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VLAAMS **SUPERCOMPUTER CENTRUM**

ANNUAL REPORT 2018

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CONTENTS

PREFACE

The VSC, the partnership between the Flemish universities and the FWO, stayed vigilant in 2018 for the needs of users. After all, challenges in the research landscape cannot remain without appropriate answers.

In 2018, the VSC's "Supercomputing as a Service" project was kicked off. With the 30 million euros awarded (end of 2017), the VSC will develop an integrated computing, data and cloud infrastructure in the following years. An operational management team is leading this project in the right direction. The extension of BrENIAC, the Flemish Tier-1, has been prepared. In addition, surveys were conducted to map the needs and expectations of users, work continued on the existing cloud pilot and pilot projects for data around iRODS and Globus were started.

71 applications were submitted for Tier-1. Of these, 65 were approved for a total of 188,488 node days and 27 starting grants were also applied for. In addition, the Tier-2 capacity was further expanded, including a machine that focuses on artificial intelligence and GPU workloads.

As always, a wide range of courses is organized for the use of Tier-1 and Tier-2. These courses are not only attended by academic users, but there is also interest from non-academic institutions and industry. In addition, a Massive Online Open Course (MOOC) was organized for the first time as part of the PRACE 5IP project. "Defensive programming and Debugging" had 750 active participants from 126 countries. The VSC also organized two PRACE Training Center (PTC) courses for the first time, in collaboration with SURFsara (Amsterdam).

The fourth VSC user day took place on 22 May 2018 at the Royal Flemish Academy of Sciences and Art in Brussels. As in previous years, national and international speakers were invited from academia and industry. More than 110 participants took part in the plenary sessions or workshops. The poster session also received an award in the form of calculation time at BrENIAC.

The VSC industrial board developed a number of actions to further promote the VSC in the non-academic world, including participation in Leuven Mindgate and a networking event from VOKA.

In short, the VSC continues to expand its services to users and is thus assured of a challenging future!

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UGent: Ewald Pauwels
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VUB: Stefan Weckx, Ward Poelmans
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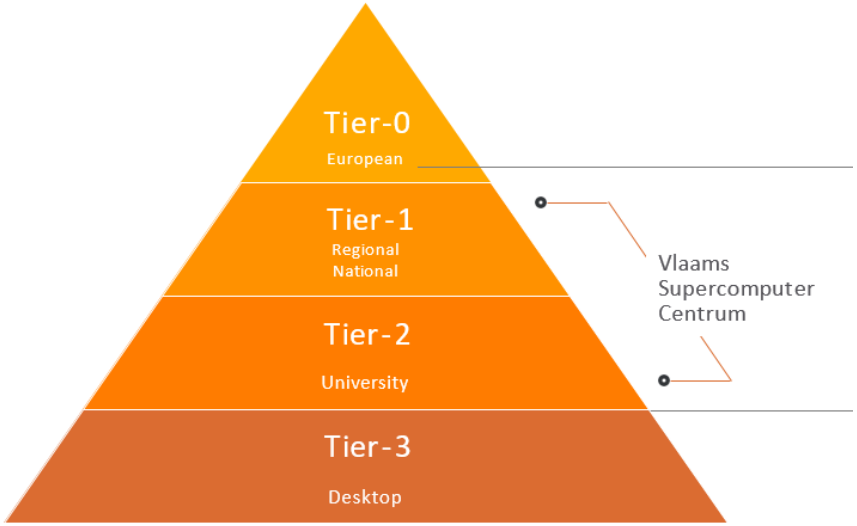
INFRASTRUCTURE

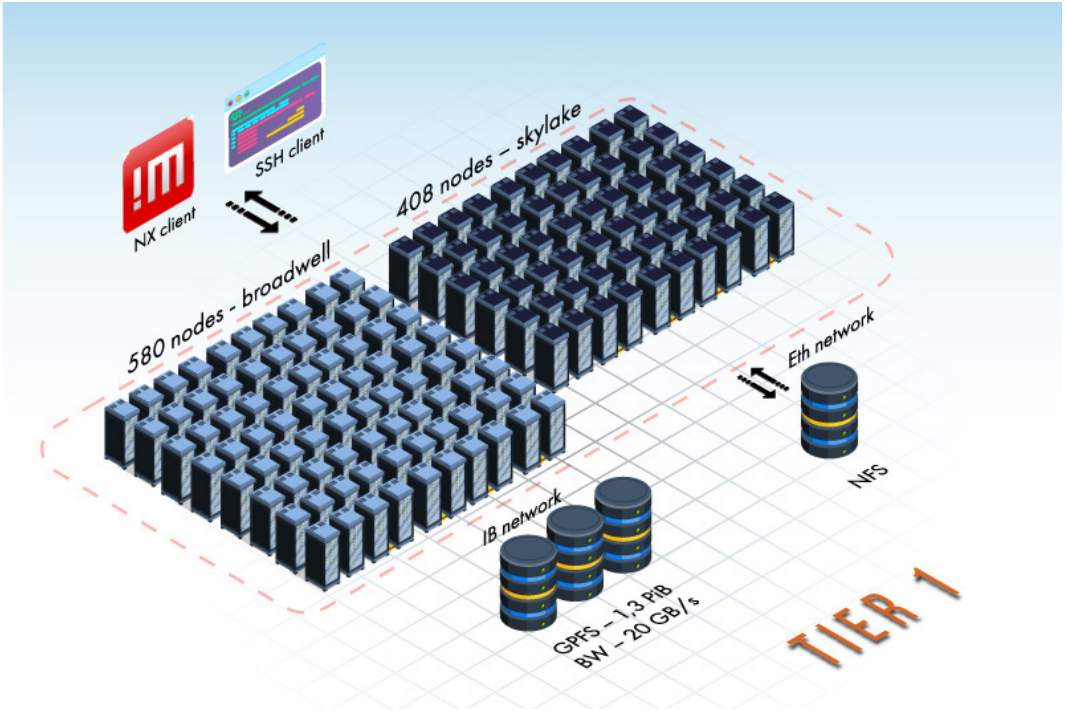
INTRODUCTION

In the European model for HPC, a distinction is made between three levels: the computing capacity that research institutions have Tier-2, the computing capacity whose needs and costs exceed an institution and which is provided at the level of a region or country Tier-1 and the super-heavy computing infrastructure Tier-0. The VSC focuses primarily on the Tier-2 and Tier-1 layers, thereby attempting to form a stepped bridge between Tier-3 and Tier-0.



TIER-1 INFRASTRUCTURE

The extension of the Tier-1 cluster was ordered at the end of 2018. This expansion consists of 408 compute nodes, each with 2 Skylake Gold 6132 processors, and is intended to bring the Flemish Tier-1 environment into the Petaflop range. This expansion will be installed at the beginning of 2019 and is the first step in the further expansion of the Flemish Tier-1 platform.



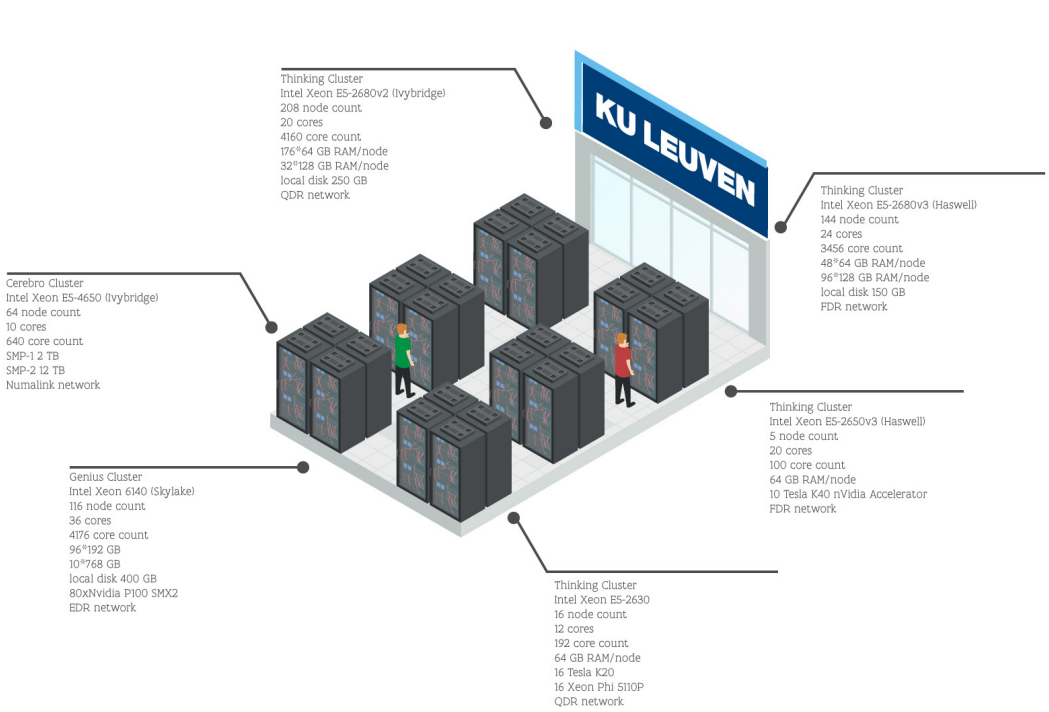
TIER-2 INFRASTRUCTURE

The VSC has developed a differentiated Tier-2 infrastructure within the various Flemish universities that is available to the academic and business world.

KU Leuven and Hasselt University

KU Leuven and UHasselt work together for the Tier-2 infrastructure.
The infrastructure consists of:

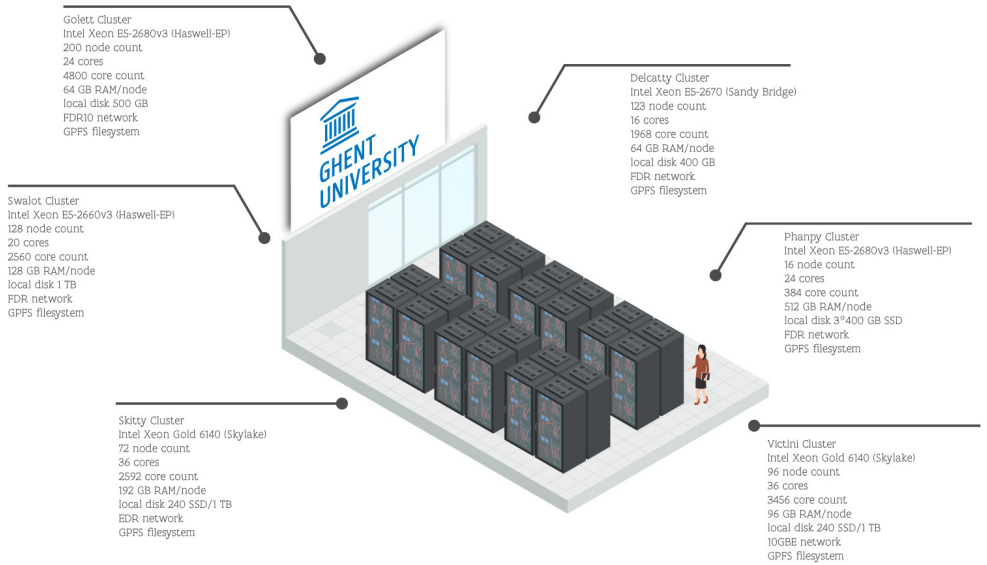
- 2 clusters, 7 partities
- 551 TF
- 11792 CPU / 355536 accelerator cores (Tesla K20/K40/P100)
- 72 TB memory



Ghent University

UGhent has been investing for several years in the development of a high-performance infrastructure. This currently consists of:

- 6 clusters
- 582 TF
- 15.760 CPU cores
- 67 TB memory



University of Antwerp

The Tier-2 infrastructure consists of:

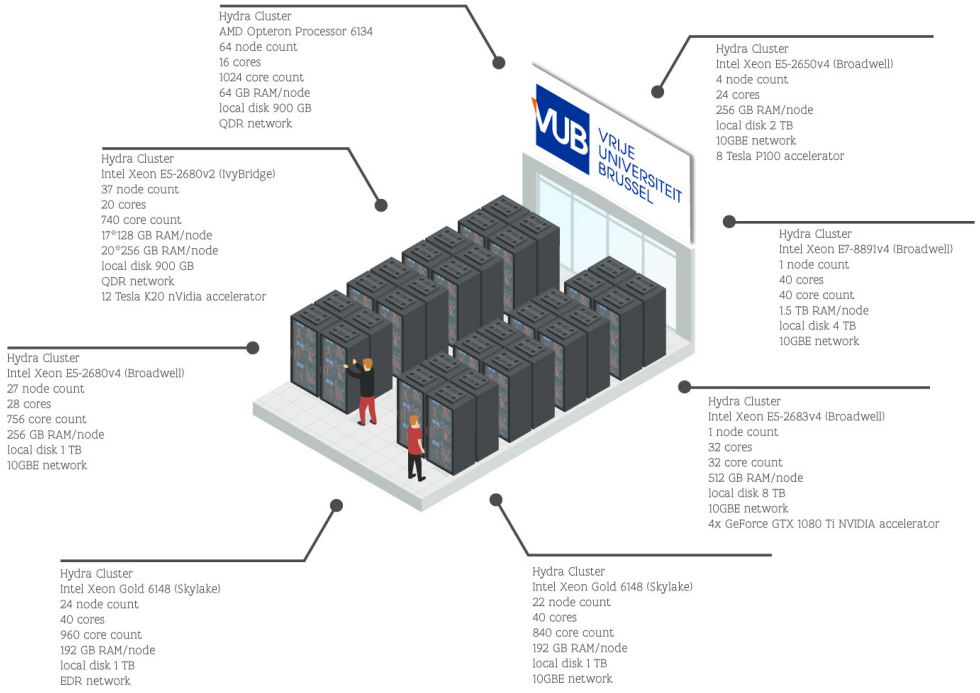
- 2 clusters (Hopper en Leibniz), divided in 4 partities
- 238 TF
- 7672 CPU cores, 7236 accelerator cores (Tesla P100 + Xeon Phi 7720P)
- 36 TB memory

Vrije Universiteit Brussel (VUB)

The Tier-2-infrastructure consists of:

- 1 cluster / 7 partities
- 17,2 TF
- 4392 CPU cores / 32256 GPGPU cores
- 29,5 TB memory

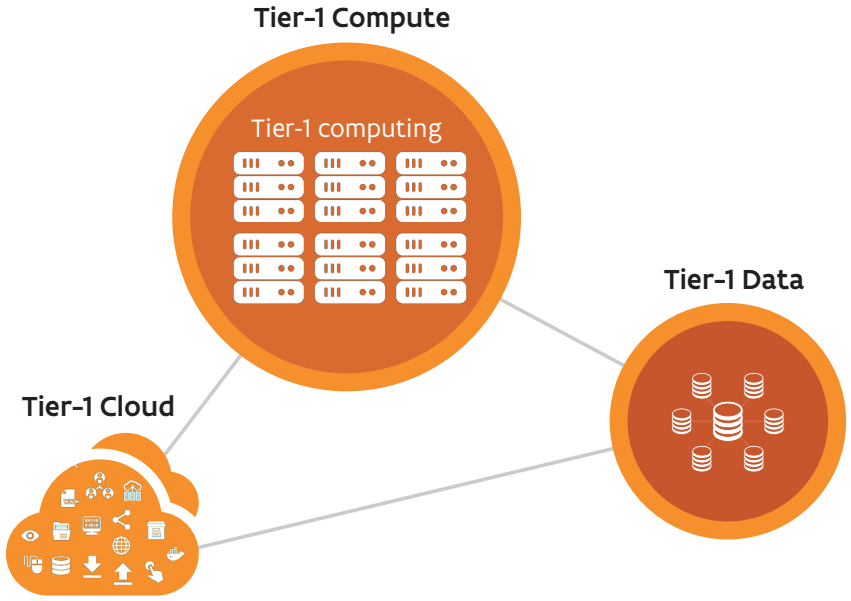
In addition to its own Tier-2 infrastructure, the VUB - together with the ULB - also manages the grid infrastructure, which is used, among other things, to process the data collected during experiments with the Large Hydron Collider (HPC) used at CERN, but also within the Flemish research community. Finally, the VUB has a test facility for cloud infrastructure.



TIER-1 SUPERCOMPUTING PLATFORM

The Tier-1 supercomputing infrastructure in Flanders has until 2018 mainly been targeted at users with serious calculation issues (typical HPC / HTC workloads). Although this platform in its current form is already very successful, the current focus on compute no longer meets all the needs of many researchers. There is also a strong demand from industry for more data processing, access and customized user environments.

The VSC therefore offers a new conceptual Tier-1 model: supercomputing as a service. Within this model we can distinguish different infrastructure components that together make it possible to offer an increased service level to the users of the VSC:

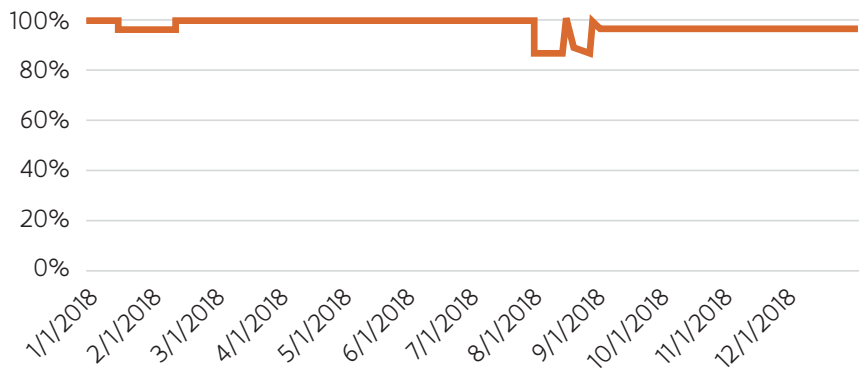


COMPUTE

Compute infrastructure remains the most important component: traditional calculation clusters that can handle large data volumes or a multitude of calculation tasks. The second Flemish Tier-1 went into production in 2016. KU Leuven is responsible for the technical exploitation of this machine and is responsible for financing the accommodation.

Tier-1 Uptime

The uptime of the system in 2018 has been good, there were no general interruptions, only a few system upgrades and maintenance work



Allocation of compute time

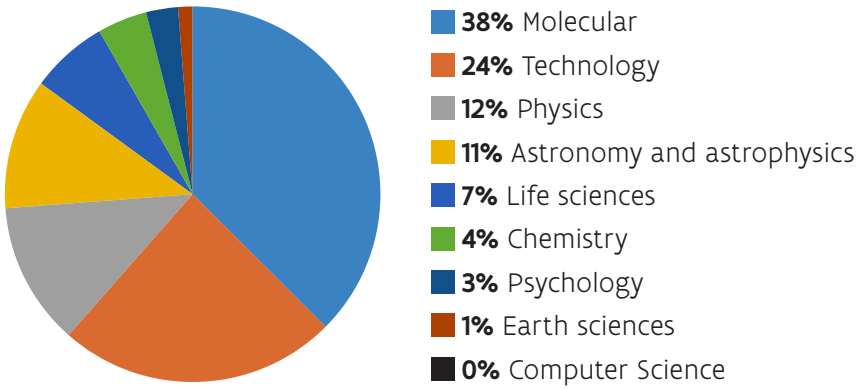
There are a number of ways in which researchers can obtain calculation time on Tier-1. A distinction is made between academic and non-academic users.

For researchers affiliated with a university, a SOC or other research institution, the following (free) access channels exist:

- Starting Grant (max. 100 node days), to try out Tier-1 and perform benchmarks or software tests, in preparation for a full-fledged project application
- Project access (500-5000 node days) based on project applications that can always be submitted, but are evaluated by the Tier-1 Allocation Board at 3 times a year.

For the assessment of the Tier-1 project applications, a "Tier-1 Allocation Board" was set up with five foreign experts. This committee evaluates the applications and decides whether the requested calculation time is granted in full, in part or not at all.

In the three rounds of 2018, a total of 71 projects were submitted for a total of 232662 node days from which 65 projects were awarded for a total of 188488 node days. Over the different project rounds, an average of 88% of the allocated time is used up. Just like with HPC clusters abroad, chemistry, physics and the engineering domains are well represented.



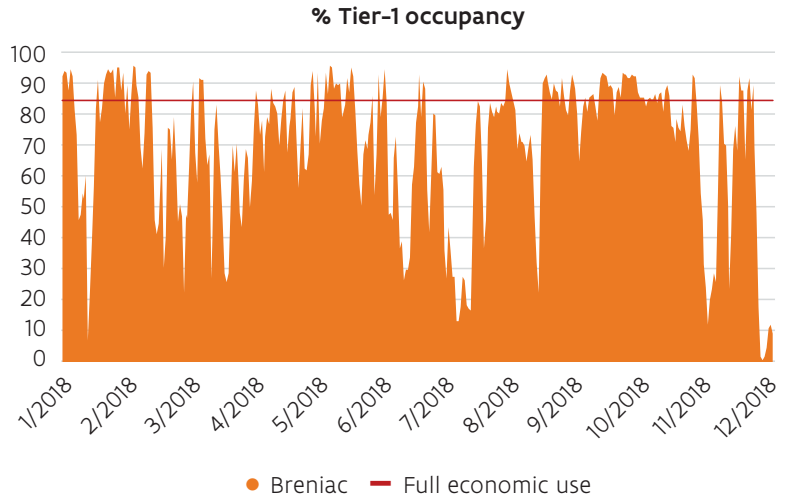
There are also two access channels for researchers from the industry to obtain Tier-1 computing time:

- Exploratory Access (max. 100 free node days)
- Full Access through an agreement with the Tier-1 housing institution and FWO on the basis of full cost charging of used computing time and used storage

The rates at which industrial users can purchase Tier-1 computing time were laid down in the Access Regulations 2018. In addition, researchers from the industry can also gain access to Tier-1 through a research project in collaboration with a public research institution such as a Flemish university.

Tier-1 occupancy

In 2018, the allocation period was extended from 6 to 8 months so that projects of 2 allocation rounds are active at all times. This change was made to ensure optimum utilization of the machine



The summer period (end of July and beginning of August) influences the occupation of the cluster but also technical interventions outside the cluster such as Belnet maintenance (14/1, 25/4 and 23/7) and maintenance on the storage systems that contains home directories of users and an unavailability of the Ldap server (25/12) needed for authentication.

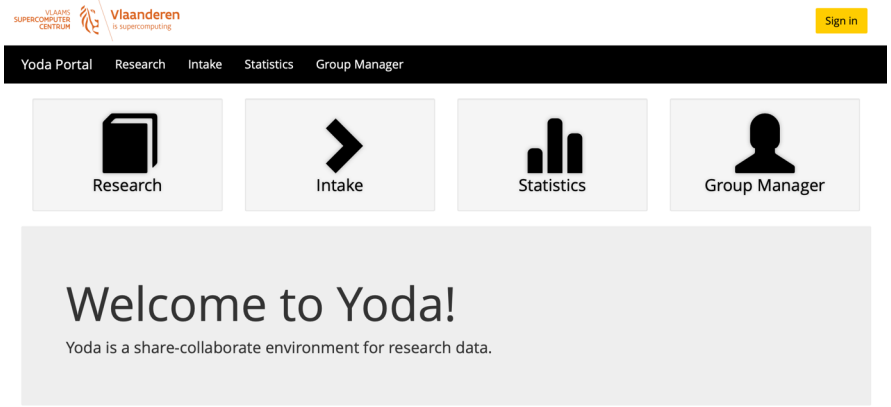
DATA

More and more users have computational work that makes intensive use of large data sets. Migrating this data to and from the compute infrastructure whenever it is to be used for a calculation is very inefficient because of the scale. It is therefore necessary to add a data component where large data sets can be stored for a longer period of time and from there also be processed efficiently.

In 2018 two VSC pilot projects were started for the Data component of the SaaS platform: around iRODS as a data management platform, and around Globus as a data transfer service.

A test setup based on iRODS 4.2.4 has been available within the VSC since 2018. This runs on a set of virtual machines at UGhent, and makes 400TB of storage available twice. This set-up is built up in a high-available way, only the iRODS (metadata) database is not. The initial focus is primarily on use testing and initial performance testing.

Data objects can be manipulated via a limited number of clients, after Single Sign-On authentication via the VSC account page. A web portal based on YoDa has also been set up. This portal is strongly focused on Research Data Management (RDM), and serves as a proof-of-concept that such a high-level service is possible. The scope of this service for the VSC is, however, limited to supercomputing related data.

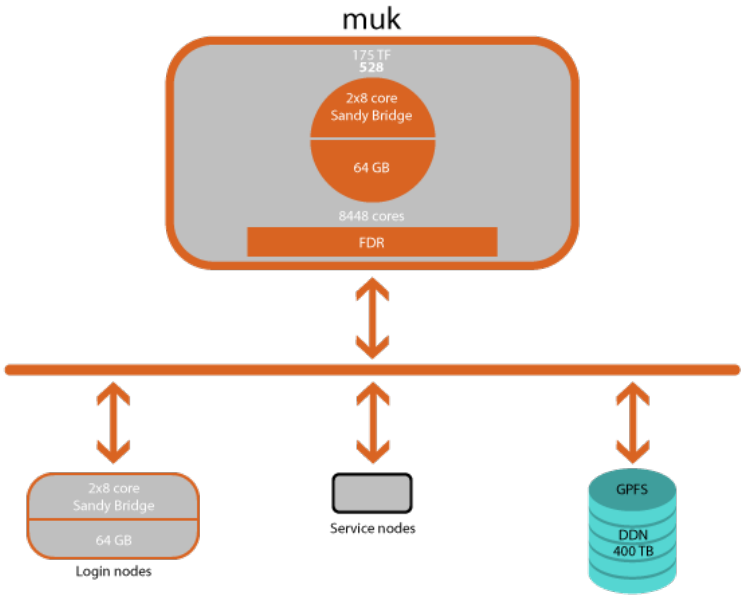


In the course of 2018, a Globus test bed was also installed on Tier-2 infrastructure at KU Leuven. Globus offers data transfer services between different data endpoints, such as scratch storage, a CIFS server and the laptop of an end user. This test set-up now successfully connects several endpoints within the Tier-2 environment of KU Leuven. This will be expanded to various Tier-1 and Tier-2 storage systems within the VSC.

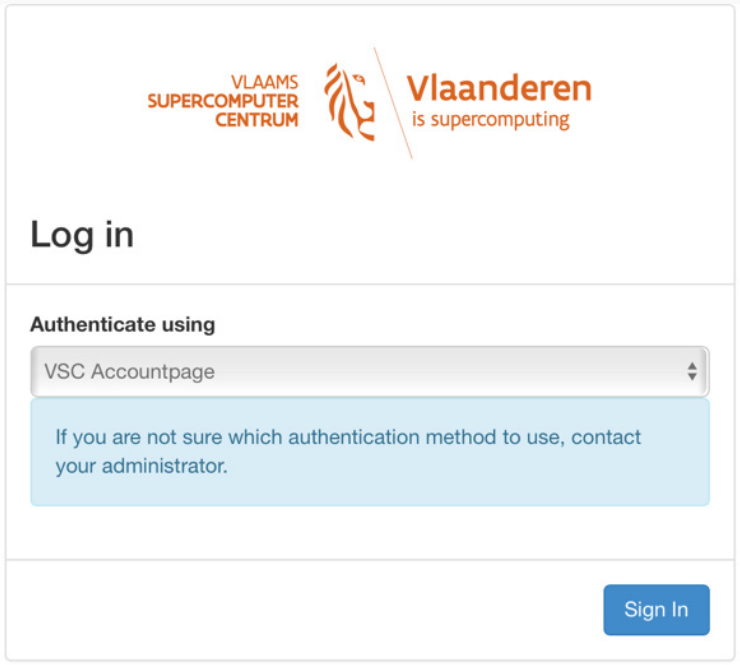
CLOUD

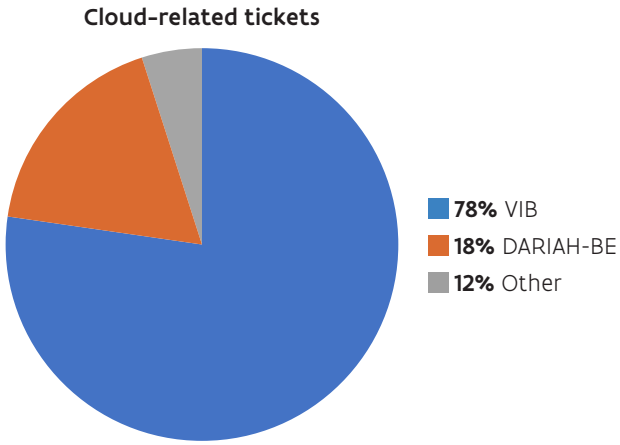
Research with datasets often also requires a flexible user environment: an environment where analyzes can be carried out in an interactive manner, tailored to the applications and the users; an environment where pre and post processing can be performed; an environment where the data can be made accessible to users in a web-based manner, can be visualized or can be consulted by employees, interested parties or users of the research or research results. To this end, an infrastructure is provided that does not focus on compute but rather on 'tailor-made' access and use of the data. Here a model can be used that closely resembles that of cloud providers.

From the beginning of 2018, a cloud test setup based on OpenNebula is available for various pilot end users of the VSC. This setup is based on the infrastructure of the decommissioned Tier-1a in Ghent, after a thorough reconversion of the still usable hardware. This setup currently includes 24 hypervisors, but can be expanded to a maximum of 192 hypervisor



Tier-1 at the UGhent (cloud infrastructure)





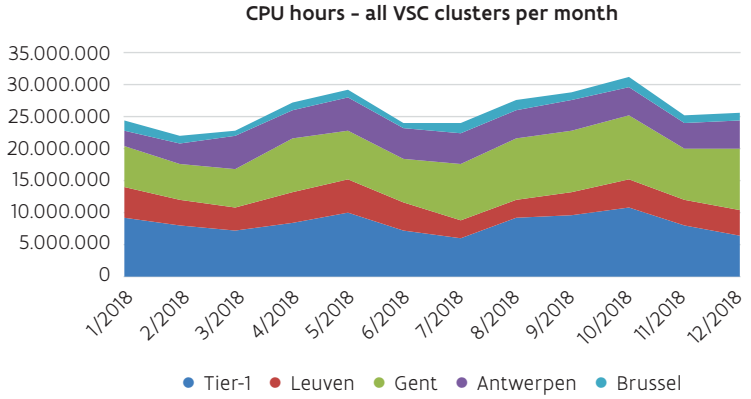
In the course of 2018, it was decided to switch to OpenStack to develop this cloud platform. This fits in better with existing (international) initiatives and the wishes of users. A VSC cloud platform based on OpenStack has been active since September 2018.

At present, access to the pilot platform is limited to a small number of groups, including VIB and DARIAH-BE. Despite the limited number of users, the demand for support is very high. The graph above shows the number of support tickets for the Cloud component, divided by user group. A total of 121,450 virtual core hours were used on both cloud test setups (OpenNebula and OpenStack).

TIER-2 INFRASTRUCTURE

EXPLOITATION AND USE

VSC has a central XDMoD infrastructure for reporting usage, which collects all data from the various clusters and generates the necessary overviews.



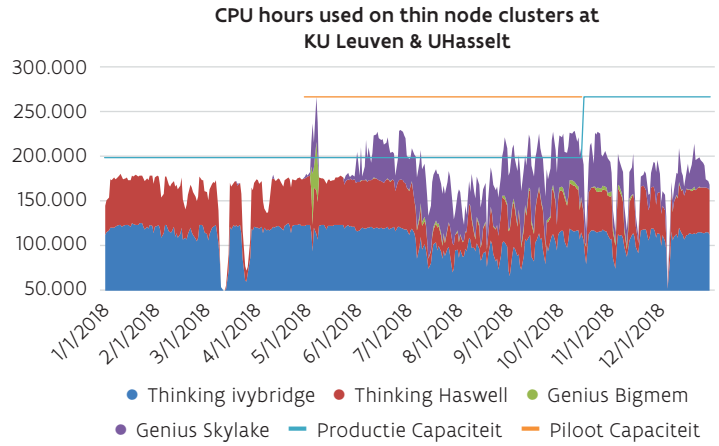
Use expressed in core hours of all VSC cluster

The figure above shows the cumulated use of the Tier-1 and Tier-2 infrastructure. A clear increase is noticeable. The total number of core hours continues to increase in 2018 through the deployment of the new Tier-1 BrENIAC and the renewal of the Tier-2 infrastructure at the various institutions.

KU Leuven and University of Hasselt

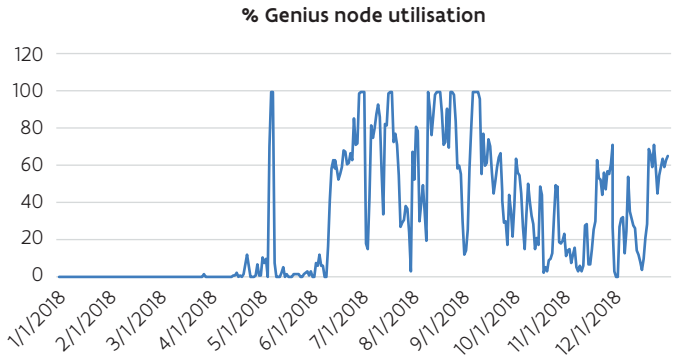
Both universities work together for the Tier-2 infrastructure. An important expansion in the Tier-2 layer was carried out in 2018. A new cluster, Genius, was taken into use. This cluster is built with the latest generation of Intel CPUs, but also has an important section with GPU devices. With this new cluster, in addition to the existing HPC workloads, the specific Machine Learning / AI workload can now also be efficiently processed. The most important characteristics of the new cluster are:

- 307 TFlops / s peak performance
- nodes with more memory (768 GB)
- 20 nodes with 4 P100 NVIDIA GPUs each
- EDR interconnect
- integration with the existing parallel file system

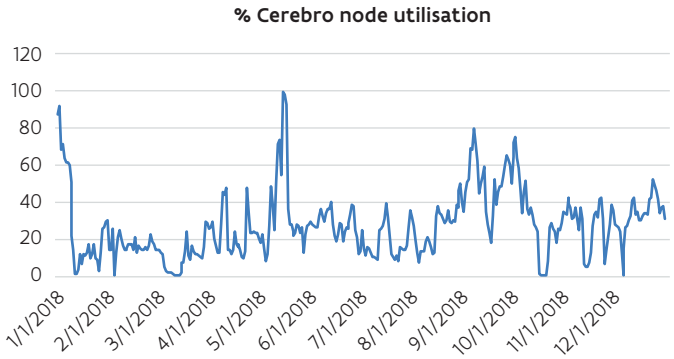


Core hours used at the KU Leuven / UHasselt thin node cluster

The previous figure shows Core hours used at the KU Leuven / U Hasselt thin node cluster provides an overview of the use of the infrastructure at KU Leuven. The graph represents the cumulative use of the various thin node clusters at KU Leuven. There is 1 important interruption in the graph. This is related to the installation of the new Genius cluster. The cluster was integrated with the existing cluster at storage level. The clusters experienced a high occupancy rate during the rest of the year. Genius was opened in the pilot phase from 1 June to 18 October. Approximately 640 users, spread over many research domains, have counted on these Thin node clusters.



Use of accelerators



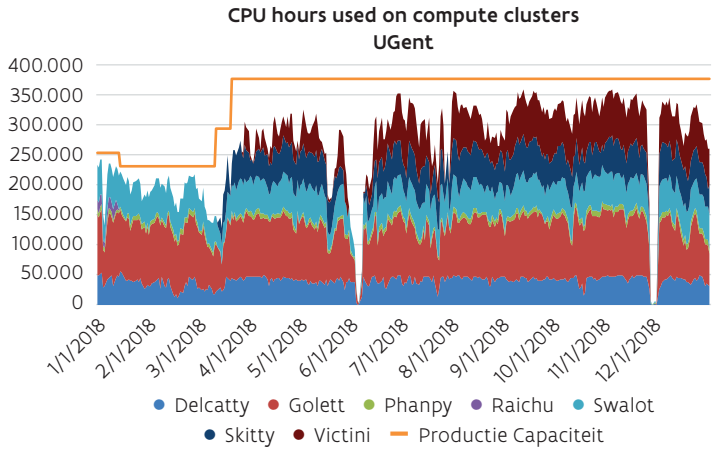
Use of shared memory

In addition to the thin node computing cluster, there is also a shared memory machine and an arrangement with accelerators at KU Leuven. The use of these machines is expressed in node hours and not in core hours. This is because the full node is often used because of the memory required or because of the accelerators. These more specialized sections are also used more often cross-site. As in the past, Cerebro has experienced typical usage peaks. Cerebro is coming to an end and was encountered by parts of the machine that were temporarily unavailable. This is not shown in the graph. To continue to support the type of abdomen, a purchase was also made at the end of 2018 for a new system (Superdome). This will only become operational in 2019.

The occupation of the GPU nodes that is shown relates to the new section installed in Leuven. The GPU nodes were made available from May 2018 in an open pilot period up to and including October 2018. The machine has been well tested by various user groups. The machine went into production from the end of October.

Ghent University

The Tier-2 infrastructure is made up of different clusters, depending on specific characteristics. Cluster raichu was decommissioned in the course of 2018, and two new clusters were taken into production: skitty and victini. The latter was also transformed into the standard cluster (instead of cluster delcatty previously).

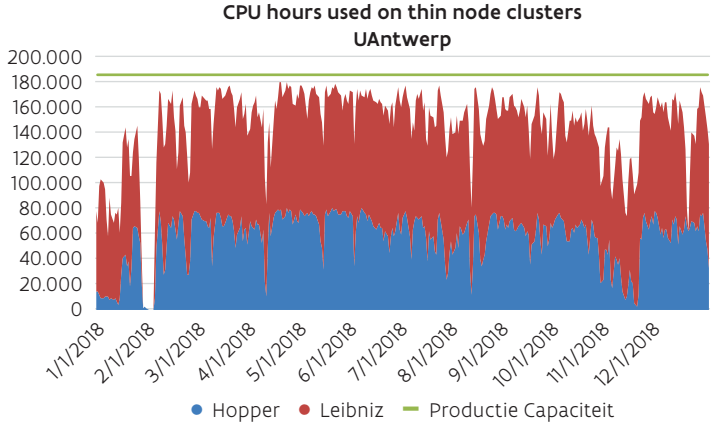


The figure above shows the cumulative use in 2018 of all calculation clusters at Ghent University. In 2018, a total of 95,559,679 core hours were used on the Tier-2 calculation clusters at Ghent University. This would correspond to 10,933 years of calculations on a single core. The average effective usage rate is 74% for all clusters in 2018. This percentage indicates how much of the theoretically available computing power was used in one year (this did not take into account down times, so the actual value is higher). The effective usage rate is quite high compared to typical HPC systems and indicates good economic use of the infrastructure.

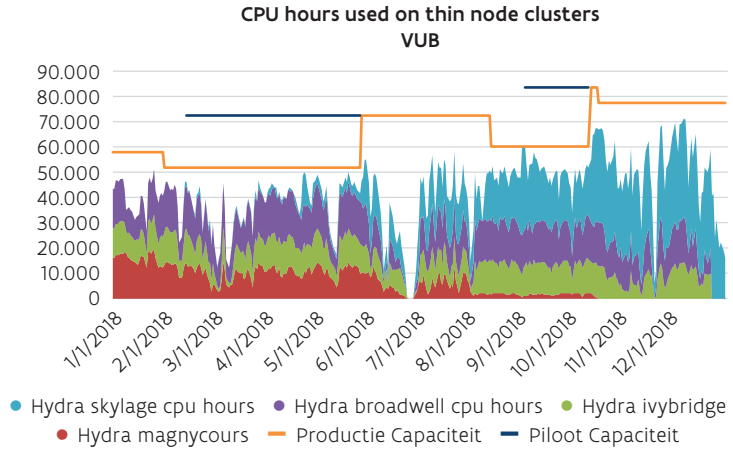
Declines in the graph above refer to downtimes due to planned maintenance work.

University of Antwerp

The graph above represents the cumulative use of the Hopper and Leibniz clusters at the University of Antwerp. At the end of January / beginning of February there was a planned interruption for a software upgrade of the storage system and network switches. At the same time, the switch to CentOS 7 of the clusters was completed. In addition, there was a small interruption on Leibniz in the second half of December due to network problems. Leaving aside these interruptions, the clusters are very well occupied.

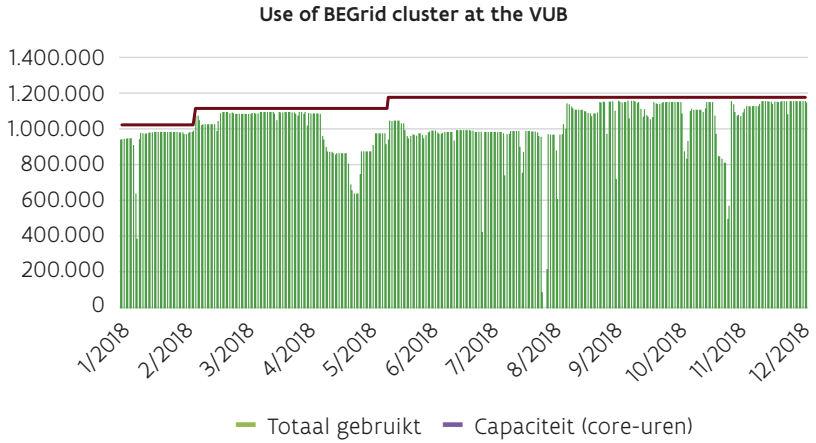


Vrije Universiteit Brussel (VUB)



All AMD nodes were taken out of production in 2018 and a partition with Intel Skylake nodes was added: 22 nodes with 10 GbE connection, the rest with Infiniband EDR. There was 1 scheduled maintenance in June and in addition there were problems with cooling or storage a few times. The improvement work of 2017 was continued. In the maintenance of June a major reorganization of the storage happened to be more in line with the other VSC sites. In addition, numerous small technical improvements have been made to make the cluster more user-friendly and stable. Part of the cooling has also been replaced.

The Hydra cluster performs both jobs that use all calculation scores in a node and jobs that do not use all cores, but that do require the full node due to memory requirements. In addition, a number of nodes have been reserved for interactive work by a number of research groups. Because such a mix distorts the occupancy rate according to core hours or node days, the standard reporting method for the other universities, the total number of available core hours was not indicated on the graph.



BEgrid 19-29 and BEgrid 47-50 are the different parts of the BEgrid cluster at the VUB. During the course of 2018, additional worker nodes were added in several phases: 20 new Intel Broadwell nodes for a total of 1120 extra job slots. In addition, the storage was also expanded to 5PB. There was a planned downtime for routine maintenance work in August and another due to work on the electricity supply in November. In addition, there were also only unplanned downtimes, among other things because of problems with fileserver (June), cooling problems (July).

ALLOCATION OF TIER-2 COMPUTE TIME

Each university uses its own procedure for allocating calculation time on the Tier-2 infrastructure and whether or not a small part of the costs is passed on to the academic researcher. For industrial / external users, all used computing time is always fully charged. To gain access to one of the Tier-2 compute clusters in the four VSC hubs (Antwerp, Brussels, Ghent, Leuven), the user must have a VSC userid. This can be requested on https://account.vscentrum.be. This website and database also centralizes all user information across the institutions over storage quota, membership of user groups, virtual organizations, etc.

The researchers from UAntwerpen and its association have completely free access to the Tier-2 infrastructure. Research groups can, on a voluntary basis, make a financial contribution.

Researchers at the VUB can count on the HYDRA cluster after they have been granted access to it by the data center. The grid cluster is available upon request from the person in charge of this infrastructure. The use of the Tier-2 infrastructure is free of charge.

The UGhent researchers and its association have full free access to their own Tier-2 infrastructure. Research groups can, on a voluntary basis, make a financial contribution with a (slightly) higher fair share as the direct return-on-invest.

The KU Leuven / UHasselt clusters work with a credit accounting system that is included in the scheduling software. New users get calculation time to become familiar with the system and to perform initial tests. This makes the entry threshold for researchers to switch to the Tier-2 infrastructure as low as possible. Credits can then be requested via a simple procedure and at minimal cost. The credits divide the available calculation time between different projects and have a responsibilizing effect. When performing a calculation task, the project is indicated on which the credits are charged. The principal investigator is the manager of the project. He can give researchers access to the calculation time and also monitor the calculation time used.

By using central accounts, users can also count on other sites, taking into account the applicable modalities. Below is a brief overview of the cross-site calculation.

		Compute time in corehours			
		UAntwerpen	VUB	UGent	KULeuven / UHasselt
Site	UAntwerpen		49	250	0
	VUB	16419		35901	3
	UGent	238899	0,6		1797642
	KU Leuven / UHasselt	53839		641681	

This so-called “cross-site” use is closely monitored.

In addition to the cross-site use of Tier-2 infrastructure, the grid infrastructure, managed by VUB / ULB, is also used extensively by researchers from different institutions: VUB, UAntwerpen and UGhent.

The remaining calculation time on the grid infrastructure is used by researchers from ULB and UCL.

Most researchers use the so-called "glide in" mechanism. This involves "pilot jobs" that, once active on a worker node, will get the "payload" elsewhere. For the calculation of the percentages mentioned above, only the calculation time of the "pilot jobs" is taken into account, not the individual "payloads". In addition, it should be noted that in the case of a grid, a user's workflow may be spread across different sites in different countries and the above percentages therefore represent only part of the actual used computing time.

USERS SUPPORT

The user support consists of different components:

- **Answering questions from users (help desk);**
- **Meetings with users / specific support;**
- **Training and outreach (see sections 'training' and 'outreach').**

Answering user questions

Below is an overview of the tickets that end up at the help desk. There is no central VSC help desk. Each institution answers the questions and problems of its own users (ie users who have requested an account in the institution concerned), both with regard to their own Tier-2 infrastructure and the central Tier-1, but also to external users who use the VSC infrastructure. If necessary, questions regarding the Tier-1 will be contacted with the help desk at KU Leuven (for the second Tier-1). For the questions a distinction is made between

- Questions about accounts;
- Questions about software
- Other questions.

The table below provides an overview of the number of tickets handled, per category and per institution.

	KU Leuven / UHasselt	UGent	UAntwerpen	VUB
Tier-2 + grid				
Accounts	834	339	70	297
Software	620	247	296	406
Overig	1027	963	120	297
Tier-1				
Accounts	31	0		
Software	89	0		
Overig	128	101	8	
Totaal	**2729**	**1650**	**494**	**1000**

Meetings with users / specific support

On the one hand, an attempt is made to involve as many researchers as possible in the HPC story by looking at whether and how they can make the transition from their desktop to the HPC infrastructure or simply use their own desktop more efficiently.

For existing users, this can also help with the transition from Tier-2 to Tier-1 and possibly to Tier-0. On the other hand, attempts are made to provide researchers with specific support.

Some examples:

- Optimizing existing workflows;
- Analysis / optimization of code;
- Give input to writing research projects.

In addition, user meetings take place at each institution in which a delegation of users is represented. Here we make a selection of the aforementioned support for each institution.

KU Leuven and University of Hasselt

The daily support handles questions i.v.m. accounts, basic usage of the cluster and software installations. These questions come from users from groups that have been using the cluster for a long time. Making the VSC infrastructure known to new research groups is a permanent task. But also within groups that are already using the cluster, specific actions can help to stimulate cluster use. This allows more computational work to be performed more efficiently in a shorter time compared to local infrastructure such as workstations and desktops. New researchers are made familiar with the use of the cluster in the regular introduction sessions or through a one-to-one consultation. The latter are very important to help new researchers get started all year round. After a two-hour consultation, the researcher usually has enough information to be productive on the cluster, provided some general knowledge of Linux and HPC. If a new group wishes to start on the cluster, specific workshops are also organized.

A number of specific support measures were continued in 2018. For Hasselt University, the emphasis was mainly on attracting new user groups and some faculties received special support.

Ghent University

Various user meetings were organized throughout the year in response to specific questions from researchers. In order to convince as many (potential) users as possible of the importance and the added value of supercomputing, the VSC was presented internally and various tours were organized in the UGent data center:

- 5/02/2018, Information session FWO call 2018 for Research Grants, Research Projects and SBO
- 29/03/2018, general presentation and tour for students of the course 'networks and IT' (Sint-Lievenscollege Business, Ghent)
- 5/11/2018, guided tour for members of Zeus WPI, the student association for computer sciences (UGent)

UGent's Atmospheric Physics research group is conducting computational climate research in collaboration with KMI, both on Tier 1 and Tier 2 infrastructure of UGent. To highlight this partnership, cluster-on-wheels 'ditto' was exhibited at the Open Days of the KMI, 29-30 September 2018. Although this mini-cluster is a demonstration device, it was very present as an eye-catcher (and noise maker) on the climate center exhibition of the KMI Open Days.

University of Antwerp
On the one hand, we handle questions from existing users and try to organize that calculation work as optimally as possible and to perform it as efficiently as possible by working proactively. A well-maintained software stack and supporting tools play an important role in this. On the other hand, we also make the VSC known to other researchers to point out the potential benefits of using the central infrastructure. For this we will specifically visit the researchers / research groups.

Every year two intro sessions are organized, which from 2016 consist of 3 parts: "Linux introduction", "Supercomputers for starters" and "HPC introduction". After all, it is not only necessary to be able to work with the environment, but also to have the necessary background knowledge. In early 2018, the fifth "HPC Tips & Tricks" was also given on "Code modernization - Two real world case studies and Intel tools for finding performance bottlenecks".

In addition, the necessary attention is paid to keeping the documentation on the VSC website up-to-date. In the second half of 2018, the switch was made to a new ticketing system.

In 2018, among other things, we organized a new session at the Institute of Tropical Medicine, sat around the table with the Port of Antwerp and examined with researchers from the transport economy department how they can make the switch to the Tier 2 infrastructure. In addition, other research groups from departments that are already active in the infrastructure such as Biology, Bioscience Engineering, Medicine and Health Sciences, Linguistics, and Applied Engineering Sciences have found their way.

In addition, there is guidance for master students in the use of the information structure, and support with applications for calculation time on Tier-1 and with computational aspects of (inter-university) project applications.

In addition to the courses within the VSC, courses are also provided in the regular program, namely "Scientific computing environments" and "(Parallel) programming".

A user group has been active at the UAntwerpen since 2006, which meets twice a year. The user group consists of representatives from 12 groups and directions.

Vrije Universiteit Brussel
In addition to continuing monitor existing users at Tier-2 and Tier-1 level, efforts were made to actively identify new potential Tier-1 users and to initially encourage them to apply for a starting grant for computing time. The expansion of the HPC team in 2017 allowed us to focus more on supporting our users. This resulted in considerably more used CPU time than in 2017 and a much better follow-up of the use of the cluster. For the Tier-2 level, the focus was on researchers from the humanities in particular, for whom the use of Tier-2 infrastructure would mean a major step. Because of specific, Windows-based software, a solution was offered for these researchers within the cloud environment. The VUB has an HPC user committee that meets every six months, with feedback from the VSC, and which monitors the use and needs for HPC. The user committee comprises members from all faculties, from the data center and from the research policy department. In terms of courses, the courses "Introduction to Linux", "Introduction to the use of HPC at the VUB" and "Introduction to GRID computing" are organized twice a year. User meetings were also organized with a number of groups to identify their specific needs and / or problems with HPC:

STAFF

Given that the infrastructure of the VSC Tier-2 and Tier-1 infrastructure is installed in the various university data centers, the staff is also employed at the various universities.

SUBSIDIZATION

On the one hand, every university needs staff to operate the Tier-2 infrastructure and support end-users. 20 FTE are subsidized for this. On the other hand, the institute that houses the Tier-1 is also awarded FTE's. To this end, 2 FTEs were awarded in 2018 for the operation of the Tier-1a (UGent) and 2 FTEs for Tier-1b (KU Leuven). In addition, 2 FTEs are added for the expansion of the Tier-1 services. This FTE will be deployed in 2018 to staff the operational management team. In 2018 this team will be responsible for the realization of the Tier-1 project, "Supercomputing as a service".

Because every university has a different personnel policy and uses different remuneration principles, a fixed amount of 95,000 euros is paid for each FTE.

Institution	number of subsidized FTEs for Tier-2 exploitation and support
UGent	5
UAntwerpen	4
VUB	3
UHasselt	2,5
KU Leuven	6

Institution	number of subsidized FTEs for Tier-1 operation and operational management
UGent	2,6
UAntwerpen	0,6
KU Leuven	2,6

EFFECTIVE STAFF DEPLOYMENT

To exploit, maintain and support the various Tier-2 and Tier-1 setups, on the one hand more manpower is required than is provided for within the subsidy. On the other hand, a range of expertise is needed that cannot be built up within one limited team. To meet this, the HPC technicians and support staff can call on other experts who work in the IT services of the different universities. The universities use 35.7 FTE for the HPC exploitation and support.

Institution	Number of FTEs used for HPC	Number of heads involved in HPC exploitationand support
UGent	9,4	14
UAntwerpen	5,4	9
VUB	5,0	14
UHasselt	2,3	3
KU Leuven	13,5	21
Totaal	35,5	61

PROFILES

To effectively operate and support an HPC infrastructure, there are several IT profiles required:

- infrastructure managers: they are responsible for the installation of the infrastructure in de datacentra
- system admins: they install and manage the basis software on the HPC machines
- users support: for the basic users support
- scientific or advanced supporters: they optimise the users software on the HPC infrastructures
- project leaders: direct leadership of the HPC teams or larger HPC projects
- outreach: they promote scientific computing and HPC to academic and industrial users.

	Infrastructure management	System Administration	Basic user support	Scientific or advanced support	Management	Outreach
KU Leuven	10	12	7	7	8	4
UAntwerpen	1	3	6	4	2	2
UGent	5	7	5	5	2	3
UHasselt			2	2	2	2
VUB	4	4	8	4	4	3
Total	20	26	28	22	17	14

OUTREACH

The VSC has the ambition to operate as a service center where companies can go if they want to incorporate innovative computational techniques into their business. Whereas for the academic world the VSC primarily is an infrastructure provider, it is primarily a knowledge center for the industry and private sector with the main aim of informing and convincing industry of the possibilities of HPC within their sector. The differentiated VSC infrastructure that is available is regarded as a "production" environment for the academic world, while in service provision to the industry it is used as a stepping stone to prepare own investments or integrate HPC into the production process .

Consulting and training, the second and third pillar of the VSC services, are of greater importance to the industry than the available shared infrastructure, which can be deployed in the exploration phase, but often less suitable as a production environment.

SERVICES TO COMPANIES

The VSC wants to support Flemish companies and other non-academic institutions in their innovation process by providing a broad expertise. To stimulate the use of scientific and technical calculations in the Flemish academic and business world, the VSC has elaborated an extensive service package.

Awareness raising

The VSC takes part in events that are organized in different sectors, in order to show the possibilities of HPC to the business community. Through presentations, demos and marketing material, the VSC wants to make its services known to the business community and also highlight the possibilities of HPC. To make this concrete, a portfolio of references and testimonials is being worked on.

In addition, the VSC itself also tries to play a role in community building by organizing events itself where networking is possible between all stakeholders of the HPC domain.

Training

Training is an important part of the functioning of the VSC. Training events are organized on a regular basis that are also open to users from the business world. Topics include Linux, (parallel) programming languages and paradigms and code optimization. Application-oriented training for specific domains such as materials science, numerical fluid dynamics, data science and machine learning are also covered.

The VSC offers tailor-made training courses that are popular with academic users. However, there is also interest from non-academic institutions and industry.

Examples are SCK-CEN, the Hydraulic Engineering Laboratory, VITO, EnergyVille, AGT, NXP and Cegeka, BASF.

Consultancy

The VSC consultants can help put the companies in contact with experts and have the infrastructure to set up experiments, demos and proof of concepts. They can also offer support in dimensioning their own infrastructure needs and set them on their way to introduce computational techniques into their production process.

The VSC experts analyze the specific needs of a company and examine how supercomputing can offer added value for this company. The VSC offers an intake interview to determine which services in the VSC network best meet those needs.

Through its contacts with users from academic institutions and from industry, the VSC can discover opportunities for collaboration. Within the network, the VSC can connect the company with a suitable top-level research partner in the Flemish academic landscape and act as a mediator.

Infrastructure

Companies can purchase computing time at internationally competitive prices on the state-of-the-art supercomputing infrastructure within the VSC network. Users receive step-by-step support to start computational tasks, and a special help desk is available to resolve usage-related questions and assist users with the installation of specific software.

The following table provides a more detailed overview of the VSC services to the business world and non-academic institutions for the years 2016-2018.

	Consultancy			Training			Infrastructure use					
							Tier-2			Tier-1		
3E	2016						2016	2017	2018	2016	2017	2018
01ortho								2017				
Ablynx					2017							
Aeronomie			2018									
AM-TEAM		2017	2018									
Analizo		2017										
ApheaBio		2017									2017	
Bekaert					2017		2016	2017	2018	2016		
Diabatix	2016						2016	2017	2018		2017	2018
European Organisation for Research and Treatment of Cancer (EORTC)			2018						2018			

	Consultancy			Training			Infrastructure use					
							Tier-2			Tier-1		
Federale Politie		2017						2017				
FEOPS										2016		
Flanders Make								2017	2018			
FluidDA	2016											
Havenbedrijf Antwerpen			2018									
Hogere Zeevaartschool Antwerpen					2017							
ILVO	2016				2017		2016	2017	2018	2016		
IMDC	2016				2017		2016	2017	2018			
imec							2016	2017	2018	2016		
iMinds	2016			2016								
Inbiose					2017			2017	2018			
INBO							2016	2017	2018			
Instituut Tropische Geneeskunde		2017	2018	2016	2017	2018	2016	2017	2018			
IRCEL		2017				2018	2016	2017	2018			
KMI	2016			2016		2018				2016		
Materialise			2018			2018						
Promat		2017										

	Consultancy			Training			Infrastructure use					
							Tier-2			Tier-1		
Royal Belgian Institute of Natural Sciences			2018						2018			
Royal Museum for Central Africa			2018		2017			2017	2018			
Saudi Aramco Systems					2017							
SCK.CEN	2016	2017										
Siemens				2016						2016		
UMICORE	2016									2016	2017	2018
UZ Gent	2016											
UZ Leuven	2016	2017	2018		2017	2018	2016	2017	2018			
VIB					2017		2016	2017	2018	2016	2017	
VITO		2017					2016	2017	2018			
VMM		2017					2016	2017	2018			
Volvo					2017							
Von Karman Instituut (VKI)		2017			2017			2017	2018			
Waterbouwkundig Laboratorium							2016	2017	2018			
Woestijnvis			2018						2018			

INDUSTRIAL BOARD

The Industrial Board can strengthen the exchange of ideas and expertise between knowledge institutions and industry. It develops initiatives to inform companies and non-profit institutions about the added value that HPC provides in developing and optimizing services and products and promotes the services that the VSC provides to companies such as consultancy, research collaboration, training and computing power.

The VSC Industrial Board developed a number of campaigns in 2018 to promote the VSC. Thanks to the VSC Industrial Board, the VSC was able to present itself at the following events:

Leuven Mindgate | 1/3/2018 "High Performance Computing voor de Maakindustrie: de supercomputer en haar toepassingsmogelijkheden"

Leuven MindGate was founded by 29 leading knowledge institutions, companies and government institutions from the Leuven region and aims to achieve cross-fertilization between the various organizations and to put the region in the spotlight internationally. Leuven MindGate regularly organizes theme sessions. A specific session on the use of High Performance Computing in the manufacturing industry was set up together with Flanders Make. The possibilities of VSC were presented as well as how companies can make concrete use of the services of the VSC.

Voka Limburg | 2/10/2018

On October 2, VOKA C.E.O.-Limburg organized its network event "Come give gas." The VSC was able to explain various concrete use cases to those present.

Furthermore, the focus of the VSC Industrial Board in 2018 was primarily on elaborating use cases and testimonials from VSC users to show and promote the added value of the VSC and its services through concrete applications in various domains. New testimonials are regularly posted on the VSC LinkedIn account.

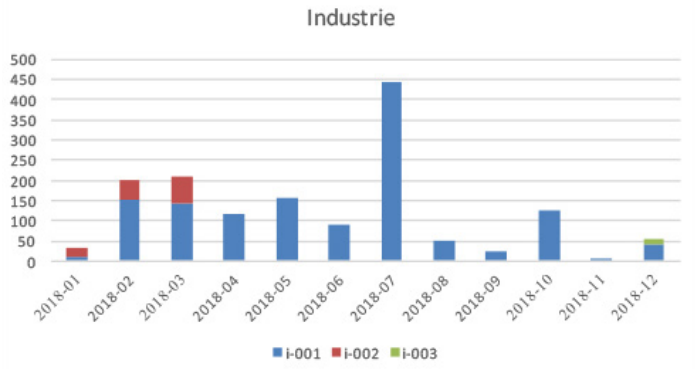
Finally, work continued in 2018 on the "Start to VSC" project, the step-by-step plan to facilitate the access of new industrial users to VSC. To support the step-by-step plan, a number of tools must be worked out: a standard contract, FAQ for users, a checklist for IT departments, a document with the most important safety specifications, a list of used software, an overview of use cases.

TIER-1 USE BY COMPANIES

To date, agreements have been concluded with four companies for the structural reduction of calculation time on the Tier-1: one company in the renewable energy sector, one in the pharmaceutical sector, an engineering firm and a company active in materials technology.

Several other companies are already active on the Tier-1 and Tier-2 computing infrastructure, but in an exploratory phase, in order to be able to properly assess whether the scale of this infrastructure can offer added value for their business activities.

The image below offers an (anonymous) overview of the use of calculation time on Tier-1 BrENIAC by industry in 2018



USE TIER-2 BY COMPANIES AND NON-ACADEMIC INSTITUTIONS

Not only researchers from the institutions of the VSC consortium use the Tier-2 infrastructure. Strategic research centers, recognized Flemish scientific institutions and federal science institutions, government bodies and companies also make use of the VSC services and Tier-2 infrastructure, An overview can be found above.

PUBLICATION TO COMPANIES AND OTHER KNOWLEDGE INSTITUTIONS

Also in 2018, the focus was on direct contact and enthusiasm for companies to use supercomputing and the VSC services. When exchanging best practices between the HPC centers of the SESAME Net consortium, it turned out that through this type of smaller events, in which personal contacts with industry are central, companies can be better convinced of the added value of supercomputing. Several user meetings and kickstart events were organized, mostly on-site.

VSC was also actively present at various network events to promote supercomputing. In addition, various industry use cases were prepared and published on the VSC website, and distributed via, among others, the SESAME Net channel.

Some outreach events from 2018:

Genius AI event | 23/4/2018
The new Tier-2 machine at KU Leuven has specialized technology that can be optimally used for the new AI applications. To highlight this, an event was organized in which the CTO of HPE Dr. Eng Lim Goh gave the keynote, followed by different perspectives on AI and machine learning by professors from Leuven (prof. Dr. Ir. Yves Moreau, prof. Danny De Schreye, Prof. Thomas Hertog and Dr. Bart Thijs).

This event was open to all users of the HPC and those interested in AI. The new machine was highlighted and was also picked up in specialized international media.

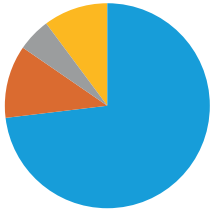
Leuven AND & festival | 2-5/5/2018
During the Leuven art and science festival, Craftworks, an IT company within the Cronos group, took part in the "Genius painter" exhibition. The supercomputer was used for this purpose and it was possible to explain to a wide audience how new technologies are being applied and what the role of the VSC is.

ISC - NVIDIA Booth talk | 26/6/2018
During the booth presentation of NVIDIA, the main producer of GPU devices, the new machine of the VSC was presented at the European supercomputer conference.

TRAINING

The VSC spends the necessary time supporting and training researchers who use the infrastructure. It is important that calculations are performed efficiently in order to increase the scientific competitive position of the universities in the international research landscape. Training courses organized by the VSC are intended not only for researchers affiliated with Flemish universities and their respective associations, but also for researchers working in the Strategic Research Centers, the Flemish scientific research institutions and the industry.
The courses can be divided into four categories that either indicate the required prior knowledge or clarify that these are domain-specific topics:

- **Introductory**
- **Intermediate**
- **Advanced**
- **Specialist courses & workshops**



Introductory courses are intended for all users of the infrastructure and are highly recommended for those who do not yet have the necessary skills. The local VSC employees lead these sessions. This also gives researchers the opportunity to get to know the people who answer the questions asked at the help desk. This removes the impersonal and anonymous nature of e-mail traffic.
To follow the sessions at the intermediate level, the introductory courses are required as prior knowledge. These sessions also deal with more specific topics. The majority of these courses are intended for users who develop software themselves, either for calculation-intensive applications or for pre- and post-processing of data. Because these courses are more specialized and intensive than the introductory courses, they are not offered on every VSC site. Users are therefore encouraged to attend the courses at another site.
Advanced level courses require even more experience and are more domain specific than the intermediate courses. The VSC uses external teachers for these courses. They are often connected to PRACE Advanced Training Centers (PATC) or they come from the industry. Only two or three such courses are organized each year.
In 2018, the VSC organized two PRACE Training Center (PTC) courses for the first time in collaboration with SURFsara (Amsterdam). These trainings are given by VSC staff who participated in the PRACE train-the-trainer program.
Some courses do not fit into either of these three levels: either they are too domain specific or they cover the full introductory to advanced level. This explains the term “specialist”. For this too, recourse is often made to external specialists.

The VSC also offers tailor-made training courses, both for research groups and for knowledge institutions and industry. In this case it is usually a standard course, supplemented with domain-specific modules that are specially developed for this. In 2018, training sessions were conducted by Cegeka, NXP and BASF, and VITO again appealed to the VSC.
New forms of learning are also used. The VSC developed a Massive Open Online Course (MOOC) for "Defensive programming and Debugging" for PRACE (5th Implementation Phase, work package 4). The first edition of this MOOC started on November 5, 2018 and had 750 active participants from 126 countries. A second edition is planned for May 2019.

VSC staff can also offer support to teachers who want to use the VSC infrastructure for regular courses. In 2018 this was the case for three courses. Of course there are also teachers who train their students themselves.

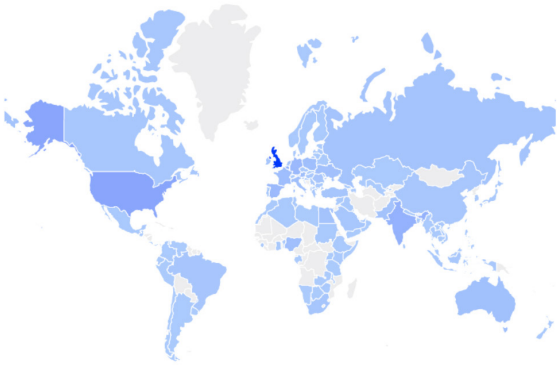
Of course, existing training courses are always kept up-to-date with recent developments, but new topics are also selected and worked out annually for training. The VSC website announces the training offer, so that the information is available to all interested parties. The announcements are distributed to the users of the infrastructure via internal mailing lists. Targeted mailings draw attention to specific training courses if they can be useful for a limited target group or for potential users.

MOOC demographics

118 landen

TOP 5

GB 32%
Amerika 6%
België 5%
India 4%
Duitsland 3%



EVENTS

VSC USERS DAY 2018

The VSC User Committee organized the annual VSC User Day in Brussels, on 22 May 2018. More than 110 participants registered for this event. The foreign speaker, Dr. Ulrich Rühe from CERFACS and the University of Erlangen-Nuernberg, opened the day with a lecture on "Ultrascalable algorithms for complex flows". In the other plenary sessions Jan Fostier (UGent) presented "Processing Genomics Data: High Performance Computing meets Big Data" and Joris Coddé, CTO Diabatix also demonstrated "Why HPC and artificial intelligence engineering go hand in hand".

Both in the morning and in the afternoon choices could be made from one of the workshops: "VSC for starters", "Start to GPU", "Code optimization" or "Code debugging".

The ambitious VSC project "Supercomputing as a service" was presented and the day ended with an award ceremony for the best poster from the poster session where researchers presented their HPC-related research and for which the public was encouraged via 1-minute presentations. This approach has ensured that many participants were clearly interested in the numerous posters.

The completed evaluation forms were unanimously positive.

PARTICIPATION IN NATIONAL AND INTERNATIONAL EVENTS, CONGRESSES AND WORKSHOPS

Organized by VSC

- AI event - Genius | April 23, Leuven
- VSC Users day | May 22, Brussels

Organized by other organization

- EOSC hub kick-off meeting | January 9-12, Amsterdam, the Netherlands
- Workshop on Cloud Services for Synchronization and Sharing | January 29-31, Krakow, Poland
- Easybuild User meeting | January 30-February 1, Amsterdam, the Netherlands
- FOSDEM'18 Co-organization of HPC, Big Data and Data Science devroom | 3-4 February, Brussels
- Leuven Mindgate: "High Performance Computing for the manufacturing industry: the supercomputer and its application possibilities" | March 1, Leuven
- Spectrum Scale (GPFS) User Group 2018 | April 18-19, London, UK
- EOSC hub week 2018 | April 16-20, Spain
- HPE Reimagine 2018 | April 24, 2018
- 25th Quattor workshop | April 25-27, Orsay-Ville, France
- And & Leuven | 2-5 May, Leuven
- CÉCI Scientific Day | May 4, Namur
- NEC users group | May 14-16, Aachen, Germany
- PRACEdays | May 28 to June 1, Ljubljana, Slovenia
- HP-Cast | June 22-23, Frankfurt, Germany
- ISC 2018 | June 24-28, Frankfurt, Germany
- PRACE meeting WP4 | 4-5 September 2018, Amsterdam, the Netherlands
- Slurm User Group meeting 2018 | September 25-26, Madrid, Spain
- PRACE meeting WP3 | 26-27 September 2018, Brussels
- Voka Limburg | October 2, Zolder, Belgium
- Workshop "Call PRACE Tier-0" | October 4, Gosselies
- Belnet Conference | October 10, Brussels
- EasyBuild HPC-SIG workshop | October 22, Birmingham, UK
- 26th Quattor workshop | October 29-31, Ghent
- HP-Cast | November 9-10, 2018, Dallas, USA
- Supercomputing 2018 | November 11-16, 2018, Dallas, USA
- HPE - Customer Experience Day | November 15, Diegem
- PRACE: Parallel & GPU programming in Python @ SURFsara | December 10-11, Amsterdam, the Netherlands
- FWO Kennismakers | December 14, Antwerp

The VSC sponsored the Flemish Programming Competition every year. The purpose of this is to increase name recognition among students and staff members, especially among association partners.

INTERNATIONAL COOPERATION

PRACE EN EUROHPC

The VSC is, through Belgian membership, part of PRACE. PRACE offers the possibility to use Tier-0 calculation time. Access to Tier-0 calculation time is organized through calls for project proposals. These proposals are assessed according to "excellent science" standards. The projects that are ranked best receive the requested calculation time. At the 17th call, a team around Prof. Giovanni Lapenta (KU Leuven) was awarded 35 million core hours on the German SuperMUC supercomputer. Flemish researchers are made aware of the existence of these calls, by means of messages on the VSC website. And to better inform the researchers about writing PRACE Tier-0 applications, Cenaero, together with CECI and VSC, organized a workshop "Call PRACE Tier-0" on 4 October 2018. John Clifford, Peer Review Officer at PRACE, has told more about "PRACE Peer Review Process: How to prepare a good Project Access proposal". In addition, there were lectures from users: Prof. Giovanni Lapenta (KU Leuven), Koen Hillewaert (Cenaero) and Prof. Philippe Chatelain (UCLouvain).

The MOOC "Defensive Programming and Debugging" started on November 5, 2018. This MOOC was developed by UHasselt and KU Leuven, in collaboration with Future Learn. There were 1342 registrations from 118 countries. Both the workshop and the MOOC are part of the contribution to the "PRACE fifth implementation phase project", or PRACE 5IP for short. Cenaero and KU Leuven are the Belgian participants in this project.

In the meantime, the EuroHPC train continues at high speed. Working groups set out the guidelines for the future European supercomputers (petascale and pre-exascale), identified the needs of the various research communities, formed consortia for possible exploitation, etc.

Also within Belgium there was a lot of discussion between all parties about a possible participation. The final decision on this is foreseen for the beginning of 2019.

Geert Van Grootel (EWI) represents Belgium on the Governing Board of the EuroHPC Joint Undertaking (JU), with Laurent Ghys (BELSPO) as substitute. The JU is the body that controls the EuroHPC event. It supports the activities through, among other things, tenders and open calls. The JU is operational from 2019 until (at least) 2026. The budget for that period is approximately 1 billion euros.

Meanwhile, PRACE is also considering his/her role within the European HPC landscape with the arrival of EuroHPC.

EGI

The VSC is actively present at the European Grid Infrastructure event (EGI). The VUB grid cluster is integrated in the EGI federated e-Infrastructure and with the support of international virtual organizations it offers the possibility for researchers from Flanders to use this European computing infrastructure. High-energy physicists from the University of Antwerp, UGent and VUB in particular make use of this. Some examples are:

- The grid cluster supports the international collaboration "IceCube". Researchers from VUB and UGent are active in this.
- A new international research group "SoLid", with researchers from UGent, UAntwerpen and VUB, among others, studying neutrino oscillations at a very short distance from the core of a reactor at SCK-CEN in Mol, was started. This research group, with support from the VUB grid team, uses the EGI grid middleware to easily share data across participating universities.
- In addition, the WeNMR project is also an active user of the grid cluster.
- Two new collaborations were started in 2018: LOFAR (low frequency radio astronomy) and AUGER (high energy comic radiation).
- In January 2018, the VUB also joined the EOSC hub project as a member and helps with the work package "Federated Service Management".

SESAME NET

The VSC is a partner in the SESAME Net project awarded to the consortium within the EU Horizon 2020 program. SESAME Net stands for 'Supercomputing Expertise for SMAll and Medium Enterprise Network' and its main objectives are to support, expand and promote a network of HPC knowledge and HPC experience in Europe, but especially to spread best practices around HPC use by industry. The primary target group are SMEs.

In 2018, the number of members of SESAME Net increased to 32 partners, now including PRACE and several other European centers of excellence in the HPC periphery as project partners: Energy oriented Center of Excellence for computing applications (EoCoE, https: //www.eocoe) .eu) and Performance Optimization and Productivity, A Center of Excellence in HPC (https://pop-coe.eu).

The third SESAME Network Annual Assembly took place on March 9, 2018.

SESAME Net also participated in several outreach activities, including PRACE days 2018 (May 29-31, Ljubljana) and an interregional matchmaking event to promote HPC among SMEs (March 22, Zagreb), facilitated by WATIFY, an awareness campaign of the European committee to support companies with their digital transformation.

SUCCESS STORIES

NICOLE VAN LIPZIG
CLIMATE CHANGE

Regional climate models (RCMs) offer scientifically justified, quantitative estimates about the future climate change of a country or a region. Prof. Nicole van Lipzig from KU Leuven shares her success story with the help of the VSC infrastructure, in which she explains the climate process and its social consequences and lets society understand how extreme weather can change in the future.

Click on the screen to play the video

OLIVIER GOURGUE
TIDAL MARSHES

With the help of VSC supercomputers, Olivier Gourgue, of the Department of Biology, at the University of Antwerp, studies the interaction between tidal flows, sediment transport and vegetation in coastal areas. In his study he describes the importance of the tidal marshes for people, birds and the fish that live there because they protect us against the major floods.

Click on the screen to play the video

KATLEEN WILS
EARTHQUAKES

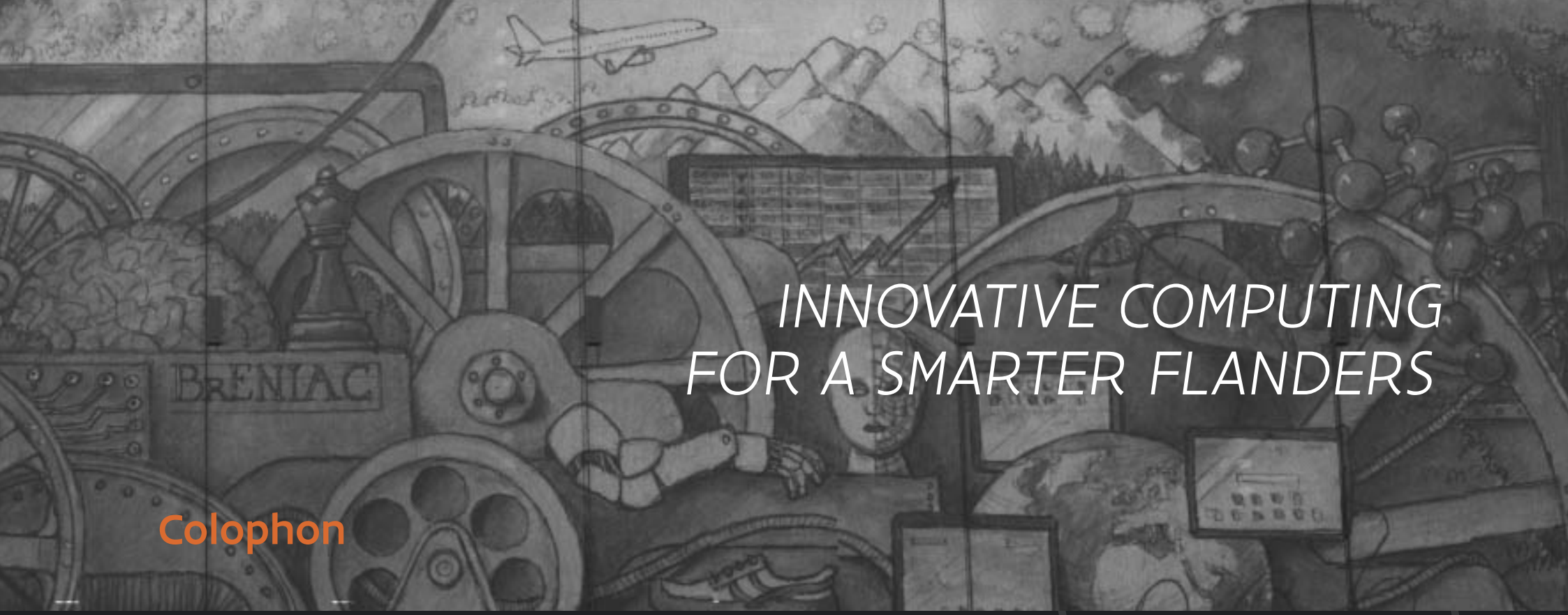
PhD student Katleen Wils from Ghent University uses the VSC supercomputer to learn about earthquakes and the earthquake cycle, including the movements that occur between the earthquakes.

Click on the screen to play the video

CHRISTOPHE VANDEVIVER **CRIMINOLOGY**

Christophe Vandeviver of the Ghent University, criminological research department, has carried out groundbreaking research in new domains thanks to the HPC infrastructure at the Flemish Supercomputer Center. He investigated how burglars select targets and what makes a target stand out for a burglar. With the help of the super computers of the VSC, he has modeled half a million houses and mapped out which house properties make them stand out for a burglar. He also discovered that when burglars travel further, they try to make it worthwhile and select more lucrative goals.

Click on the screen to play the video



INNOVATIVE COMPUTING FOR A SMARTER FLANDERS

Colophon

The Flemish Supercomputer Centre (VSC) is a virtual centre making supercomputer infrastructure available for both the academic and industrial world. This centre is managed by the FWO in partnership with the five Flemish university associations.

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