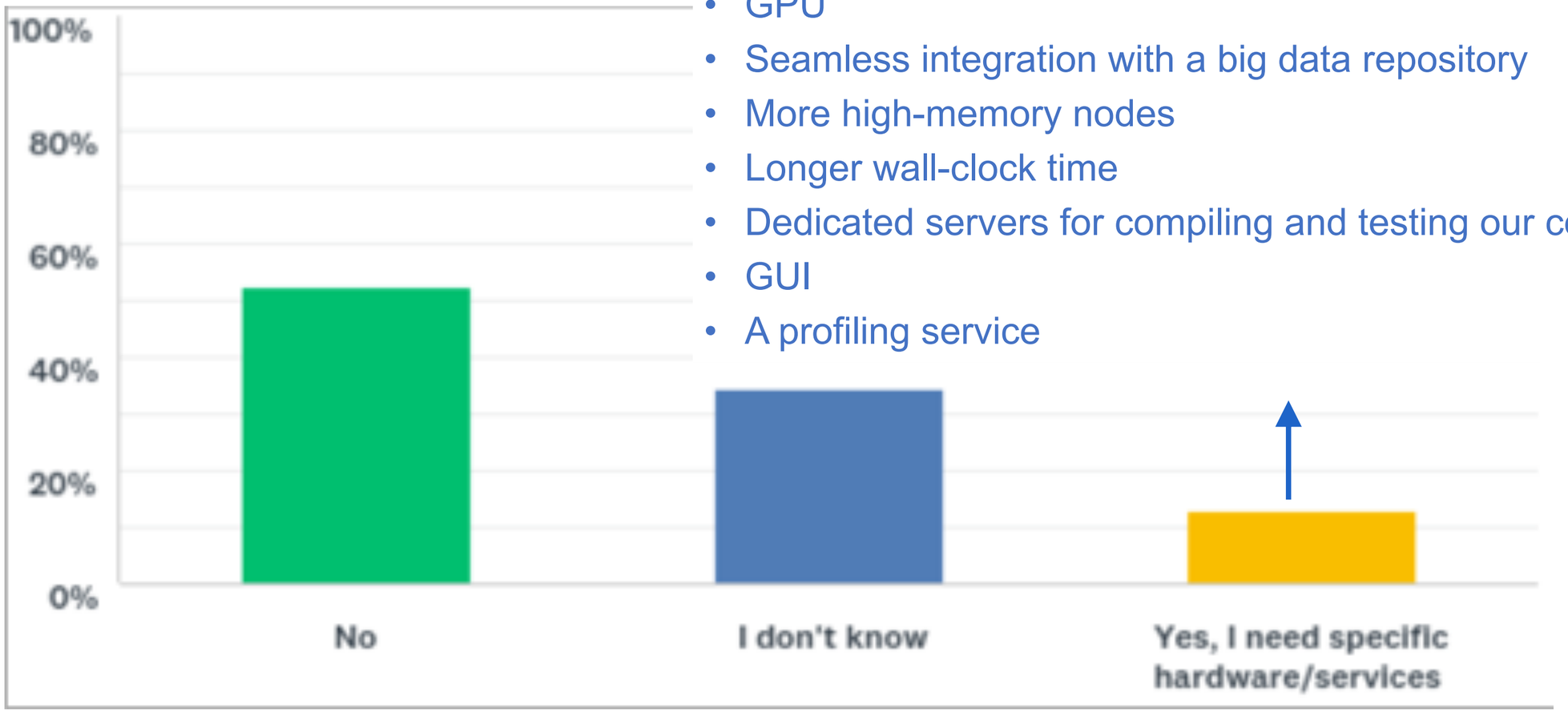


# REVIEW OF USER POLL RESULTS

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




- GPU
- Seamless integration with a big data repository
- More high-memory nodes
- Longer wall-clock time
- Dedicated servers for compiling and testing our code
- GUI
- A profiling service

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# REVIEW OF USER POLL RESULTS

**How could we further improve HPC-UGent services?**

Documentation

- Expert items from the (defunct) userwiki, e.g. compile Java programs
- Documentation better geared towards beginners
- Update and expand HPC manual
- More hands-on experience
- Monthly Q&A session
- Graphical scheme of clusters and storage organization

# REVIEW OF USER POLL RESULTS

**How could we further improve HPC-UGent services?**

User experience

- Shorter queue times
- Way to estimate queue time
- Quota overview page of all clusters, including Tier-1 scratch quota
- Longer wall-clock time

Infrastructure

- More clusters
- GPU

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# REVIEW OF USER POLL RESULTS

**How could we further improve HPC-UGent services?**

Data

- Faster data transfer across campus
- Easier sharing of data between users collaborating on a project
- Lower latency on shared file systems
- VSC-wide shared storage capabilities, shared between institutes
- More storage volume per user

Training

- More programming courses

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# REVIEW OF USER POLL RESULTS

**How could we further improve HPC-UGent services?**

Policy

- Higher priority for multi-node jobs on MPI clusters

Software

- Possibility to perform MATLAB calculations on multiple nodes

User support

- Speed up software installation
- Debugging and profiling of codes as a service

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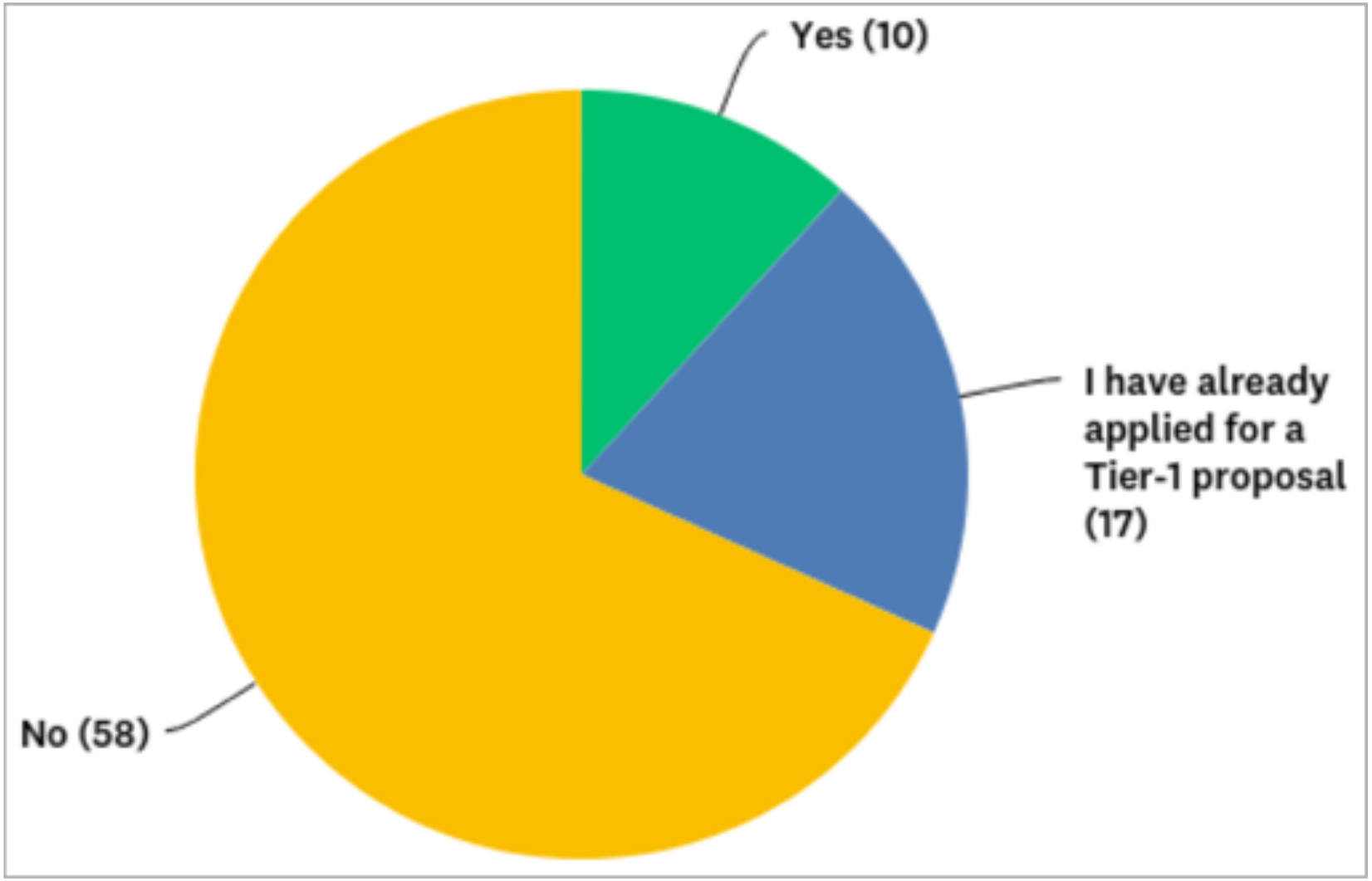
# REVIEW OF USER POLL RESULTS

**Would you be interested in applying for a Tier-1 proposal?**

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Dr. Ewald Pauwels
Scientific coordinator HPC @ Ghent University
Vice-coordinator VSC

HPC-UGent

E hpc@ugent.be

www.ugent.be/hpc

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