

# ANNUAL REVIEW HPC-UGENT

2021



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# 1 ABOUT HPC-UGENT

**In scientific computing\*, computers are used to solve complex problems. (\*aka: supercomputing or high-performance computing - HPC)**

## 1.1 Our mission

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

HPC-UGent is part of the central ICT department of Ghent University, and is a strategic partner of the Flemish Supercomputer Center (VSC - <http://vscentrum.be/>).

## 1.2 Our vision

HPC-UGent offers a professional scientific computing environment that is stable, user-friendly, and serves the diverse purposes of researchers from Ghent University, industry and other research institutions.

We provide a structural training curriculum for new and advanced users, and provide supporting course material.

We present a supercomputing portfolio that is well known within Ghent University and beyond, and we establish ourselves in the international community via contributions to centralised solutions, such as EasyBuild (<https://easybuild.io>).

## 1.3 Personnel

In 2021, the HPC-UGent team consists of 9 people:

Álvaro Simón García, Andy Georges, Ewald Pauwels, Kenneth Hoste, Kenneth Waegeman, Stijn De Weirdt, Wouter Depypere, Balázs Hajgató and Bart Verheyde.

Tasks include:

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

Additionally, several consultants (Inuits) are also regularly engaged to help solve software installation requests, for OpenStack Cloud and sysadmin expertise and for python expertise: Pavel Grochal, Jakub Zárýbnický, Denis Kristak, Peter Hardon, Martin Sakin.

## 2 INFRASTRUCTURE

### 2.1 Overview

The Ghent University compute infrastructure (Tier-2) consists of several specialised clusters, jointly called Stevin, hosted in the S10 datacenter.

In 2021, the following changes to the Tier-2 infrastructure were applied:

- Cluster *doduo* was taken in production. This is an AMD-based CPU cluster with an HDR-100 InfiniBand network supporting MPI jobs. It replaces cluster *golett* which was decommissioned in 2020.
- Cluster *phanpy* reached its end of life and was taken offline. The big-memory functionality of this cluster is maintained by active cluster *kirlia*.
- New GPU cluster *accelgor* was initialized and introduced for testing by selected pilot users.
- New job command wrappers were introduced (`qsub`, `qstat`, `qdel`, etc.) on all Tier-2 clusters as a frontend to the Slurm scheduler system. These job wrappers largely follow the Torque PBS way of submitting jobs (this job scheduler was abandoned), which are heavily used in the user documentation. These wrappers will allow HPC-UGent to facilitate maintainability, and to more easily support additional features in the future.

Beyond the Tier-2 level, HPC-UGent devoted **a lot** of time in 2021 to preparing and maintaining infrastructure for the Flemish Supercomputer Center VSC at the Tier-1 level. Over the last few years, the VSC has been gradually reworking its offer of infrastructure components, including Data and Cloud in addition to more ‘traditional’ Compute infrastructure.

Two new components are being hosted by Ghent University and considerable effort from the HPC-UGent team has gone into their development:

- VSC Tier-1 Cloud component  
This Infrastructure as a Service platform enables ‘on-demand’ resources in a more flexible and cloud-like manner for power users that can deploy resources such as virtual machines and storage systems, and adapt these to their scientific use case. The system was officially taken in production in a product launch on 20 May 2021. <https://www.vscentrum.be/cloud>
- VSC Tier-1 Compute component ‘Hortense’  
This is the new Tier-1 HPC system of the VSC, designated follow-up for Tier-1 system BrENIAC. Majority of effort in 2021 went into meetings with the vendor, legal actions and dealing with a.o. COVID-19 related delays in getting the system ready.  
Pilot access to Tier-1 system Hortense was opened on 23 November 2021. <https://www.vscentrum.be/compute>

More information on the actions and developments for these VSC components are provided in the VSC year report 2021: <https://www.vscentrum.be/publications>

## 2.1.1 Compute clusters

Cluster name	#nodes	CPU / GPU per node	Usable memory per node	Local disk per node	Network interconnect
<b>Phanpy</b>	16	2 x 12-core Intel E5-2680v3 (Haswell-EP @ 2.5 GHz)	480 GiB  Decommissioned on 18 March 2021	3 x 400 GB (SSD, striped)	FDR InfiniBand
<b>Swalot</b>	128	2 x 10-core Intel E5-2660v3 (Haswell-EP @ 2.6 GHz)	116 GiB	1 TB	FDR InfiniBand
<b>Skitty</b>	72	2 x 18-core Intel Xeon Gold 6140 (Skylake @ 2.3 GHz)	177 GiB	1 TB	EDR InfiniBand
<b>Victini</b>	96	2 x 18-core Intel Xeon Gold 6140 (Skylake @ 2.3 GHz)	88 GiB	1 TB	10 Gb ethernet
<b>Joltik</b>	10	2 x 16-core Intel Xeon Gold 6242 (Cascade Lake @ 2.8 GHz)  4x NVIDIA Volta V100 GPUs (32GB GPU memory)	256 GiB	800 GB SSD	Double EDR InfiniBand
<b>Kirlia</b>	16	2 x 18-core Intel Xeon Gold 6240 (Cascade Lake @ 2.6 GHz)	738 GiB	1.6 TB NVME	HDR-100 InfiniBand
<b>Doduo</b>	128	2x 48-core AMD EPYC 7552 (Rome @ 2.2 GHz)	250 GiB  In production on 6 April 2021	180 GB SSD	HDR-100 InfiniBand
<b>Accelgor (pilot)</b>	9	2x 24-core AMD EPYC 7413 (Milan @ 2.2 GHz)  4x NVIDIA Ampere A100 GPUs (80GB GPU memory)	500 GiB	180 GB SSD	HDR-100 InfiniBand



## 2.1.2 Shared storage

Partition	Total storage space
<b>\$VSC_HOME</b>	90 TB
<b>\$VSC_DATA</b>	1.9 PB
<b>\$VSC_SCRATCH</b>	1.7 PB
<b>\$VSC_SCRATCH_KYUKON</b>	
<b>\$VSC_SCRATCH_ARCANINE</b>	70 TB NVME

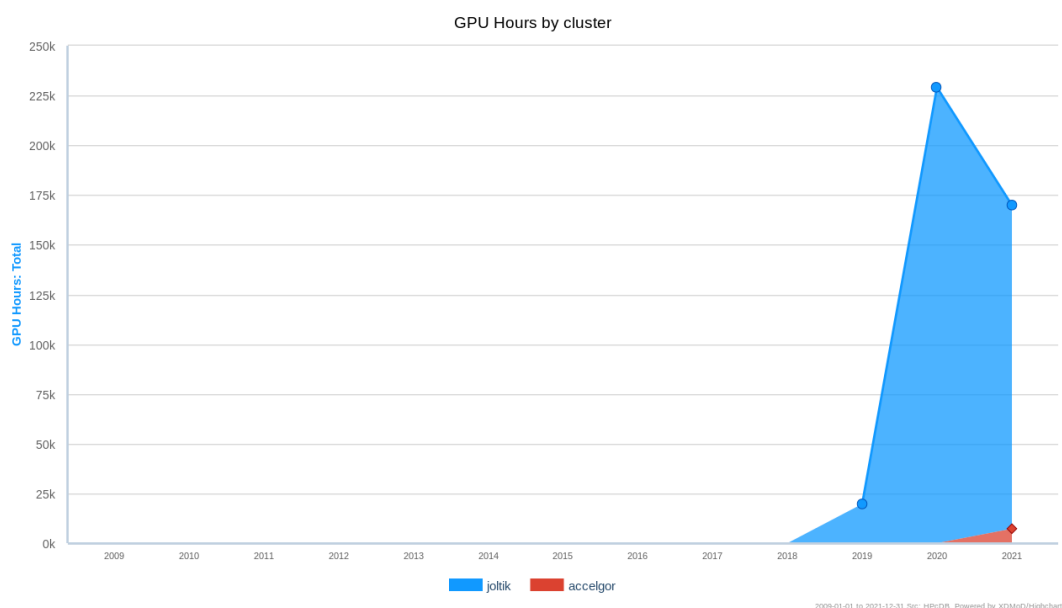
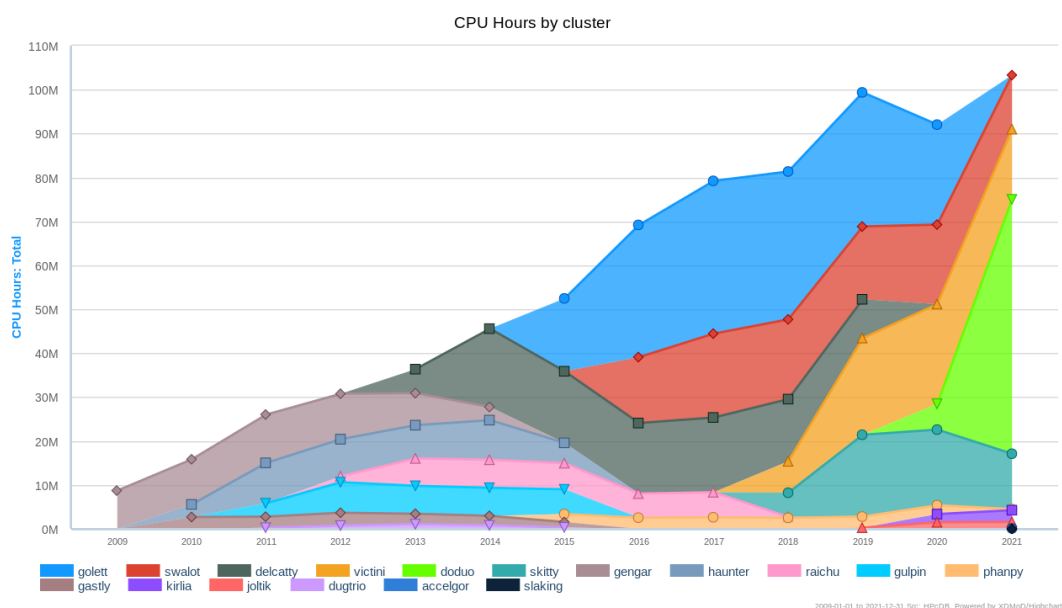


## 2.2 Usage

In the graphs below, the used or available compute time on the compute clusters is typically expressed in *CPU hours* or *GPU hours*.

- 1 GPU hour corresponds to the work done by a graphical processing unit for one hour of time.
- Modern CPU processors contain many cores that are capable of running a computational task. Since the number of cores varies a lot between processor types and production years, 1 CPU hour is used here to mean the work done by one core in a CPU processor for one hour of time.

### 2.2.1 Historical perspective on used compute time



These plots give a historical perspective on the amount of compute time that is used every year, coloured according to the cluster that does the work. All clusters together, since the start in 2009, have now produced more than 740 million CPU core hours (equivalent to 84.506 years of compute work on one core) and 419 thousand GPU hours.

## 2.2.2 Consumed compute time in 2021

### 2.2.2.1 Consumed compute time per compute cluster

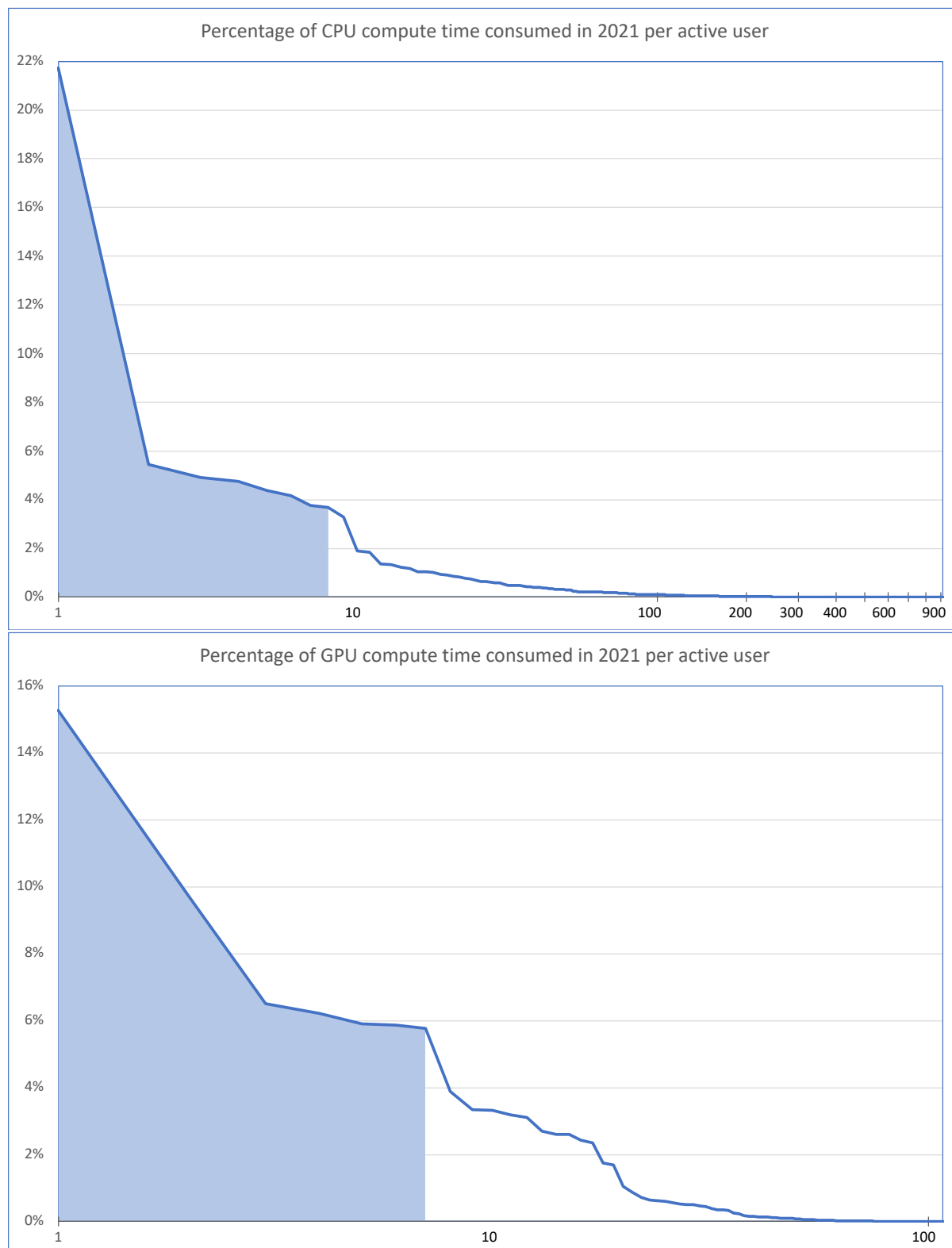
Cluster name	Compute time consumed		Effective use percentage	
	<i>CPU hours</i>	<i>GPU hours</i>	<i>CPU</i>	<i>GPU</i>
<b>Phanpy</b>	242 117		34%	
<b>Swalot</b>	16 066 093		72%	
<b>Skitty</b>	16 632 156		73%	
<b>Victini</b>	20 292 526		67%	
<b>Kirlia</b>	3 540 566		70%	
<b>Doduo</b>	77 542 561		72%	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

In 2021, a total of 136 822 484 CPU core hours (this corresponds to 15 619 core years) and 252 205 GPU hours have been consumed on the Tier-2 compute clusters of Ghent University.

The effective use percentage expresses how much of the theoretically available compute power in one year ( $\#nodes \times \#cores/node$  or  $\#GPUs/node$ ) was used. Downtimes were not taken into account, so the percentages represent a lower bound.



## 2.2.2.2 Consumed compute time versus active users



In 2021, 915 persons actively used CPU compute time on the Tier-2 compute clusters of Ghent University, 109 persons actively used GPU compute time. Both for CPU and GPU, the user base typically contains a limited number of power users in addition to regular users with a lower usage profile. The plots above graph per user (x axis) what percentage of all compute time produced in 2021 this user consumed. The blue area indicates the 50% level of all Tier-2 CPU/GPU compute time consumed.

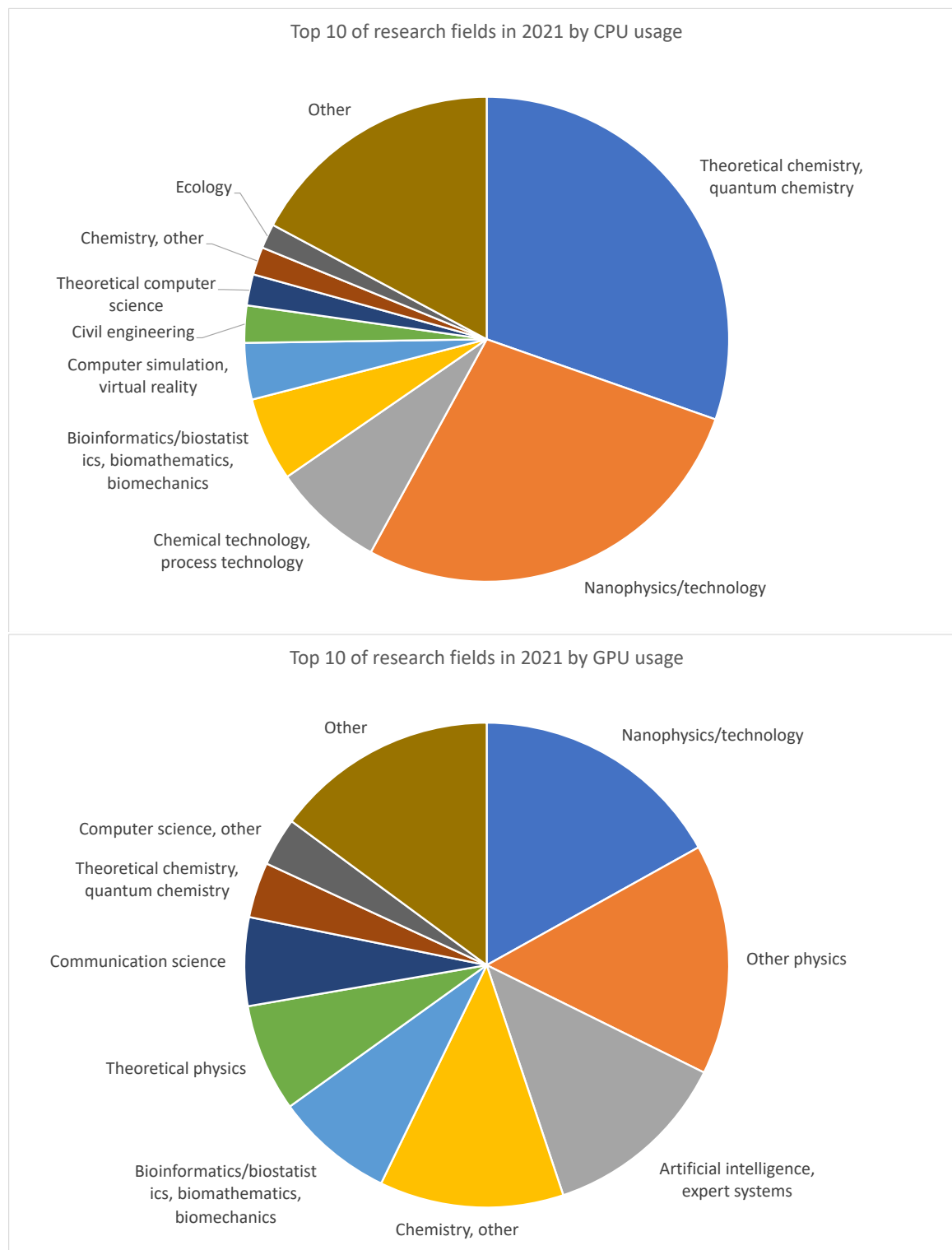
Everyone can get access to the Tier-2 compute clusters of Ghent University. The conditions that apply depend on the affiliation of the researcher. Researchers affiliated with Flemish university associations (constituting the Flemish Supercomputer Center – VSC) get free access. Other Flemish or federal research institutes can get access for their researchers on a contract basis, with 1500 euro worth of compute time given out free of charge per year. Industry can buy compute time in a pay-what-you-use model.

Breakdown of consumed compute time by affiliation		
	<i>CPU time</i>	<i>GPU time</i>
<b>UAntwerpen</b>	0.10%	0.01%
<b>VUB</b>	0.39%	2.68%
<b>UGent</b>	98.62%	96.86%
<b>KULeuven / UHasselt</b>	0.51%	0.00%
<b>Other research institutes</b>	0.30%	0.00%
<b>Industry</b>	0.08%	0.46%
<b>Total</b>	<b>100.00%</b>	<b>100.00%</b>

Master or Bachelor students enrolled in a Flemish university association can also get access to the Tier-2 compute clusters of Ghent University. Several teachers effectively rely on the infrastructure for training purposes, stimulating several students to become a user. Master students often rely on the infrastructure to perform research included in their Master thesis.

Number of students/researchers versus breakdown of consumed compute time by category		
	<i>CPU time</i>	<i>GPU time</i>
<b>Ma/Ba students</b>	17.55%	11.83%
<b>Researchers</b>	82.45%	88.17%
<b>Total</b>	<b>100.00%</b>	<b>100.00%</b>

### 2.2.2.3 Consumed compute time versus research field



These are the research fields that users enter when requesting their account to access HPC-UGent resources. No doubt, there is overlap between certain fields and some users have not listed a research field at all. As such, the above distributions merely gives an indication of the top research fields that actively use scientific computing, and which ones actively use either CPU or GPU resources.

## 3 TRAINING AND SUPPORT

### 3.1 Training overview and evaluations



The COVID-19 pandemic, but mostly all the work required to deliver the VSC Tier-1 Compute and Cloud components considerably impacted the possibility and resources to organize trainings in 2021.

#### 3.1.1 PRACE OpenFOAM Seasonal School

Trainer: Matej Forman (OpenFOAM training coordinator, ESI Group)

This course was co-organized by PRACE, KU Leuven and Ghent University. All sessions took place online. A host of national and international attendants took part, making use of the HPC-UGent infrastructure for the hands-on sessions.

Date	#participants
20/04/2021	30
21/04/2021	
27/04/2021	
28/04/2021	

Not enough feedback was received via a poll to perform a significant quantitative analysis. Some participants took the time to send a personal review of the course, providing more direct meaningful feedback.

One representative review:

*“Overall I find the course very useful, informative. Starting from the registration process, creating an account on the server and during the session all the technical problems were solved by the UGent HPC team and they were very supportive with the prompt response.”*

*“Course mentor was an expert in his domain that had helped to understand the details of the OpenFoam software. It was well defined and the content was well*

*distributed. I have achieved the 4 points goal which mentor asked at the beginning of the course.”*

*“There are no critics as such, but the mentor can update the presentation to include the more recent changes in the software versions. I will definitely attend [an] advanced course if it is offered in near future.”*

Country/institute of participants		
Belgium	23	
KU Leuven		8
UAntwerpen		1
UGent		8
ULB		4
VIB		1
VKI		1
Czech Republic	1	
Czech Technical University Prague		1
Germany	1	
Greece	1	
National and Kapodistrian University of Athens		1
Spain	1	
Jaume I University		1
Turkey	3	
Middle East Technical University		2
Sivas University of Science and Technology		1
<b>Total</b>	<b>30</b>	

## 3.2 Lectures and community meetings

### 3.2.1 Tier1 information session

Learn more about the VSC Tier-1 infrastructure and how to write a good proposal.

Date	#participants
11/01/2021	28

### 3.2.2 HPC-UGent user meeting

Purpose of this meeting is to inform all users about future plans for the HPC-UGent infrastructure, and to bring together users and the HPC-UGent team.

Featured presentations

- Ewald Pauwels, HPC-UGent  
“Overview of HPC-UGent activities, future plans, VSC opportunities”  
“Review of user poll results, Q&A”

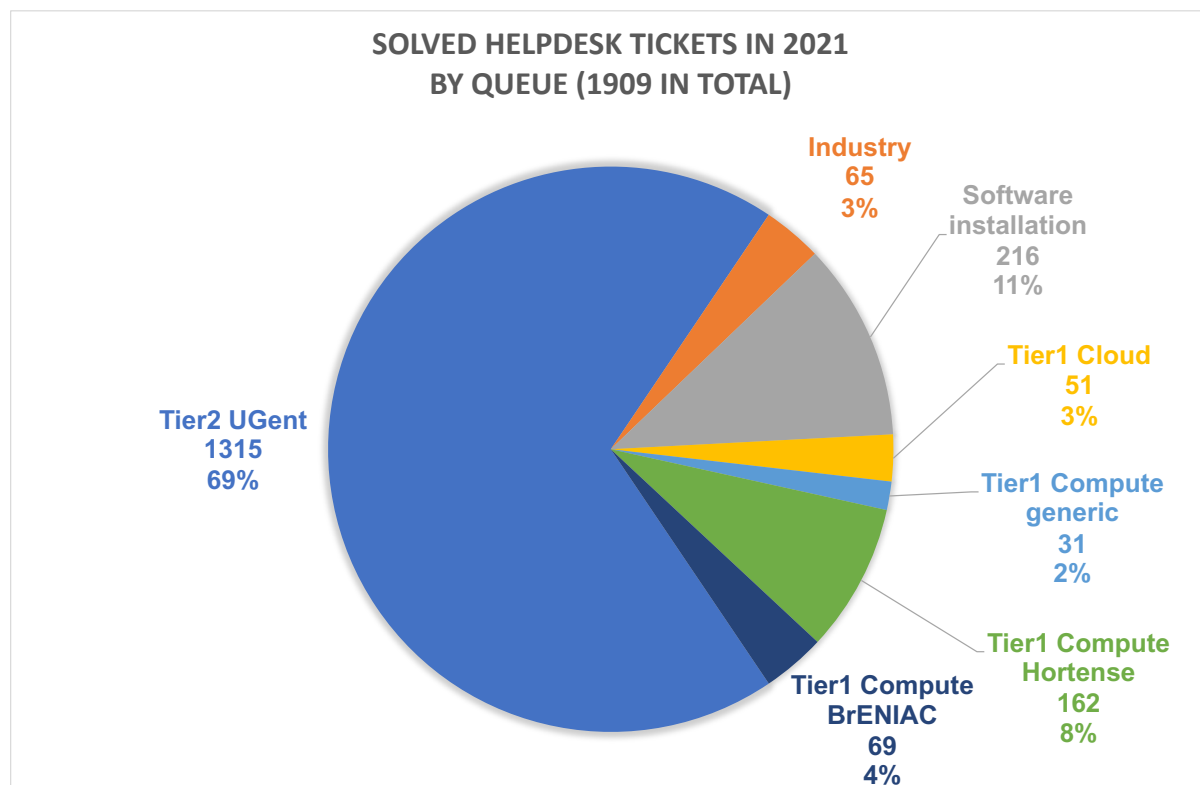
- Nick Vereecke  
Research group of virology & PathoSense  
Department virology, parasitology and immunology  
Faculty of vererinary medicine, UGent  
“Linking Nanopore sequencing & High-Performance Computing”

Date	#participants
28/06/2021	40

### 3.3 Helpdesk

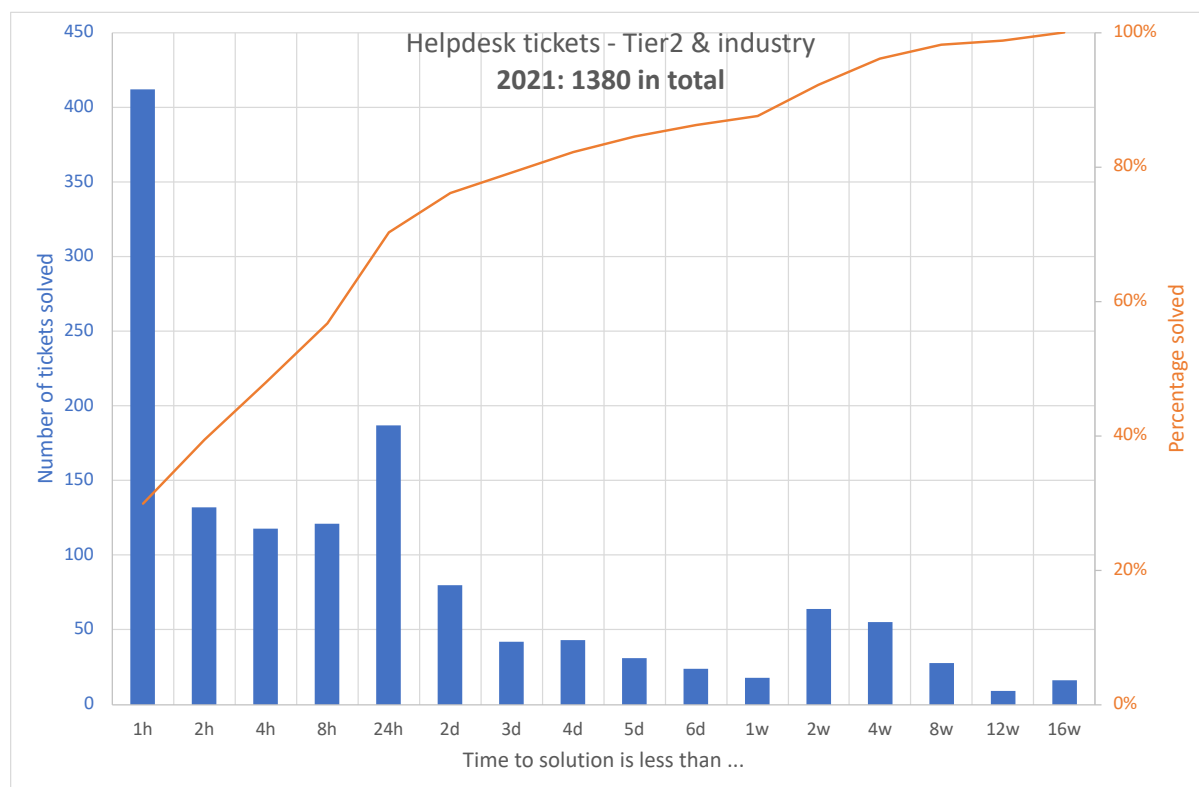
#### 3.3.1 Number of tickets

In all, 1909 tickets were resolved in 2021, distributed over 7 different helpdesk queues. These queues were installed to better deal with the support questions relating to different infrastructure platforms and services, whether within Ghent University or VSC. The tickets in the Tier1 Compute BrENIAC queue were resolved by the VSC colleagues from KU Leuven, relating to the BrENIAC Tier1 Compute infrastructure.

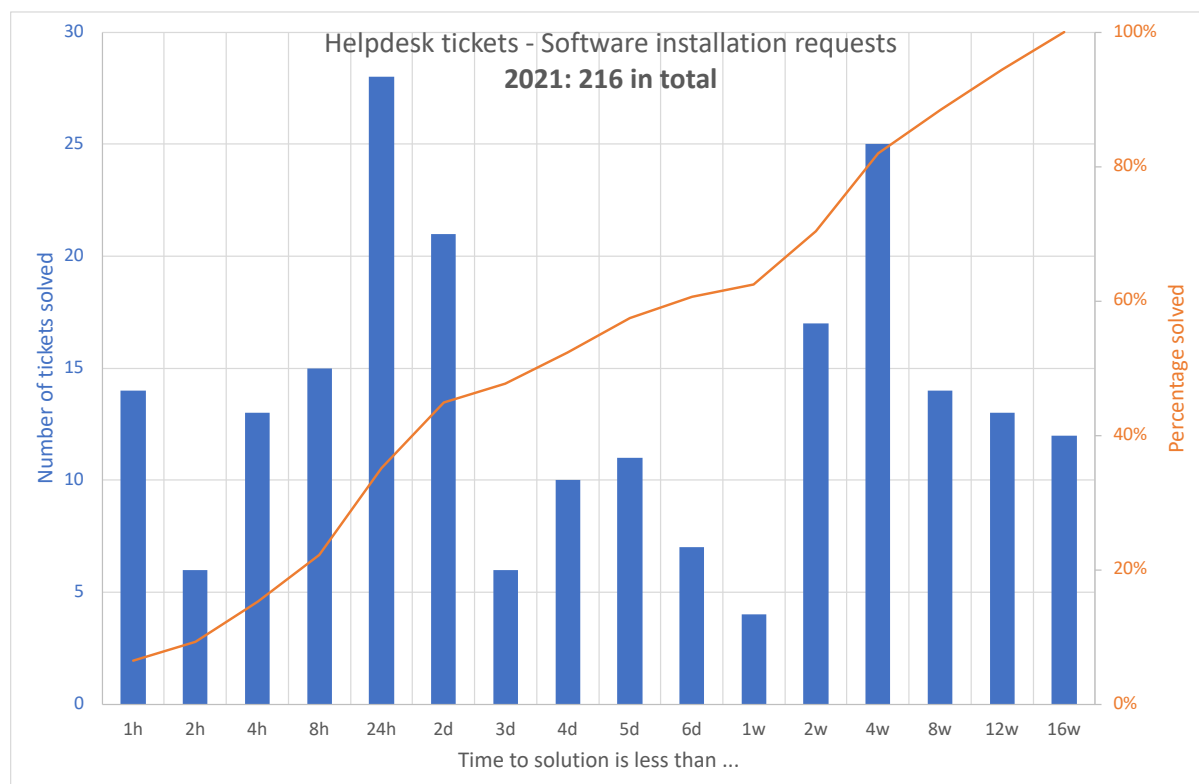




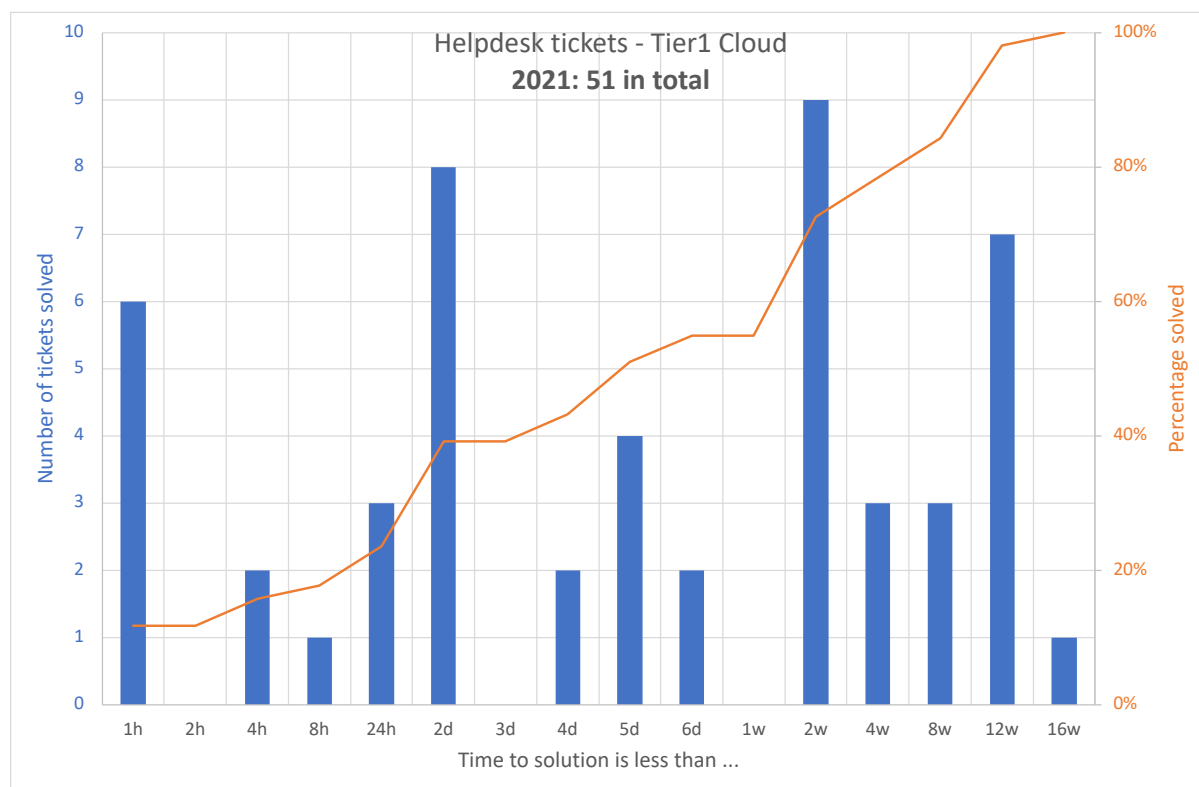
### 3.3.2 Average time to resolution – Tier2 and industry



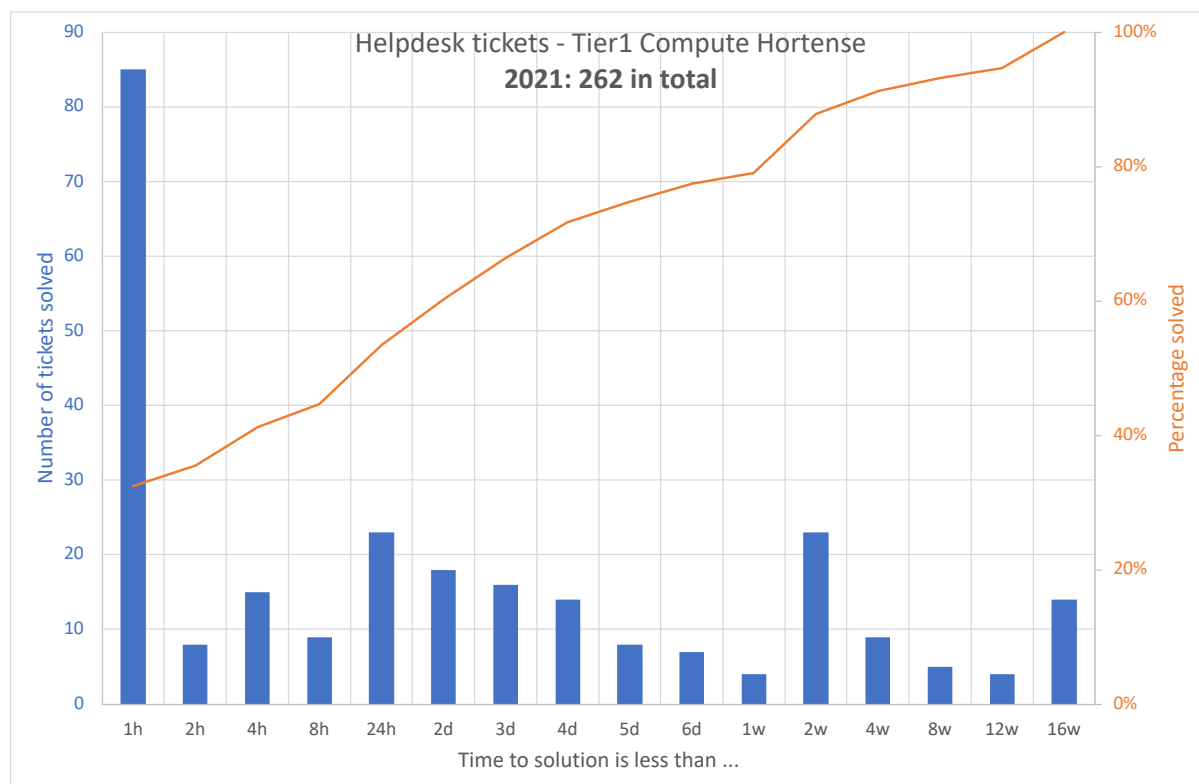
### 3.3.3 Average time to resolution – software installation requests



### 3.3.4 Average time to resolution – Tier1 Cloud

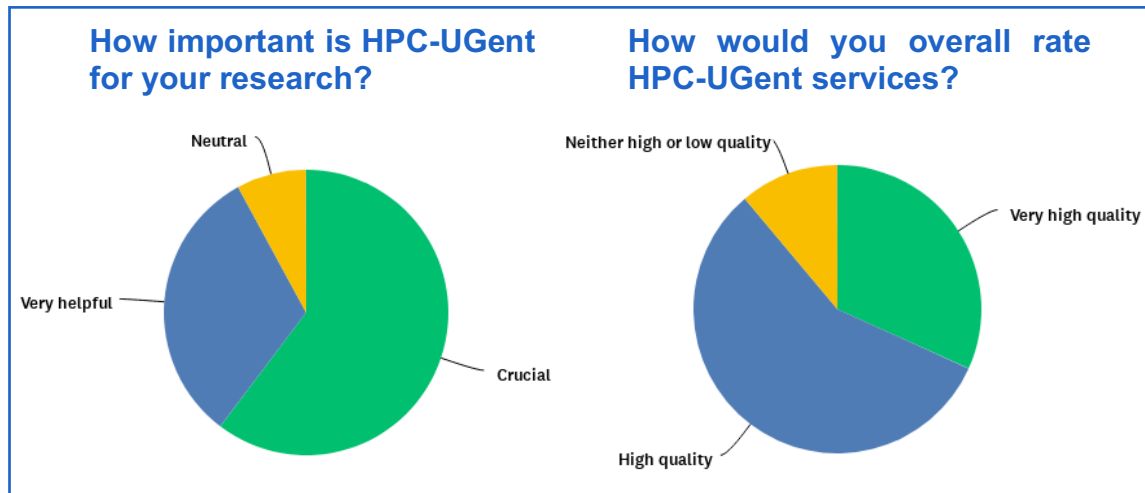


### 3.3.5 Average time to resolution – Tier1 Compute

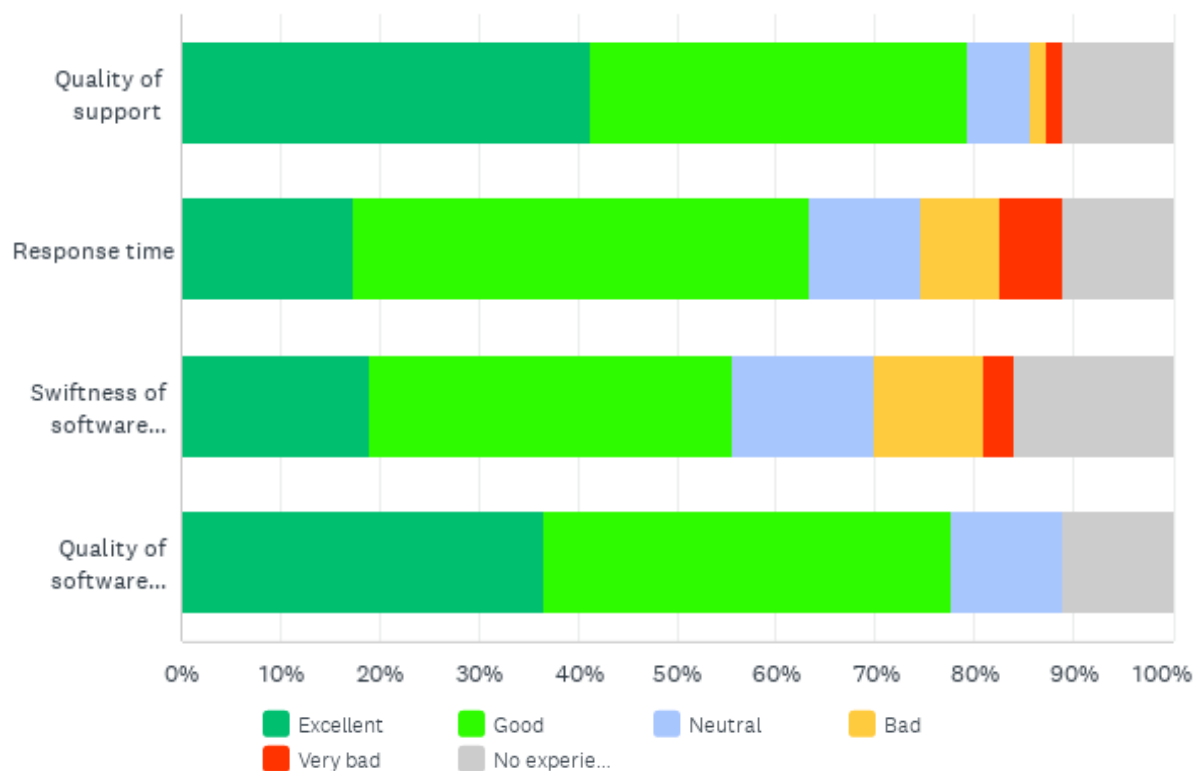


### 3.4 User evaluation

In order to improve HPC-UGent services, all current users were asked to complete a user survey. This survey was anonymous, short (average completion time 2 minutes) and in all 63 users responded. A selection of questions and responses is shown.



#### Please rate the following aspects related to HPC-UGent user support



At least 9 out of 63 respondents are not happy with the 'response time' and 'swiftiness of software installation'. Clearly, the HPC-UGent helpdesk is suffering from lack of staffing in comparison with the volume of work.

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

	#responses	%
No – The current compute platform suffices	31	49%
I don't know	23	37%
Yes – I need specific hardware/services	9	14%
<ul style="list-style-type: none"> <li>• More GPU hardware</li> <li>• Specific scientific software packages</li> <li>• No queue time</li> <li>• Support/training for local server/cloud install</li> <li>• Keep remote desktops</li> <li>• Cluster job scheduling (sic)</li> </ul>		

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

#### Infrastructure

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

#### 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

#### 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 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

## 4 OUTREACH

### 4.1 Within Ghent University

Date	Event
12/01/2021	<i>"Roadmap: compute resources for education"</i> FEA computer committee, Faculty of Engineering and Architecture
4/02/2021 25/03/2021 1/07/2021 23/09/2021 10/12/2021	The HPC-UGent team regularly meets with the UGent data stewards. The scope here is broader than the typical HPC-UGent community of users, comprising all UGent researchers and all infrastructure and services of the ICT department (DICT).
23/03/2021	<i>"Roadmap HPC-UGent"</i> DICT Systems group and Infrastructure office
26/04/2021	<i>"Introduction to High-Performance Computing (HPC)"</i> Guest lecture for Information Technology and Data Processing course, Ghent University.
11/05/2021	<i>"HPC-shares / Globus / HPC webportal"</i> Demo session for UGent data stewards and related stakeholders
9/11/2021	<i>"DICT storage platforms – Applied"</i> Short Sessions on Hot Topics (SSHT) – Faculty of Economics and Business Administration
26/11/2021	<i>"Data storage @ UGent"</i> Webinar for Faculty of Engineering and Architecture

### 4.2 To policy makers, industry and general public

Date	Event
12/02/2021	DICT – IDLab/imec Information exchange on compute infrastructure upkeep
19/08/2021	TechTransfer and industry meetup BlueBridge/Upskill project Zeebrugge
16/09/2021	Visit to UGent datacenter and supercomputers by Mathieu Michel, Belgian state secretary for digitization
7/10/2021	VSC lunch session on A.I. Keynote presentation <i>"Artificial Intelligence and GPUs"</i>

8/11/2021	Industry road tour VSC – HPC meets AI Presentation “ <i>Introduction of VSC</i> ” Enabled by AI4growth, EuroCC, UGent 3Square, Zwijnaarde
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### 4.3 Within international HPC community

Date	Event
7/01/2021 4/02/2021 4/03/2021 1/04/2021 6/05/2021 3/06/2021 1/07/2021 5/08/2021 2/09/2021 17/09/2021 7/10/2021 15/10/2021 4/11/2021 19/11/2021 2/12/2021	Monthly “ <i>European Environment for Scientific Software Installations (EESSI)</i> ” update meetings Online <a href="https://github.com/EESSI/meetings/wiki">https://github.com/EESSI/meetings/wiki</a>
14/01/2021	LUMI kickoff event Belgium Online <a href="https://www.vscentrum.be/lumi">https://www.vscentrum.be/lumi</a>
25-29/01/2021	6th EasyBuild User Meeting (EUM'21) Online <a href="https://easybuild.io/eum21/">https://easybuild.io/eum21/</a> Co-organization of meeting Keynote presentation “ <i>EasyBuild State of the Union</i> ” Co-lead in “ <i>CernVM-FS tutorial</i> ”
6-7/02/2021	FOSDEM'21 Brussels, Belgium Co-organization and support of “ <i>HPC, Big Data and Data Science devroom</i> ” <a href="https://archive.fosdem.org/2021/schedule/track/hpc_big_data_and_data_science/">https://archive.fosdem.org/2021/schedule/track/hpc_big_data_and_data_science/</a>
9/03/2021 23/03/2021 30/03/2021 18/06/2021	“ <i>Introductory tutorial on EasyBuild for the LUMI User Support team (LUST)</i> ” Online Co-organization of training, in collaboration with CSCS (Finland) <a href="https://easybuilders.github.io/easybuild-tutorial/2021-lust/">https://easybuilders.github.io/easybuild-tutorial/2021-lust/</a>



15-17/03/2021	Slurm Training for University of Antwerp and VSC partners Online
29/03/2021	EasyBuild Tech talk “FlexiBLAS” – Martin Köhler (Max Planck Institute Magdeburg) <a href="https://github.com/easybuilders/easybuild/wiki/EasyBuild-tech-talks-III:-FlexiBLAS">https://github.com/easybuilders/easybuild/wiki/EasyBuild-tech-talks-III:-FlexiBLAS</a> Online
25/06/2021	ISC 2021 Online Co-organization of ISC'21 EasyBuild tutorial “Maintaining a Modern Scientific Software Stack Made Easy with EasyBuild” <a href="https://easybuilders.github.io/easybuild-tutorial/2021-isc21/">https://easybuilders.github.io/easybuild-tutorial/2021-isc21/</a>
17/08/2021	EasyBuild Tech talk “AMD Rome & Milan” - Evan Burness + Jithin Jose (Microsoft Azure) <a href="https://github.com/easybuilders/easybuild/wiki/EasyBuild-tech-talks-IV:-AMD-Rome-&amp;-Milan">https://github.com/easybuilders/easybuild/wiki/EasyBuild-tech-talks-IV:-AMD-Rome-&amp;-Milan</a> Online
28-29/09/2021	EasyBuild maintainer summit 2021 <a href="https://github.com/easybuilders/easybuild/wiki/Notes-from-EasyBuild-maintainer-summit-2021">https://github.com/easybuilders/easybuild/wiki/Notes-from-EasyBuild-maintainer-summit-2021</a> Online
13-17/12/2021	EESSI hackathon <a href="https://github.com/EESSI/meetings/wiki/EESSI-hackathon-Dec'21">https://github.com/EESSI/meetings/wiki/EESSI-hackathon-Dec'21</a> Online
20/12/2021	EasyBuild Tech talk “MPItrampoline” - Erik Schnetter <a href="https://github.com/easybuilders/easybuild/wiki/EasyBuild-tech-talks-V:-MPItrampoline">https://github.com/easybuilders/easybuild/wiki/EasyBuild-tech-talks-V:-MPItrampoline</a> Online

#### 4.4 Within the context of the EuroCC project

Date	Event
2/02/2021	Kick-off meeting EuroCC Belgium Online
11/02/2021 26/10/2021	WP30.3/30.4 meeting EuroCC Belgium Online

29/04/2021	Castiel Competences - outcomes of the Competence Task Force work Online
4/05/2021 6/07/2021 11/10/2021	National Competence Center meeting Belgium Online
20/05/2021 27/05/2021 3/06/2021 7/06/2021 17/06/2021 21/06/2021 24/06/2021	NCC competence pitches Online
21/05/2021	Castiel - Workshop on two studies around the Competence topic Online
8/06/2021	AMD-EuroCC Half-Day Workshop Online
17/06/2021	NCC Belgium competence pitch Online
22-23/06/2021	EuroCC/CASTIEL joint conference Online
14/09/2021	Castiel - Introduction of Intel to EuroCC Network
21/09/2021	Castiel - Workshop on HPDA: use cases and experiences from Finland and Italy Online
12-14/10/2021	EuroCC and Castiel – first Joint Undertaking review Online
28/10/2021	EuroCC mentoring workshop on industry engagement Online
12/11/2021	Sarus and Firecrest workshop (NCC Switzerland) Firecrest workshop (NCC Switzerland) Online
25/11/2021	EuroCC Workshop on HPC, HPDA and AI Applied to Industrial Use Cases Online

Highlight:



### EuroCC Belgium

Within the EuroCC project under the European Union's Horizon 2020 program (H2020), participating countries are tasked with establishing a single National Competence Centre (NCC) in the area of high-performance computing (HPC) and high-performance data analytics (HPDA). Each NCC will coordinate activities in all HPC-related fields at the national level and serve as a contact point for customers from industry, science, (future) HPC experts, and the general public alike.

For Belgium, the NCC is a consortium of 12 entities:

- CECI: the 5 French speaking Universities (<http://www.ceci-hpc.be/>)
- VSC: the 5 Flemish speaking Universities (<https://vscentrum.be/>) also Tier-1 operator for Flanders
- Cenaero: Research center (<http://www.cenaero.be/>) Tier-1 operator for Wallonia
- Innoviris: Research & Innovation hub (<https://innoviris.brussels/>)

The objectives of EuroCC Belgium are:

- Support usage of high-performance computing and data analytics
- Set up a full training offer
- Set up a framework to ease access to HPC/HPDA for industry
- Identify available competences at national and European level
- Facilitate access to systems, scientific and technical expertise and knowledge pools
- Set up communication and dissemination actions

### **Role of HPC-UGent**

HPC-UGent represents Ghent University in this consortium and is joint task-leader of WP30.5, set on mapping HPC/Big Data/AI technical competences within Belgium. UGent is further involved as a contributor in WP30.3 focusing on 'Technology Transfer/Business Development' and WP30.4 'Collaboration with Industry'.

Link: <https://www.enccb.be>